Compression, inversion, and approximate PCA of dense kernel matrices at near-linear computational complexity

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November 15, 2017

Abstract: Dense kernel matrices $\Theta \in \mathbb{R}^{N \times N}$ obtained from point evaluations of a covariance function $G$ at locations $\{x_i\}_{1 \leq i \leq N}$ arise in statistics, machine learning, and numerical analysis. For covariance functions that are Green’s functions of elliptic boundary value problems and approximately equally spaced sampling points, we show how to identify a subset $S \subset \{1, \ldots, N\} \times \{1, \ldots, N\}$, with $\#S = O(N \log(N) \log^d(N/\epsilon))$, such that the zero fill-in incomplete Cholesky factorisation of $\Theta_{i,j} \mathbf{1}_{(i,j) \in S}$ is an $\epsilon$-approximation of $\Theta$. This block-factorisation can provably be obtained in complexity $O(N \log(N) \log^d(N/\epsilon))$ in space and $O(N \log^2(N) \log^{2d}(N/\epsilon))$ in time. The algorithm only needs to know the spatial configuration of the $x_i$ and does not require an analytic representation of $G$. Furthermore, an approximate PCA with optimal rate of convergence in the operator norm can be easily read off from this decomposition. Hence, by inverting the order of the Cholesky decomposition we also obtain a solver for elliptic PDE with complexity $O(N \log(N) \log^d(N/\epsilon))$ in space and $O(N \log^2(N) \log^{2d}(N/\epsilon))$ in time.

Keywords: Cholesky decomposition, covariance function, gamblet transform, kernel matrix, sparsity, principal component analysis.

2010 Mathematics Subject Classification: 65F30 (42C40, 65F50, 65N55, 65N75, 60G42, 68Q25, 68W40)

1 Introduction

1.1 Sparse factorisation of dense kernel matrices

Symmetric positive-definite matrices of the form

$\Theta_{i,j} := \iint_{\Omega} v_i(x) G(x, y) v_j(y) \, dx \, dy$

play an important role in many different parts of applied mathematics. In numerical analysis, these matrices arise as discretised integral operators and are obtained by integrating the Green’s function $G$.
of a partial differential operator against test functions \( \{ v_i \} \), (Hsiao, 2006; Sauter and Schwab, 2011). In computer graphics, the radiosity equation describing the illumination of a scene is an integral equation of the above kind (Gortler et al., 1993). In machine learning, replacing the Gram matrix of the measurement vectors by a kernel matrix of the above form often allows one to implicitly work in an infinite-dimensional feature space (Schölkopf and Smola, 2002). Kernel matrices also play a central role in scattered data approximation (Wendland, 2005), i.e. function interpolation based on unstructured localised measurements. Finally, since covariance matrices of Gaussian processes are kernel matrices, such matrices also play a central role in spatial-statistical methods such as Kriging (Stein, 1999).

The above examples typically require matrix-vector multiplication by \( \Theta \) or \( \Theta^{-1} \), the computation of \( \det(\Theta) \), or the computation of a matrix square root \( \Theta^{1/2} \) in order to sample from the normal distribution \( N(0, \Theta) \). Since integral operators are typically nonlocal, the resulting matrices will generally be dense. When \( \Theta \) is an \( N \times N \) matrix, standard Gaussian elimination methods to compute the inverse and determinant would be of \( O(N^3) \) complexity and even a matrix-vector multiplication involving \( \Theta \) has complexity \( O(N^2) \). For large \( N \), this is prohibitively expensive, making it necessary to exploit the problem’s underlying structure.

Let \( \Omega \subset \mathbb{R}^d \) be a bounded domain with Lipschitz boundary and let, for an integer \( s > d/2 \), the operator \( \mathcal{L}: H^s_0(\Omega) \to H^{-s}(\Omega) \) be bounded and local in the sense that

\[
\int_{\Omega} u \mathcal{L} v \, dx = 0 \quad \text{for all } u, v \in H^s(\Omega) \text{ with } \text{supp}(u) \cap \text{supp}(v) = \emptyset.
\]

We furthermore define \( G := \mathcal{L}^{-1} \). The most common instances of such operators, and the ones we have mostly in mind, are elliptic partial differential operators of order \( 2s \) with Dirichlet boundary conditions. Let now \( \{ x_i \}_{i \in I} \) be a set of \( N \) points in \( \Omega \) that are approximately uniformly distributed in the sense that, for some \( \delta \in (0, 1) \),

\[
\frac{\max_{x_i \in \Omega} \min_{i \in I} \text{dist}(x_i, x)}{\min_{i \neq j \in I} \left( \text{dist}(x_i, \{ x_j \} \cup \partial \Omega) \right)} \leq \frac{1}{\delta}.
\]

We then define \( \Theta \in \mathbb{R}^{I \times I} \) by

\[
\Theta_{i,j} := \int_{\Omega} \delta_{x_i} G (\delta_{x_j}) \, dx,
\]

where \( \delta_{x_i} \in H^{-s} \) follows from \( s \geq d/2 \). Matrices of this kind appear in many areas of computational physics, machine learning, and statistics. In the first case, they arise due to the ubiquity of elliptic partial differential equations in the description of physical systems, while in machine learning and statistics, matrices like \( \Theta \) arise as covariance matrices of smooth Gaussian random fields. In particular — modulo their behavior at the boundary, which we will discuss later — many members of the popular Matérn family of covariance functions fall into this class (Whittle, 1954, 1963; Fasshauer, 2012). Since \( \Theta \) is a dense matrix, directly computing these quantities using dense matrix algebra and Cholesky factorisation will result in computational complexity of \( O(N^2) \) or \( O(N^3) \), which is prohibitive for large numbers of data points. The main result of this paper shows that despite involving dense \( N \times N \) matrices, the above-mentioned quantities can be computed in near-linear time:
Figure 1.2: The original dense matrix is plotted entrywise on the left. The sparsity pattern is visualised
on the right.

Theorem 1.1. There exist index sets $S_\rho \subset I \times I$ of size $\#(S_\rho) = O(N \log(N)\rho^d)$ and a permutation
matrix $P \in \mathbb{R}^{I \times I}$ depending only on $\{x_i\}_{i \in I}, \Omega$ (but not on the entries of $\Theta$) such that, defining

$$\Gamma := P^T \Theta P,$$

and

$$\Gamma_{i,j}^{(\rho)} := \begin{cases} 
\Gamma_{i,j} & \text{for } (i,j) \in S_\rho \\
0 & \text{otherwise},
\end{cases}$$

and letting $L_\rho$ be the zero-fill-in incomplete Cholesky factorisation (q.v. Algorithm 2) of $\Gamma_\rho$, we have

$$\|L_\rho L_\rho^T - \Gamma\| \leq \text{poly}(N) \exp(-\gamma \rho)$$

for $\gamma$ and poly independent of $N, \rho$. Furthermore, this factorisation can be computed in computational
complexity $O(N \log^2(N)\rho^d)$. In particular, a sparse $\varepsilon$-approximate Cholesky factor $\Gamma$, i.e. a lower-
triangular matrix $L_\varepsilon$ such that

$$\|L_\varepsilon L_\varepsilon^T - \Gamma\| \leq \varepsilon,$$

can be computed with complexity of $O(N \log(N)\log^d(N/\varepsilon))$ in space and $O(N \log^2(N)\log^2d(N/\varepsilon))$
in time.

The sparsity pattern is obtained hierarchically. First, the measurement locations are divided into
subsets $\{x_j\}_{j \in J(k)}$, sampled at resolution $\approx 2^{-k}$, for $1 \leq k \leq q$ (see Figure 1.3). The $x_i$ are then ordered
from $J(1)$ to $J(q)$. By reordering the rows and columns of $\Theta$ in this way, we obtain $\Gamma$. Next, for $i \in J(k)$
and $j \in J(l)$ we let $(i,j) \in S \iff \text{dist}(x_i, x_j) \leq \rho 2^{-\min(k,l)}$. This procedure is illustrated in Figure 1.4

| Algorithm 1: Standard dense Cholesky decomposition. | Algorithm 2: Incomplete sparse Cholesky decomposition with nonzero entries (nnz) in $S$. |
|-----------------------------------------------------|---------------------------------------------------------------|
| **Data:** $A \in \mathbb{R}^{N \times N}$ symmetric | **Data:** $A \in \mathbb{R}^{N \times N}$ symmetric, \text{nnz}(A) \subset S \subset \{1, \ldots, N\}^2 |
| **Result:** $L \in \mathbb{R}^{N \times N}$ lower triangular | **Result:** $L \in \mathbb{R}^{N \times N}$ lower triangular, \text{nnz}(L) \subset S |
| for $i \in \{1, \ldots, N\}$ do | for $i \in \{1, \ldots, N\}$ do |
| $A_{i,i} \leftarrow \sqrt{A_{i,i}}$ | $A_{i,i} \leftarrow \sqrt{A_{i,i}}$ |
| for $j \in \{i+1, \ldots, N\}$ do | for $j \in \{i+1, \ldots, N\}$ : $(i,j) \in S$ do |
| for $k \in \{j, \ldots, N\}$ do | for $k \in \{j, \ldots, N\}$ : $(k,i), (k,i) \in S$ do |
| $A_{k,j} \leftarrow A_{k,j} - \frac{A_{k,i}A_{i,j}}{A_{i,i}}$ | $A_{k,j} \leftarrow A_{k,j} - \frac{A_{k,i}A_{i,j}}{A_{i,i}}$ |
| return LowerTriangularPart($A$); | return LowerTriangularPart($A$); |
Figure 1.3: The measurement points are divided into subsets sampled on different scales, $J^{(1)}$, $J^{(2)}$, and $J^{(3)}$.

Figure 1.4: The upper panels show the interaction lengths on the different levels. The lower panels show the corresponding entries being added to (the lower-triangular part of) $\Gamma^\rho$.
Finally, once we have obtained $\tilde{\Gamma}$, we simply apply ordinary Cholesky factorisation (Algorithm 1), but skip any elementwise update that involves a write or read operation outside of $S^o$, as in Algorithm 2. Once the sparse Cholesky factorisation is computed, the application of the forward and inverse operator to a vector, the computation of the determinant, and sampling from $\mathcal{N}(0,L^oL^{oT})$ can all be done in complexity $O(N\log(N)\log^d(N/\varepsilon))$.

We prove Theorem 1.1 using gamblet multiresolution analysis as introduced by Owhadi (2017) and Owhadi and Scovel (2017), which we will, to some degree, generalize. We will also explain in more detail how the above algorithm is related to and inspired by the gamblet transform. Another purpose of this paper is to further illustrate interplays between Gaussian random fields, Gaussian elimination, statistical inference, numerical homogenisation and multiresolution methods. For example, we will show that the screening effect (Furrer et al., 2006; Stein, 2002), which is well known in the spatial statistics community, is intimately linked to numerical homogenisation and provides a natural explanation of the sparse approximation described in this paper. Beyond Theorem 1.1, we will prove that a similar effect also holds in the case of $s \leq d/2$, provided that $P$ is replaced by a simple averaging scheme. By reversing the order of elimination, we obtain a sparse factorisation of discretisations of the operator $L$, leading to fast solver for elliptic PDE with complexity $O(N\log(N)\log^d(N/\varepsilon))$ in space and $O(N\log^2(N)\log^d(N/\varepsilon))$, which is not surprising since the gamblets were originally developed to rapidly invert such operators. Finally, inheriting a similar property from gamblets, the matrices $L_{1,k}^p, (L_{1,k}^p)^T$ are near-optimal rank-$k$ approximations to $\Gamma$, making them a sparse approximate PCA.

1.2 Existing methods

Kernel-based approaches are ubiquitous in applied mathematics and there is a rich literature on methods designed to avoid the $O(N^3)$ bottleneck incurred by vanilla solvers that are based upon Gaussian elimination. Here we provide a non-exhaustive overview of existing techniques, loosely sorted by field of application and underlying ideas.

The simplest way of approximating large kernel matrices is subsampling, on the basis that subsampled data points may contain enough information to achieve the desired accuracy. Furthermore, if parts of the domain require more accurate estimates, points in these regions can be adaptively sampled at a higher rate. In the Gaussian process statistics community, this approach is frequently referred to as the selection of an active set of training variables (Rasmussen and Williams, 2006). From the point of view of the kernel matrix, subsampling the data just amounts to subampling rows and columns. Some algorithms proposed for this purpose rely on greedy selection combined with a cheap estimator for the quality of the approximation (Smola and Schölkopf, 2000; Bach and Jordan, 2003; Fine and Scheinberg, 2001). When solving integral equations arising in PDEs, the user usually has more flexibility in choosing the mesh of the discretisation than the statistician has in choosing the measurement locations of the training data. From this point of view, (adaptive) mesh generation amounts to subsampling an infinite amount of data (Feischl et al., 2015).

Subsampling schemes, which correspond to subsampling the rows and columns of the covariance matrix, can also be seen as low-rank approximations, with the additional restriction that the low-dimensional subspace must be spanned by a set of vectors of the standard basis. Although individual measurements define non-adapted bases, fixed-rank Kriging can be used to produce adapted bases (Cressie and Johannesson, 2008). In some problems, the prior knowledge of a good separable approximation of the kernel function may inform the choice of a low-rank model. An initial subsampling procedure can also be combined with an eigendecomposition (Williams and Seeger, 2001; Santin and Schaback, 2016) to improve the accuracy of the low-rank approximation. This approach is in some sense similar to that of Halko et al. (2011), where a random projection followed by an SVD is used to obtain low-rank approximations of matrices. Another probabilistic algorithm is given by Rahimi and Recht (2008) and relies on the inverse kernel trick together with random projections to approximate the kernel matrix by the Gram matrix of a low-dimensional feature map. Chalupka et al. (2013) compare approximation methods for Gaussian process regression and Stein (2014) shows that low-rank models can perform poorly even in presence of strong correlation between neighbouring points.

A way to overcome the limitations of low-rank approximations is to recognise that long-range correlations tend to be of lower rank than short-range correlation. Therefore, adapting the rank of the approximation to submatrices may be a better strategy. Using this idea in the context of particle simula-
tions, the pioneering work of Greengard and Rokhlin (1987) shows that it is possible to apply dense kernel matrices to vectors in $O(N)$ time, with rigorous error estimates. The concept of hierarchical matrices was developed (Hackbusch and Khoromskij, 2000; Hackbusch, 1999; Hackbusch and Börm, 2002; Börm et al., 2003) as an abstraction of those ideas. Hierarchical matrices provide a framework for efficiently computing with matrices that have large low-rank submatrices and have been successfully used as fast solvers for PDEs (Bebendorf, 2016, 2008). Despite their various favorable properties (including the existence of rigorous error estimates for a wide range of problems), the spread of these methods appears to have remained limited in the statistics community. Nevertheless, as recently described by Ambikasaran et al. (2016), these methods are well suited for many standard problems arising in Gaussian process statistics.

Although the approximation methods discussed above are all based on low-rank properties, there is another class of methods, often called covariance tapering, that artificially imposes sparsity by truncating long-range correlations (Furrer et al., 2006). This apparently crude approximation is empirically known to perform well (Chilès and Delfiner, 2012; Armstrong, 1998: Journel and Huijbregts, 1978). Furrer et al. (2006) asserts that the success of covariance tapering (despite the presence of large scale correlations) could be heuristically explained by a screening effect. The idea of this phenomenon, analysed theoretically by Stein (2002), is that strongly correlated random variables corresponding to distant points in space may become weakly correlated after conditioning on their neighbours (through a process of shielding). The iterative conditioning of a Gaussian process can be shown to be equivalent to computing the Cholesky decomposition of its covariance matrix and, as a result, screening is also a well-known phenomenon in the sparse Cholesky decomposition literature, where it forms the basis of nested dissection type algorithms (George, 1973). As opposed to artificially sparsifying the covariance matrix, Lindgren et al. (2011) use the correspondence between Matérn kernels and stochastic partial differential equations as observed by Whittle (1954, 1963). They construct a fine mesh, on which they discretise the elliptic PDE associated to the Matérn covariance function considered. By performing a nested dissection Cholesky decomposition of the stiffness matrix $L$, they obtain a computationally tractable form of $L^{-1}$, which is then used as a covariance operator. Here, the sparsity is inherited from the locality of the associated partial differential operator. Similar approaches based on direct approximation of the PDE associated to the Matérn kernel have been proposed by Roininen et al. (2011, 2013, 2014) in the context of Bayesian inverse problems. In a similar spirit, Stuart (2010) proposes the use of negative powers of “Laplacian-like” operators, where the size of the (possibly fractional) exponent parametrises possible a-priori beliefs regarding the smoothness of the target of estimation. Recent work in Spantini et al. (2017) shows that sparse generalised precision matrices even allow for the efficient representation of non-Gaussian random fields. This is achieved by generating sparse transport maps that map an i.i.d. Gaussian to the desired distribution. The above-mentioned idea of “conditional sparsity” leads to the next class of methods, which is often referred to as the method of inducing variables. As was observed in Quiñonero-Candela and Rasmussen (2005), these methods, implicitly or explicitly, cover a wide range of techniques for the sparse approximation of Gaussian processes. In fact, according to Quiñonero-Candela and Rasmussen (2005), many techniques for approximate estimation with a given prior in fact amount to exact estimation with an approximate prior. This approximate prior is usually such that marginalisation with respect to a few latent variables (which can, but need not, correspond to individual measurements) results in a sparse conditional distribution. The methods of Schwaighofer and Tresp (2003) and Snelson and Ghahramani (2006) fit into this framework. Titsias (2009) provides a variational approach for choosing induction variables. Stein et al. (2004) approximates densities via factorisations of conditional densities.

In a similar spirit, in Banerjee et al. (2008), predictive processes, suggested as approximations of the true process, arise from conditioning the initial process on parts of the data. Katzfuss (2016) applies this approximation hierarchically to obtain near-linear complexity approximations of the true process. Nychka et al. (2015) use hierarchies of basis functions that do not interact across scales. This idea is similar to that of using banded truncations of wavelet-transformed kernel matrices. Sang and Huang (2012) combine a low-rank model for global features with a tampered sparse covariance for small-scale interactions.

Hierarchical and multiresolution bases were introduced much earlier in numerical approximation theory (Daubechies, 1992; Mallat, 2009). We refer in particular to Beylkin et al. (1991) for the introduction of sparse wavelet based representations of integral operators. For a given approximation quality $\epsilon > 0$, this allows for compression of the integral matrix in a form that enables matrix-vector multiplication.
with complexity $O(N \log N)$ (for the standard form of the wavelet representation) or $O(N)$ (for the non-standard form).

Beylkin and Coult (1998), Beylkin (1998), and Gines et al. (1998) show how to exploit the sparsity-preserving property of the fine-to-coarse Cholesky decomposition of wavelet-based matrix representations of differential and integral operators. These methods rely on wavelets having a sufficiently high number of vanishing moments (i.e. their $L^2$ orthogonality with polynomials of a given order). For a large class of boundary integral operators, Dahmen et al. (2006) prove the optimal asymptotic complexity of wavelet-based compression; see also Stevenson (2009) for a recent overview. Gantumur and Stevenson (2006) and Harbrecht and Schneider (2006) discuss the details of the implementation of such schemes.

1.3 Our contribution and outline of the paper

Using the estimates of Owhadi and Scovel (2017), we will show that kernel matrices obtained from local measurements of Green’s functions, and represented in a multiresolution basis, have exponentially localised Cholesky factors. Given an symmetric positive-definite operator $T$ mapping a Banach space $B$ into its dual space $B^*$, the gamblet transform developed by Owhadi and Scovel (2017) computes operator adapted wavelets (so-called gamblets) that enable a block-diagonalisation of $T$ into sparse blocks of uniformly bounded condition number. These operator-adapted wavelets define a multiresolution decomposition of $B$ obtained through the transformation of a multiresolution decomposition of $B^*$ (i.e. a hierarchy of linearly nested elements of $B^*$). By removing the vanishing moments conditions on the multiresolution decomposition of $B^*$ — which Owhadi and Scovel (2017) use to prove that the blocks are uniformly well conditioned — we will extend the results of Owhadi and Scovel (2017) and show that, assuming the continuity of the Green’s function, a simple subsampling scheme can be used to produce the multiresolution decomposition of $B^*$ (required by the gamblet transform and our method). Therefore, the multiresolution representation of the kernel matrix used by our method corresponds to a simple permutation of its rows and columns and allows to compute an $\varepsilon$-accurate Cholesky factorisation of the kernel matrix just by subsampling and incomplete Cholesky factorisation, in complexity $O(N \log^2(N) \log^{2d}(N/\varepsilon))$ in time and $O(N \log(N) \log^d(N/\varepsilon))$ in space. As a result, given a target approximation error $\varepsilon$, only $O(N \log(N) \log^d(N/\varepsilon))$ entries need to be read (known) and those entries are solely determined by the locations of the evaluation points — in particular, they are independent of the underlying kernel. Furthermore, by stopping the factorisation at step $k$, one obtains the $k$ first components of a sparse approximate PCA of the covariance operator. Finally we will show that by inverting the order of elimination, one obtains a sparse factorisation of the precision matrix $\Theta^{-1}$. This leads to a direct solver for elliptic PDEs with rough coefficients, with complexity $O(N \log^2(N) \log^{2d}(N/\varepsilon))$ in time and $O(N \log^d(N) \log^{d^2}(N/\varepsilon))$ in space.

In Section 2 we introduce algorithms based on the exponential localisation of Cholesky factors and describe their emergence from the interplay between statistical estimation, Gaussian elimination and numerical homogenisation. In Section 3, we rigorously prove the decay of the Cholesky factors and the overall complexity of our algorithm under general conditions. In particular, we show that matrices obtained from Green’s functions of elliptic boundary value problems fulfill those general conditions if the density of the samples is homogeneous. In Section 4, we provide numerical illustrations of the exponential decay. Our numerical results are based on the popular Matérn kernels which, although strictly speaking not within the scope our our theoretical results, exhibit the exponential decay predicted by our theory, with the exception of points close to the boundary. Surprisingly, this also holds true for Matérn kernels corresponding to fractional order PDEs. We summarise our results in Section 5 and discuss their relations to other available numerical methods for the treatment of kernel matrices. To conclude, we provide a brief outlook on related topics for further investigation.

The scripts and Matlab functions that were used to create the numerical experiments described in this paper can be found at https://github.com/f-t-s/nearLinKernel.git
2 Description of the Algorithm

2.1 Setting

Let $\Theta \in \mathbb{R}^{I \times I}$ be a $I \times I$ symmetric positive-definite matrix. Assume that $\Theta$ is obtained as the Gram matrix of a positive-definite kernel $G: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$, i.e.

$$
\Theta_{i,j} := \int \int \phi_i(x)G(x,y)\phi_j(y) \, dx \, dy.
$$

where the $\phi_i$ are test functionals compact and disjoint support. In this section, we will use the one dimensional Matérn kernel with smoothness $1/2$ (i.e. $G(x,y) := \exp\left(-|x-y|/\rho\right)$) as our running example to describe the sequence of ideas leading to our algorithm. We will also use Dirac delta functions as test functionals, i.e. $\phi_i := \delta_{x_i}$ with a point cloud of $\{x_i\}_{1 \leq i \leq N} \subset [0,1]$ such that $x_1 = 0$, $x_N = 1$ and such that the ratio between the minimal and maximal spacing between consecutive points is bounded from above by $\delta_{\text{mesh}}$.

Inverting the resulting Gram matrix $\Theta$ by the standard Cholesky decomposition has computational complexity $O(N^3)$ in time and $O(N^2)$ in space. This is frequently referred to as the $O(N^3)$-bottleneck in Gaussian process statistics.

2.2 Disintegration of Gaussian measures and the screening effect

We will now show that the representation of the Gram matrix as the covariance matrix of centered Gaussian random vector can be used to used to improve the complexity of the standard Cholesky decomposition. Recall that, since $\Theta$ is symmetric and positive, there exists a centered Gaussian random vector $X$ with covariance matrix $\Theta$, i.e.

$$
E[X X^T] = \Theta.
$$

Recall that many integration problems in probability can be simplified by disintegration of measure. Consider for instance the problem of computing the expectation $f(X)$ by Monte Carlo methods. For an $X$-measurable random variable $Y$ we can write, using the tower property:

$$
E[f(X)] = E[E[f(X)|Y]].
$$

This means that instead of sampling the random variable $X$ directly, one can first sample $Y$ and then sample $(X|Y)$. The question at this point is, of course, whether this yields any reduction in complexity. Assume for instance that $Y$ is the Gaussian obtained by subsampling the $X$ at entries $i \in J$ and assume that $J$ is limited to a single element, i.e. $J = \{j\}$ for an element $j$ such that $x_j$ is close to $\frac{1}{2}$. Observe that $Y$ is then just a scalar Gaussian random variable, which can be easily sampled. We will now need the following standard fact about Gaussian random vectors (see Gallier (2010), and see Owhadi and Scovel (2015) for a generalisation):

**Lemma 2.1** (Conditioning of Gaussian random variables). Let $X$ be a centered Gaussian random vector on $\mathbb{R}^{n_1+n_2}$ with covariance matrix $C$. Assume that $X = (X_1, X_2)$ and the corresponding block decomposition of $C$ is

$$
C = \begin{pmatrix}
C_{1,1} & C_{1,2} \\
C_{2,1} & C_{2,2}
\end{pmatrix}
$$

For $x_2 \in \mathbb{R}^{n_2}$ it holds true that

$$
E[X_1|X_2 = x_2] = C_{1,2}C_{2,2}^{-1}x_2,
$$

$$
\text{Cov}[X_1X_1^T|X_2 = x] = C_{1,1} - C_{1,2}C_{2,2}^{-1}C_{2,1}.
$$

Let $Z = X - Y$ and consider the problem of sampling the Gaussian vector $(Z|Y)$. For our example, it can be observed that the conditional covariance between $Z_{x_1}$ and $Z_{x_2}$ given $Y$, i.e. $\text{Cov}[ZZ^T|Y]_{1,2}$, will be close to zero if $x_1$ and $x_2$ are on opposite sides of $x_j$. This implies that $\text{Cov}[ZZ^T|Y]$ has less than $N^2/2$ non-negligible entries. Since the main cost in sampling a Gaussian vector consists in inverting its covariance matrix, sampling from $(X|Y)$ might be considerably easier than sampling from $X$. 

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Observe that, by conditioning on \( Y \), we halve the number of nonzero entries in the covariance matrix. What happens to the other entries of \( \mathbb{E} \left[ \mathbb{E} \left[ XX^T | Y \right] \right] \)? Fixing the value at \( x_i \) seems to prevent values on opposite sides of it from communicating with each other. Given that the Matérn kernel is the Green’s function of a PDE (Whittle, 1954, 1963; Fasshauer, 2012) this should not come as a surprise, since conditioning on \( Y \) essentially creates two independent boundary value problems. Simple linear algebra shows that this effect can always be expected if the precision matrix \( \Theta^{-1} \) is (approximately) banded. This effect is a particular instance of the screening effect, long known in the spatial statistics community and analysed by Stein (2002). This screening effect can be understood as a spatial Markov property under which random variables at separate locations become independent after conditioning on the variables located in between them. The idea of exploiting conditional sparsity is not new and has been used to define inducing variables (Quiñonero-Candela and Rasmussen, 2005; Schwaighofer and Tresp, 2003) and predictive process approximation (Banerjee et al., 2008; Katzfuss, 2016).

### 2.3 Sparse Cholesky decomposition of dense matrices: fade-out instead of fill-in

The next idea leading to our algorithm is the equivalence of Cholesky decomposition and disintegration of Gaussian measures. The importance of this equivalence appears to have remained overlooked in the literature (apart from few instances such as Bickson (2008), where the equivalence between Cholesky decomposition and Bayesian belief propagation is explicitly used to develop a fast message passing algorithm for linear problems). In order to clarify this equivalence, we will continue working with our running example and assume that \( X^T = (Y^T, Z^T) \). Defining \( \Theta_{11} := \mathbb{E} [YY^T] \), \( \Theta_{12} := \mathbb{E} [YZ^T] \), and \( \Theta_{22} := \mathbb{E} [ZZ^T] \), we can then write

\[
\mathbb{E} [XX^T] = \begin{pmatrix} \Theta_{11} & \Theta_{12} \\ \Theta_{21} & \Theta_{22} \end{pmatrix} = \begin{pmatrix} \text{Id} & 0 \\ \Theta_{21} \Theta_{11}^{-1} & \text{Id} \end{pmatrix} \begin{pmatrix} \Theta_{11} & 0 \\ 0 & \Theta_{22} - \Theta_{21} \Theta_{11}^{-1} \Theta_{12} \end{pmatrix} \begin{pmatrix} \text{Id} & \Theta_{11}^{-1} \Theta_{12} \\ 0 & \text{Id} \end{pmatrix} = \begin{pmatrix} \text{Id} & 0 \\ \text{E}[Z|Y = \text{Id}] & \text{Id} \end{pmatrix} \begin{pmatrix} \text{Cov}[Y] & 0 \\ 0 & \text{Cov}[Z|Y] \end{pmatrix} \begin{pmatrix} \text{Id} & \text{E}[Z|Y = \text{Id}]^T \\ 0 & \text{Id} \end{pmatrix}.
\]

The last equality uses Lemma 2.1 and the abuse of notation \( \mathbb{E} [Z|Y = \text{Id}]_{i,j} := \mathbb{E} [Z_i|Y = e_j] \). Note that the above decomposition is the result of the first step of a (block-)Cholesky decomposition of \( \Theta \).

What happens if we pick a bisective ordering \( i_1, i_2, \ldots \) of the elements of \( I \) such that \( x_{i_1} \approx 1/2 \), \( x_{i_2} \approx 1/4 \), \( x_{i_3} \approx 3/4 \) and so on? Figure 2.1 shows that as we proceed with the Cholesky decomposition of \( \Theta \), the matrix becomes sparser. Instead of fill-in (i.e. the introduction of new nonzero entries), we observe a fade-out (i.e. the vanishing of previously nonzero entries).

Of course, our one-dimensional example has a very simple topology. How should we proceed when our test functions are living on a two-dimensional grid? The answer is to use a quadsection ordering as presented in Figure 2.2. We note that the orderings we proposed for the decomposition of \( \Theta \) are exactly the reverse of the well-known nested dissection orderings for the sparse Cholesky decomposition of sparse matrices (George, 1973; Lipton et al., 1979; Gilbert and Tarjan, 1987).

Indeed, this should not be surprise. Define \( A := \Theta^{-1} \) and assume that \( LL^T = \Theta \) is the Cholesky decomposition of \( \Theta \). Then

\[
A = (LL^T)^{-1} = L^{-T}L^{-1} \implies PAP = PL^{-T}PPL^{-1}P = (PL^{-T}P)(PL^{-T}P)^T,
\]

where \( P \) is the permutation matrix reversing the order of indices. Note that multiplying from left and right by \( P \) turns upper-triangular matrices into lower-triangular matrices and vice versa, while keeping the number of nonzero/nonsmall entries fixed. Therefore, the Cholesky decomposition of \( A \) with reverse elimination ordering is given by \( (PL^{-T}P)(PL^{-T}P)^T \).

Furthermore, we can write \( L^{-1} = L^{-1}L^T A = L^T A \). If \( A \) is sparse and has at most \( l \) entries per column, then multiplication of \( L^T \) with \( A \) will increase the number of nonzero entries by at most a factor of \( l \). Therefore, the sparsity of the Cholesky factors of \( \Theta \) with one ordering implies the sparsity of the Cholesky factors of \( A \) with the reverse order. We note that the converse is not true, as one can see by considering our one-dimensional example with the canonical ordering.

It is important to observe that the step \( \min(i, j) \) is the first time when the entry \( \Theta_{i,j} \) is used in the Cholesky decomposition. Therefore, if we know that \( \text{Cov} \left[ X_i, X_j \right] \{ \text{min}(i, j) \} \approx 0 \), we need neither
update nor even know the value $\Theta_{i,j}$. However, the set on which this is the case is only determined by the sparsity pattern of the precision matrix, not its actual value. Since this pattern is oftentimes known a-priori based upon its underlying geometric structure, it can be obtained before running the actual decomposition. This allows for the sparse factorisation of $\Theta$ in subquadratic space and subcubic time complexity if we have a good nested dissection ordering for the sparsity graph of $(\Theta)^{-1}$.

Algorithm 3: Sparse factorisation via reverse nested dissection ordering.

**Data:** A covariance matrix $\Theta \in \mathbb{R}^{I \times I}$, and a graph $(I, E)$ such that $\Theta_{i,j}^{-1} = 0$ for all $\{i, j\} \notin E$, as well as a thickness parameter $t$.

**Result:** A permutation matrix $P$ and a sparse lower-triangular matrix $L$, such that $PLL^T P^T = \Theta$.

Obtain reverse nested dissection ordering $P$ with separator thickness $t$. Denote its separator set by $T$.

Define the sparsity set $S := \{(i, j) | i$ and $j$ are connected in $(V, E)$ after removal of $\{k \in T | k < \min(i, j)\}\}$. Initialise the sparse matrix $M$ as all zero.

for $(i, j) \in S$ do

if $\Theta_{i,j} \neq 0$ then

$M_{i,j} \leftarrow \Theta_{i,j}$

else

$M_{i,j} \leftarrow \text{eps}$

end if

end for

$L \leftarrow \text{no fill-in incomplete Cholesky factorisation of } M$, with permutation $P$.

Here, the “thickness” $t$ of the dissection acts as a tuning parameter that we adjust depending on the expected bandwidth of the precision matrix. The algorithm, by the same argument given by George (1973) for the factorisation of sparse matrices, has $O(N^3/2)$ complexity in time and memory and $O(N \log N)$ complexity when using a two-dimensional regular mesh with $t$ fixed. Thus, this simple and apparently novel algorithm already beats the $O(N^3)$ bottleneck in spatial statistics, for sparse precision matrices. We refer to Lipton et al. (1979) and Gilbert and Tarjan (1987) for extensions of the nested dissection idea to more general graphs. Lipton et al. (1979) showed that the efficiency of nested dissection depends crucially on the existence of good separators, in the sense that many sparse graphs without good separators are not amenable to nested dissection. While there is a rich literature on methods aimed at preventing fill in when applying Cholesky decomposition to sparse matrices, we are not aware of any prior work where Cholesky decomposition was used as a mean to induce sparsity. The process of conditioning, which is implicit in our algorithm, can be seen as a particular choice of inducing points according to Quiñonero-Candela and Rasmussen (2005) or knot locations according to Katzfuss (2016) (where, however, the connections to sparse orderings for the Cholesky decomposition do not appear to have been observed). A closely related paper is Katzfuss (2016) which proposes a multiresolution sparse approximation of Gaussian processes, but does not use such approximations to obtain sparse matrix factorisations. Katzfuss (2016) describes good performance results in the one-dimensional setting, attributes them to the screening effect and suggests to choose the knots close to the boundaries of a partition of the space (in a way that is similar to nested dissection). However, Katzfuss (2016) does not seem to mention that nested dissection orderings and sparse precision matrices would imply an exact sparse representation of the Gaussian process, also in higher dimensions. In closely related work, Lindgren et al. (2011) first approximate the precision matrix by a discretisation of the differential operator corresponding to the Matérn covariance function. Then they use Cholesky decomposition with a nested dissection ordering to obtain the a sparse representation of the covariance operator. Based on the above arguments, for sufficiently regular sampling locations, one can instead obtain a sparse approximation by applying Cholesky factorisation with the reverse of their ordering to the covariance matrix. This avoids the explicit approximation of the precision matrix, although it might prove less stable when dealing with an inhomogeneous density of sampling points.

So far we have proposed an algorithm for the Cholesky decomposition of kernel matrices with sparse inverses and a few problems remain to be addressed:
Figure 2.1: Sparsification by Bisection. As the Cholesky decomposition progresses, the entries of the remaining values (shown on a log$_{10}$-scale) diminish.

Figure 2.2: Sparsification by Quadsection. The top row shows the magnitude of the entries of $\Theta$ (in log$_{10}$ scale) as the quadsective Cholesky decomposition progresses. The bottom row shows (in yellow) the positions of the indices that have been eliminated.

(i) Good nested dissection orderings do not always exist. In fact, the complexity of the algorithm given above is $O(N^{3/2})$ for two-dimensional meshes and deteriorates rapidly for higher-dimensional meshes.

(ii) The covariance matrix is usually not the inverse of a discretised partial differential operator (i.e. a sparse matrix) but is oftentimes obtained by sampling and taking local averages of the Green’s function of a partial differential equation. Can the precision matrix still be approximated by a sparse matrix?

The solutions to these problems can be found in the recent literature on numerical partial differential equations, as we will see in the next section.

2.4 Compression, inversion and approximate PCA using gamblets

In order to resolve the above-mentioned difficulties, we will use the theory of gamblets, recently introduced by Owhadi (2017) and generalised by Owhadi and Scovel (2017). Although their setting is similar to ours, it is originally motivated by the problem of solving

$$\mathcal{L}u = f,$$

where $\mathcal{L}$ is the inverse of $G$ in the sense that $\mathcal{L} \int G(x,y)f(y) = f(x)$ (i.e., from the statistical point of view, $\mathcal{L}$ is the precision operator associated to the covariance function $G$). For the sake of clarity, we will temporarily adopt the more restricted setting of Owhadi (2017), where $\mathcal{L}$ is a second-order elliptic partial
differential operator in divergence form, i.e. \( \mathcal{L}u(x) = -\text{div} (a(x)\nabla u(x)) \). We note that many covariance functions with finite smoothness are the Green’s functions of such partial differential operators. For instance, the popular Matérn kernel with smoothness \( \nu \) in dimension \( d \) is the Green’s function of an elliptic partial differential equation of order \( 2\nu + d \) on \( \mathbb{R}^d \), when \( \nu + d \) is an integer (Whittle, 1954, 1963; Lindgren et al., 2011; Hou and Zhang, 2017; Fasshauer, 2012).

The Galerkin (e.g. finite element) discretisation of the above equation leads to large sparse systems of linear equations. Iterative solvers such as conjugate gradient descent or the Gauss–Seidel smoother can exploit the sparsity of the discrete system. However, their convergence rate depends on the condition number of the matrix, which for partial differential equations grows as a negative power of the mesh size. Multi-grid methods (Fedorenko, 1961; Brandt, 1977; Hackbusch, 1978, 2013) are a popular way of circumventing this problem via multiscale approximations iteratively communicating via interpolation/restriction operators (the main difficulty is the identification of good interpolation operators).

Other (e.g. finite element) discretisation of the above equation leads to large sparse systems of linear equations. Iterative solvers such as conjugate gradient descent or the Gauss–Seidel smoother can exploit the sparsity of the discrete system. However, their convergence rate depends on the condition number of the matrix, which for partial differential equations grows as a negative power of the mesh size. Multi-grid methods (Fedorenko, 1961; Brandt, 1977; Hackbusch, 1978, 2013) are a popular way of circumventing this problem via multiscale approximations iteratively communicating via interpolation/restriction operators (the main difficulty is the identification of good interpolation operators).

Owhadi (2017) formulates the identification of good interpolation operators and the problem of computing with incomplete information as zero-sum adversarial games played against the missing information. Optimal strategies for such games are mixed (randomised) strategies, which form a saddle point for the underlying minimax problem (Owhadi and Scovel, 2017), and are identified by placing an optimal prior distribution on the solution space of the differential operator. Using this prior, the problem of estimating fine scale features of the solution based on computation on a coarser grid can then be cast as a Bayesian estimation problem.

Statistical approaches to numerical analysis are not new (Poincaré, 1987; Diaconis, 1988; Sul’din, 1959; Larkin, 1972; Sard, 1963; Kimeldorf and Wahba, 1970; Shaw, 1988; O’Hagan, 1991, 1992). However, they have in the past received little attention, and the possibilities offered by combining numerical uncertainties/errors with model uncertainties/errors (Chkrebtii et al., 2016; Owhadi, 2015; Hennig et al., 2015; Perdikaris et al., 2016; Raisi et al., 2017b; Cockayne et al., 2017) are stimulating the reemergence of such methods (Skilling, 1992; Chkrebtii et al., 2016; Schober et al., 2014; Owhadi, 2015; Hennig, 2015; Hennig et al., 2015; Briol et al., 2015; Conrad et al., 2016; Raisi et al., 2017a,b; Owhadi, 2017; Cockayne et al., 2016; Perdikaris et al., 2016; Owhadi and Scovel, 2017; Cockayne et al., 2017) where solutions of PDEs and ODEs are randomised and numerical errors are interpreted in a Bayesian framework as posterior distributions. This reemerging field is sometimes referred to as probabilistic numerics (Hennig et al., 2015) or Bayesian numerical analysis (Diaconis, 1988; Owhadi, 2015) from the Bayesian perspective or computational information games from the game-/decision-theoretic perspective (Owhadi, 2015; Owhadi and Scovel, 2017).

From a Bayesian perspective, the process of randomization in probabilistic numerical methods (Cockayne et al., 2017) corresponds to placing a prior a distribution on the solution space of \( \mathcal{L} \) (i.e. a prior probability distribution on the true solution \( u \)) and conditioning on a family of linear measurements \( [\phi_i^{(k)}, u] \) encoding the process of computing with partial information at a given resolution. From the decision-theoretic perspective this prior distribution is obtained as an optimal mixed strategy for the adversarial recovery of \( u \) given the measurements \( [\phi_i^{(k)}, u] \) (Owhadi, 2015; Owhadi and Scovel, 2017).

Here, \( \langle \cdot, \cdot \rangle \) denotes the duality product between an element of a Banach space (second variable) and an element of its dual (first variable). Following Owhadi (2015, 2017), in the case of multisolution methods for elliptic PDE, these functionals can be chosen as indicators functions on the elements of a nested partition of the physical domain such that (1) for some \( \delta > 0 \) and \( h \in (0,1) \), each \( \tau_i^{(k)} \) is contained in a ball of diameter \( h^k \) and contains a ball of diameter \( \delta h^k \), and (2) each \( \tau_i^{(k)} \) is the union of some elements \( \tau_j^{(k+1)} \).

Note that the nesting of the subsets \( \tau_i^{(k)} \) implies that of the functionals \( \phi_i^{(k)} \), i.e. there exists matrices \( \pi^{(k,l)} \) such that \( \phi_i^{(k)} = \sum_j \pi^{(k,l)}_{i,j} \phi_j^{(l)} \), for \( k < l \). When the relative error in operator norm \( [\mathcal{L}u, u]^{\frac{1}{2}} \) is used as a loss function for the adversarial recovery problem mentioned above, the optimal mixed strategy is solely determined by the operator norm (in particular it is independent from the functionals \( \phi_i^{(k)} \)). This optimal mixed strategy (optimal prior) is the Gaussian field with covariance function \( G \) (Owhadi and Scovel, 2017), defined as a linear isometry mapping the dual of the solution space, endowed with the dual norm of the operator norm, onto a Gaussian space.

The corresponding best guess for the solution \( u \), given the measurements \( \phi_i^{(k)} \) is therefore the conditional expectation \( \mathbb{E}[u| \phi_i^{(k)}, u] \). Defining the so-called gamblets \( \psi_i^{(k)} := \mathbb{E}[u| \phi_i^{(k)}, u] = \delta_{i,j} \) as the
elementary conditional expectations assigned to \( \phi^k_i \), one can write \( \mathbb{E}[u|\phi^k_i, u] = \sum_j [\phi^k_j, u] \psi^k_j \).

Now, we want to split the solution space in a direct sum of gamblets on different levels. To this end, for \( k \geq 2 \), introduce the matrices \( W^{(k)} \) such that \( \text{im}(W^{(k)}) = \ker(\pi^{(k-1)}) \) and \( \sum_j W_{i,j}^{(k)} \phi^k_j = 0 \) for all \( i \) and \( l \). As shown in Owhadi (2017), the \( W^{(k)} \) can be chosen such that the diameter of the support of \( \phi_i^{(k),\chi} := \sum_j W_{i,j}^{(k)} \phi_j^k \) is of order \( h^{k} \). Then we define \( \chi_k := \sum_j W_{i,j}^{(k)} \psi^k_j \). The results in (Owhadi, 2017, Theorem 3.11) show that the \( \psi^k_i, \chi^k \) decay exponentially, at the \( h^{k} \) scale, away from \( \tau^k_i \) and that the stiffness matrices \( A^{(k)}_{i,j} := [\mathcal{L}\phi^k_i, \phi^k_j] = \langle \mathcal{L}\phi^k_i, \phi^k_j \rangle_{L^2}, B^{(k)}_{i,j} := [\mathcal{L}\chi^k_i, \chi^k_j] = \langle \mathcal{L}\chi^k_i, \chi^k_j \rangle_{L^2} \) are exponentially decaying as

\[
A^{(k)}_{i,j} \leq C \exp \left( -\frac{\gamma \min \{ \text{dist}(\tau^k_i, \tau^k_j) \} }{h^k} \right),
\]

\[
B^{(k)}_{i,j} \leq C \exp \left( -\frac{\gamma \min \{ \text{dist}(\tau^k_i, \tau^k_j) \} }{h^k} \right).
\]

Furthermore Owhadi (2017, Theorem 4.17) shows that the matrices \( A^{(k)} \) and \( B^{(k)} \) have uniformly bounded condition numbers. Using these results Owhadi (2017) obtains an near linear time hierarchical algorithm for the nested computation of gamblets and for solving elliptic PDE with rough coefficients.

In Subsection 2.3 we have argued that the \textit{screening effect} of conditioning translates to sparse Cholesky decompositions. Therefore it seems promising to use the estimates of Owhadi (2017) and Owhadi and Scovel (2017) to obtain sparse Cholesky decompositions of covariance matrices.

The \( \phi^k_i,\chi \) define a multiresolution decomposition of \( \text{span}\{\phi^l_i\} \). It follows directly from the definition of the gamblets that, for \( l > k \),

\[
\mathbb{E}\left[ [\phi^l_i,\chi, u] | [\phi^k_j, u] = \delta_{i,j} \right. \text{ for all } j] = [\phi^l_i,\chi, \phi^k_j].
\]

Furthermore, some basic linear algebra yields that

\[
\text{Cov}\left[ [\phi^k_i,\chi, u] | [\phi^k_j, \phi^k, u] | [\phi^k_j, \phi^k, u] \right. \text{ for all } i, j] = (B^{(k)})^{-1}.
\]

Define the matrices \( H^{(k)} \) by \( \phi^k_i,\chi = \sum_j H^{(k)}_{i,j} \phi^q_j \) and the \( q \times 1 \) block matrix \( (H_{i,j})_{i,j} := H_{i,j}^k \), for \( k \leq l \). Let us for simplicity assume that the \( W \) and \( \pi \) are such that \( \mathcal{H} \) is an orthogonal matrix. Define the \( q \times q \) block matrix \( \Gamma \) as \( \Gamma^{l,k}_{i,j} := (H^{(k)} \Theta H^{(l)} \mathcal{T})_{i,j} \). We obtain the following algorithm:
Algorithm 4: Sparse block-factorisation via Gamblet transform.

**Data:** A covariance matrix $\Theta$, and a multiresolution basis $\mathcal{H}$.

**Result:** An exponentially localised triangular block matrix $L$ and a block-diagonal, exponentially localised matrix $D$ such that the condition numbers of the blocks $D_{k,k}$ are uniformly bounded, the exponentially localised lower-triangular block-diagonal Cholesky factor of $D$, $L^D$, such that $\Theta = \mathcal{H}^T L D L^T \mathcal{H} = \mathcal{H}^T L L^D L^D, T \mathcal{H}$, and a matrix $\Psi$ that contains in its columns a discretisation of the gamblets associated to the operator $A$.

Initialise $L$ as a block-identity matrix (an identity matrix divided into blocks according to the levels of $\mathcal{H}$), $D$ as a block-zero matrix (an all zero matrix divided into blocks according to the levels of $\mathcal{H}$);

$\Gamma \leftarrow \Theta \mathcal{H}^T$;

for $k \leftarrow 1$ to $q-1$ do

\begin{align*}
L_{k,k}^D & \leftarrow \text{CHOL} (\Gamma_{k,k}); \\
D_{k,k} & \leftarrow \Gamma_{k,k}; \\
\Gamma_{k+1,q,k+1,q} & \leftarrow \Gamma_{k+1,q,k+1,q} - \Gamma_{k+1,q,k} \left( L_{k,k}^D \Gamma_{k,k} \right)^{-1} \Gamma_{k,k+1,q}; \\
\Psi & \leftarrow LH; \\
L_{q,q}^D & \leftarrow \text{CHOL} (\Gamma_{q,q}); \\
D_{q,q} & \leftarrow \Gamma_{q,q};
\end{align*}

The estimates of Owhadi and Scovel (2017) show that, up to exponentially small entries, the matrices in the above algorithm will be sparse according to a pattern known a priori. Therefore a fast (near-linear complexity) version of Algorithm 4, can be obtained by restricting the computation the the known sparsity patterns and the resulting factorisation allows for near-linear time inversion of $\Theta$. Furthermore, the columns of $\Psi$ have the form $\psi_{i,j} = \left[ \phi_{i}^{(q)}, \psi_{j}^{(k)} \right]$, if the index $j$ is part of the $k$th level of the multiresolution basis. Hence, they contain a discretisation of the gamblets $\psi_{i,j}^{(k)}$. As mentioned in Owhadi and Scovel (2017) and exploited for low-rank compression of operators in Hou and Zhang (2017), the gamblets provide an approximation of the principal components of the operator $G$. In particular, in Hou and Zhang (2017) it was conjectured that gamblets can also be computed directly from the covariance operator. Algorithm 4, with computation restricted to the near-sparsity patterns, provides a method for achieving this computation in near linear time based on and following the initial basis transformation. Algorithm 4 has nearly linear complexity if computation is reduced to the patterns of approximate sparsity of the gamblets, furthermore the relationship to the \textit{gamblet transform} of Owhadi (2017) and Owhadi and Scovel (2017) is transparent. We will see in the next section that, analogously to the nested dissection, the decay estimates for gamblets also imply the sparsity of the hierarchical Cholesky decomposition. This leads to the following, simpler algorithm:

Algorithm 5: Zero fill-in Cholesky on $S$ in multiresolution basis

**Data:** A covariance matrix $\Theta \in \mathbb{R}^{I \times I}$, a multiresolution basis $\mathcal{H}$ (ordered from coarse to fine) and a set $S \subseteq I \times I$

**Result:** A sparse lower-triangular matrix $L$ such that $\Theta = \mathcal{H}^T L L^T \mathcal{H}$

Initialise $\Gamma$ by $\Gamma_{i,j} = \Theta_{i,j}$, for $(i,j) \in S$ and $\Gamma_{i,j} = 0$, else;

$\Gamma \leftarrow \mathcal{H}^T \mathcal{H}$;

$L \leftarrow \text{ICHOL}(\Gamma, S)$;

Here, ICHOL $(\Gamma, S)$ denotes the Cholesky factorisation, where every read or write operation involving entries of the complement of $S$ is skipped, as described in Algorithm 8. Typically, if the size of the support of $\phi_{i}^{(k)}$ is of the order of $h^k$, then choosing the sparsity pattern $S$ as

$$S_{\rho} := \left\{ (i,j) \in J^{(k)} \times J^{(l)} \mid \text{dist} \left( \text{supp} \left( \phi_{i}^{(k)} \right), \text{supp} \left( \phi_{j}^{(l)} \right) \right) \leq \rho h^{\min(k,l)} \right\},$$

this leads to a matrix $L$ of size $S_{\rho} \times S_{\rho}$.
results in the exponential decay of the approximation error $\|\Gamma - LL^T\|$ as a function of $\rho$. Let $i^{(k)}$ be the last index on level $k$ of the multiresolution basis. Then define the $L^k := L_{i^{(k)},i^{(k)}}$. The operator $L^{(k)}L^{(k)T}$ then provides us with a low-rank approximation of the operator $\Theta$ corresponding to the one obtained by projecting onto the space spanned by the gamblets $\psi_{i,k}^{(k)}$, at scale $k$. We note that if we only want the principal components of this approximate sparse PCA, we can simply stop the Cholesky decomposition prematurely. As in Algorithm 3, we only need compute those entries of $\Gamma$ that lie on the sparsity pattern.

Although the complexity of the nested dissection algorithm deteriorates for $d > 1$, the proposed incomplete Cholesky decomposition remains of $O(N \text{polylog}(N))$ complexity in any spatial dimension $d$ (with the order of the polylog depending on $d$).

In Owhadi and Scovel (2017), the results of Owhadi (2017) were generalised to the abstract setting of bounded operators on Banach spaces (including arbitrary continuous linear bijections from $H^s$ to $H^{-s}(\Omega)$). Although the proof of exponential decay of gamblets provided in Owhadi and Scovel (2017) allows for very general measurement functions $\phi^{(k)}_i$ (including Dirac masses, indicator functions and higher-order polynomials, see also Hou and Zhang (2017) for strongly elliptic PDEs with higher-order polynomials as measurement functions), the proof Owhadi and Scovel (2017) that the matrices $B^{(k)}$ have uniformly bounded condition numbers rely on vanishing moments of the underlying multiresolution basis. That is, they rely on the property that

$$\int_{\Omega} p \sum_{j \in I^{(k)}} \left( W^{(k)} \pi^{(k,q)} \right)_{i,j} \phi^{(q)}_j \, dx = 0$$

for all $p \in \mathcal{P}_{2s-1}$ and for $\text{diam}(\Omega^{(k)}_i) \approx h^k$, if $\Theta$ arises from the Green’s function of an elliptic partial differential operator of order $2s$. This has a number of disadvantages:

(i) The user, who might be given $\Theta$ just in the form of a matrix, has to specify the estimated order of the differential operator $a$-priori. Furthermore, for unstructured grids, the construction of $\pi$ and $W$ might be complex.

(ii) The matrices $H^{(k)}$ might need to have columns with many nonzero entries, corresponding to averages over large regions. While in the integral equations arising in numerical analysis it is usually possible to evaluate the Green’s function at arbitrary points, allowing to use exponentially convergent quadrature formulae (Harbrecht and Schneider, 2006; Gantumur and Stevenson, 2006), this need not be the case in statistical applications, where unstructured grids are common. Therefore, the computation of the relevant entries of $\Gamma$ to machine precision will typically not be possible in near-linear time.

(iii) The dependence on vanishing polynomials makes it more difficult to identify measurement functions on geometries other than $\mathbb{R}^d$.

2.5 A simple algorithm: subsampling, reordering and zero-fill in incomplete Cholesky decomposition

The explicit requirement that measurement functions have vanishing polynomial moments is an unnecessary limitation. We will, in Section 3.5.1, generalize the results of Owhadi and Scovel (2017) by relaxing the condition that measurement functions have vanishing polynomial moments used in Section 3.5.1 to show that the condition numbers of $B^{(k)}$ are uniformly bounded. Under this generalization, the piecewise constant measurement functions of Owhadi (2017) can be proven to be sufficient for operators of arbitrary order. Furthermore, as a consequence of this generalization, in situations where pointwise measurements are defined (i.e., solutions are continuous), subsampling can be used as trivial aggregation scheme. If the grid spacing on the finest level is of order $h^s$, then coarse measurement functions on level $k$ are then obtained from a subset of measurement functions with grid spacing of order $h^k$, as illustrated in Figure 2.4.

Therefore the basis transform $\mathcal{H}$ in the above algorithm reduces to a permutation matrix and the orthogonalized gamblets are simply a subset of the original gamblets on the same level.

$$\left\{ \chi_i^{(k)} \right\}_{i \in J^{(k)}} = \left\{ \psi_i^{(k)} \right\}_{i \in I^{(k)}} \setminus \left\{ \psi_i^{(k-1)} \right\}_{i \in I^{(k-1)}}.$$
Figure 2.4: Aggregation by Subsampling: This figure, taken from Owhadi and Scovel (2017), shows the simple form that the $\pi(k,l)$ and $W^{(k)}$ take under subsampling.

As in the introductory example of Section 1, if the $\phi_i^{(q)}$ are localised around points $\{x_i^{(q)}\}_{i \in I^q} \subset \Omega \subset \mathbb{R}^d$ with spacing $\approx h^q$, then we can split $I := I^{(q)}$ into disjoint sets $J^{(k)}$ for $1 \leq k \leq q$ such that, for a constant $\delta_{\text{mesh}}$,

$$\max_{x \in \Omega} \min_{j \in J^{(k)}} \text{dist}(x, x_j) \leq h^{-k};$$

$$\min_{i,j \in \cup_{1 \leq l \leq k} J^{(l)}} \text{dist}(x_i, x_j) \geq \delta_{\text{mesh}} h^{-k}.$$

Then, $H$ is simply given by the permutation matrix $P$, which orders the indices from $J^{(1)}$ to $J^{(q)}$, with arbitrary ordering within each $J^{(k)}$. As in the introduction, we define $S_\rho := \{(i,j) \in J^{(k)} \times J^{(l)} \mid \text{dist}(x_i, x_j) \leq \rho h^{\min(k,l)}\}$.

Our algorithm is now straightforward:

**Algorithm 6:** Zero fill-in Cholesky on $S$, typically applied to an $S$ similar to $S_\rho$ as defined above.

**Data:** A covariance matrix $\Theta \in \mathbb{R}^{I \times I}$, a permutation matrix $P$ and a set $S \subset I \times I$

**Result:** A sparse lower-triangular matrix $L$ such that $\Theta = P^T L L^T P$

Initialise $\Gamma$ by $\Gamma_{i,j} = \Theta_{i,j}$, for $(i,j) \in S$ and $\Gamma_{i,j} = 0$, else;  
$\Gamma \leftarrow P \Gamma P^T$;  
$L \leftarrow \text{ICHOL}(\Gamma, S)$;

Here, ICHOL $(\Gamma, S)$ is the Cholesky factorisation of $\Gamma$ ignoring operations involving entries $(i,j) \notin S$. We note that, as before, we can obtain the first $k$ components of an approximate sparse PCA of $G$, by stopping the Cholesky algorithm after $k$ iterations.

In Theorem 3.53, we show that for kernel matrices arising from elliptic boundary values with order $s > d/2$, $S$ and $P$ can be chosen such as to provide an $\varepsilon$-accurate Cholesky factorisation in complexity $\mathcal{O}(N \log^2(N) \log^{2d}(N/\varepsilon))$ in time and $\mathcal{O}(N \log(N) \log^d(N/\varepsilon))$ in space.
2.6 Reordering revisited, and a simple algorithm for solving elliptic PDE with rough coefficients

Just as in our first approach to finding an ordering for the sparsifying Cholesky decomposition of the dense matrix $\Theta$ turned out to be the reverse of the well-known nested dissection ordering, the multiresolution ordering used in Algorithm 6 is reminiscent of the minimum degree heuristic of George and Liu (1989). The minimum degree heuristic consists in the elimination, at each step, of the remaining index with the lowest degree, according to the sparsity graph. After restricting $\Theta$ to the hierarchical sparsity pattern used in Algorithms 4 and 6, our elimination ordering actually corresponds to a maximum, or reverse minimum degree ordering. The difference with the case of nested dissection, however, is that the graph by which we are choosing our maximum degree ordering is not the graph given by the nearest neighbour relations between the degrees of freedom. Once we have found this hidden graph according to which the maximum degree ordering leads to near-optimal results, we may again ask if we can invert the precision matrix using the reverse ordering. Indeed, just as in the case of the nested dissection ordering, one can show that the Cholesky decomposition of $\Theta^{-1}$ is exponentially localised when performed in the minimum degree ordering according to $S$.

From the point of view of the numerical resolution of PDEs one usually starts with the precision operator $\mathcal{L}$. Using a Galerkin method (Braess, 2007; Bernardi et al., 2004), the equation

$$\mathcal{L} u = f$$

can be discretised by introducing a finite-dimensional subspace $V$ of the solution space $\im \mathcal{L}^{-1}$, and looking for $u_V \in V$ such that

$$\langle v, \mathcal{L} u_V \rangle_{L^2} = \langle v, f \rangle_{L^2} \quad \text{for all } v \in V.$$  

This is just a finite dimensional system of linear equations which, picking a basis of $V$, can be written as

$$Ax = b.$$  

If $A^{-1}$ were a Gram matrix of the Green’s function, then our results would immediately imply a near linear Cholesky factorisation of $A$. Since the results of Owhadi and Scovel (2017) hold for the discrete operator defined by the numerical discretization of $\mathcal{L}$ (using a stable method), our incomplete Cholesky with a minimum degree ordering on $S$ also provides a simple near-linear complexity algorithm for solving elliptic PDE with rough coefficients. Although the fine-to-coarse multiresolution Cholesky decomposition was suggested by Gines et al. (1998), their theoretical results relied on multiresolution bases with order $p + 1$ vanishing moments to achieve algebraic localisation of order $p + 1$. In contrast, we can prove exponential decay without any need for vanishing moments. Again, we are lacking a sufficiently strong stability estimate for the incomplete Cholesky factorisation to prove rigorously the error estimates for the element-wise Cholesky factorisation. It seems as if such an estimate would also be required for the approach following Gines et al. (1998), but we could not find it in the literature.

3 Analysis of the Algorithm

3.1 Setting and notation

In this subsection we present the abstract setting, in which we will prove the exponential decay of Cholesky decompositions. Let $I^{(q)} \equiv I$ be an index set and $\Theta^{(q)} \equiv \Theta \in \mathbb{R}^{I^{(q)} \times I^{(q)}}$ be a symmetric positive-definite matrix. Assume that we are given families of index sets $I^{(1)}, \ldots, I^{(q-1)}$ and matrices $\pi^{(k,l)} \in \mathbb{R}^{I^{(k)} \times I^{(l)}}$ such that $\pi^{(k,l)} \pi^{(l,s)} = \pi^{(k,s)}$, $\pi^{(k,l)} = \pi^{(l,k)} T$, and $\pi^{(k,k)} = \text{Id}_{I^{(k)}}$. Let $J^{(1)}, \ldots, J^{(q)}$ and $J := \bigcup_{1 \leq k \leq q} J^{(k)}$, where we order the indices from $J^1$ to $J^q$ and let $W^{(k)} \in \mathbb{R}^{J^{(k)} \times I^{(k)}}$. Now define $\Theta^{(k)} := \pi^{(k,q)} \Omega^{(q)} \pi^{(q,k)}$ and $A^{(k)} := \Theta^{(k)} \pi^{(k,l)}$. Also define, for $k \leq l$, $H^{(k,l)} := W^{(k)} \pi^{(k,l)}$ and

$$H^{(k,l)} := \begin{pmatrix} H^{(1,l)} \\ \vdots \\ H^{(k,l)} \end{pmatrix}$$

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notations will allow us to keep track of the order of averaging and inversion of the various submatrices. With the notation from Section 3.1, for any Lemma 3.1. In this subsection, we will, based on algebraic properties, formulate the block Cholesky decomposition. 3.2 The Cholesky decomposition. Following, all block matrices will be with respect to $J^{(k)}$, $J^{(l)}$ and for such block matrices we will write $M_{r,s,n,m}$ for the concatenation of the blocks $M_{k,l}$ for $k \in \{r, \ldots, s\}$ and $l \in \{n, \ldots, m\}$. The above notations will allow us to keep track of the order of averaging and inversion of the various submatrices appearing in our algorithm.

At this point we only assume $\Theta$ to be positive definite. Over the course of this section we will prove the exponential decay of its Cholesky factors, by gradually introducing additional structure: (i) In Section 3.2, we will obtain a representation of a block-Cholesky decomposition of $\Gamma = \Gamma^{(q)}$ based on its linear algebraic structure. (ii) In Section 3.3, we introduce a notion of hierarchical pseudodistance, which assigns to each pair of indices in $J \times J$ a notion of distance, adapted to the scale of the two indices. Using the fact that it fulfills a generalised triangle inequality, we can show that the Cholesky factors of $\Gamma$ are exponentially decaying, under conditions on the exponential decay and condition numbers of submatrices forming the characterisation obtained in Section 3.2. Those conditions will be satisfied based on the properties of gamblets presented in Owhadi and Scovel (2017).

(iii) In Section 3.4, we prove the error- and complexity estimates for the incomplete Cholesky factorisation implied by the exponential decay of the Cholesky factors. (iv) In Section 3.5 we extend the theory developed by Owhadi (2017) and Owhadi and Scovel (2017) to drop the requirement of vanishing moments in the proof of bounded condition numbers. We then use this theory to prove that the conditions identified in Section 3.3 are fulfilled for kernel matrices arising from appropriate measurement functionals of Green’s functions associated to elliptic boundary value problems. (v) In Section 3.6, we put together the results of our previous section for three important classes of kernel matrices. (vi) In Section 3.7, we comment on two byproducts of our theory and algorithm, notably the factorisation of precision matrices and the approximate sparse PCA.

3.2 The Cholesky decomposition

In this subsection, we will, based on algebraic properties, formulate the block Cholesky decomposition in the basis given by the matrices $\mathcal{H}^{(k,l)}$. As a first step we consider only two scales:

Lemma 3.1. With the notation from Section 3.1, for any $1 \leq n \leq q$, we have the following matrix identity:

$$\Gamma^{(n)} = \begin{pmatrix} \Gamma^{(n)}_{1:1,k}\Gamma^{(n)}_{1:k+1:k} \Gamma^{(n)}_{1:k+1,1:k} \Gamma^{(n)}_{1:k+1,1:k+1} \end{pmatrix} = LDL^T$$

with

$$L = \begin{pmatrix} \text{Id}_{J^{(1,k)}} & 0 & \text{Id}_{J^{(1,k)}} & 0 \\ \Gamma^{(n)}_{k+1:n,1:k} & \Gamma^{(n)}_{k+1:n,1:k}^{-1} & \text{Id}_{J^{(1,k+1,n)}} \end{pmatrix} = \begin{pmatrix} \text{Id}_{J^{(1,k)}} & 0 \end{pmatrix} B^{(n)}_{k+1:n,1:k} \text{Id}_{J^{(1,k+1,n)}}$$

and

$$D = \begin{pmatrix} \Gamma^{(n)}_{1:k,1:k} & 0 \\ 0 & \Gamma^{(n)}_{k+1:n,1:k} - \Gamma^{(n)}_{k+1:n,1:k} \text{Id}_{J^{(1,k+1,n)}}^{-1} \Gamma^{(n)}_{1:k,1:k} \end{pmatrix} = \begin{pmatrix} \Gamma^{(n)}_{1:k,1:k} & 0 \\ 0 & \text{Id}_{J^{(1,k+1,n)}}^{-1} \end{pmatrix}$$

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Proof. The first equality for $L$ and $D$ is just the ordinary block Cholesky factorisation. For the second inequality, we define $M_{1,1} := B_{[1:k],[1:k]}$, $M_{1,2} := B_{[1:k],[k+1:n]}$, $M_{21} := B_{[k+1:n],[1:k]}$ and $M_{22} := B_{[k+1:n],[k+1:n]}$. Now we can verify by simple matrix multiplication that

$$
\begin{pmatrix}
B_{1,1} & B_{1,2} \\
B_{2,1} & B_{2,2}
\end{pmatrix}
\begin{pmatrix}
(B_{1,1} - B_{1,2}B_{2,2}^{-1}B_{2,1})^{-1} & -B_{1,1}^{-1}B_{1,2} (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1} \\
-B_{2,2}^{-1}B_{2,1} (B_{1,1} - B_{1,2}B_{2,2}^{-1}B_{2,1})^{-1} & (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1}
\end{pmatrix}
= \text{Id}
$$

From this we can conclude

$$
\Gamma^{(n)} = \begin{pmatrix}
(B_{1,1} - B_{1,2}B_{2,2}^{-1}B_{2,1})^{-1} & -B_{1,1}^{-1}B_{1,2} (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1} \\
-B_{2,2}^{-1}B_{2,1} (B_{1,1} - B_{1,2}B_{2,2}^{-1}B_{2,1})^{-1} & (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1}
\end{pmatrix}.
$$

Inserting the above into the Schur complement yields

$$
\Gamma^{(n)}_{[k+1:n],[k+1:n]} - \Gamma^{(n)}_{[1:k],[1:k]} \left( \Gamma^{(n)}_{[1:k],[1:k]} \right)^{-1} \Gamma^{(n)}_{[1:k],[k+1:n]} = (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1} - B_{2,2}^{-1}B_{2,1}B_{1,1}^{-1}B_{1,2} (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1} = (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1} + B_{2,1}^{-1} (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2}) (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1} = B_{2,2}^{-1} (B_{2,2} - B_{2,1}B_{1,1}^{-1}B_{1,2})^{-1} = B_{2,2}^{-1}.
$$

This proves the characterisation of $D$, and the expression for $L$ follows from an analogous calculation.

We remind the reader of the following well-known quotient property of the Schur complement:

**Lemma 3.2** (Quotient property: Crabtree and Haynsworth (1969)). Given a block matrix

$$
N := \begin{pmatrix} A & B \\ C & D \end{pmatrix}
$$

Write its Schur complement with respect to the block $A$ as

$$(N/A) := D - CA^{-1}B.
$$

Then for a block matrix

$$
M := \begin{pmatrix} A & B \\ D & E \\ C & F \end{pmatrix}
$$

we have

$$
\left( \begin{pmatrix} A & B \\ D & E \end{pmatrix} / A \right) = \left( \begin{pmatrix} A & B \\ C & F \end{pmatrix} / A \right).
$$

**Remark 3.3.** In terms of jointly Gaussian vectors $(X, Y, Z)$, the quotient property is the following tower rule for covariance:

$$
\text{Cov}[Z|X,Y] = \text{Cov}[(Z|X)|(Y|X)].
$$

Now we can proceed to prove the following theorem:

**Theorem 3.4.** We have the following decomposition:

$$
\Gamma^{(q)} = LDL^T
$$

with $L$ and $D$ defined as:

$$
D = \begin{pmatrix}
B_{1,1}^{(1)} & 0 & \cdots & \cdots & 0 \\
0 & B_{2,2}^{(1)} & \ddots & 0 & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\vdots & 0 & \cdots & B_{q-1,q-1}^{(q-1)} & 0 \\
0 & 0 & \cdots & 0 & B_{q,q}^{(q)}
\end{pmatrix},
$$

$$
L = \begin{pmatrix}
B_{1,1}^{(1)} & 0 & \cdots & \cdots & 0 \\
0 & B_{2,2}^{(1)} & \ddots & 0 & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\vdots & 0 & \cdots & B_{q-1,q-1}^{(q-1)} & 0 \\
0 & 0 & \cdots & 0 & B_{q,q}^{(q)}
\end{pmatrix}.
$$
and

\[
L = \begin{pmatrix}
\text{Id} & 0 & \cdots & 0 \\
B_{2,2}^{(2)} & \text{Id} & \cdots & 0 \\
& \ddots & \ddots & \vdots \\
& & \ddots & \text{Id} \\
B_{q,q}^{(q)} & B_{q,1}^{(q)} & \cdots & \text{Id}
\end{pmatrix}^{-1} = \begin{pmatrix}
\text{Id} & 0 & \cdots & 0 \\
L_{2,1} & \text{Id} & \cdots & 0 \\
& \ddots & \ddots & \vdots \\
& & \ddots & \text{Id} \\
L_{q,1} & L_{q,2} & \cdots & L_{q,q-1} \text{Id}
\end{pmatrix},
\]

where

\[
L_{i,j} := \sum_{k=1}^{j} \Gamma_{i,k}^{(q)} B_{k,j}^{(q)} = \sum_{k=1}^{j} \Gamma_{i,k}^{(q)} \left( \Gamma^{(q)} \right)^{-1}_{k,j}.
\]

This decomposition is in particular the one obtained by successive block-Cholesky factorisation of \( \Gamma^{(q)} \).

Proof. Applying Lemma 3.1 to \( \Gamma^{(n)} \) with \( k = n - 1 \) successively successively for \( n \) ranging from \( q \) to 2, we obtain the following decomposition:

\[
\begin{pmatrix}
\Gamma_{1,1}^{(q)} & \cdots & \Gamma_{1,q-1}^{(q)} & \Gamma_{1,q}^{(q)} \\
\vdots & \ddots & \vdots & \vdots \\
\Gamma_{q-1,1}^{(q)} & \cdots & \Gamma_{q-1,q-1}^{(q)} & \Gamma_{q-1,q}^{(q)} \\
\Gamma_{q,1}^{(q)} & \cdots & \Gamma_{q,q-1}^{(q)} & \Gamma_{q,q}^{(q)}
\end{pmatrix}
\begin{pmatrix}
0 \\
-\Gamma_{1,1}^{(q-1)} - \Gamma_{1,q-1}^{(q)} - \Gamma_{1,q}^{(q)} \\
\vdots \\
-\Gamma_{q-1,1}^{(q-1)} - \Gamma_{q-1,q-1}^{(q)} - \Gamma_{q-1,q}^{(q)} \\
\Gamma_{q,q-1}^{(q)} - \Gamma_{q,q}^{(q)}
\end{pmatrix}
\begin{pmatrix}
0 \vdots 0 \\
0 \vdots 0 \\
\vdots \\
0 \vdots 0 \\
0 \text{Id}
\end{pmatrix}
\]

Now we want to characterise the triangular factors in the above equation. Using the well-known charac-
terisation of inverses of elementary triangular matrices, we obtain:

\[
\begin{pmatrix}
\text{Id} & B_{1,2}^{(2)} & 0 \\
0 & \text{Id} & \vdots \\
0 & \ldots & \text{Id}
\end{pmatrix}
\cdots
\begin{pmatrix}
B_{1,q-1}^{(q-1)} & B_{q-1,q-1}^{(q-1),-T} & 0 \\
0 & \ldots & 0 \\
0 & \ldots & \text{Id}
\end{pmatrix}
\begin{pmatrix}
\text{Id} & B_{1,q}^{(q)} & 0 \\
0 & \ldots & 0 \\
0 & 0 & \text{Id}
\end{pmatrix}
=\begin{pmatrix}
B_{1,q}^{(q),-T} & B_{q,q}^{(q),-T} & 0 \\
0 & \ldots & 0 \\
0 & 0 & \text{Id}
\end{pmatrix}
\]

This provides us with the first characterisation of the triangular factors of the decomposition. To obtain the second factor, we calculate

\[L D L^T = \Gamma^{(q)} \iff L^T = D^{-1} L^{-1} \Gamma^{(q)}\]

from this follows the second characterisation of L. To show that this is the same factorisation that would be obtained by a block-Cholesky factorisation, we can deduce from the quotient property of Schur complements that the block-Cholesky factorisation leads to the same diagonal part. Since the Cholesky factorisation is unique, this shows that the factorisation obtained by the block-Cholesky algorithm is the same as the one we obtained above.

3.3 Exponential decay

Up until now, we have only used the algebraic structure of the operator in order to find an alternative expression of its block-Cholesky decomposition in a given basis.

These expressions are useful because they provide a method for employing the decay estimates obtained in Owhadi (2017) and Owhadi and Scovel (2017) to prove that these matrices are nearly sparse. Most theories on the propagation of sparsity or exponential decay of matrices under operations like multiplication use the distance induced by the sparsity graph of the initial sparse matrix.

One difficulty that we have to deal with is that interactions between i, j in J depends on the levels of the two indices. In particular, our notion of distance can not fulfill the triangle inequality, since the indices on the coarsest level are interacting with every other index. When modelling the kind of decay featured by gamblets, we can enforce the triangle inequality between indices i, j, s only if the coarsest level involved is one of the endpoints. This restricted triangle inequality turns out to be the right compromise to model the decay of gamblets, while still allowing to control its propagation under multiplication and inversion.

Definition 3.5. A function d: I^{(q)} × I^{(q)} → \mathbb{R} is called a hierarchical pseudometric if

(i) \(d(i,j) \geq 0\) for all \(i,j \in I^{(q)}\);
(ii) \(d(i,i) = 0\) for all \(i \in I^{(q)}\);
(iii) \(d(i,j) = d(j,i)\) for all \(i,j \in I^{(q)}\);
(iv) for all \(1 \leq k \leq q\), the restriction of d to \(J^{(k)} \times J^{(k)}\) is a metric;
(v) for all $1 \leq k \leq m, l \leq q$ and $i_k \in I^{(k)}, j_l \in I^{(l)}, s_m \in I^{(m)}$, we have $d(i_k, j_l) \leq d(i_k, s_m) + d(s_m, j_l)$.

The estimates in Owhadi (2017) and Owhadi and Scovel (2017), as generalised in the next section, imply that the following conditions hold true for a wide range of kernel matrices. We will for now take them for granted and elaborate on their scope in the next section.

**Condition 3.6 (Localised conditional expectations).** We say that $\Gamma$ has localised conditional expectations for constants $C, \gamma$ with respect to the hierarchical pseudometric $d$, if, for all $1 \leq k < l \leq q$ and $i, j \in J$,

$$\left| \left( \Gamma^{q}_{k+1:q,1:k} \Gamma^{(k),-1} \right)_{i,j} \right| \leq C \exp(-\gamma d(i,j)) \quad (3.1)$$

and for all $1 \leq k \leq q$:

$$\left| \left( \Gamma^{(k),-1} \right)_{i,j} \right| \leq C \exp(-\gamma d(i,j))$$

**Condition 3.7 (Hierarchically bounded condition numbers).** We say that $\Gamma^{(q)}$ has hierarchically uniformly bounded condition number if there exists a $\kappa > 0$ such that

$$\text{cond} \left( B^{(k)}_{k,k} \right) \leq \kappa \text{ for all } 1 \leq k \leq q.$$  

We note that (3.1) immediately implies the exponential localisation of $L$ as in Theorem 3.4 according to $d$.

**Lemma 3.8.** Assume $\Gamma$ satisfies (3.1) with constants $\gamma, C$. Then we have

$$(L_{i,j}) \leq \tilde{C} \exp(-\gamma d(i,j))$$

where $\tilde{C} := \max(1, C)$

**Proof.** We can show the result blockwise. Clearly, it holds true for the blocks on and above the diagonal. For the blocks below, we notice that

$$L_{k,l} := \sum_{m=1}^{l} \Gamma^{(q)}_{k,m} B^{(l)}_{m,l} = \left( \Gamma^{(q)}_{1:q,1:l} \Gamma^{(l),-1} \right)_{k,l}$$

where the $k$ and $l$ are blocks, not entries. This is a submatrix of the matrix in equation (3.1), and hence has the desired decay. \qed

As a next step, we will want to show that the matrix $D$ has a Cholesky decomposition that decays according to $d$. To this end, we will need to preserve the locality of $B^{(k)}_{k,k}$ under inversion. There exist, in fact, a number of results saying, roughly, that well-conditioned localised matrices have localised inverses. These kinds of results have partly been phrased in a more abstract setting as the closedness of certain algebras (Jaffard, 1990; Krishtal et al., 2015), or more concretely providing non-asymptotic decay estimates (Demko et al., 1984). A general strategy by which those results are proven, is to use approximation theory to approximate the function $x \mapsto x^{-1}$ by polynomials of order $N$, up to a term of order $c^{-N}$. Then, one can control the spread of the localisation when applying the polynomial to the original matrix. In the following we will need some very minor extensions of existing results of this kind.

First we need to find a way to control the localisation of the product of localised matrices. To this end, define:

$$c_{1,I,d}(\gamma) := \sup_{j \in J} \sum_{i \in I} \exp(-\gamma d(i,j))$$

and define $c_{l,d} := c_{1,I,d}$. We then need the following lemma (Jaffard, 1990), and which we only reprove for the sake of providing the constants.
Lemma 3.9. Let $I_k$ be index sets for $1 \leq k \leq n + 1$ and let $d: I_1 \cup \cdots \cup I_n \times I_1 \cup \cdots \cup I_n \to \mathbb{R}_{\geq 0}$ satisfy the following triangle-type inequality for $i_k \in I_k$:

$$d(i_1, i_{n+1}) \leq \sum_{k=1}^{n} d(i_k, i_{k+1})$$

Let $A_k \in \mathbb{R}^{I_k \times I_{k+1}}$ for $1 \leq k \leq n$ be such that $|A_{i,j}| \leq C_k \exp(-\gamma d(i,j))$. Then

$$\left(\prod_{k=1}^{n} A_k\right)_{i,j} \leq \left(\prod_{k=1}^{n} C_k\right) \left(\prod_{k=2}^{n} c_{I_k, I_{k+1}, d} (\gamma/2)\right) \exp\left(-\frac{\gamma}{2} d(i,j)\right).$$

Proof. Set $i_1 \colonequals i$, $i_{n+1} \colonequals j$. We then have

$$\left(\prod_{k=1}^{n} A_k\right)_{i,j} \leq \left(\prod_{k=1}^{n} C_k\right) \sum_{i_2, \ldots, i_{n-1} \in I} \exp\left(-\gamma \sum_{k=1}^{n} d(i_k, i_{k+1})\right) \leq \left(\prod_{k=1}^{n} C_k\right) \exp\left(-\frac{\gamma}{2} d(i_1, i_{n+1})\right) \sum_{i_2, \ldots, i_{n-1} \in I} \exp\left(-\frac{\gamma}{2} \sum_{k=1}^{n} d(i_k, i_{k+1})\right) \leq \left(\prod_{k=1}^{n} C_k\right) \left(\prod_{k=2}^{n} c_{I_k, I_{k+1}, d} (\gamma/2)\right) \exp\left(-\frac{\gamma}{2} d(i,j)\right).$$

Now, we can proceed by proving the exponential decay of inverses by polynomial approximation of $x \mapsto x^{-1}$. Again, the proof is essentially taken from Jaffard (1990), we only keep track of constants. The results of Demko et al. (1984) are not immediately applicable since our matrices are not banded, but only exponentially localised.

Lemma 3.10. For any symmetric positive-definite $A \in \mathbb{R}^{I \times I}$ with $A_{i,j} \leq C \exp(-\gamma d(i,j))$,

$$(A^{-1})_{i,j} \leq \frac{\|A\| + \|A^{-1}\|}{2} \exp\left(-\frac{2 \log(1 - r)}{2} + \log(C)\right) \leq \frac{\|A\| + \|A^{-1}\|}{2} \exp\left(-\frac{2 \log(1 - r)}{(1 + \log(C)) - \log(r)} + \log(C)\right) \leq \frac{\|A\| + \|A^{-1}\|}{2} \exp\left(-\frac{2 \log(1 - r)}{(1 + \log(C)) - \log(r)} + \log(r) \frac{\gamma}{2} d(i,j)\right) \leq \frac{\|A\| + \|A^{-1}\|}{2(1 - r)^2} \exp\left(-\frac{2 \log(1 - r)}{(1 + \log(C)) - \log(r)} + \log(r) \frac{\gamma}{2} d(i,j)\right)$$

where $C_R \colonequals \max\left\{1, \frac{2C}{\|A\| + \|A^{-1}\|}\right\}$ and $r \colonequals \frac{1 - \frac{\|A\| + \|A^{-1}\|}{2}}{1 + \frac{\|A\| + \|A^{-1}\|}{2}}$.

Proof. Define $R \colonequals \text{Id} - \frac{2}{\|A\| + \|A^{-1}\|} A$. Then we have $\|R\| \leq \frac{1 - \frac{\|A\| + \|A^{-1}\|}{2}}{1 + \frac{\|A\| + \|A^{-1}\|}{2}} =: r$. Writing now:

$$A = \frac{2}{\|A\| + \|A^{-1}\|} (\text{Id} - R) \implies A^{-1} = \frac{\|A\| + \|A^{-1}\|}{2} \sum_{k=0}^{\infty} R^k$$

using positive definiteness of $A$, we obtain:

$$R_{i,j} \leq \max\left\{1, \frac{2C}{\|A\| + \|A^{-1}\|}\right\} \exp(-\gamma d(i,j))$$

Define $C_R \colonequals \max\left\{1, \frac{2C}{\|A\| + \|A^{-1}\|}\right\}$. Based on Lemma 3.9, we have

$$R_{i,j}^k \leq (c_{I,d}(\gamma/2))^{k-1} C_R^k \exp\left(-\frac{\gamma}{2} d(i,j)\right)$$
Combining the above estimates leads us to the estimate:
\[
\frac{2}{\|A\| + \|A^{-1}\|} (A^{-1})_{i,j} \leq (n+1) (c_{I,d} (\gamma/2))^{n-1} C_R^n \exp \left( - \frac{\gamma}{2} d(i,j) \right) + r^{n+1} \frac{1}{1-r}
\]
\[
\leq \exp \left( (1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) (n+1) - \frac{\gamma}{2} d(i,j) \right) + \exp (- \log(1-r) + \log(r)(n+1))
\]

If we want to balance the two terms, we would like to choose:
\[
n + 1 = \frac{\gamma}{2} d(i,j) - \log(1-r) + \log(r) (n+1)
\]
yielding
\[
\exp \left( (1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) (n+1) - \frac{\gamma}{2} d(i,j) \right) + \exp (- \log(1-r) + \log(r)(n+1))
\]
\[
= \exp \left( - \log(1-r) (1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) + \log(r) \frac{\gamma}{2} d(i,j) \right)
\]
\[
\frac{(1 + \log (c_{I,d} (\gamma/2)) + \log (C_k))}{(1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) - \log(r)}
\]

Since we have the constraint to choose \( n + 1 \) as an integer strictly bigger than 0, we have to increase \( n + 1 \) by up to a value smaller than one, compared to the above. This can be estimated by multiplying with another factor of \( - \log(1-r) (1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) \), leading to the first two inequalities of the result. By optimising over \( (1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) \), we obtain the result. \( \square \)

With the above tools, we can now prove the exponential decay of the Cholesky factors of \( D \). The following lemma appears in similar form in Benzi and T˚ uma (2000) for the case of banded matrices and in Krishtal et al. (2015), without explicit constants.

**Lemma 3.11.** Let \( B \in \mathbb{R}^{I \times I} \simeq \mathbb{R}^{N \times N} \) be symmetric and positive definite with \( B_{i,j} \leq C \exp (- \gamma d(i,j)) \) for a pseudometric \( d \) on \( I \). Then the Cholesky decomposition of its inverse \((B)^{-1} = LL^T\) is such that

\[
L_{i,j} \leq \sqrt{\frac{\|B\| (\|B\| + \|B^{-1}\|)}{2(1-r)^2}} \exp \left( \frac{\log(r)}{(1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) - \log(r)} \frac{\gamma}{2} d(i,j) \right)
\]

where \( C_R := \max \{ 1, 2C, \frac{2C}{\kappa} \} \) and \( r := \frac{1-\kappa}{1+\kappa} \).

Results similar to the one above have already been used to prove the near-sparsity of well-conditioned (near-)sparse matrices in Benzi and T˚ uma (2000) and Krishtal et al. (2015). We provide a separate proof because the first result is restricted to banded matrices and the second does not provide decay constants.

**Proof.** We will show the result by looking showing that for all \( 1 \leq k \leq N \), the \( k^{th} \) column of \( L \) when considered as an element of \( \mathbb{R}^{I \times I} \) by zero padding, satisfies the exponential decay. Define, \( S^{(k)} := B_{k:n,k:n} - B_{k:n,k-1} (B_{1:k-1,1:k-1})^{-1} B_{1:k-1,k:n} \). Then \( L_{[k:N],k} = \frac{S^{(k)} \Gamma}{\sqrt{S^{(k)} \Gamma}} \). Using Lemma 3.1, we see that \( S^{(k)} (B_{[k:n],[k:n]})^{-1} \), and hence it follows from Lemma 3.10 that

\[
\left( S^{(k)} \right)_{i,j} \leq \frac{\|B\| + \|B^{-1}\|}{2} \exp \left( \frac{\log(r)}{(1 + \log (c_{I,d} (\gamma/2)) + \log (C_k)) - \log(r)} \frac{\gamma}{2} d(i,j) \right)
\]

Here we made use of the facts that the spectrum of \( B_{k:n,k:n} \) is contained in the spectrum of \( B \), that the maximal and minimal eigenvalue of \( B \) appear interchangeably or in the form of the condition number, and that the right-hand side of the above estimate is increasing in \( r \) and \( C_R \). Using the estimate \( S^{(k)}_{k,k} \geq \frac{1}{\|S^{(k)}\|_{\infty}} \geq \frac{1}{\|B\|} \), we obtain the result. \( \square \)
With the above preparation we can now show the near sparsity of the Cholesky decomposition of a near sparse matrix. For all Cholesky decompositions in the following, we use an elimination ordering $\prec$ on $J$, such that for $i \in J^{(k)}, j \in J^{(l)}$, and $k < l$, we have $i \prec j$.

**Theorem 3.12.** Let $\Gamma$ be fulfill Condition 3.6 with respect to the hierarchical pseudometric $d$, with constants $\gamma, C$, and let it fulfill Condition 3.7, with constant $\kappa$. Define furthermore $C_R := \max \{1, 2C, \frac{2C}{\kappa}\}$ and $r := \frac{1 - \kappa}{1 + \kappa}$ and:

$$\tilde{C}_k := \sqrt{\|\Gamma^{-1}\| (\|\Gamma\| + \|\Gamma^{-1}\|)}$$

and

$$\tilde{\gamma} = \frac{\log(r)}{(1 + \log(c_{J,d}(\gamma/2)) + \log(C_k)) - \log(r)}$$

Then the matrix block $D_{k,k}$ of the matrix $D$ as in Theorem 3.4 has a Cholesky decomposition $D_{k,k} = \bar{L}^{(k)}_{L}^{(k) T}$ such that

$$|\bar{L}_{i,j}^{(k)}| \leq \tilde{C}_k \exp(-\tilde{\gamma}d(i,j))$$

And the element-wise Cholesky decomposition $\Gamma = \bar{L}^{T}$ is localised as:

$$|\bar{L}_{i,j}| \leq \max_k \{c_{J,i,d}(\gamma/2)\} C \exp(-\frac{\gamma}{2}d(i,j))$$

**Proof.** The decay of $D_{k,k}$ follows by applying Lemma 3.11 to the matrices $B_{k,k}^{(k)}$. The decay of $\bar{L}$ follows then by writing the blocks $\bar{L}_{k,l} = L_{k,l} \bar{L}^{(l)}$, where $L_{k,l}$ is chosen as in Theorem 3.4 and applying Lemma 3.9.

**Remark 3.13.** We point out that the exponential decay of the Cholesky factors can be shown if in Condition 3.6, only exponential decay of the matrices $A^{(k)}$ is provided. This can be done by looking at the characterisation of $L$ as the inverse of a block- lower-triangular matrix in Theorem 3.4. We note that this implies that $L^{-1}$ is exponentially decaying. By writing $L = \text{Id} + \sum_{k=1}^{\infty} (-1)^k L^{-k}$ as its Neumann series and noticing that this series converges after the first $q$ elements because of the nilpotency of $L^{-1} - \text{Id}$, we can obtain the exponential decay of $L$ using Lemma 3.9.

### 3.4 Computational complexity and error estimates

#### 3.4.1 Computational complexity of the incomplete factorisation

In the above section we have proven conditions, under which the Cholesky decomposition of a matrix is exponentially localised. While this is already enough to obtain a compression of the matrix by truncating the exponential tail of the entries, it is not a-priori sufficient to provide us with a linear algorithm. For the Cholesky-decomposition, however, sparsity of the resulting factorisation translates very naturally to low algorithmic complexity. We remind ourselves that the algorithm for Cholesky decomposition is as follows:

**Algorithm 7:** Cholesky decomposition

```plaintext
input : A positive-definite $N \times N$ matrix $\Theta$
output: A lower-triangular $N \times N$ matrix $L$.
for $i \leftarrow 1$ to $N$ do
    for $j \leftarrow i$ to $N$ do
        $L_{i,j} \leftarrow \Theta_{i,j}$
for $i \leftarrow 1$ to $N$ do
    for $j \leftarrow i + 1$ to $N$ do
        $L_{[j:N],j} \leftarrow L_{[j:N],j} - L_{[j:N],i} L_{j,i} / L_{i,i}$
        $L_{i:N,i} \leftarrow L_{[i:N],i} / \sqrt{L_{i,i}}$
```
Assume now that we want to restrict computation to a subset $S \subset J \times J$. Defining $S_\ell(i) \equiv \{(i, j) \in S \mid i \leq j\}$, $S_\ell(i) \equiv \{(i, j) \in S \mid i < j\}$, $S_{\ell+1}(i) \equiv \{(i, j) \in S \mid i \geq j\}$, and $S_{\ell}(i) \equiv \{(i, j) \in S \mid i > j\}$, we can compute the Cholesky decomposition restricted to $S$, as:

\textbf{Algorithm 8:} Cholesky decomposition restricted to $S$

\begin{verbatim}
input : A positive-definite $N \times N$ matrix $\Theta$ and a sparsity set $S$
output: A lower-triangular $N \times N$ matrix $L$, with support contained in $S$
for $i \leftarrow 1$ to $N$ do
  for $j \in S_{\ell}(i)$ do
    $L_{i,j} \leftarrow \Theta_{i,j}$
for $i \leftarrow 1$ to $N$ do
  for $j \in S_{\ell}(i)$ do
    $L_{S_{\ell}(i),j} \leftarrow L_{S_{\ell}(i),j} - L_{S_{\ell}(i),l}L_{j,l}/L_{i,i}$
    $L_{S_{\ell}(i),i} \leftarrow L_{S_{\ell}(i),i}/\sqrt{L_{i,i}}$
\end{verbatim}

We first analyse the computational complexity of the algorithm.

\textbf{Lemma 3.14.} The restricted Cholesky decomposition can be computed in $O(\#S) = O\left(\sum_{i=1}^{N} \#S_{\ell}(i)\right) = O\left(\sum_{i=1}^{N} \#S_{\ell}(i)\right)$ space- and $O\left(\sum_{i=1}^{N} \sum_{j \in S_{\ell}(i) \#S_{\ell}(j)}\right) = O\left(\sum_{i=k}^{N} \sum_{j \in S_{\ell}(k) \#S_{\ell}(j)}\right)$ time complexity.

\textbf{Proof.} The first equality can be read directly from the pseudocode for Algorithm 8. For the second equality, we notice that the index $(k, j)$ is updated during the line $L_{S_{\ell}(i),i} \leftarrow L_{S_{\ell}(i),i}/\sqrt{L_{i,i}}$, whenever $j \in S_{\ell}(k)$. Each such $j$, in turn, appears in the innermost loop whenever $i \in S_{\ell}(j)$. \hfill $\square$

In order to apply the result to our Cholesky decomposition, we define for $i \in J^{(k)}$ the downward ball of radius $\rho$:

$$B_{\rho,\downarrow}(i) := \{ j > i \mid d(i, j) < \rho \}.$$  

With this notation, the complexity of the incomplete Cholesky decomposition is easily described as follows:

\textbf{Corollary 3.15.} The incomplete Cholesky decomposition as described in Theorem 3.12 has memory usage bounded above by $\sum_{i \in J^{(k)}} \#B_{\rho,\downarrow}(i)$ and the number of read and write operations it needs to perform is bounded from above by $\sum_{i \in J^{(k)}} \sum_{j \in B_{\rho,\downarrow}(i)} \#B_{\rho,\downarrow}(j)$.

\textbf{Proof.} The result follows since $B_{\rho,\downarrow}(i) = S_{\ell}(i)$, for $S := \{(i, j) \mid d(i, j) \leq \rho\}$. \hfill $\square$

In order to bound this complexity, we need to make further assumptions regarding the size of the $B_{\rho,\downarrow}(i)$. A possible condition under which we obtain near-linear complexity is the following:

\textbf{Condition 3.16.} We say that $J, d$ fulfill the low dimensionality condition if there exist $C_{d, d > 0}$, such that for all $1 \leq k \leq q$, $i \in J^{(k)}$ and $\rho > 0$, we have

$$\#J^{(k)} \cap B_{\rho,\downarrow}(i) \leq C_{d}d^d$$

\textbf{Condition 3.17.} We say that $J, d$ fulfill the balance condition, if there exists a $C > 0$, such that for all $1 \leq l \leq q$ and $i \in J^{(k)}$, we have

$$\#B_{\rho,\downarrow}(i) \cap J^{(l)} \leq C \frac{\#J^{(l)}}{\#J^{(k)}}$$

Under the above conditions, the complexity of the incomplete Cholesky decomposition is near linear:

\textbf{Theorem 3.18.} Assume that $J, d$ fulfill Conditions 3.16 and 3.17. The memory cost of the decomposition in Theorem 3.12 is bounded above by $qCC_{d}d^{d}\#J$ and the number of read and write operations it performs is bounded by $(qCC_{d}d^{d})^{2} \#J$.
Proof. For \(i \in J^{(k)}\), \(B_{\rho,i}(i) = \bigcup_{j \in J^{(k)} \cap B_{\rho,i}(j)} B_{0,i}(j)\). Therefore, for \(i \in J^{(k)}\) and \(l \geq k\),

\[
\#J^{(l)} \cap B_{\rho,i} \leq CCd\rho^d \frac{\#J^{(l)}}{\#J^{(k)}}.
\]

From this we conclude

\[
\sum_{i \in J} \sum_{j \in B_{\rho,i}(i)} \sum_{k=1}^{q} \sum_{l=1}^{\#N} \#B_{\rho,i}(j) \leq \sum_{k=1}^{q} \sum_{l=1}^{\#N} \sum_{r=1}^{J^{(l)}} \sum_{l=1}^{J^{(r)}} \#B_{\rho,i}(j) \leq \sum_{k=1}^{q} \sum_{l=1}^{\#N} \sum_{r=1}^{J^{(l)}} \sum_{l=1}^{J^{(r)}} qCCd\rho^d \frac{\#J^{(r)}}{\#J^{(k)}} = qCCd\rho^d \#J.
\]

By applying the above argument twice, we obtain the bound on the time complexity:

\[
\sum_{i \in J} \sum_{j \in \#B_{\rho,i}(i)} \#B_{\rho,i}(j) = \sum_{k=1}^{q} \sum_{l=1}^{\#N} \sum_{r=1}^{J^{(l)}} \sum_{l=1}^{J^{(r)}} \#B_{\rho,i}(j) \leq \sum_{k=1}^{q} \sum_{l=1}^{\#N} \sum_{r=1}^{J^{(l)}} \sum_{l=1}^{J^{(r)}} qCCd\rho^d \frac{\#J^{(r)}}{\#J^{(k)}} \leq qCCd\rho^d \#J.
\]

\[\square\]

Remark 3.19. We point out that the above theorem does not treat the question of how to trace the sparsity pattern during the algorithm. This can however be done using standard tree-like constructions and we will comment more on this topic in the next section.

### 3.4.2 Stability of the incomplete factorisation

In this section, we want to prove a stability result for the incomplete Cholesky factorisation that allows us to bound the error propagation over the course of the factorisation. Naively applying perturbation bounds for Schur complements on every step leads to a multiplicative error of order \(cN\) for some constant \(c\) and is thus not enough to guarantee stability. In order to rigorously prove the stability, we will rely on two main ideas. First, on each scale \(k\), sufficiently separated parts of \(J^{(k)}\) will not interact with each other that is the nonzero sets of the respective columns of the sparsity pattern are disjoint. Therefore, when eliminating these indices, no amplification of error is taking place. Second, for points that are very close to each other, a minor increase of the sparsity pattern can introduce dense submatrices into the sparsity pattern. These blocks can be dealt with by applying only once the error estimate for the dense Cholesky factorisation. Because of the these two mechanisms, the number of factors of \(c\) can be reduced to a manageable amount. Since the first mechanism improves with \(\rho\) becoming small and the latter improves with \(\rho\) becoming large, the power of \(c\) can be bounded uniformly in \(\rho\).

**Definition 3.20** (Supernodes). Let \(J = \bigcup_{i=1}^{q} J^{(k)}\) be an index set and \(S \subset J \times J\) a symmetric sparsity pattern. A supernodal decomposition consists of an ordering \(\prec\) of the elements of \(J^{(q)}\), called the supernodal ordering and a set of disjoint subsets \(N^{(k)}_m \subset J^{(k)}\) of each of the \(J^{(k)}\) such that for \(i \prec j\) and \(i, j \in N^{(k)}_m\), we have:

\[
(i, j) \in S \implies (i, j) \in S.
\]

the subsets \(N^{(k)}_m\) are then called supernodes (on level \(k\)).

**Remark 3.21.** Each supernode corresponds submatrix of the sparsity pattern \(S\) with a dense lower-triangular part, which in turn can be seen as a grouping of similar behaving nodes together to one
representative node. While we are using it for theoretical purposes, supernodes have been used for efficient implementations of sparse Cholesky factorisation, since the inclusion of dense submatrices allows for the use of highly optimised dense matrix BLAS in the implementation Rothberg and Gupta (1994); Liu et al. (1993).

**Definition 3.22** (Multicolor ordering). Let \( J = \bigcup_{k=1}^{q} J^{(k)} \) be an index set and \( S \subset J \times J \) a symmetric sparsity pattern with a supernodal decomposition given by \( \{ \mathcal{N}_i^{(k)} \}_{1 \leq i \leq n_k} \) and the corresponding supernodal ordering. Assume that each \( J^{(k)} \) can be written as the disjoint union of \( n_k \) supernodes \( \{ \mathcal{N}_i^{(k)} \}_{1 \leq i \leq n_k} \). Let us now assume that for all \( k \), each \( \mathcal{N}_i^{(k)} \) can be colored in one of \( p \) colors, such that supernodes \( \mathcal{N}_n^{(k)} \) of the same color do not interact, i.e.

\[
i \in \mathcal{N}_n^{(k)}, j \in \mathcal{N}_n^{(k)} \implies (i, j) \notin S.
\]

Then, a multicolor ordering \( \prec \) of the elements of \( J \) is an ordering as follows:

(i) Indices are labeled from coarse to fine. First all \( i \in J^{(1)} \) then all \( i \in J^{(2)} \) etc.

(ii) On each level, indices are ordered by color. First all the indices contained in red supernodes, then all blue supernodes etc.

if \( \prec \) is also a valid supernodal ordering for the supernodes \( \{ \mathcal{N}_i \}_{1 \leq i \leq n_k} \), it is called a *supernodal multicolor ordering*.

**Remark 3.23.** Again, while we are merely using it as a theoretical device, the above ordering can be seen as a generalisation of the well-known red-black ordering. In particular it can be seen as a level-wise application of blockwise multicolor ordering as in Iwashita and Shimasaki (2003). While this ordering would also be suitable to induce parallelisation into the factorisation, the resulting independence between different supernodes will allow us obtain to better control the error propagation in the incomplete factorisation.

For a factorisation using a multicolor ordering with \( p \) colors, the amount of error propagation can be bounded in terms of \( p \). To this end, we will introduce a slightly strengthened version of condition 3.7.

**Condition 3.24** (Strengthening of hierarchically bounded condition numbers). We say that \( \Gamma^{(q)} \) has

\[
\frac{\lambda_{\max}\left(\Gamma_{[k,q],[k,q]}^{(q)}\right)}{\lambda_{\min}\left(\frac{\Gamma_{[k,q],[k,q]}^{(q)}}{\Gamma_{[1,k],[1,k]}^{(q)}}\right)} \leq \kappa,
\]

where \( \Gamma_{[k,q],[k,q]}^{(q)}/\Gamma_{[1,k],[1,k]}^{(q)} \) denotes the Schur complement.

**Lemma 3.25.** Let \( J = \bigcup_{k=1}^{q} J^{(k)} \) be an index set, \( S \subset J \times J \) a symmetric sparsity pattern and \( \prec \) a supernodal multicolor ordering with \( p \) colors. Let \( L \) be a lower-triangular matrix with zero entries outside of \( S \) such that \( LL^T \) fulfills 3.24 with constant \( \kappa \), i.e.

\[
\frac{\lambda_{\max}\left((LL^T)_{[k,q],[k,q]}\right)}{\lambda_{\min}\left((LL^T)_{[k,q],[k,q]} / (LL^T)_{[1,k],[1,k]}\right)} \leq \kappa.
\]

Then, if \( \|\Gamma - LL^T\|_{\text{Fro}} \leq \frac{\lambda_{\min}(LL^T)_{[k,q],[k,q]}}{4(\frac{3}{2} + 2\kappa + 8\kappa^2)^q} \), algorithm 8 terminates without incurring a nonpositive pivot and the resulting factor \( L \) satisfies:

\[
\|\bar{L}L^T - LL^T\|_{\text{Fro}} \leq \left(\frac{3}{2} + 2\kappa + 8\kappa^2\right)^q \left(\|\Gamma - LL^T\|_{\text{Fro}}\right)\]

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In order to prove this, we introduce some notation: We define $S^k$ as the $k+1 : N \times k+1 : N$ block of $LL^T$ after the first $k$ outer iterations of algorithm 8. In particular, we define $S^0 := LL^T$ and notice that for $(i,j) \in S$, we have:

$$S^k_{i,j} = \left((LL^T)_{k,N,k,N} / (LL^T)_{1,k,1,k}\right)_{i,j},$$

that is $S^k$ is equal to the Schur complement of $LL^T$ on $S$. Analogously, we define $\tilde{S}^k$ as the $k+1 : N \times k+1 : N$ block of $\Gamma$ after the application of the first $k$ outer iterations of algorithm 8. Finally, we define the difference $E^k := \tilde{S}^k - S^k$.

As a first step, we will consider error propagation under the elimination of one color on one level:

**Lemma 3.26.** Let $J = \bigcup_{k=1}^p J^{(k)}$ be an index set, $S \subset J \times J$ a symmetric sparsity pattern and $S$ a supernodal multicolor ordering with $p$ colors. Assume that algorithm 8 has completed the first $k-1$ outer iterations without encountering a nonpositive pivot and that it the $k$th through $l$th iterations are the iterations corresponding to some color on some level. Let furthermore $\lambda_{\text{max}}$ denote the maximal eigenvalue of $S^{(k)}$ and $\lambda_{\text{min}}$ denote the minimal eigenvalue of $S^{(k)}$. Then we have, for all $k \leq m \leq l$:

$$\|S^m - \tilde{S}^m\|_{\text{Fro}} \leq \left(\frac{3}{2} + 2\frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} + 8\frac{\lambda_{\text{max}}^2}{\lambda_{\text{min}}^2}\right)\|S^k - \tilde{S}^k\|_{\text{Fro}}$$

**Proof.** The key observation is that for all $k \leq m \leq l$ applying $m$ outer iterations of algorithm 8 or $m$ outer iterations of algorithm 7 to $\tilde{S}^m$ and $S^m$ yields the same result, when restricted to $S$. Therefore,

$$\|S^m - \tilde{S}^m\|_{\text{Fro}} \leq \left\|S_{m,N,m,N}^k - (S^k + E^k)_{m,N,k,m} (S^k + E^k)^{-1} S_{k,m,m}^k - (S^k + E^k)_{m,N,m,m} \right\|_{\text{Fro}}$$

As we have seen in the above lemma, the perturbation analysis of the elimination of all nodes of a given color, on a given node can be done by only involving the perturbation bounds for Schur complements once. We proceed with the proof of Lemma 3.25:

**Proof of Lemma 3.25.** The result follows from the iterative application of Lemma 3.26. As a first step we note that, for $\lambda_{\text{min}}, \lambda_{\text{max}}$ as in Lemma 3.26, we have $\lambda_{\text{max}}/\lambda_{\text{min}} \leq \kappa$. Therefore, we can inductively apply Lemma 3.26 to see that $\|E^k\|_{\text{Fro}}$ stays bounded from above by $\lambda_{\text{min}}/2$ and we thus obtain the error bound in the lemma.

In order to apply the above results, we need to assume one additional geometric condition on our space:

**Condition 3.27** (Ball packing). We say that an index set $J = \bigcup_{k=1}^p J^{(k)}$ together with a hierarchical pseudodistance fulfills the ball-packing condition with constant $C_b$, if for all $1 \leq k \leq q$ any ball of radius $r$ with respect to $d$ in $J^k$ contains at most $C_b$ disjoint balls of radius $r/6$.

**Lemma 3.28.** Let $J, d$ fulfill condition 3.27 with constant $C_b$. Then there exists a $p$ depending only on $C_b$ such that the following holds true: For any sparsity pattern $S \subset S \subset J \subset \{(i,j) \mid d(i,j) \leq \rho\}$ there exists a sparsity set $S \subset \tilde{S} \subset \{(i,j) \mid d(i,j) \leq 2\rho\}$ such that there exists a $p$-color supernodal multicolor ordering for $J, d, \tilde{S}$. 

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Proof. We will prove the result constructively. As a first step, we want to group the degrees of freedom on each level $k$ into supernodes. To this end, select a set $\{x_i\}_{1 \leq i \leq n} \subset J^{(k)}$ such that

$$J^{(k)} \subset \bigcup_{i=1}^{n} B_{2\rho}(x_i)$$

and

$$i \neq j \implies J^{(k)} \cap B_\rho(x_i) \cap B_\rho(x_j) = \emptyset.$$  

The selection of such $x_i$ is always possible, by iteratively adding $x_i$ and using the triangle inequality to show that $J^{(k)}$ needs to be fully covered once no $x_i$ can be added any more. By assigning now each $y \in J^{(k)}$ to one of the $B_{2\rho}(x_i)$ that contains it, we obtain a family of subsets $\{N_i\}_{1 \leq i \leq n}$. A multicolor ordering then ordering corresponds to a graph coloring of the undirected Graph $G$ with vertices $\{N_i\}$ and edges $\{(N_i, N_j) \mid \{x \in N_i, y \in N_j, (x, y) \in S\}$. For a graph of maximal degree $d$, it is well known Husfeldt (2015) that the greedy coloring algorithm achieves a $d+1$ coloring in complexity linear in the numbers of edges and vertices. Therefore, in order to bound the number of colors, it is enough to bound the maximal degree of $G$. To this end, we observe that if two supernodes $N_i$ and $N_j$ with corresponding center $x_i$ and $x_j$ are connected in $G$, then we must have $B_\rho(x_i) \subset B_\rho(x_j)$. Therefore, the maximal degree $d$ is bounded above as $d \leq C_6 - 1$ yielding a multicolour ordering with $p = C_6$ colors that can be found in linear time. Let us now assume, we have ordered the degrees of freedom according to the multicolor ordering. For definiteness, let us also assume that the ordering is such that degrees of freedom belonging to the same supernode are eliminated consecutively. Assume now that, for some $l$, there exist $i, \tilde{i} \in N_l$ and $j \in J$ such that $i \prec j$ and $(i, j) \in S$. The triangle inequality of $d$ implies that

$$d(i, j) \leq d(\tilde{i}, i) + d(i, j) \leq 4\rho + \rho = 5\rho,$$

where the last inequality follows, since the diameter of each supernode is bounded above by $4\rho$ and we have $S \subset \{(i, j) \mid d(i, j) \leq \rho\}$ for the original sparsity set. Therefore, by adding all the missing $(\tilde{i}, j)$ to $S$ we obtain a $\tilde{S} \subset \{(i, j) \mid d(i, j) \leq 5\rho\}$ that turns our ordering into a supernodal multicolor ordering with $C_6$ colors. 

\[ \Box \]

3.4.3 Summary

With the above results, we are in the position to provably bound both the approximation error and computational complexity of the incomplete Cholesky factorisation.

**Theorem 3.29** (Computational efficiency of ICHOL). Let $J := \bigcup_{k=1}^{b} J^{(k)}$, and a hierarchical pseudometric $d$ on $J$ fulfills conditions 3.16, 3.17 and 3.27 with constants $C_g, d, C_g, C_h$, respectively. Furthermore $\Gamma$ fulfill the conditions 3.24 with constant $\kappa$ and 3.6 with constants $\gamma, C_\gamma$. Assume that there exist a constants $\alpha, C_\alpha$ such that $\frac{1}{\max(1, \lambda_{min}(\Gamma))} \leq C_\alpha N^\alpha$ and that $\log(N) \approx q$

Then there exist constants $\rho_{\min}, C_\gamma$, and $\gamma$, depending only on $C_g, d, C_\gamma, \alpha, C_\alpha, C_h$, and $\kappa$, such that, for $\rho \geq \rho_{\min}(\log(N) + 1)$, there exists a sparsity set $\{(i,j) \mid d(i,j) < \rho\} \subset S \subset \{(i,j) \mid d(i,j) < 5\rho\}$ such that, possibly after reordering within the levels $J^{(k)}$, algorithm 8 applied to $\Gamma, \tilde{S}$ terminates and yields a factor $L$ with the approximation property

$$\log\left(\frac{1}{\|LL^T - \Gamma\|_{\text{Fro}}}\right) \leq C_\gamma \log(N) - \gamma\rho.$$  

In particular, this allows to compute a factorisation $LL^T$ that constitutes an $\varepsilon$-approximation of $\Gamma$ in complexity $O\left(N \log(N) \log^d(N/\varepsilon)\right)$ and $O\left(N \log^2(N) \log^{2d}(N/\varepsilon)\right)$ in space and time, respectively.

**Remark 3.30.** We note that we have not dealt with the complexity of the construction of $S$, yet, which we will do in a more concrete setting in section 3.6.

**Proof.** As a first step, we note that because of the condition 3.27, we can find a sparsity pattern $S$ as described above and a $C_6$-color supernodal multicolor ordering by applying Lemma 3.28 to the initial pattern $\{(i,j)|d(i,j) < \rho\}$. In the following $C$ and $\beta$ will be generic constants depending on $C_g, d, \gamma,$
Thus, for \( \rho \geq \frac{1}{2} (C + \beta \log(N)) \) we have

\[
\left\| L^S_{[k], [q]} \right\|_{H^b} \leq \lambda_{\min} \left( \frac{\Gamma(q)}{[k], [q]} / \Gamma(q)_{[1], [1]} \right) / 2.
\]

Therefore, for \( \rho \geq \frac{1}{2} (C + \beta \log(N)) \) we have

\[
\left\| L^S_{[k], [q]} \right\|_{H^b} \leq \lambda_{\min} \left( \frac{\Gamma(q)}{[k], [q]} / \Gamma(q)_{[1], [1]} \right) / 2.
\]

Thus, \( L^S L^S \) fulfills condition 3.24 with constant \( 4 \kappa \). Let \( L \) denote lower-triangular factor obtained by applying algorithm 8 to \( \Gamma(q) \) using the multicolor ordering and the supernodal sparsity pattern \( S \). Then, for a possibly larger \( C, \beta \),

\[
\left\| L^S L^S - L L^T \right\| \leq C N^3 \exp(\tilde{\gamma} \rho)
\]

given that we also have \( \rho > \frac{\beta}{2} (1 + \log(N)) \). Taking \( \rho_{\min} \) large enough to ensure that \( \rho \) satisfies both lower bounds, we obtain the result. \( \square \)

### 3.5 Validity of the conditions

In Owhadi and Scovel (2017), the authors give very general conditions under which the above conditions on exponential decay and bounded condition numbers are fulfilled. Following Owhadi and Scovel (2017), the abstract setting will consist of a Banach space \( B \) and its topological dual \( B^* \), an continuous operator \( G : B^* \to B \) and its continuous inverse \( L \). For an arbitrary operator \( T : V \to W \), we denote by \( C_T := \sup_{v \in V} \| T v \|/ \| v \| \) its continuity constant. We furthermore assume that we are given families of elements of \( B^* \), \( \{ \phi_i(k) \}_{i \in I(k)} \) for \( 1 \leq k \leq q \) and that these are nested in the sense that there exist matrices \( \pi(k, l) \in \mathbb{R}^{l \times q} \) for all \( 1 \leq k \leq l \leq q \) such that \( \phi_i(k) = \sum_{j \in I(l)} \pi_{i,j}(k,l) \phi_j(l) \). Finally, we assume that we are given index sets \( J(k) \) and matrices \( W(k) \in \mathbb{R}^{J(k) \times J(k)} \), for \( 1 \leq k \leq q \), such that \( \im(W(k)T) = \ker(\pi(k-1,k)) \) and \( W(k)W(k)T = \text{Id}_{J(k)} \). For a Banach space \( V \) and its topological dual \( V^* \), we denote by \( [\cdot, \cdot] : V \times V^* \to \mathbb{R} \) its duality product. In the following, we will deal with the following three examples. The first example is already treated in full, in (Owhadi and Scovel, 2017, Example 2.27), which is why we will mention it only briefly.

**Example 3.31 (Piecewise Polynomials).** For \( s, d \in \mathbb{N} \), let \( \Omega \subset \mathbb{R}^d \) be an open, bounded domain with Lipschitz boundary and \( B = H^s_0(\Omega) \). Let \( (h, d_{\text{mesh}}) \in (0,1) \) and let \( \{ \tau^k \}_{t \in T(k)} \) be convex, uniformly Lipschitz domains that form a nested partition of \( \Omega \), i.e., \( \Omega = \cup_{t \in T(k)} \tau^k_t \) is a disjoint union except for the boundaries and each \( \tau^k_t \) can be written as the (up to boundaries) disjoint union of members of \( \{ \tau^k \}_{t \in T(k+1)} \). Note that we can choose \( \pi(k-1,k) \) such that \( \|\pi(k-1,k)\|_2 \leq C_\Phi \). Assume that, for all \( t \in T(k) \), there exists \( x^k_t \) such that

\[
B_{d_{\text{mesh}}} \left( x^k_t \right) \subset \tau^k_t \subset B_{d_{\text{mesh}}} \left( x^k_t \right).
\]

Let for every \( t \in T(l) \), \( \{ \phi_{i,t} \}_{1 \leq i \leq \binom{s+d-1}{d}} \) be an \( L^2 \left( \tau^k_t \right) \) orthonormal basis of \( \mathcal{P}_{s-1} \left( \tau^k_t \right) \), the space of \( d \)-variate polynomials on \( \tau^k_t \) of degree at most \( s - 1 \). Then define \( I(k) := \left\{ 1, \ldots, \binom{s+d-1}{d} \right\} \times T(k) \) and let \( \phi_{i,t} \big|_{\tau^k_t} := \phi_{i,t} \), for \( (i, t) \in I(k) \). Choose \( W(k) \) such that, for all \( j \in J(k) \), there exists some \( t \in T(k-1) \) so that \( \text{supp}(\phi_{j,k}) \subset \tau^k_{t,k-1} \). Now define \( \Omega_{\beta} := \bigcup_{t \in T(l)} B_{2d_{\text{mesh}}} \left( x^k_t \right) \cap \Omega \). For \( i(k) = (s, t) \in I(k) \) and \( j = (s, \tau) \in I(l) \), we then define the pseudometric \( d \) as follows:

\[
d \left( (i(k), j(l)) \right) := \inf \left\{ n_{1}\beta_{1}^{(r_1)} = t_1, p_2^{(r_2)} \in I(l), \ldots, p_n^{(r_n)} = t_n, \min(k, l) \leq r_1 \cdots r_n + 1, \Omega_{\beta}^{(r_n)} \cap \Omega_{\beta}^{(r_n+1)} \neq \emptyset \right\},
\]
In statistical applications, most often the kernel function is continuous and evaluated at a set of measurement points. In this case, we can use subsampling as an averaging scheme, allowing for a near linear complexity algorithm without the use of quadrature formulae. For the following two example, we introduce an additional domain \( \Omega' \supset \Omega \), which will be the physical domain of the partial differential operator, as opposed to \( \Omega \).

**Example 3.32** (Radon measures with compact support). For \( s > d/2 \), let \( \Omega \subset \Omega' \subset \mathbb{R}^d \), define \( \mathcal{B} := H_0^s(\Omega') \) and let \( \Omega \) be bounded with uniformly Lipschitz boundary. For \( h, \delta_{\text{mesh}} \in (0,1) \) and \( q \in \mathbb{N} \) let \( \{ x_i^{(1)} \}_{i \in I^1} \subset \cdots \subset \{ x_i^{(q)} \}_{i \in I^q} \subset \Omega \) for nested index sets \( I^{(1)} \subset \cdots \subset I^{(q)} \) be a hierarchy of point sets, such that

1. \( \sup_{x \in \Omega} \min_{i \in I^{(k)}} \text{dist} \left( x, x_i^{(k)} \right) \leq h^k \)
2. \( \inf_{i \neq j \in I^{(k)} \setminus I^{(k-1)}} \text{dist} \left( x_i^{(k)}, \partial \Omega \cup x_j^{(k)} \right) \geq 2\delta_{\text{mesh}} h^k \)

Let the constants \( \alpha_{\text{min}}, \alpha_{\text{max}} \) be such that \( 0 < \alpha_{\text{min}} \leq \alpha_{\text{max}} < \infty \) and define \( \phi_i^{(k)} := \mu_i^{(k)} \) to be pairwise distinct Radon measures such that the mass of \( \mu_i^{(k)} \) restricted to \( B_{\delta_{\text{mesh}} h^s/2}(x_i^{(k)}) \) is bounded from below by \( \alpha_{\text{min}} \) and the mass of \( \mu_i^{(k)} \) is bounded from above by \( \alpha_{\text{max}} \). Let the sets of radon measures be nested, \( \{ \mu_i^{(l)} \}_{i \in I^{(l)}} \subset \cdots \subset \{ \mu_i^{(1)} \}_{i \in I^{(1)}} \) and define

\[
\tau_{i,j}^{(k,l)} := \begin{cases} 
1, & \mu_j^{(k)} = \mu_j^{(l)} \\
0, & \text{else}
\end{cases}
\]

Furthermore define \( J^k := I^{(k)} \setminus I^{(k-1)} \) (where \( I^{(0)} = \emptyset \)) and

\[
W_{i,j}^{(k)} := \delta_{i,j}.
\]

The definition of \( \pi \) and \( W \) in are illustrated in Figure 2.4. Now define \( \Omega_i^{(k)} := B_{2h^k}(x_i^{(k)}) \cap \Omega \). For \( i^{(k)} \in I^{(k)} \) and \( j \in I^{(l)} \), we then define the pseudometric \( d \) as follows:

\[
d \left( i^{(k)}, j^{(l)} \right) := \inf \left\{ m \left| p_1^{(r_1)} = i^{(k)}, p_2^{(r_2)} \in I^{(r_2)}, \ldots, p_{n+1}^{(r_{n+1})} = j^{(l)}, \min(k,l) \leq r_1 \ldots r_{n+1}, \Omega^{(s_m)} \cap \Omega^{(s_{m+1})} \neq \emptyset \right\}.
\]

In some cases, the underlying PDE might not have enough regularity allow for pointwise evaluations of the Green’s function. In this case, the question of whether subsampling can be used as an aggregation scheme becomes more difficult to answer. In order to treat this case, we present a third possible setting.

**Example 3.33** (Averaging over Patches). For \( s, d \in \mathbb{N} \), let \( \Omega \subset \Omega' \subset \mathbb{R}^d \), define \( \mathcal{B} := H_0^s(\Omega') \) and let \( \Omega \) be bounded with uniformly Lipschitz boundary. For \( h, \delta_{\text{mesh}} \in (0,1) \) and let \( \{ \tau_i^{(k)} \}_{i \in I^{(k+1)}} \) be convex, uniformly Lipschitz domains that form a nested partition of \( \Omega \), i.e. \( \Omega = \cup_{i \in I^{(k)}} \tau_i^{(k)} \) is a disjoint union except for the boundaries and each \( \tau_i^{(k)} \) can be written as the (up to boundaries) disjoint union of members of \( \{ \tau_i^{(k)} \}_{i \in I^{(k+1)}} \). Assume that, for all \( i \in I^{(k)} \), there exists \( x_i^{(k)} \) such that

\[
B_{\delta_{\text{mesh}} h^s} \left( x_i^{(k)} \right) \subset \tau_i^{(k)} \subset B_{h^s} \left( x_i^{(k)} \right).
\]

Then define \( \phi_i^{(k)} := \frac{1}{\sqrt{\left| \tau_i^{(k)} \right|}} \)

\[
\tau_{i,j}^{(k,l)} := \begin{cases} 
\sqrt{\frac{\left| \tau_j^{(k+1)} \right|}{\left| \tau_j^{(k)} \right|}}, & x_j^{(k+1)} \subset \tau_i^{(k)} \\
0, & \text{else}
\end{cases}
\]

and define \( W^{(k)} \), as described in (Owhadi, 2017, Construction 4.13), such that
(i) for all $1 \leq k < l \leq q$, $i \in I^{(k)}$, and $j \in J^{(k+1)}$, and $\left\langle \phi_i^{(k)}, \phi_j^{(k+1)} \right\rangle_{L^2} = 0$;
(ii) for all $1 \leq k \leq q$ and $j \in J^{(k)}$, there exists $i \in I^{(k-1)}$ such that $\text{supp} \phi_j^{(k)} \subset \tau_i^{(k-1)}$;
(iii) $W^{(k)} W^{(k),T} = \text{Id}_{J^{(k)}}$.

Now define $\Omega_1^{(k)} := B_{2h^k}(x_i^{(k)}) \cap \Omega$. For $i^{(k)} \in I^{(k)}$ and $j \in I^{(l)}$, we then define the pseudometric $d$ as follows:

$$d(i^{(k)}, j^{(l)}) := \inf \left\{ n | p_1^{(r_1)} = t, p_2^{(r_2)} = s, \ldots, p_{n+1}^{(r_{n+1})} = t, \min(k, l) \leq r_1 \ldots r_{n+1}, \Omega_m^{(s_m)} \cap \Omega_{m+1}^{(s_{m+1})} \neq \emptyset \right\}.$$

We note that the last case was already treated in Owhadi (2017) and Owhadi and Scovel (2017, Example 2.26) for the case $s = 1$. In the following we extend the results there, by showing that the polynomial order of the $\phi_i^{(k)}$, need not match the order of the PDE.

### 3.5.1 Bounded condition numbers without vanishing moments

Hou and Zhang (2017) requires polynomial measurement functions $\phi_i^{(k)}$ of order $s - 1$ to prove the exponential decay of strongly elliptic differential operators of order $2s$. Although Owhadi and Scovel (2017) does not require polynomial measurement functions (or vanishing moments) to obtain the exponential decay of gamblits for elliptic operators of order $2s$, a vanishing moments condition is implicitly used to obtain a uniform bound on $\text{cond}(B^{(k)})$. Vanishing moments conditions have also been used to compress integral operators with wavelets (DeVore and Kuno, 2009; Beylkin et al., 1991; Gines et al., 1998; Beylkin and Coult, 1998; Beylkin, 1998).

In the following, we will generalize the proof that $\text{cond}(B^{(k)})$ is uniformly bounded (Owhadi and Scovel, 2017) by relaxing conditions requiring vanishing moments. We thus obtain an easy to implement multisolution decomposition algorithm that does not require the prior construction of hierarchies of measurement functionals $\phi_i^{(k)}$ with vanishing moments; with this generalization a simple subsampling strategy can be used to produce the $\phi_i^{(k)}$.

As in Owhadi and Scovel (2017), conditions for uniform boundedness of $\text{cond}(B^{(k)})$ are as follows:

**Condition 3.34.** There exists some constants $C_\phi \geq 1$ and $H \in (0, 1)$ such that:

(i) $\frac{1}{C_\phi} H^k \leq \frac{\|\phi_i^{(1)}\|}{|x|}$ for $k \in \{1, \ldots, q\}$, $x \in \mathbb{R}^{f^{(k)}}$ and $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$, and $x \in \mathbb{R}^{f^{(k)}}$

(ii) $\frac{\|\phi_i^{(1)}\|}{|x|} \leq C_\phi$ for $\phi = \sum_{i \in I^{(1)}} x_i \phi_i^{(1)}$ and $x \in \mathbb{R}^{f^{(1)}}$

(iii) $\|\phi_i^{(k-1)}\|_2 \leq C_\phi$ for $k \in \{2, \ldots, q\}$

(iv) $\frac{1}{C_\phi} H^k \leq W^{(k)} W^{(k),T} \leq C_\phi J^{(k)}$ for $k \in \{2, \ldots, q\}$

and

**Condition 3.35.** The constants $C_\phi$ and $H$ in Condition 3.34 satisfy also:

(i) $\inf_{\phi \in \Phi^{(k-1)}} \frac{\|\phi - \phi'\|}{|x|} \leq C_\phi H^{(k-1)}$ for $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$, $k \in \{2, \ldots, q\}$, and $x \in \mathbb{R}^{f^{(k)}}$

(ii) $\frac{\|\phi_i^{(1)}\|}{|x|} \leq C_\phi H^{(k-1)}$ for $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$, $k \in \{2, \ldots, q\}$, and $x \in \ker(\pi^{(k-1),j})$

Conditions 3.34 play the role of an inverse Poincaré inequality, a global Poincaré inequality as well as bounds on the aggregation ant orthogonalisation matrices. The first part of Condition 3.35 ensures that the operator is approximated better and better by its projection onto $\Phi^{(k)}$ for growing $k$. We note that the second part of Condition 3.35 is a type of Poincaré inequality that actually implies the approximation property. The bounded condition numbers of $B^{(k)}$ can be seen as arising from the balance between the inverse Poincaré inequality, which describes how higher eigenvalues of $L$ become visible under refinement of the mesh, and the Poincaré inequality, which describes how lower eigenvalues are factored out by the orthogonalisation procedure. The proof of the inverse Poincaré inequality depends only on localisation and scaling and will, for partial differential operators of order $2s$, generally yield $H = h^{2s}$. The Poincaré inequality however depends crucially on vanishing moments of order $s - 1$, in order to obtain the scaling $H = h^{2s}$, as was observed by Owhadi and Scovel (2017). This leads to the problem that the order of the
obtain that

\[ \text{Summarising we have obtained that} \]

modify Lemmas 10.11 and 10.12 of Owhadi and Scovel (2017) as follows. For achieved for \( z \) (Owhadi and Scovel, 2017, Eq. 15.4) (Owhadi and Scovel, 2017, Eq. 15.3) (Under Conditions 3.35 and 3.36 it holds true that there exists a constant Theorem 3.37.
The remaining part of the proof is similar to that of Theorem 10.9 of Owhadi and Scovel (2017). In order to prove the slightly stronger condition 3.24, we need to skip multiple scales at once:

\[ (\text{i}) \text{ for all } k \leq l, \phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}, \text{ and } x \in \mathbb{R}^{I^{(l)}} \]

\[ \inf_{y \in \mathbb{R}^{I^{(k-1)}}, |y| \leq C_k |x|} \frac{\| \phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)} \|_2}{|x|} \leq C_k H^{k-1} \]

for \( \phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}, k \in \{2, \ldots, q\}, \) and \( x \in \mathbb{R}^{I^{(k)}}. \)

The following theorem is proved by a modification of (Owhadi and Scovel, 2017, Theorem 9.10).

**Theorem 3.37.** Under Conditions 3.35 and 3.36 it holds true that there exists a constant \( C \) depending only on \( C_k \) such that \( C^{-1} I^{(1)} \leq A^{(1)} \leq C H^{-2} I^{(1)}, \) Cond(\( A^{(1)} \)) \( \leq C H^{-2}, \) and \( C^{-1} H^{-2(k-1)} J^{(k)} \leq B^{(k)} \leq C H^{-2k} J^{(k)} \) for \( k \in \{2, \ldots, q\}. \) In particular, \( \text{Cond}(B^{(k)}) \leq C H^{-2}. \)

**Proof.** The proof of Theorem 3.37 is similar to that of Theorems 9.10 and 10.9 of Owhadi and Scovel (2017), but there are two important modifications. First observe that condition 3.36 is sufficient to obtain (Owhadi and Scovel, 2017, Eq. 15.4) \( (z^T B^{(k)} z) \leq C_k^2 H^{-2(k-1)} |A^{(k)}| W^{(k)}, T \) because the infimum in (Owhadi and Scovel, 2017, Eq. 15.3) \( (z^T B^{(k)} z) = \inf_{y \in \mathbb{R}^{I^{(k)}}} \sum_{j \in I^{(k)}} z_j \chi_j (k) \sum_{i \in I^{(k)}} y_i \psi_i^{(k-1)} \|z\|^2 \) is achieved for \( y = 0. \) Second, following (Owhadi and Scovel, 2017, Lemma 10.10), to bound \( \|P(k)\|_2 \) we modify Lemmas 10.11 and 10.12 of Owhadi and Scovel (2017) as follows. For \( x \in \mathbb{R}^{I^{(k)}} \) and \( y \in \mathbb{R}^{I^{(k-1)}}, \) we have \( P(k) = P(k)(x - \pi^{(k,k-1)} y) + P(k)\pi^{(k,k-1)} y. \) Using \( P(k) = \pi^{(k,k-1)} A^{(k-1)} \pi^{(k-1,k)} \Theta^{(k)} \) we obtain that \( P(k)\pi^{(k,k-1)} y = \pi^{(k,k-1)} y \) and \( |P(k)(x - \pi^{(k,k-1)} y)| \leq \pi^{(k,k-1)} A^{(k-1)} \pi^{(k-1,k)} \Theta^{(k)} \|x - \pi^{(k,k-1)} y\|_{\Theta^{(k)}}. \) Choosing \( y \) as in Condition 3.36 and using \( \|\pi^{(k,k-1)} y\|_2 \leq C_k \) we deduce that \( \|P(k)\|_2 \leq C_k^2 |x| \) and \( |x - \pi^{(k,k-1)} y|_{\Theta^{(k)}} \leq C_k H^{k-1} |x|. \) As in the proof of (Owhadi and Scovel, 2017, Lemma 10.11) observe that \( \|\pi^{(k,k-1)} A^{(k-1)} \pi^{(k-1,k)} \Theta^{(k)}\|_2^2 = \lambda_{\max}(\pi^{(k,k-1)} A^{(k-1)} \pi^{(k-1,k)}) \) and as in (Owhadi and Scovel, 2017, Eq. 10.34) bound \( \lambda_{\max}(\pi^{(k,k-1)} A^{(k-1)} \pi^{(k-1,k)}) \) by \( \|\pi^{(k,k-1)}\|_2^2 \lambda_{\max}(A^{(k-1)}) \leq C_k^2 H^{-2(k-1)}. \) Summarising we have obtained that

\[ \|P(k)\|_2 \leq C_k^2 + C_k^3. \]

The remaining part of the proof is similar to that of Theorem 10.9 of Owhadi and Scovel (2017).

In order to prove the slightly stronger condition 3.24, we need to skip multiple scales at once:

**Corollary 3.38.** Assume that conditions 3.35 and 3.36 hold and that we additionally have:

(i) for all \( 1 \leq k < l \leq q, \|\pi^{(k,l)}\|_2 \leq C_k; \)

(ii) for all \( 1 \leq k < l, \phi = \sum_{i \in I^{(l)}} x_i \phi_i^{(l)}, \text{ and } x \in \mathbb{R}^{I^{(l)}}, \)

\[ \inf_{y \in \mathbb{R}^{I^{(k-1)}}, |y| \leq C_k |x|} \frac{\| \phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)} \|_2}{|x|} \leq C_k H^{k-1}. \]

Then, defining \( B^{(k,l)} \in \mathbb{R}^{\chi_{k-1} J^{(n)} \times \chi_{k-1} J^{(n)}} \) as the block matrix obtained from the blocks \( W^{(m)} \pi^{(m,l)} A^{(l)} \pi^{(l,m)} W^{(n)}, T \) for \( k \leq n, m \leq l, \) we obtain \( \lambda_{\min}(B(k,l)) \geq C^{-1} H^{-2(k-1)} J^{(k,l)}. \)

**Proof.** The result follows from Theorem 3.37 by considering the scales from \( k \) to \( l \) as one scale with \( \pi^{(k,l)} \) playing the role of \( \pi^{(k-1,k)} \) in Theorem 3.37 and the \( k-l+1 \times 1 \) block matrix \( (\pi^{(l,k)} W^{(k)}, T, \pi^{(l,k)} W^{(k+1)}, T, \ldots, \pi^{(l,k)} W^{(l)}, T)^T \) playing the role of \( W(k) \) in Theorem 3.37.
Theorem 3.39. Let $\Omega \subset \Omega' \subset \mathbb{R}^d$ and let $\Omega$ be bounded with uniformly Lipschitz boundary and let $G$ be a continuous bijection from $H^{-s}(\Omega')$ to $H_0^s(\Omega')$ with inverse $L$. For $h, \delta_{\text{mesh}} \in (0, 1)$ and $1 \leq k \leq q \in \mathbb{N}$ let $\{x_i^{(k)}\}_{i \in I^k}$ sets of points in $\mathbb{R}^d$, such that

(i) $\sup_{x \in \Omega} \min_{i \in I^k} \text{dist} \left( x, x_i^{(k)} \right) \leq h^k$
(ii) $\inf_{i, j \in I^k} \text{dist} \left( x_i^{(k)}, \partial \Omega \cup x_j^{(k)} \right) \geq 2\delta_{\text{mesh}} h^k$

Let furthermore be $0 < \alpha_{\min} \leq \alpha_{\max} < \infty$ and define $\phi_{i}^{(k)} := \mu_i^{(k)}$ to be a Radon measure with mass bounded from below by $\alpha_{\min}$ and from above by $\alpha_{\max}$, such that $\text{supp} \left( \mu_i^{(k)} \right) \subset B_{h^k}(x_i^{(k)})$ and $\phi_{i}^{(q)} \in (H_0^{-s}(\Omega'))$.

Now define the functions

$$S_{\min}^{(k)}(r) := \min_{i \in I^{(k)}} \left\| \phi_i^{(k)} \right\| \left( H_0^s(B_{r}(x_i^{(k)})) \right)^*$$

and

$$S_{\max}^{(k)}(r) := \max_{k \leq l \leq q, i \in I^{(l)}} \left\| \phi_i^{(l)} \right\| \left( H_0^s(B_{r}(x_i^{(l)})) \right)^*$$

Then we have, for constants $C_{\phi}$ and $r$ depending only on $s$, $d$, $\Omega$, $\Omega'$, $G$, $h$, $\delta_{\text{mesh}}$, $\alpha_{\max}/\alpha_{\min}$,

(i) $\frac{1}{C_{\phi}} S_{\min}^{(k)}(\delta_{\text{mesh}} h^k) \leq \left\| \phi_i^{(k)} \right\| \text{ for } k \in \{1, \ldots, q\}, x \in \mathbb{R}^d \text{ and } \phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)} \text{ and } x \in \mathbb{R}^{I^{(k)}}$.

(ii) $\left[ \left\| \phi_i^{(k)} \right\| \right]_{k \leq l \leq q} \leq C_{\phi} S_{\max}^{(l)}(r)$ for $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ and $x \in \mathbb{R}^{I^{(k)}}$.

(iii) $\inf_{y \in \mathbb{R}^{I^{(k)}} \text{ with } \left\| \phi_i^{(k)} \right\| \leq C_{\phi} S_{\max}^{(k)}(r) \text{ for } \phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}, k \in \{1, \ldots, q\}, k \leq l \leq q$.

Proof. For part (ii), we notice by choosing $r$ such that $\Omega \subset B_{r-2/2}(0)$, we obtain:

$$\sup_{v \in H^s_0(\Omega')} \frac{\left\| \phi_i^{(k)} \right\|_2^2}{\left\| H^s_0(\Omega') \right\|_2} \leq \sup_{v \in H^s(\Omega' \cap B_{r-1/2}(x_i^{(k)}))} \frac{\left\| \phi_i^{(k)} \right\|_2^2}{\left\| v \right\|_2} \leq \frac{C}{\left\| v \right\|_2} \frac{\left\| \phi_i^{(k)} \right\|_2^2}{\left\| v \right\|_2} \leq C \sup_{v \in H^s_0(\Omega' \cap B_{r-1/2}(x_i^{(k)}))} \frac{\left\| \phi_i^{(k)} \right\|_2^2}{\left\| v \right\|_2} \frac{\left\| v \right\|_2}{\left\| v \right\|_2} \leq C_S^{(k)}(r)$$

Here, the constant $C$ follows from the application of a continuous extension theorem for Sobolev spaces, which can be obtained from the classical extension theorem to $H_0^s(\mathbb{R})$ (Adams and Fournier, 2003) by application of a cutoff function. Now to prove part one, we can write, following Owhadi and Scovel (2017, Proposition 4.17):

$$\left\| \phi \right\|_{H^{-s}(\Omega')} \geq \sum_{i \in I^{(k)}} v_i H_0^s \left( B_{\text{mesh}, h^k}(x_i) \right) \left( \frac{2}{B_{\text{mesh}, h^k}(x_i)} \right) \left( x_i^{(k)} \phi_i^{(k)} \right) \geq S_{\min}^{(k)} \left( \delta_{\text{mesh}} h^k / 2 \right)^2 \left\| x \right\|^2$$

Next we prove part (iii). The proof will be similar to the proof of the first part of Condition 3.35, as found in the proof of (Owhadi and Scovel, 2017, Proposition 4.17).

By using a standard covering argument there exist $h_0(\Omega)$, and constants $0 < c_{\min}(\Omega) \leq c_{\max}(\Omega)$ such that for every $x_i^{(k)}$ with $h^k \leq h_0$ there exists a matrix $T \in \mathbb{R}^{d \times d}$ such that $c_{\min} \leq \sigma_{\min}(T) \leq \sigma_{\max}(T) \leq c_{\max}$ such that

$$\Omega_i^{(k)} := T \left( \left[ 0, \frac{(2s+1)h^{k-1}}{\delta} \right]^d \right)$$
where $\delta = \delta(2s,d)$ is chosen according to Lemma 3.40. Therefore, by Lemma 3.40 there exists a $0 < \rho_{\text{max}}(\Omega, s)$ and $C(\Omega, s)$ such that for all $k$ with $h^{k-1} \leq h_0$ and $i \in I^{(l)}$ we have $\text{diam}(\Omega_i^{(k)}) \leq \rho_h h^{k-1}$ and there exists $u_{i,k} \in \mathbb{R}^{I^{(k-1)}}$ such that $|u_{i,k}| \leq \alpha_{\text{max}}/\alpha_{\text{min}} C$ and

$$\int_{\Omega_i^{(k)}} p(x) \left( \phi_i^{(k)} - \sum_{i \in I^{(k-1)}} w_{i,j}^{(k-1)} \phi_j^{(k-1)} \right) = 0,$$

for all $p \in P_{2s-1}$. We observe that there exists a constant $C_{\text{packing}}(d, \rho, \delta_{\text{mesh}})$, such that

$$\# \{ j | B_{\rho_h h^{k-1}}(x_i^k) \cap B_{\rho_h h^{k-1}}(x_j^k) \neq \emptyset \} \leq C_{\text{packing}}$$

Based on the above preparation, we want to prove the inequality for a given scale $k$. By estimating the remaining level by the Poincaré inequality on $\Omega$, we can restrict ourselves to the $k$, for which $h^{k-1} \leq h_0$. We set

$$y_i := x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)}$$

and compute:

$$\left\| \phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)} \right\|_{L^2_{\Omega}}^2 = \left\| \sum_{i \in I^{(l)}} x_i \phi_i^{(l)} - x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)} \phi_j^{(k-1)} \right\|_{L^2_{\Omega}}^2$$

$$= \sup_{v \in H_0^2(\Omega')} \left( 2 \sum_{i \in I^{(k-1)}} \int_{\Omega} \left( x_i \phi_i^{(l)} - x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)} \phi_j^{(k-1)} \right) dx - \|v\|_{H_0^2(\Omega')}^2 \right)$$

$$\leq \sup_{v \in H_0^2(\Omega')} \left( 2 \sum_{i \in I^{(k-1)}} \int_{\Omega} \left( x_i \phi_i^{(l)} - x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)} \phi_j^{(k-1)} \right) dx - \|v\|_{H_0^2(\Omega)}^2 \right)$$

$$\leq \sup_{v \in H_0^2(\Omega')} \left( 2 \sum_{i \in I^{(k-1)}} \int_{B_{\rho_h h^{k-1}}(x_i^k)} v \left( x_i \phi_i^{(l)} - x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)} \phi_j^{(k-1)} \right) dx - \frac{1}{2C_{\text{packing}}} \|v\|_{H_0^2(B_{\rho_h h^{k-1}}(x_i^k))}^2 \right)$$

$$= \sup_{v \in H_0^2(\Omega')} \left( 2 \sum_{i \in I^{(k-1)}} \inf_{p \in P_{2s-1}} \int_{B_{\rho_h h^{k-1}}(x_i^k)} (v - q) \left( x_i \phi_i^{(l)} - x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)} \phi_j^{(k-1)} \right) dx \right)$$

$$- \frac{1}{2C_{\text{packing}}} \|v\|_{H_0^2(B_{\rho_h h^{k-1}}(x_i^k))}^2$$

Now, using the Bramble–Hilbert lemma (Bramble and Hilbert, 1970) in its version for convex domains (Dekel and Levitan, 2004), we obtain from the above for a constant $C(\Omega, \rho)$

$$\cdots \leq \sup_{v \in H_0^2(\Omega')} \left( 2 \sum_{i \in I^{(k-1)}} \left\| x_i \phi_i^{(l)} - x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)} \phi_j^{(k-1)} \right\|_{H^1(B_{\rho_h h^{k-1}}(x_i^k))} \right)$$

$$- \frac{1}{2C_{\text{packing}}} \|v\|_{H_0^2(B_{\rho_h h^{k-1}}(x_i^k))}^2$$

$$\leq \left( \sum_{i \in I^{(k-1)}} \left\| x_i \phi_i^{(l)} - x_i \sum_{j \in I^{(k-1)}} w_{j,i}^{(k)} \phi_j^{(k-1)} \right\|_{H^1(B_{\rho_h h^{k-1}}(x_i^k))}^2 \right)^{1/2},$$

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where we used Young’s inequality in the last step. Using the triangle inequality, we obtain:

\[ \cdots \leq C h^{2(k-1)s} (|x|^2) \max \left\{ \left\| \phi_i^{(k)} \right\|_{H^s(B_{2\rho h^{k-1}}(x_i^{(k)}))}^2, \left\| \phi_i^{(k-1)} \right\|_{H^s(B_{2\rho h^{k-1}}(x_i^{(k)}))}^2 \bigg| i \in I^{(l)} \right\} \cup \left\{ \left\| \phi_i^{(k-1)} \right\|_{H^s(B_{2\rho h^{k-1}}(x_i^{(k)}))}^2 \bigg| i \in I^{(l)}, j \in I^{(l-1)} \right\} \]

Now, we can compute:

\[
\| \phi \|_{H^s(B_{2\rho h^{k-1}}(x_i^{(k)}))}^s = \sup_{v \in H^s(B_{2\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|v\|_{H^s(B_{2\rho h^{k-1}}(x_i^{(k)}))}} \\
\leq h^{-d/2} \sup_{v \in H^s(B_{2\rho h^{k-1}}(x_i^{(k)}))} \|v(h^{-k-1})\|_{H^s(B_{\rho h}(x_i^{(k)}))} \\
\leq C h^{-d/2} \\|E[h^{-k-1}]\|_{H^s(B_{\rho h}(x_i^{(k)}))}
\]

Here, \( E \) is the bounded extension operator from \( H^s(B_{\rho h}(x_i^{(k)})) \) to \( H^s(B_{2\rho h}(x_i^{(k)})) \). By defining \( \tilde{v} := E[h^{-k-1}] \), we obtain:

\[
\| \phi \|_{H^s(B_{\rho h^{k-1}}(x_i^{(k)}))}^s \leq C h^{-d/2} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|\tilde{v}\|_{H^s(B_{2\rho h}(x_i^{(k)}))}} \\
\leq C h^{-d/2} h^{-k-1} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|\tilde{v}(h^{-k-1})\|_{H^s(B_{2\rho h}(x_i^{(k)}))}} \\
= C h^{-d/2} h^{-k-1} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, \tilde{v}(h^{-k-1})]}{\|\tilde{v}(h^{-k-1})\|_{H^s(B_{2\rho h}(x_i^{(k)}))}} \\
\leq C h^{-d/2} h^{-k-1} \| \phi \|_{H^s(B_{\rho h^{k-1}}(x_i^{(k)}))}^s
\]

plugging this into our estimate of the dual norm, we obtain:

\[
\left\| \phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)} \right\|_{*}^2 \leq C h^{-d/2} h^{-k-1} S_{\max}^{(k)} (r h^{-k-1})
\]

with \( r := 2 \rho \).

**Lemma 3.40.** Let \( m, d \in \mathbb{N} \), \( 0 < \alpha_{\min} \leq \alpha_{\max} < \infty \) and \( r > 0 \) be given. Then there exist constants \( c(m, d, \alpha_{\min}, \alpha_{\max}, r) \), \( \delta(m, d, r) \), and \( n(m, d, \delta_{\text{mesh}}) \) such that for all point sets \( \{x_i\}_{i \in I^{(l)}(0)} \subset \mathbb{R}^d \) with max \( x \in [0, (m+1)\delta] \) \( \min \{ \text{dist}(x, x_j) \} \leq h \) and all families of Radon measures \( \{ \mu_i \}_{i \in I^{(l)}(0)} \) with mass between \( \alpha_{\min} \) and \( \alpha_{\max} \) and \( \text{supp}(\mu_i) \subset B_{\rho h}(x_i) \), there exists a finite subset \( \{\nu_i\}_{i \in I} \subset \{\mu_i\}_{i \in I} \) and \( w \in \mathbb{R}^n \) such that:

\[
[\mu_0, p] + \sum_{i=1}^n w_i [\nu_i, p] = 0 \quad \text{for all } p \in \mathcal{P}_{m-1} \left([0, h/\delta]^d\right)
\]

and \( \|w\|_2 \leq \epsilon^{-1} \).

**Proof.** We first prove the result in the case, in which \( x_0 = 0 \) and \( \mu_i := \delta_{x_i} \). In this case, the problem has the following form:

\[
p(0) + \sum_{i=1}^n w_i p(y_i) = 0 \quad \text{for all } p \in \mathcal{P}_{m-1} \left([0, h/\delta]^d\right).
\]
Recall that the problem of interpolating values at \([1, \ldots, m]d\) with polynomials in \(\bigotimes_{k=1}^{d} P_{m-1}(\mathbb{R})\) is uniquely solvable; in particular its Vandermonde matrix \(V(m,[1, \ldots, m]^d)\) is invertible. By the continuity of polynomials, there exists a \(0 < \delta(m,d) < 1/4\), \(0 < \varepsilon(m,d)\) such that
\[
\varepsilon \leq \min \left\{ \sigma_{\min}(V(m,[1, \ldots, m]^d + (z_1, \ldots, z_m))) \mid \sup_{1 \leq i \leq m} |z_i| < \delta \right\}.
\]
That is, under perturbation of the grid smaller than \(\delta\), the minimal singular value of \(V\) stays bounded below by \(\varepsilon > 0\). Note that the result of the lemma is invariant under rescaling of \(\{x_i\}_{i \in \mathbb{N}}\) and \(h\) by \(\frac{k}{h}\), obtaining \(\tilde{h} := \frac{k}{h} h \equiv \delta\) and \(\tilde{x}_i := \delta x_i\). Then for each \(z \in [1, \ldots, m]^d\) there exists an \(\tilde{x}_z \in \{\tilde{x}_i\}_{i \in J}\) such that \(|\tilde{x}_z - z| \leq \delta\). We choose those elements our interpolation points and observe that we obtain the weights \(w_i\) as \(w := -V^{-1}(1,0 \ldots 0)\). In particular we have correspondingly \(|w|_2 \leq \frac{1}{\varepsilon}\). This shows the result for Dirac measures. In order to extend the result to localised Radon probability measures, we initially proceed as in the above proof. In the very end, we can then rescale with a factor depending only on \(r,s,d\) to “shrink the Radon measures to points”, until the generalised Vandermonde matrix is invertible. General but uniformly bounded masses can easily be incorporated by possibly including a factor of \(\alpha_{\max}/\alpha_{\min}\) in the norm estimate of \(w\). \(\square\)

**Remark 3.41.** We note that the above described techniques to prove the bounds on the condition numbers are far more flexible than those based on vanishing moments. With our approach, the projection used in the proof and the projector used in the algorithm are decoupled, which allows us to use computationally nontrivial projectors in the proof, without needing to implement them in the algorithm.

If \(s > d/2\), bounds on the \(S_{\max}\) and \(S_{\min}\) are particularly easy to establish:

**Theorem 3.42.** In the setting of Example 3.32, we have, for a constant depending only on \(s, d, \Omega, \Omega', G, h, \delta_{\text{mesh}}, \) and \(\alpha_{\max}/\alpha_{\min}\),
\[
C^{-1} \alpha_{\max}^{-1} \prec A^{(1)} \prec \alpha_{\min}^{-1} h^{-2(s-d/2)}
\]
and
\[
C^{-1} \alpha_{\max}^{-1} h^{-2(k-1)(s-d/2)} \prec B^{(k)} \prec C \alpha_{\min}^{-1} h^{-2k(s-d/2)},
\]
which results in
\[
\text{cond}(A^{(1)}) \leq C^2 \frac{\alpha_{\max}}{\alpha_{\min}} h^{-2(s-d/2)} \quad \text{and} \quad \text{cond}(B^{(k)}) \leq C^2 \frac{\alpha_{\max}}{\alpha_{\min}} h^{-2(s-d/2)}.
\]
Moreover, for \(B^{(k,l)}\) defined as in Corollary 3.38, we have:
\[
C^{-1} \alpha_{\max}^{-1} h^{-2(k-1)(s-d/2)} \prec B^{(k,l)}.
\]

**Proof.** Since obviously \(\|\pi^{(k-1,k)}\| = 1\) and \(W^{(k)} W^{(k),T} = \text{Id}\), we need to show that the first two parts of Condition 3.34 and Condition 3.36 hold. We will use Theorem 3.39 and hence need to find bounds on \(S_{\min} \) and \(S_{\max}\). The result follows directly from Theorem 3.39, provided we can bound \(S_{\min}\) from below and \(S_{\max}\) from above. Indeed, we have for some \(i,k\):

\[
S_{\max}^{(k)} \left( r h^{(k-1)} \right) \leq \alpha_{\max} \sup_{v \in H_0^s(B_{r h^{(k-1)}(x_i^{(k)})})} \frac{\|v\|_{C^0(B_{r h^{(k-1)}(x_i^{(k)})})}}{\|v\|_{H_0^s(B_{r h^{(k-1)}(x_i^{(k)})})}} \leq \alpha_{\max} r^{-s-d/2} h^{(k-1)(s-d/2)} \sup_{v \in H_0^s(B_{r h^{(k-1)}(x_i^{(k)})})} \frac{\|v\|_{C^{(1)}(B_{r h^{(k-1)}(x_i^{(k)})})}}{\|v\|_{H_0^s(B_{r h^{(k-1)}(x_i^{(k)})})}} \leq \alpha_{\max} C r^{-s-d/2} h^{(k-1)(s-d/2)},
\]

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where the last estimate follows from the Sobolev embedding into Hölder spaces. In order to prove the lower bound on $S_{\min}$, let $\eta \in H_0^s(B_1(0))$ be such that $\eta \geq 0$ on $B_1(0)$ and $\eta \geq 1$ on $B_{1/2}(0)$. We then have

$$
\left\| \phi_i^{(k)} \right\|_{H^{-1}(B_{\delta_{mesh}h^k}(x_i^{(k)}))} \geq \frac{\left[ \phi_i^{(k)}, \eta \left( x_i^{(k)} + 1/ (\delta_{mesh}h^k) \cdot \right) \right]_{H_0^s(B_{\delta_{mesh}h^k}(x_i^{(k)}))}}{\eta \left( x_i^{(k)} + 1/ (\delta_{mesh}h^k) \cdot \right)_{H_0^s(B_{\delta_{mesh}h^k}(x_i^{(k)}))}} \geq \frac{\alpha_{\min}}{\| \eta \|_{H_0^s(B_1(0))}} \left( \delta_{mesh}h^k \right)^{s-d/2} \alpha_{\min},
$$

from which follows $S_{\min}(\delta_{mesh}h^k) \geq C\alpha_{\min}h^{(s-d)/2}$. The inequality for $B^{(k,a)}$ follows in an analogous way from Corollary 3.38.

Next we prove the bounded condition numbers in the case of averaging, by a similar argument.

**Theorem 3.43.** In the setting of Example 3.33, there exists a constant $C$ depending only on $s$, $d$, $\Omega$, $\Omega'$, $C_G$, $C_{G^{-1}}$, and $\delta_{mesh}$ such that

$$
C^{-1}h^{d/2} \prec A^{(1)} \prec A_{\min}^{-1}h^{-2s}
$$

and

$$
C^{-1}h^{d/2}h^{-2(k-1)(s-d)/2} \prec B^{(k)} \prec A_{\min}^{-1}h^{-2ks},
$$

which results in

$$
\text{cond}(A^{(1)}) \leq C^2h^{-d/2}h^{-2s},
$$

$$
\text{cond}(B^{(k)}) \leq C^2h^{-d/2}h^{-2s}.
$$

Moreover, for $B^{(k,l)}$ defined as in Corollary 3.38, we have:

$$
C^{-1}A_{\max}^{-1}h^{d/2}h^{-2(k-1)(s-d)/2} \prec B^{(k,q)}.
$$

**Proof.** By a simple calculation we see that $\|\pi^{(k-1,k)}\| = 1$ and by construction $W^{(k)}W^{(k)}T = \text{Id}$. Again we need to show that the first two parts of Condition 3.34 and Condition 3.36 hold. We want to use Theorem 3.39 but we first notice that the $\phi_i^{(k)}$ are normalised in $L^2$, not in $L^1$, as is appropriate for the Radon measures used in Theorem 3.39. Therefore, we apply Theorem 3.39 to the rescaled $\phi_i^{(k)}$, normalised in the $L^1$-norm.

$$
S_{\max}^{(k)} \left( r h^{k-1} \right) \leq \frac{1}{\delta_{mesh}h^{kd}} \sup_{v \in H_0^s(B_{r h^{k-1}}(x_i^{(k)}))} \| v \|_{L^1(B_{r h^{k-1}}(x_i^{(k)}))},
$$

$$
S_{\max}^{(k)} \left( r h^{k-1} \right) \leq \frac{1}{\delta_{mesh}h^{kd}} \max \frac{1}{r h^{k-1}h^{k-1}(s-d)/2} \sup_{v \in H_0^s(B_{r h^{k-1}}(x_i^{(k)}))} \frac{\| v \|_{L^1(B_{r h^{k-1}}(x_i^{(k)}))}}{\| v \|_{H_0^s(B_{r h^{k-1}}(x_i^{(k)}))}},
$$

where the last estimate follows from the Sobolev embedding into Hölder spaces. In order to prove the lower bound on $S_{\min}$, let $\eta \in H_0^s(B_1(0))$ be such that $\eta \geq 0$ on $B_1(0)$ and $\eta \geq 1$ on $B_{1/2}(0)$. We then have

$$
\left\| \phi_i^{(k)} \right\|_{H^{-1}(B_{\delta_{mesh}h^k}(x_i^{(k)}))} \geq \frac{\left[ \phi_i^{(k)}, \eta \left( x_i^{(k)} + 1/ (\delta_{mesh}h^k) \cdot \right) \right]_{H_0^s(B_{\delta_{mesh}h^k}(x_i^{(k)}))}}{\eta \left( x_i^{(k)} + 1/ (\delta_{mesh}h^k) \cdot \right)_{H_0^s(B_{\delta_{mesh}h^k}(x_i^{(k)}))}} \geq \frac{\alpha_{\min}}{\| \eta \|_{H_0^s(B_1(0))}} \left( \delta_{mesh}h^k \right)^{s-d/2} \alpha_{\min}.\]
covariance operator $G$ the way from Corollary 3.38. B for all $i$

decomposition introduced in Kornhuber and Yserentant (2016a,b). We note that, by generalising the arguments in
this section, we will present the recent abstract results of exponential localisation of gamblets obtained
3.5.2 Exponential decay of gamblets

In the setting of Example 3.31, we have, for a constant depending only on $s$, $d$, $\Omega$, $G$, and $\delta_{\text{mesh}},$

$$C^{-1} \prec A^{(1)} \prec h^{-2s}$$

and

$$C^{-1} h^{-2(k-1)s} \prec B^{(k)} \prec Ch^{-2ks},$$

which results in

$$\text{cond}(A^{(1)}) \leq C^2 h^{-2s},$$

$$\text{cond}(B^{(k)}) \leq C^2 h^{-2s}.$$}

Moreover, for $B^{(k,l)}$ defined as in Corollary 3.38, we have:

$$C^{-1} \alpha_{\text{max}}^{-1} h^{d/2} h^{-2(k-1)(s-d/2)} \prec B^{(k,l)}.$$

3.5.2 Exponential decay of gamblets

In this section, we will present the recent abstract results of exponential localisation of gamblets obtained in Owhadi and Scovel (2017), which in turn are a generalisation of the subspace iteration method introduced in Kornhuber and Yserentant (2016a,b). We note that, by generalising the arguments in Owhadi (2017) to higher-order equations, exponential decay for higher-order elliptic PDE was obtained by Hou and Zhang (2017) under the additional condition of strong ellipticity, independently of Owhadi and Scovel (2017).

The first ingredient for the proof exponential decay in Owhadi and Scovel (2017) will be a domain decomposition

Construction 3.45. Let $\{B^{(k)}_i\}_{i \in I^{(k)}}$ be a family of subspaces of $\mathcal{B}$, such that $\mathcal{B} := \sum_{i \in I^{(k)}} B^{(k)}_i$ and
for all $i \in I^{(k)}$, there exists $v_i^{(k)} \in B_i^{(k)}$ such that $\left[\phi_i^{(k)}, v_i^{(k)}\right] = \delta_{i,j}$.

We define $\mathcal{W}^{(k),\perp} := \{v \in \mathcal{B} \mid [\phi_i^{(k)}, v] = 0 \text{ for all } i \in I^{(k)}\}$ and $\mathcal{W}_i^{(k),\perp} := B_i \cap \mathcal{W}^{(k),\perp}$. We define $P_i^{(k)}$ as the $(\cdot, \cdot)$-orthogonal projection of $\mathcal{B}$ onto $\mathcal{W}_i^{(k),\perp}$ and define $P^{(k)} := \sum_{i \in I^{(k)}} P_i^{(k)}$.

As before, we define the gamblets $\psi_i^{(k)} := \mathbb{E}[u|\phi_i^{(k)} = \delta_{i,j}]$, for $u$ a centered gaussian vector with covariance operator $G$. Define the undirected graph $G^{(k)} := (I^{(k)}, E^{(k)})$ such that $\{(i,j)\} \in E$ if there

$$\geq 2 \frac{\delta_{\text{mesh}}^2}{\|\eta\|_{H^s_0(B_i(0))}} \|H^s_0(B_i(0))\|_{H^s_0(B_i(0))},$$

from which follows $S_{\text{min}}^{(k)}(\delta_{\text{mesh}} h^{k}) \geq C h^{k(s-d/2)}$. By applying Theorem 3.39 and scaling back to normalisation with respect to $L^2$, we obtain

(i) $\|\phi\|_{\mathcal{B}} \leq C h^{-d/2}$ for $k \in \{1, \ldots, q\}$, $x \in \mathbb{R}^{I^{(k)}}$ and $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ and $x \in \mathbb{R}^{I^{(k)}}$.

(ii) $\|\phi\|_{\mathcal{B}} \leq C h^{-d/2}$ for $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ and $x \in \mathbb{R}^{I^{(k)}}$.

(iii) $\inf_{y \in \mathbb{R}^{I^{(k-1)}}, |y| \leq C h^{k-1}} |\phi - \sum_{i \in I^{(k-1)} \setminus \{\cdot\}} y_i \phi_i^{(k-1)}| \leq C h^{(k-1)s-d/2}$, for $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$, $k \in \{2, \ldots, q\}$. The result follows then, by applying Theorem 3.37. The inequality for $B^{(k,q)}$ follows in an analogous way from Corollary 3.38.

Finally, for Example 3.31, from (Owhadi and Scovel, 2017, Proposition 2.17) and (Owhadi and Scovel, 2017, Theorem 2.13) and an analogous application of Corollary 3.38 we have:

**Theorem 3.44.** In the setting of Example 3.31, we have, for a constant depending only on $s$, $d$, $\Omega$, $G$, and $\delta_{\text{mesh}},$

$$C^{-1} \prec A^{(1)} \prec h^{-2s}$$

and

$$C^{-1} h^{-2(k-1)s} \prec B^{(k)} \prec Ch^{-2ks},$$

which results in

$$\text{cond}(A^{(1)}) \leq C^2 h^{-2s},$$

$$\text{cond}(B^{(k)}) \leq C^2 h^{-2s}.$$
exist $v_i \in B_i^{(k)}$ and $v_j \in B_j^{(k)}$ such that $\langle v_i, v_j \rangle \neq 0$. Let $d^{(k)}(\cdot, \cdot)$ denote the corresponding graph distance. Define $\psi_i^{(k),0}$ as the solution to:

$$\begin{align*}
\text{Minimize } & \|\psi\| \\
\text{Subject to } & \psi \in B_i^{(k)} \text{ and } \left[\phi_j^{(k)}, \psi\right] = \delta_{i,j} \quad \forall i,j.
\end{align*}$$

Then Owhadi and Scovel (2017, Theorem 6.4.) states:

**Theorem 3.46.** If $\lambda_{\min}(P) > 0$, then for all $n > 0$ there exists a $\psi_i^{(k),n} \in \sum_{j: d^{(k)}(i,j) \leq n} B_j$, such that

$$\|\psi_i^{(k)} - \psi_i^{(k),n}\| \leq \left(\frac{\text{cond}(P) - 1}{\text{cond}(P) + 1}\right)^n \|\psi_i^{(k),0}\|.$$ 

Owhadi and Scovel (2017) give methods for the estimation of $\text{cond}(P)$, which result in proofs of exponential decay. In the case where $B$ is a Sobolev space, the following construction is used.

**Construction 3.47** (Construction 2.19 in Owhadi and Scovel (2017)). Let $h, \delta_{\text{mesh}} \in (0, 1)$, for $1 \leq k \leq q$, let $\tau_i^{(k)}$ be a partition of the Lipschitz domain $\Omega \subset \mathbb{R}^d$ into convex, uniformly Lipschitz sets such that contain a ball of radius $\delta_{\text{mesh}} h^k$ and are contained in a ball of radius $h^k$, with $\text{supp} \left(\phi_i^{(k)}\right) \subset \tau_i^{(k)}$. For $i \in I^{(k)}$, let $\Omega_i^{(k)} \subset \Omega$ such that $\Omega_i^{(k)}$ contains $\tau_i$ and $\text{dist} \left(\Omega_i^{(k)} \cap \Omega, \tau_i^{(k)}\right) \geq h^k$. Then we can define $B_i^{(k)} := H_h^0 \left(\Omega_i^{(k)}\right)$.

In order to prove exponential decay, the following condition is needed.

**Condition 3.48** (Condition 2.23 in Owhadi and Scovel (2017)). Given Construction 3.47 with $\delta_{\text{mesh}}$, $h \in (0, 1)$. And define

$$\mathfrak{W}^{(k),\perp} := \left\{f \in H_h^0(\Omega) \mid \phi_i^{(k)} f = 0 \text{ for all } i \in I^{(k)}\right\}.$$ 

Then we assume that there exists a constant $C(\Omega, d, \delta_{\text{mesh}}, s, \Omega, s)$, such that

$$\|D^t f\|_{L^2(\Omega)} \leq Ch^{s-t} \|f\|_{H_s^0(\Omega)} \text{ for } t \in \{0, 1, \ldots, s\}, f \in \mathfrak{W}^{(k),\perp},$$

$$\sum_{i \in I^{(k)}} \left[\phi_i^{(k)} f, f\right]^2 \leq C \left(\|f\|_{L^2(\Omega)}^2 + h^{2s} \|f\|_{H_s^0(\Omega)}^2\right), f \in H_h^0(\Omega),$$

$$|x|^2 \leq Ch^{-2s} \left\|\phi_i^{(k)} f\right\|_{H^{-s}(\Omega)} \text{ for all } i \in I^{(k)}.$$ 

Under these conditions (Owhadi and Scovel, 2017, Theorem 6.20) proves exponential decay of Gamblets:

**Theorem 3.49.** Given a bounded measurable open subset of $\Omega \subset \mathbb{R}^d$ with uniformly Lipschitz boundary, let $s \in \mathbb{N}^*$ and let $L$ be a continuous bijection from $H_h^0(\Omega)$ to $H^{-s}(\Omega)$ that is local in the sense that $[L v, w] = 0$ if $\text{supp} (v) \cap \text{supp} (w) = \emptyset$. Let $C_L$, $C_L^{-1}$ be the continuity constants of $L$. Let $\phi_i^{(k)}$ be as in Construction 3.47 and satisfy Condition 3.48. Then there exists a constant $C$ depending only on $d$, $\delta_{\text{mesh}}$, $s$, $C_L$ and $C_L^{-1}$ such that $\text{cond}(P) \leq C$ and $\|\psi_i^{(k),0}\| \leq C$.

Using the above-cited theorems, we are now ready to prove the hierarchical exponential decay.

**Theorem 3.50.** For $s > d/2$, and $h, \delta_{\text{mesh}} \in (0, 1)$, consider the situation of Example 3.32, with $\Omega = \Omega'$. Let $C_L$, $C_L^{-1}$ be the continuity constants of $L$ and its inverse. Then we have, for constant $C, \gamma$ depending only on $s$, $d$, $\Omega$, $\Omega'$, $\delta_{\text{mesh}}$, $C_L$, $C_L^{-1}$, and $\alpha_{\max}/\alpha_{\min}$, that Condition 3.6 holds.
Proof. When looking into the proof of Theorem 3.49 in Owhadi and Scovel (2017) one notices that the fact that the $\Omega_i^{(k)}$ is derived from a partition $\tau_i^{(k)}$ is not essential and the proof holds equally for $\Omega_i^{(k)}$ as introduced above. We note that the exponential decay of gamblets as in the statement of Theorem 3.46 is invariant under scaling of $\phi_i^{(k)}$. Hence, to better fit to the notation in Owhadi and Scovel (2017, Proposition 13.3), we can instead treat the case of $\phi_i^{(k)} := \frac{1}{k^{d/2}} \phi_i^{(k)}$. After this rescaling, the proof of the second and third estimate in Condition 3.48 is analogous to the case of Dirac measures treated in Owhadi and Scovel (2017, Proposition 13.3). In order to show that Condition 3.48 holds, we note that for $f$ to integrate to zero against a Radon measure with support localised in $B_{\rho}(x_i^{(k)})$ it has to have positive and negative values in $B_{\rho}(x_i^{(k)})$. Therefore, by the intermediate value theorem, it has to achieve the value 0 somewhere in $B_{\rho}(x_i^{(k)})$. Thus, the proof of the Poincaré inequality can be reduced to the one found in Owhadi and Scovel (2017, Proposition 13.3) for Dirac measures.

Therefore, one obtains the estimate

$$\|\psi_i^{(k)} - \psi_i^{(k),n}\| \leq C \exp^{-\gamma n}$$

Therefore we have

$$\left| \left( \Gamma_{i,k+1,q}^{(g)}, \Gamma_{i,j}^{(k),-1} \right) \right|_{l,1} \leq \left[ \phi_i^{(l)} \psi_j^{(k)} \right] \leq C \exp (-\gamma d(i,j))$$

and

$$\left| \left( \Gamma_{i,j}^{(k),-1} \right) \right| = \left| \langle \psi_i^{(k)}, \psi_j^{(k)} \rangle \right| \leq C \exp (-\gamma d(i,j)). \qed$$

**Theorem 3.51.** For $h, \delta_{\text{mesh}} \in (0,1)$ consider the situation of Example 3.31, with $\Omega = \Omega'$ and let $L$ be a continuous bijection from $H_0^2(\Omega)$ to $H^{-s}(\Omega)$ that is local in the sense that $[L \ell, \nu] = 0$ if $\text{supp} (\nu) \cap \text{supp} (\nu') = \emptyset$. Let $C_L, C_{L^{-1}}$ be the continuity constants of $L$ and its invers. Then we have, for constants $C, \gamma$ depending only on $s, d, \Omega, \Omega', \delta_{\text{mesh}}, C_L, C_{L^{-1}}$, and $\delta_{\text{mesh}}$, $C_L, C_{L^{-1}}$, that Condition 3.6 holds.

**Proof.** The result follows directly from Owhadi and Scovel (2017, Theorem 2.24) and Owhadi and Scovel (2017, Theorem 2.24) and the argument in Theorem 3.50. \qed

**Theorem 3.52.** For $h, \delta_{\text{mesh}} \in (0,1)$ consider the situation of Example 3.33, with $\Omega = \Omega'$ and let $L$ be a continuous bijection from $H_0^2(\Omega)$ to $H^{-s}(\Omega)$ that is local in the sense that $[L \ell, \nu] = 0$ if $\text{supp} (\nu) \cap \text{supp} (\nu') = \emptyset$. Let $C_L, C_{L^{-1}}$ be the continuity constants of $L$ and its invers. Then we have, for constants $C, \gamma$ depending only on $s, d, \Omega, \Omega', \delta_{\text{mesh}}, C_L, C_{L^{-1}}$, and $\delta_{\text{mesh}}$, $C_L, C_{L^{-1}}$, that Condition 3.6 holds.

**Proof.** The result follows directly from Owhadi and Scovel (2017, Theorem 2.24) and Owhadi and Scovel (2017, Theorem 2.24) and the argument in Theorem 3.50. \qed

### 3.6 The final result

The combined results of the last subsection will now lead to proof of the correctness and runtime estimate of our algorithm.

**Theorem 3.53.** Consider the situation of Examples 3.32, 3.31, or 3.33 with $\Omega = \Omega'$. Then, there exist constants $C, C_\gamma, \rho_{\text{min}}$ depending only on $s, d, \Omega, \delta_{\text{mesh}}, \alpha_{\text{min}}, \alpha_{\text{max}}, C_L, C_{L^{-1}}$, and $h$ such that, for $\rho \geq \rho_{\text{min}} \log(N)$, there exists a sparsity set $S \subset J \times J$ such that

$$\{(i,j) \mid d(i,j) < \rho\} \subset S \subset \{(i,j) \mid d(i,j) < 5\rho\}$$

and an ordering $\prec$ on $J$ Algorithm 8 applied to $\Gamma$ with the elimination ordering $\prec$ and sparsity pattern $S$ has the following approximation property:

$$\log \left( \frac{1}{\|LL^\Gamma - \Gamma\|_{\text{Fro}}} \right) \leq C_\gamma \log(N) - \gamma \rho.$$
and has complexity of at most $CN\log^2(N)\rho^{2d}$ in time and $CN\log(N)\rho^d$ in space. In particular, algorithm $S$ computes an $\epsilon$ accurate approximate Cholesky factorisation in $O\left(N\log^2(N)\log^d(N/\epsilon)\right)$ complexity in time and $O\left(N\log(N)\log^d(N/\epsilon)\right)$ in space.

**Proof.** The result follows directly by putting together the results of the last section. From Theorems 3.50, 3.51, and 3.52, it follows that the Condition 3.6 on hierarchical exponential decay is satisfied. Similarly, from Theorems 3.42, 3.44, and 3.43 it follows that Conditions 3.7, 3.24 on bounded condition numbers are satisfied. It follows from a simple sphere packing argument that $d$ fulfills the Conditions 3.16, 3.17, and 3.27. Therefore, we can conclude by applying Theorem 3.29 to obtain the error estimate. Here we used Theorems 3.42, 3.44, and 3.43 to obtain the polynomial bounds on the norms of $\Gamma$ and $\Gamma^{-1}$. The complexity estimate then follows from theorem 3.18.

**Corollary 3.54.** In the above theorem, $d(\cdot, \cdot)$ can be replaced with

$$d'(i, j) := h^{-\min(k,l)} \text{dist}(x^{(k)}_i, x^{(l)}_j)$$

for all $i \in J^{(k)}, j \in J^{(l)},$ for a possibly different constant.

**Proof.** The corollary follows directly from the above theorem, since $d(i, j) \leq Cd(i, j)$, for a constant $C$, depending only on $s, d, \Omega, \Omega'$, $\delta_{\text{mesh}}$, $\alpha_{\min}, \alpha_{\max}, C_L$, and $C_{L^{-1}}$.

Of course, in general we cannot expect an ordering sparsity pattern to be given to us, but will have to compute it given knowledge of the triples $\{i, x_i, \text{dist}(x_i, \partial \Omega)\}_{i \in J}$. The next theorem proves that this can be done efficiently.

**Theorem 3.55.** Let $\delta \in (0, 1)$ and $\Omega \subset \mathbb{R}$ be fixed. Then there exists a $\delta$ depending only on $\delta$ and $\Omega$ such that for every set of points $\{x_i\}_{i \in J}, \#J = N$ with

$$\sup_{x \in \Omega} \min_{i \in J} \text{dist}(x, x_i)/(\min_{i \neq j \in J} \text{dist}(x_i, x_j)) \leq \frac{1}{\delta},$$

there exists a $q = O(\log(N))$ and a decomposition $J = \bigcup_{k=1}^{q} J^{(k)}$ such that, for a $C$ depending only on $\Omega$, we have for all $1 \leq k \leq q$: 

(i) $\sup_{x \in \Omega} \min_{i \in J^{(k)}} C 2^{-k};$

(ii) $\min_{i \neq j \in J^{(k) \setminus J^{(k-1)}}} \geq \delta 2^{-k},$

where $J^{(k)} := \bigcup_{i=1}^{k} J^{(i)}$. Furthermore, this decomposition, as well as a sparsity set $S$ as described in Theorem 3.53 (for $h = 1/2$), can be constructed in computational complexity $O(Nq^2\rho^{2d}).$

**Proof.** We claim that the decomposition $J = \bigcup_{k=1}^{q} J^{(k)}$ can be obtained from Algorithm 10. Let $C$ be as in Algorithm 10. Then, for $C2^{-k} \geq \min_{i \in J^{(k)}} d(x_i, x_j)$, we have

(i) $\sup_{x \in \Omega} \min_{i \in J^{(k)}} \leq C 2^{-k};$

(ii) $\min_{i \neq j \in J^{(k) \setminus J^{(k-1)}}} \geq \frac{C}{2} 2^{-k}.$

by construction. Let $\tilde{k}$ be the maximal such $k$. But then, we know that $q = \tilde{k} + 1$, which implies

(i) $\sup_{x \in \Omega} \min_{i \in J^{(k)}} \leq 2C2^{-q};$

(ii) $\min_{i \neq j \in J^{(k) \setminus J^{(k-1)}}} \geq \frac{C}{2} 2^{-q}.$

To estimate the computational complexity of Algorithm 10, we note that the number of times that the innermost for loop is iterated can be bounded from above as $O(Nq)$ by a simple sphere packing argument. The most expensive operation in this loop is the $O(\log(N))$ reordering of the heap, leaving us with a computational complexity of $O(Nq^2\log(N))$. Once the ordering has been found, one can use Algorithm 11 to obtain the sparsity pattern $S_\rho$. Then, as described in Lemma 3.28 a multicolor ordering and supernodal pattern can be obtained. By using sphere-packing arguments and the complexity estimate on greedy graph coloring Husfeldt (2015), one can show that this can also be done in complexity $O(Nq^2\rho^{2d}).$

**Remark 3.56.** Although the third and fourth step are necessary for our proof of stability to work and allow to leverage optimised dense linear algebra and parallelisation, they do not seem necessary to achieve a stable algorithm, in practice.
3.7 Additional consequences of the result

3.7.1 Sparse Cholesky decomposition of the stiffness matrix

In numerical analysis, instead of being given the matrix $\Theta$, many times one starts out with the inverse $A$, in the form of a discretised differential operator. In this case, the compression of the operator is not the main concern, since it will usually be banded according to the physical distance of the meshpoints. However, even though the original matrix might be sparse, it’s Cholesky factors won’t be sparse because of the fill-in phenomenon. While there exist numerous approaches to finding orderings that reduce fill in, we are not aware of any such ordering that results in a provably near-linear algorithm on meshes of dimension $d > 1$. Often, the analysis of fill-in is based on graph theoretic approaches which, as in nested dissection ordering (George, 1973; Lipton et al., 1979; Gilbert and Tarjan, 1987) or minimal degree ordering (George and Liu, 1989). These methods however only exploit the algebraic structure implied by the position of the nonzero entries, without taking the values of these nonzero entries into consideration, a property that is very rigid with respect to small perturbations of the precision matrix. Instead, when interpreting the dense inverse matrix as a covariance operator corresponding to a smooth function prior to $h$, it is very natural that the sparsity inducing effect of elimination should enjoy a certain robustness. This allows to replace the separators used in nested dissection by smaller “approximate” separators, leading to near-linear algorithms. Thus, probabilistic interpretation of the fade-out occurring during the decomposition of the inverse operator $\Theta$ also gives a more complete understanding of the fill-in effect encountered when decomposing $A$. We have the following theorem:

**Theorem 3.57.** Assume that $\Theta$ has a Cholesky decomposition $\Theta = LL^T$, with:

$$|L_{i,j}| \leq C \exp(-\gamma_L d(i,j))$$

And that the inverse $A := (\Theta)^{-1}$ decays as

$$|A_{i,j}| \leq C \exp(-\gamma_A d(i,j)).$$

Furthermore assume that $d(\cdot, \cdot)$ fulfills Conditions 3.16 and 3.17. Now define $P$ as the permutation matrix reversing the order of variables. Then the Cholesky decomposition of $PAP$ is exponentially localised as:

$$|\tilde{L}_{i,j}| \leq qC^2 \bar{C} (\gamma_A, \gamma_L) \exp(- (\gamma_A \gamma_L) / 4d(P[i],P[j]))$$

where by a slight abuse of notation, $P[i]$ is defined as the $j$, such that $Pe_i = e_j$, and $q$ denotes the number of levels of $d$. Furthermore, the Cholesky of $PAP$ restricted to $\{i,j | d(P[i],P[j]) \leq \rho\}$ can be computed in the same time and space complexity as the one of $\Theta$ restricted to $\{(i,j) | d(i,j) \leq \rho\}$

**Proof.** We have:

$$A = (LL^T)^{-1} = L^{-1}L^{-T} \implies PAP = (PL^{-1}P)^{-T}PL^{-1}P.$$ 

We note that $PL^{-1}P$ is an upper-triangular matrix. Therefore, we know that the Cholesky factors of $PAP$ are given by $(PL^{-1}P)^{-T}$. To show the required localisation, we have to show the localisation of $L^{-1}$. We have however

$$L(L^TA) = Id \implies L^{-1} = L^TA$$

Now, we note that when using the usual block structure induced by the multiresolution basis, the blocks $(L^T)^{k,l}$ for $l < k$ are zero. Hence, by the triangle inequality of $d(\cdot, \cdot)$, $L^{-1}$ is decaying exponentially as described above. As before, this shows the exponential accuracy of the restricted Cholesky factorisation. The space and time complexity follows then from Lemma 3.14 by noticing that, under the reverse ordering, $S_I(i)$ and $S_I(i)$ are interchanged. □

In the context of elliptic PDE, we furthermore obtain the following bound

**Theorem 3.58.** Consider the situation of Examples 3.32 3.31 or 3.33 with $\Omega = \Omega'$. Then, there exist constants $C, C', \gamma, \rho_{\min}$ depending only on $s, d, \Omega, \delta_{\text{mesh}}, \alpha_{\min}, \alpha_{\max}, C_{\mathcal{L}}, C_{\mathcal{L}^{-1}},$ and $h$ such that, for $\rho \geq \rho_{\min} \log N$, there exists a sparsity set $S \subset J \times J$ such that

$$\{(i,j) | d(i,j) < \rho\} \subset S \subset \{(i,j) | d(i,j) < 5\rho\}$$

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and an ordering $\prec$ on $J$ Algorithm 8 applied to $\Gamma^{-1}$ with the elimination ordering $\prec$ and sparsity pattern $S$ has the following approximation property:

$$\log \left( \frac{1}{||LL^T - \Gamma \gamma||_{\text{Fro}}} \right) \leq C_\gamma \log(N) - \gamma \rho.$$ 

and has complexity of at most $CN \log^2(N) \rho^{2d}$ in time $CN \log(N) \rho^d$ in space. In particular, algorithm 8 computes an $\varepsilon$-accurate approximate Cholesky factorisation in $O(N \log^2(N) \log^{2d}(N/\varepsilon))$ complexity in time and $O(N \log(N) \log^3(N/\varepsilon))$ in space.

Proof. The result is proven analogue to Theorem 3.53. The main differences are that for Condition 3.24 an estimate from above for $\lambda_{\max}(A^{(k)})$ is required, which is obtained the same way as the upper bound on $\lambda_{\max}(B^{(k)})$. Furthermore, the construction of the supernodal $S$ in Lemma 3.28 since the parents of a degree of freedom under one ordering are the children or the same degree of freedom under the under ordering.

Corollary 3.59. In the above theorem, $d(\cdot, \cdot)$ can be replaced with

$$d(i, j) := h^{-\min(k, l)} \text{dist}(x_i^{(k)}, x_j^{(l)}) \text{ for all } i \in J^{(k)}, j \in J^{(l)},$$

for a possibly different constant.

Proof. The corollary follows directly from the above theorem, since $d(i, j) \leq C d(i, j)$, for a constant $C$, depending only on $s, d, \Omega, \Omega', \delta_{\text{mesh}}, \alpha_{\min}, \alpha_{\max}, C_{\text{F}},$ and $C_{\rho}$. 

In the a scenario in which the stiffness matrix is given, we typically know the order of the operator. Furthermore, since the stiffness matrix is sparse, the application of averaging-based multiresolution with vanishing moments will be possible in near-linear time. Therefore, while subsampling-based sparse Cholesky decomposition as in Theorem 3.53 is an option, we can also use a multiresolution basis as in Owhadi and Scovel (2017)[Example 2.27]. The results in this reference, which also motivated the present work, directly yield Conditions 3.7 and 3.6.

3.7.2 The rank-revealing property of sparsifying Cholesky decomposition

As already noted in Owhadi (2017), the upper and lower bounds on $\text{cond}(B^{(k)})$ and orthogonality in the operator inner product suggest that gamblets have some similarity to an eigenspace decomposition, with the difference that they can be computed in near-linear time. While they are not orthogonal in operator inner product suggest that gamblets have some similarity to an eigenspace decomposition, with the difference that they can be computed in near-linear time. While they are not orthogonal in $L^2$, as one would expect from an eigendecomposition, it was shown in Owhadi and Scovel (2017) that the minimum angle between gamblets on different scales is bounded uniformly from below, which can be seen as a sort of “approximate orthogonality”. Hou and Zhang (2017) generalised the construction of Owhadi (2017) to higher-order elliptic operators (independently of Owhadi and Scovel (2017)) and proposed its use for the compression of Green’s operators. Since the sparsifying Cholesky decomposition is intimately related to the gamblet transform, it inherits the PCA-like behaviour of the gamblets. Consider the following low-rank variant of the Cholesky decomposition where $i^{(l)}$ denotes the largest index $i$, such that $i \in I^{(l)}$. $j$.

**Algorithm 9:** Low rank Cholesky decomposition

```plaintext
input : A positive-definite $N \times N$ matrix $\Theta$ and a maximum level $k$

output: A lower-triangular $N \times N$ matrix $L$

for $i \leftarrow 1$ to $i^{(l)}$
  for $j \leftarrow i$ to $N$
    $L_{i,j} \leftarrow \Theta_{i,j}$
  for $i \leftarrow 1$ to $i^{(l)}$
    for $j \leftarrow i + 1$ to $i^{(l)}$
      $L_{j,N,j} \leftarrow L_{j,N,j} - L_{i,N,i} L_{j,i} L_{i,i}$
      $L_{i,N,i} \leftarrow L_{i,N,i} / \sqrt{L_{i,i}}$
```

We have the following estimates for the truncation error of the low-rank Cholesky decomposition.
Lemma 3.60. Let $L$ be the output of Algorithm 9 applied to $\Gamma$. With the notation of Corollary 3.38, we have:

$$\|L^{(i)}L^{(i)}T - \Gamma\| \leq CH^{2l}J^{(l+1),-1} \leq \frac{1}{\lambda_{\min}(B^{(l+1,q)})}$$

Proof. We recognise that Algorithm 9 is equivalent to the assuming that after the outer iterations for $i$ up to $i^{(i)}$, the remaining block on the lower right is zero. This can equally be achieved by subtracting this lower right block from $\Gamma$, to begin with. It turns out that this lower right block is the Schur complement $\Gamma^{[l+1,q],[l+1,q]} - \Gamma^{[l+1,q],[1,l]} (\Gamma^{[1,l],[1,l]})^{-1} \Gamma^{[1,l],[l+1,q]} = B^{(l+1,q),-1}$.

This immediately provides us with a bound for the low-rank approximation error, in the setting of Theorems 3.42, 3.43 and 3.44:

Corollary 3.61. Under the conditions of Theorems 3.42, 3.43, or 3.44 we have $\|L^{(i)}L^{(i)}T - \Gamma\| \leq C\alpha_{\max}h^{2l(s-d/2)}$, $\|L^{(i)}L^{(i)}T - \Gamma\| \leq C\alpha_{\max}h^{d/2}h^{2l(s-d/2)}$, or $\|L^{(i)}L^{(i)}T - \Gamma\| \leq C\alpha_{\max}h^{d/2}h^{2l(s-d/2)}$, respectively.

4 Implementation and Numerical Results

4.1 Constructing the sparsity pattern

For the numerical experiments in this section, we constructed our measurement locations as random perturbations of a regular grid, which makes it very easy to construct the hierarchical ordering and sparsity pattern. For the sake of completeness, in this section we provide algorithms that allow construction of the sparsity pattern given the $N$ triples $\{i,x_i,\text{dist}(x_i,\partial\Omega)\}_{i \in J}$, in near-linear time. Algorithm 10 constructs the necessary multiscale ordering:
Algorithm 10: Constructing the hierarchy.

**input**: \(N\) triples \(\{i, x_i, \text{dist}(x_i, \partial \Omega)\}_{i \in J}\)

**output**: A partition of \(J\) in \(q\) subsets \(J^{(q)}, \ldots, J^{(1)}\)

for \(i \in J\) do
\[
\begin{align*}
&s[i].\text{Id} \leftarrow i; \\
&s[i].\text{level} \leftarrow 0; \\
&s[i].x \leftarrow x_i; \\
&s[i].d \leftarrow \text{dist}(x_i, \partial \Omega); \\
&s[i].C \leftarrow \emptyset; \\
&s[i].p \leftarrow i; \\
\end{align*}
\]
// The set of ‘‘children’’-nodes
// The ‘‘parent’’-node

\(H \leftarrow \text{BINARY_HEAP}(s, ‘d’, ‘descending’);\) // constructs a binary heap of the structs \(s\) ordered by \(d\), with the maximal \(d\) at the root

\(C \leftarrow \text{ROOT}(H).d\) // The function \(\text{ROOT}\) obtains the root of the heap

\(q \leftarrow 0;\)
while \(H \neq \emptyset\) do
\[
\begin{align*}
&\text{while } \text{ROOT}(H).d \leq C2^{-q} \text{ do} \\
&\quad i \leftarrow \text{ROOT}(H).\text{Id}; \\
&\quad \text{REMOVE_ROOT}(H) \text{ // removes the present root from the heap.} \\
&\quad s[i].\text{level} \leftarrow q; \\
&\quad \text{if } q = 1 \text{ then} \\
&\quad \quad s[i].C \leftarrow J; \\
&\quad \text{for } j \in s[i].p.C \text{ do} \\
&\quad \quad \text{if } \text{dist}(s[j].x, s[i].x) < s[j].d \text{ then} \\
&\quad \quad \quad s[j].d \leftarrow \text{dist}(s[j].x, s[i].x) \text{ // We assume that this update causes the} \\
&\quad \quad \quad \text{heap to restore its ordering, which has complexity } O(\log(N)). \\
&\quad \quad \text{if } \text{dist}(s[j].x, s[i].x) \leq C2^{-q+1} \text{ then} \\
&\quad \quad \quad x[j].p \leftarrow i; \\
&\quad \quad \text{if } \text{dist}(s[j].x, s[i].x) \leq C2^{-q} \text{ then} \\
&\quad \quad \quad x[i].C \leftarrow x[i].C \cup j; \\
&\quad q \leftarrow q + 1; \\
&\end{align*}
\]
for \(i \in J\) do
\[
\begin{align*}
&k \leftarrow s[i].\text{level}; \\
&J^{(k)} \leftarrow J^{(k)} \cup i \text{ // Sorting the nodes into the different } J^{(k)}
\end{align*}
\]

After having obtained the hierarchy, it is easy to construct the basic sparsity pattern
\[
S^\rho := \left\{ (i, j) \in i \in J^{(k)}, j \in J^{(l)} \left| \text{dist}(x_i, x_j) \leq \rho 2^{-\min(k,l)} \right. \right\}.
\]

For simplicity, we assume that \(\rho \geq 2C = 2 \min_{i \in J} \text{dist}(x_i, \partial \Omega).\)
Algorithm 11: Constructing the sparsity pattern.

\[ \text{input : The sets } \{J^{(k)}\}_{1 \leq k \leq q} \text{ and the } \{x_i\}_{i \in J}, \text{ ordered by membership in the } \{J^{(k)}\}_{1 \leq k \leq q} \]

\[ \text{output: } N \text{ sets } S_i := \{j \in J : (i, j) \in S^\rho\}, \text{ sorted by membership in } \{J^{(k)}\}_{1 \leq k \leq q} \]

\[ \text{for } i \in J \text{ do} \]
\[ p[i] \leftarrow i /\text{ Initialising } \text{‘parent’-nodes} \]
\[ d[i] \leftarrow \infty /\text{ Initialise distance to parent} \]

\[ \text{for } i \in J^{(1)} \text{ do} \]
\[ \text{for } j \in J \text{ do} \]
\[ \quad \text{if } \text{dist}(x_i, x_j) < d[j] \text{ then} \]
\[ \quad \quad p[j] \leftarrow i; \]
\[ \quad \quad d[i] \leftarrow \text{dist}(x_i, x_j); \]
\[ \quad \text{if } \text{dist}(x_i, x_j) \leq \rho 2^{-1} \text{ then} \]
\[ \quad S_i \leftarrow S_i \cup j; \]

\[ \text{for } 2 \leq k \leq q \text{ do} \]
\[ \text{for } i \in J^{(k)} \text{ do} \]
\[ \quad \text{for } j \in S_{p[i]} \text{ and } \text{dist}(x_j, x_{p[i]}) \leq \rho 2^{-(k-1)} \text{ do} \]
\[ \quad \text{if } \text{dist}(x_i, x_j) < d[j] \text{ then} \]
\[ \quad \quad p[j] \leftarrow i; \]
\[ \quad \quad d[i] \leftarrow \text{dist}(x_i, x_j); \]
\[ \quad \text{if } \text{dist}(x_i, x_j) \leq \rho 2^{-k} \text{ then} \]
\[ \quad S_i \leftarrow S_i \cup j; \]

Once the hierarchical ordering and the sparsity pattern \(S^\rho\) are obtained, a supernodal multicolor ordering can be obtained as described in the proof of Lemma 3.28. Since we empirically observe stability of the algorithm, even without a supernodal or multicolor ordering (cf. Section 4.3.3), we do not describe this algorithm in further detail but note that it can also be done in \(O(Nq^2\rho^2d)\) computational complexity.

Note that Algorithms 10 and 11 require only knowledge of the pairwise distances between points and the distance of points to the boundary of \(\Omega\). Therefore, other than algorithms based on, for example, quadtrees or octtrees, our algorithm is oblivious to the ambient dimension.

We further note that when dealing with covariance matrices that do not correspond to a boundary value problem, like the Matérn family, improved results can be obtained by including points on the boundary in each of the \(J^{(k)}\) (cf. Section 4.3.5). For our numerical experiments, we will use the Matérn family of covariance kernels.

### 4.2 The Matérn family

The Matérn family of kernels, originally introduced by Matérn (1960), is used in many branches of statistics and machine learning to model random fields with finite order of smoothness (Guttorp and Gneiting, 2006; Rasmussen and Williams, 2006). It is defined as

\[ G(x, y) := \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu|x-y|}}{l} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu|x-y|}}{l} \right), \]

where \(K_\nu\) is the modified Bessel function of second kind (Abramowitz and Stegun, 1964, Section 9.6) and \(\nu, l\) are parameters describing the degree of smoothness, and the length-scale of interactions, respectively (Rasmussen and Williams, 2006). For \(\nu = p + 1/2\), \(p \in \mathbb{N}\), the Matérn kernel take a particularly simple form (Rasmussen and Williams, 2006), yielding for example:

\[ G_{1/2}(x, y) = \exp \left( -\frac{|x-y|}{l} \right) \]

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\[ G_{\frac{3}{2}}(x,y) = \left(1 + \sqrt{3} \frac{|x-y|}{l} \right) \exp \left(-\frac{\sqrt{3}|x-y|}{l} \right) \]
\[ G_{\nu/2}(x,y) = \left(1 + \sqrt{\nu} \frac{|x-y|}{l} + 5 \frac{|x-y|^2}{l^2} \right) \exp \left(-\frac{\sqrt{\nu}|x-y|}{l} \right). \]

Stein (1999) strongly recommends the Matérn family as a model for spatial statistics for its capability to allow for small-scale structure as opposed to, say, the Gaussian covariance function.

When considered as function on \( \mathbb{R}^d \times \mathbb{R}^d \), the Fourier transform of the Matérn kernel is given by
\[
\hat{G}(s) = \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^\nu}{\Gamma(\nu)^{2\nu}} \left( \frac{2\nu}{l^2} + 4\pi^2 |s|^2 \right)^{-(\nu + d/2)}. \]

As was observed by Whittle (1954, 1963), this makes the Matérn kernel the Green’s function of (possibly fractional) order 2(\(\nu + d/2\)). Accordingly, the Matérn kernel has found uses in meshfree methods for PDEs (Schaback, 2007; Cockayne et al., 2016; Raissi et al., 2017b) and Bayesian inverse problems involving PDEs (Dunlop et al., 2016; Roininen et al., 2014).

Recently it has been observed that in large applications, featuring a simple low-dimensional geometry, for example the surface of the earth in spatial statistics, it can be beneficial to work directly with the underlying PDE. While it is conceptually more difficult to solve a PDE than to evaluate a closed form for example the surface of the earth in spatial statistics, it can be beneficial to work directly with the PDEs (Dunlop et al., 2016; Roininen et al., 2014).

When considered as function on \( \mathbb{R}^d \times \mathbb{R}^d \), the Fourier transform of the Matérn kernel is given by
\[
\hat{G}(s) = \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^\nu}{\Gamma(\nu)^{2\nu}} \left( \frac{2\nu}{l^2} + 4\pi^2 |s|^2 \right)^{-(\nu + d/2)}. \]

As was observed by Whittle (1954, 1963), this makes the Matérn kernel the Green’s function of (possibly fractional) order 2(\(\nu + d/2\)). Accordingly, the Matérn kernel has found uses in meshfree methods for PDEs (Schaback, 2007; Cockayne et al., 2016; Raissi et al., 2017b) and Bayesian inverse problems involving PDEs (Dunlop et al., 2016; Roininen et al., 2014).

Stein (1999) strongly recommends the Matérn family as a model for spatial statistics for its capability to allow for small-scale structure as opposed to, say, the Gaussian covariance function.

When considered as function on \( \mathbb{R}^d \times \mathbb{R}^d \), the Fourier transform of the Matérn kernel is given by
\[
\hat{G}(s) = \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^\nu}{\Gamma(\nu)^{2\nu}} \left( \frac{2\nu}{l^2} + 4\pi^2 |s|^2 \right)^{-(\nu + d/2)}. \]

As was observed by Whittle (1954, 1963), this makes the Matérn kernel the Green’s function of (possibly fractional) order 2(\(\nu + d/2\)). Accordingly, the Matérn kernel has found uses in meshfree methods for PDEs (Schaback, 2007; Cockayne et al., 2016; Raissi et al., 2017b) and Bayesian inverse problems involving PDEs (Dunlop et al., 2016; Roininen et al., 2014).

4.3 Numerical experiments

4.3.1 The basic set-up

Uur numerical experiments use the domain \([0, 1]^2\) and a uniform grid of points created by \(q\) subdivisions of the domain, as indicated by Figure 4.1. This regular grid is used only for ease of implementation. In order to show that regularity of the grid is not necessary for our algorithm to work, we introduce in each dimension a random perturbation of \(2^{-q} \delta_x \text{Unif}(-1, 1)\), for \(q\) the number of levels. For \(q = 5\), the effect of this perturbation is shown in Figure 4.2. Ordering the points \(x_i\) from points on coarse levels to points...
on finer ones, we obtain our covariance matrix $\Gamma$ as

$$
\Gamma_{i,j} \coloneqq 2^{1-\nu} \left( \frac{\sqrt{2^\nu |x_i - y_j|}}{l} \right)^\nu K_{\nu} \left( \frac{\sqrt{2^\nu |x_i - y_j|}}{l} \right)
$$

For a tuning parameter $\rho$, we consider the sparsity set $S \coloneqq S_\rho \coloneqq \{(i,j) | \|x_i - x_j\| \leq \rho 2^{\min(\text{lev}(i),\text{lev}(j))}\}$, where $\text{lev}(i)$ is the smallest $k$ such that $i \in I^{(k)}$. In Figure 4.3, the interactions of points on different levels are visualised. The sparsified kernel matrix $\tilde{\Gamma}_\rho$ is then obtained from $\Gamma$ by setting all entries that are not in $S_\rho$, to zero. The sparse Cholesky factor $L_\rho$ is then obtained by applying the matlab function “ichol” with option “nofill” to $\tilde{\Gamma}_\rho$, which performs an incomplete Cholesky decomposition, which is equivalent to Algorithm 8. Finally, the resulting approximation of the kernel is obtained as $\Gamma_\rho \coloneqq L_\rho L_\rho^T$. The numerical results presented here are simple illustrative examples of our theoretical results obtained from artificially created measurement points. We plan to develop a fully sparsity-exploiting implementation.
We see that the difference between the approximation obtained by Algorithm 8 and truncating the exact Cholesky factors, is tabulated in Tables 4.4, 4.5 and 4.6 for the kernels investigated. As a next example we will take again the Matérn kernel with smoothness $\nu = 1$ and interaction length of $l = 0.2$. For these values, the Matérn kernel corresponds to the Green’s function of an elliptic operator of order 4. In Table 4.1, we show the resulting absolute and relative error in Frobenius operator norm and the compression ratio compared to a dense matrix, for different values of $\rho$. To show that even very long correlation length do not lead to a breakdown of our method, we try the same kernel but this time with an interaction length of $l = 0.4$. As one can see in Table 4.2, for a given $\rho$, we get similar approximation properties as in the first example. As a next example we will take again $l = 0.2$ but we will take $\nu = 2$. This corresponds to the Green’s operator of an elliptic equation of order 6. This time, the minimal value of $\rho$ that we have to choose is larger, larger condition number has to be compensated for by a decrease in truncation error. We compile our result in Table 4.3. In Figure 4.4 we have plotted the relative error in operator norm on a logarithmic scale. The first panel shows the error obtained over the entire domain. For small relative accuracy we observe a saturation of the exponential decay, which we attribute to the boundary effects discussed in Section 4.3.5. The second panel shows the relative error in operator norm of the approximation of $\Gamma$ by $\Gamma'$, where $\Gamma'$ denotes the restriction to entries $(i,j)$ such that $x_i, x_j \in [0.1, 0.9]^2$. As we can see from the second panel of Figure 4.4, the exponential decay of the error in the interior of the domain is more rapid and is not subject to this saturation effect.

### 4.3.3 Truncated versus incomplete factors

The reason for introducing supernodes and multicolor orderings in Section 3.4.2 is that they are needed to bound the difference between the approximation obtained from the Cholesky factors $L^\rho$ as computed by Algorithm 8 and the approximation obtained by computing the exact Cholesky factor $L$ and then approximating $\Gamma$ by $(L|S)(L|S)^T$. The size of this effect, compared to the the approximation error when truncating the exact Cholesky factors, is tabulated in Tables 4.4, 4.5 and 4.6 for the kernels investigated in Section 4.3.1. We see that the difference between the approximation obtained by Algorithm 8 and...
\[ \| \Gamma^\rho - \Gamma \| / \| \Gamma \| \] 
\[ \| \Gamma^\rho - \Gamma \|_{\text{Fro}} / \| \Gamma \|_{\text{Fro}} \] 
\[ \#S \] 
\[ \#S/N^2 \]

Table 4.3: Compression and accuracy for \( q = 7 \), \( l = 0 \), \( \nu = 2 \), \( \delta_x = 0.2 \) and different values of \( \rho \).

The truncation of the exact Cholesky factors is bounded from above by the approximation error incurred when using the truncation of the exact Cholesky factors, throughout our experiments. This provides strong numerical evidence that the introduction of supernodal multicolor ordering are not necessary in practise. Instead, the sparsity pattern can simply be chosen based on the distance of the measurement points and an arbitrary ordering can be used within each level.

### 4.3.4 Irregularity of the grid and points on a submanifold

In this section we want to investigate the robustness of our algorithm to the placement of the sampling points \( x_i \). Recall that our set of sampling points is initially generated as a uniform grid, which is then subject to random perturbations of magnitude \( \delta_x 2^{-q} \). In the last section, we choose \( \delta_x \) to be 0.2, which destroys the simple regular structure of the initial mesh but still prevents neighbouring points from coming too close together. In this section we are going to drastically increase the size of the perturbation, thus creating highly irregular point clouds. We will choose values of \( \delta_x \in \{0.2, 0.4, 2, 4\} \) for a kernel with \( \nu = 1 \) and \( l = 0.2 \). In Figure 4.5, the corresponding point clouds are plotted. In Table 4.7, we tabulated the resulting approximation error for \( \rho = 6 \) Note that for \( \delta_x \in \{0.2, 0.4\} \), a lower bound on \( \delta_{\text{mesh}} \) as in Examples 3.31 3.33 and 3.32 is still guaranteed. For \( \delta_x \in \{2, 4\} \), instead, very tight

| \( \rho \) | \( ||L^\rho L^\rho \text{T} - (L_S)(L_S)^\text{T}|| \) | 2.0 | 4.0 | 6.0 | 8.0 | 10.0 | 12.0 | 14.0 |
|---|---|---|---|---|---|---|---|---|
| 6.0 | 5.278e+00 | 6.671e-02 | 3.051e-03 | 5.030e-04 | 1.404e-04 | 5.183e-05 | 2.163e-05 |
| 8.0 | 8.926e+00 | 1.085e-01 | 5.753e-03 | 1.228e-03 | 4.012e-04 | 1.570e-04 | 7.474e-05 |
| 10.0 | 5.913e-01 | 6.147e-01 | 5.304e-01 | 4.098e-01 | 3.499e-01 | 3.301e-01 | 2.894e-01 |

Table 4.4: Error induced by the incomplete factorisation for \( q = 7 \), \( l = 0.2 \), \( \nu = 1 \), \( \delta_x = 0.2 \) and different values of \( \rho \).
Table 4.5: Error induced by the incomplete factorisation for \( q = 7, \ l = 0.4, \ \nu = 1, \ \delta_x = 0.2 \) and different values of \( \rho \).

| \( \rho \) | 6.0   | 8.0   | 10.0  | 12.0  | 14.0  |
|------------|-------|-------|-------|-------|-------|
| \( \| L^{\rho} - (L\|_S)(L\|_S)^T \| \) | 3.908e-02 | 6.520e-04 | 9.081e-05 | 1.393e-05 | 2.625e-06 |
| \( \| (L\|_S)(L\|_S)^T - \Gamma \| \) | 4.077e-02 | 8.555e-04 | 1.197e-04 | 1.944e-05 | 4.442e-06 |
| \( \| L^{\rho} - (L\|_S)(L\|_S)^T \| / \| L \|_Fro \) | 7.965e-01 | 7.622e-01 | 7.584e-01 | 7.167e-01 | 5.909e-01 |

Table 4.6: Error induced by the incomplete factorisation for \( q = 7, \ l = 0.2, \ \nu = 2, \ \delta_x = 0.2 \) and different values of \( \rho \).

| \( \delta_x \) | \( \| \nu - \Gamma \| \) | \( \| \nu - \Gamma \| / \| \Gamma \| \) | \( \| \nu - \Gamma \|_{\text{Fro}} / \| \Gamma \|_{\text{Fro}} \) | \#S | \#S/N² |
|---------------|-----------------|-----------------|-----------------|------|-------|
| 0.2           | 4.336e-03       | 1.560e-06       | 1.661e-02       | 1.026e-06 | 2.125e+07 | 7.675e-02 |
| 0.4           | 4.495e-03       | 1.617e-06       | 1.706e-02       | 1.063e-06 | 2.128e+07 | 7.683e-02 |
| 2.0           | 4.551e-03       | 1.648e-06       | 1.820e-02       | 1.077e-06 | 2.127e+07 | 7.682e-02 |
| 4.0           | 8.158e-03       | 2.940e-06       | 2.976e-02       | 1.933e-06 | 2.119e+07 | 7.652e-02 |

Table 4.7: Compression and accuracy for \( q = 7, \ l = 0.2, \ \rho = 5, \ \nu = 1 \) and different values of \( \delta_x \).

Figure 4.5: Different degrees of perturbation: The above plots show the measurement points \( x_i \) for \( q = 7 \) and \( \delta_x = \{0.2, 0.4, 2, 4\} \)
clustering of measurement points can occur. We note that under inclusion of moderate irregularity the accuracy of the approximation is more or less stable or even improving slightly. When increasing the perturbation to $\delta_z = 4$, we have the first notable, although small deterioration of accuracy. This however goes along with a small decrease in the size of $#S$, making the Net-detoriation, after accounting for the decrease of $#S$, even smaller. Since the choice of the ordering in our implementation happens before the perturbation is applied, this simultaneously shows robustness of the algorithm under the choice of the multiresolution ordering. One advantage of using covariance kernels, as opposed to an explicit discretisation of the underlying PDE, is that kernel-based methods adapt nicely to points that do not lie exactly in a low-dimensional Euclidean space, but instead might be clustered around a low-dimensional submanifold of a higher-dimensional space. In order to test, how our method deals with this situation, we use introduce a new parameter $\delta_z$, and add to every point $x_i \in \mathbb{R}^2$ a third component

$$x_i^{(3)} := -\delta_z \sin \left( 6x_i^{(1)} \right) \cos \left( 2x_i^{(2)} \right) + 2\delta_z 2^{-\delta_z} \varepsilon_i^{(3)},$$

where the $\varepsilon_i^{(3)} \sim \text{Unif}(-1,1)$ are independent random variables. In Figure 4.6, we plot the resulting point clouds for $q = 7$, $\delta_z = 2$ and $\delta_z \in \{0, 0.1, 0.2, 0.4\}$. Using these sets of sampling points, for a Matérn kernel with $\nu = 1$ and $\ell = 0.2$, we obtain the numerical results summarised in Table 4.8. We see that while there is a mild increase in approximation error, as $\delta_z$ is increased, we overall obtain a good approximation even for $\delta_z = 0.4$, when $z$-axis variability is almost as large as $x$- and $y$-axis variability. We further note that because of the increasing distance between points, $#S$ is also decreasing. If one were to compensate for this decrease by slightly decreasing $\rho$, the net-detoriation would be even smaller.

### 4.3.5 Detoriation of exponential decay at the boundary

Unfortunately, the Matérn family is not covered by our theoretical guarantees since it corresponds to a Green’s function on the whole space, whereas our measurement points are only dense in a bounded subset of $\mathbb{R}^2$. PDE based methods for representing the Matérn kernels, as those of Lindgren et al. (2011) and Roininen et al. (2014) need to specify boundary conditions, so that the partial differential operators has a unique inverse. As noted by Roininen et al. (2014) this choice can severely affect the resulting covariance operator, with Dirichlet or Neumann boundary conditions leading to an under- or over-estimate of the covariances near the boundary. Roininen et al. (2014) observe that Robin boundary conditions with a well chosen coefficient can yield a much better approximation of the Matérn covariance operator. Furthermore it is noted that an artificial extension of the computational domain can decrease the effect of boundary conditions. Daon and Stadler (2016) treat the problem of mitigating the boundary effects in PDE-based approaches to Gaussian processes in more detail. The authors present methods based on the optimal choice of coefficients of the Robin boundary conditions and the normalisation of the variance to decrease the influence of the boundary conditions of the covariance operator.

In contrast to these observations, the approximate covariance kernel obtained by our method is visually indistinguishable from the true covariance kernel, without any need for the user to specify boundary conditions. This is shown in Figure 4.7, where the covariances of a point in a corner of the domain are plotted. For this figure, we have chosen a large length-scale $\ell = 0.4$ and a small compression ratio $\rho = 2$, in order to maximise the effects caused by the finiteness of $\Omega = [0, 1]^2$. In the first panel of Figure 4.7, the value of the exact and approximate kernel is plotted against the distance of the evaluation points. In the second panel, the value of this kernel approximation is visualised in the physical domain.

While we do get very good approximation results even at the boundary, asymptotic decay of correlations does not happen to the same extent as in the inside of the domain. To illustrate this, the first panel

| $\delta_z$ | $\|\Gamma^p - \Gamma\|/\|\Gamma\|$ | $\|\Gamma^p - \Gamma\|_{Fro}/\|\Gamma\|_{Fro}$ | $\|\Gamma^p - \Gamma\|_{Fro}/\|\Gamma\|_{Fro} \quad #S \quad #S/N^2$ |
|--------|----------------------------|----------------------------|----------------------------|
| 0.0    | 5.049e-03                  | 1.560e-06                  | 1.885e-02                  | 2.126e+07                  | 7.677e-02                  |
| 0.1    | 6.341e-02                  | 1.648e-06                  | 1.223e-01                  | 1.077e+07                  | 7.521e-02                  |
| 0.2    | 1.204e+01                  | 1.749e-06                  | 2.203e-01                  | 1.976e+07                  | 7.137e-02                  |
| 0.4    | 1.954e+01                  | 3.550e-06                  | 5.098e-01                  | 1.722e+07                  | 6.218e-02                  |

Table 4.8: Compression and accuracy for $q = 7$, $\ell = 0.2$, $\rho = 5$, $\nu = 1$, $\delta_z = 2$ and different values of $\delta_z$. 

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Figure 4.6: Different amounts of vertical variability: The above plots show the measurement points $x_i$ for $q = 7$, $\delta_x = 2$ and $\delta_z \in \{0, 0.1, 0.2, 0.4\}$

Figure 4.7: Accurate representation of a boundary point: The first panel shows the values of the true and the approximate kernel based in $x_N$, the last point of the ordering. The second panel shows the value of the approximate kernel based in this point, in the physical domain.
Figure 4.8: Strong interactions among boundary points: The first panel shows the $i^{th}$ column of the Cholesky factor $L$ of $K$ (with $\nu = 1$, $l = 0.4$ for an $x_i$ in the interior of the domain. The second panel shows the $j^{th}$ column of $L$ for a $x_j$ on the lower, left corner of domain. Both $x_i$ and $x_j$ are on the finest level of the hierarchy. The all zero region in the first panel is caused by the elimination of these variables in the Cholesky factorisation.

The appearence of these residual long range correlations among boundary points, which appears particularily strongly if the length-scale of interaction is large, compared to the size of the domain, is not surprising. After all, our method is based on the screening effect and there are no measurements outside of $[0,1]^2$ on which we can condition to prevent communication between boundary points. While this might limit the performance of our method in the regime of very long interactions, there are a number of remedies to this problem.

(i) First, the number of boundary points is relatively small. Therefore, it is possible to include interactions among boundary points on a longer scale than interactions involving interior points, for only a small increase of algorithmic complexity. Furthermore, one might want to include more boundary points on the coarser scales, in order to increase the screening effect among boundary points. In our experiments, our measurement points are chosen with a high, constant density on the interior of the domain. In some applications, it is to be expected that the density of measurement points will decrease towards the boundary of the domain. In such a situation, by including with each level of the hierarchy an entire layer of boundary points, starting from the outer layers, one might be able to induce a stronger screening effect among measurements on the boundary.

(ii) We note that the results shown in the second panel of Figure 4.4 indicate that on the slightly smaller subdomain $[0,1,0.9]^2$ the effect of the boundary has already diminished drastically. In applications where one has access to the covariance function it is possible to introduce artificial measurement points on the boundary, in order to induce a stronger screening effect on the variables on the boundary of the domain. By making the former boundary of the domain of measurement part of the interior of an extended domain, a very accurate approximation of their covariances can be obtained. This approximation can then be used to apply the matrix $\Theta$ in near linear time, or generate normal random variables with covariance $\Theta$. To apply the inverse of the covariance matrix, the highly accurate sparse approximation of $\Theta$ obtained by the artificial measurements can be inverted using the conjugate gradient method, with the approximation $\Theta^\rho$, as obtained without artificial measurements, serving as a preconditioner.

(iii) What is the statistical meaning of $\Theta^\rho$? The weak, long range correlations among boundary points correspond to an implicit estimate of gaussian process outside of the domain of measurement. Depending on the context, these estimates might not be very reliable, thus the truncation of these correlations might actually be sensible, from a statistical point of view. In particular we note that our approximate covariance kernel does not exhibit the boundary artifacts described by Roininen et al. (2014) and Daon and Stadler (2016). On this note, it might be interesting to compare the
boundary values produced by our method with the optimal robin boundary conditions identified by Daon and Stadler (2016)

4.3.6 Fractional operators

For any given dimension \( d \), for almost all values of \( \nu \), the corresponding PDE will not be of integer order, but contain fractional derivatives. For PDE based methods that rely on the explicit discretisation of the partial differential operators, such as those of Lindgren et al. (2011), Hou and Zhang (2017), and Roininen et al. (2014), the treatment of fractional orders results in additional difficulties, both theoretically and in terms of the implementation. Our algorithm does not explitely discretise the differential operator, it is entirely agnostic to its form. While out theoretical results only cover integer order operators, in Table 4.9, we compiled the numerical results for the Matérn kernels interpolating between PDEs of order 4 and 6. As compiled in the table, we observe very similar approximation properties for both fractional and integer order PDE. As expected the the approximation ratios of the fractional Matérn kernels interpolate between the approximation ratios of the integer order kernels.

4.3.7 Sparse approximate PCA

As mentioned in Section 3.7, the factorisation obtained from Algorithm 8 also implies a sparse, approximate PCA. To show that this approximate PCA provides a near optimal rank-\( k \) approximation of the covariance operator, we define

\[
L_{\rho,j}^{(k)} := \begin{cases} 
L_{\rho}, & \text{for } j \leq \#I^{(k)} \0, & \text{otherwise.}
\end{cases}
\]

Here, \( \#I^{(k)} \) is the number of measurement points on the levels from 1 to \( k \). We then define the \( \Theta_{\rho}^{(k)} := L_{\rho}^{(k)} L_{\rho}^{(k)} \) as the rank \( \#I^{(k)} \) approximation implied by \( L_{\rho}^{(k)} \). In Figure 4.9 we have plotted the approximation error in Frobenius norm of the rank \( \#I^{(k)} \) approximation obtained from PCA and restricted Cholesky decomposition. As observed in Owhadi (2017); Hou and Zhang (2017) for gamblet based PCA, the resulting low-rank approximation has near-optimal approximation rate, as the rank is increased. While higher-order equations pose the additional difficulty of being more ill-conditioned, their quick spectral decay is helpful for spectral approximation. By truncating the Cholesky factors obtained from Algorithm 8, one obtains a combination of a multiscale approximation based on controlling the condition numbers on each scale — and a global low-rank approximation based on the decay of the eigenvalues. From a practical point of view, this gives us a way to salvage a restricted Cholesky algorithm that encounters a zero pivot, because of a choice of \( \rho \) that was too small for the given kernel. In this case, the columns of the Cholesky factor computed before the pivots became close to zero will still be a near-optimal low-rank approximation of the kernel matrix.

| \( \nu \) | \( \| \Gamma^\nu - \Gamma \| \) | \( \| \Gamma^\nu - \Gamma \|_{\text{Fro}} \) | \( \| \Gamma^\nu - \Gamma \|_{\text{Fro}}^2 \) | \#S | \#S/N^2 |
|---|---|---|---|---|---|
| 1.0 | 1.266e-03 | 4.556e-07 | 4.987e-03 | 2.995e-07 | 2.776e+07 | 1.003e-01 |
| 1.1 | 1.813e-03 | 6.423e-07 | 6.216e-03 | 4.190e-07 | 2.776e+07 | 1.003e-01 |
| 1.3 | 3.235e-03 | 1.129e-06 | 1.039e-02 | 7.312e-07 | 2.776e+07 | 1.003e-01 |
| 1.5 | 5.245e-03 | 1.811e-06 | 1.652e-02 | 1.166e-06 | 2.776e+07 | 1.003e-01 |
| 1.6 | 6.800e-03 | 2.333e-06 | 2.148e-02 | 1.498e-06 | 2.776e+07 | 1.003e-01 |
| 1.8 | 9.891e-03 | 3.362e-06 | 3.088e-02 | 2.147e-06 | 2.776e+07 | 1.003e-01 |
| 2.0 | 1.238e-02 | 4.180e-06 | 3.892e-02 | 2.662e-06 | 2.776e+07 | 1.003e-01 |

Table 4.9: Compression and accuracy for \( q = 7 \), \( l = 0.2 \), \( \rho = 6 \), \( \delta_z = 0.2 \) and different values of \( \nu \).
5 Conclusions

5.1 Comparison to prior work

We will now highlight similarities and differences between our approach and three classes of existing methods, with the purpose of describing interplays and relations.

5.1.1 Inducing points, predictive processes and MRA

It is remarkable that the sparsity-inducing screening effect has been used by numerical analysts mostly when dealing with sparse matrices arising from the discretization of differential operators. For these matrices, which correspond to precision matrices in statistics, nested dissection orderings have provided reasonably fast solvers for low-dimensional problems (George, 1973). For dense matrices representing integral equations, however, we are not aware of any prior work recognising that integral operators too can have sparse Cholesky factors when making appropriate use of the screening effect. In the context of sparse approximate inverse preconditioners, Benzi (2016) and Benzi and Tůma (2000) observe that factorised preconditioners can provide better preconditioning results for a given number of nonzero entries than direct sparse approximations of the dense inverse matrix. This kind of preconditioner has also been used by Harbrecht (2012), which we will comment on in the context of wavelet methods. However, while Benzi and Tůma (2000) observe that the ordering influences the sparsity of the inverse Cholesky factor, and that the inverse Cholesky factors of well-conditioned sparse matrices are exponentially localised, these factors are interpreted as the inverse of the Cholesky factors of the sparse matrix, to be used for preconditioning purposes. It does not seem to be observed that these factors correspond to the Cholesky factors of the dense inverse, that they can be computed directly by an incomplete factorisation of the dense matrix, and thus serve as provide an accurate sparse representation of its inverse. In the statistics community, on the other hand, notions of conditional sparsity have a long history and form the basis of scalable Gaussian process methods. These methods are known as covariance tapering (Chilès and Delfiner, 2012), inducing points (Quissonero-Candela and Rasmussen, 2005; Snelson and Ghahramani, 2006), predictive processes (Banerjee et al., 2008), and multiresolution approximation (MRA) (Katzfuss, 2016). In particular, MRA and our method have in common the idea of using successive conditioning to obtain marginals with short correlation length, which is a simple way to obtain hierarchically sparse approximations of general stochastic processes. While these methods exploit the same mathematical phenomenon that causes our Cholesky factors to be localised, they do not make the connections to the sparsity of the Cholesky factorisation of the covariance matrix. In this paper, this connection yields a simple algorithm based on the interplay with the established theory of sparse factorisations.
Rigorous bounds on the approximation error seem to play a lesser role in the statistics literature than in numerical analysis. Often, the aim of finding classes of sparse stochastic processes that show a similar behaviour to the usual dense choices is emphasised. This might stem from the fact that covariance matrices in statistics are seen as tools to analyse data, rather than as physical models such as the equations of physics that motivated much of the research in numerical analysis. Using techniques from (numerical) analysis, we provide rigorous estimates on the tradeoff between approximation error and computational complexity for a large class of matrices, with the purpose of (1) providing a tool for the numerical analysis of localised matrices and their inverses and (2) characterising conditions implying a screening effect. In doing so, we see that a near optimal screening effect can be obtained by controlling the mesh constants of the grids on the different levels, without the need to seal off the different subregions from each other in a nested-dissection approach. This is in contrast to the suggestion of Katzfuss (2016) to prefer knots close to the boundary of the subdomains. In fact, this would lead to a deteriation of the mesh constant and thus of our error bounds, requiring us to rely on the nested dissection effect, which does not lead to a near-linear time algorithm for $d > 1$.

5.1.2 Wavelet methods for integral equations

In the numerical analysis community, sparsity-oriented approaches for the treatment of integral operators have mostly been based on wavelet methods. Vanishing moments conditions of the wavelet basis appear to be an essential requirement for these methods. We say that a family of wavelets has $M$ vanishing moments if its elements on all but the coarsest level are $L^2$-orthogonal to polynomials of order up to $M - 1$. Beylkin et al. (1991) observes that the integral operators associated to pseudo-differential operators decay algebraically with order $m + 1$, according to the sparsity graph induced by the geometry of the domain. This fact leads to $O(N \log N)$ or even $O(N)$ approximation schemes. Dahmen et al. (2006) shows that by using additional adaptive compression, wavelet schemes applied to integral operators can achieve accuracy up to discretisation error in $O(N)$ computational complexity when applied to integral equations. In the wavelet community, the method closest to our approach is the LU factorisation of integral operators in wavelet bases (Gines et al., 1998), where it is observed that, when computing the LU factorisation of a differential operator or its inverse, represented in a wavelet basis with $M$ vanishing moments, the factors are algebraically localised with order $M + 1$. Since our approach also relies on the sparsity of the Cholesky decomposition of differential and integral operators represented in a multiresolution basis, the two methods are superficially similar. There are, however, several important differences: In Gines et al. (1998), the localisation is algebraic and originally comes from the vanishing moments of the multiresolution basis. Then it is observed that this localisation can be preserved during the LU-decomposition. On the other hand, our method does not need the integral operator to be sparse in the multiresolution basis. Instead, our localisation is induced by the Cholesky decomposition. In fact Owhadi and Scovel (2017) does not require the multiresolution basis to have $s$ vanishing moments (for an elliptic partial differential operator of order $2s$) to obtain exponential decay of gamblets. Furthermore, by introducing Condition 3.36 and Theorem 3.37, we are able to obtain bounded condition numbers, and thus the exponentially localised Cholesky factorisation without any vanishing moments. The reason why this behaviour was not observed by Gines et al. (1998) is that the Cholesky factorisation was performed from fine to coarse scales. In our results, motivated by probabilistic interpretations, we discover that although the sparse matrix should be factorised from fine to coarse scales, its dense inverse should be factorised from coarse to fine scales. As mentioned in the Section 2, this type of behaviour exists for both nested-dissection and minimal-degree ordering. The reverse ordering of a sparsity-preserving ordering for the sparse matrix $L$ provides a sparsity-inducing ordering for the dense inverse $\Theta$. Such sparsity-inducing Cholesky factorisations of dense matrices appear to be new.

Another difference between Gines et al. (1998) and our work is that the former relies on the fact that the fine-to-coarse incomplete Cholesky decomposition of a sparse matrix is a very good approximation of the ordinary Cholesky decomposition, which is not the case when performing the coarse-to-fine Cholesky decomposition. However, as shown here, for integral equations, the error made by approximating the true Cholesky decomposition of the truncated kernel matrix with the coarse-to-fine incomplete Cholesky factorisation cancels out with the error made by the truncation itself, up to an exponentially small term. Although (Harbrecht, 2012) also uses a coarse-to-fine incomplete Cholesky decomposition in a wavelet basis, the resulting decomposition is only used as a preconditioner for the fast inversion of a wavelet-
sparsified integral equation, and the exponential decay of the Cholesky decomposition is not observed. This leads to the curious situation that the incomplete Cholesky preconditioner is asymptotically a better approximation of the true underlying equation than the sparse approximation of the integral operator that is being inverted using this preconditioner.

5.1.3 Fast multipole methods and hierarchical matrices

Fast multipole methods and hierarchical matrices are popular scalable approaches for dealing with dense kernel matrices. The fast multipole method, developed by Greengard and Rokhlin (1987) in the context of many-particle simulations, is based on the observation that interactions between well separated groups of particles can be approximated by relatively few terms of the potential’s multipole expansion. Using these low-rank approximations over a hierarchy of scales leads to near-linear complexity algorithms.

Hierarchical matrices (Hackbusch, 1999; Hackbusch and Khoromskij, 2000; Bebendorf, 2008) can be thought of as the algebraic abstraction of the idea underlying the fast multipole method. Here, blocks that correspond to distant groups of points are modeled to have low rank. Many types of matrices and their inverses have been shown to be well approximated by hierarchical matrices, notably the stiffness matrices of elliptic partial differential operators and their inverses (Bebendorf, 2007, 2016), as well as Matérn kernel matrices (Ambikasaran et al., 2016). It turns out that from our sparse Cholesky decomposition (and also from the decomposition proposed by Gines et al. (1998)), a hierarchical matrix type approximation of \( \Theta \) or \( A \) can be derived. This can be seen by observing that the truncated Cholesky decomposition \( L^\rho L^{\rho^T} = \Theta \) can be rewritten as \( \Theta = \sum_{i=1}^{N} l_i l_i^T \), where \( l_i := L_i^0 \). Now let \( S_1, S_2 \subset I \) be two sets of indices corresponding to points in regions \( \Omega_1, \Omega_2 \), such that \( \text{diam}(\Omega_1) \approx \text{diam}(\Omega_2) \approx \text{dist}(\Omega_1, \Omega_2) \approx 2\rho b^k \). Then, for \( i \in S_1 \cap J^{(l)} \), \( l > k \), we have \( (l_i)_j = L^\rho_{i,j} = 0 \). Therefore, we have \( \# \{ i \in I \mid |l_i|^T |_{S_1 \times S_2} \neq 0 \} \leq q \rho^d \), where \( q \) is the number of levels and \( d \) the spatial dimension. Based on this argument, our sparse Cholesky decomposition and that of Gines et al. (1998) imply a near linear hierarchical matrix type approximation of \( \Theta \) and \( A \). This provides a direct link between our results and the more traditional wavelet-based methods as a sparse counterpart of the hierarchical matrix method. Of course, these two approaches can not be expected to be fully equivalent. First of all, the fact that we chose the opposite elimination ordering for the Cholesky factorisation of sparse differential operators and their dense inverse, suggests that our method will not work well on sums of differential- and integral operators. For an SVD-based hierarchical compression, on the other hand, this should not pose any problem. Therefore, it seems likely that the hierarchical matrix method is more robust, than our sparsifying Cholesky factorisation. Furthermore, at least when using the SVD or analytic formulas to obtain the hierarchical matrix approximant, it should be able to avoid the boundary artefacts that we observe in Section 4.3.5 when using the Matérn kernel. However, our method, in settings where it applies, has the advantage of constructing the sparse approximation from only linearly many entries of \( \Theta \) (the other entries do not need to be read, known or even stored) that are chosen independently of the kernel. In contrast, if no analytic multipole expansion of the kernel is available and the hierarchical matrix approximants are computed via SVD, one needs to read every entry at least once and thus can not provide a near linear algorithm. To overcome this problem, other methods have been designed to compute the low-rank approximants in near-linear time. One approach is to use quadrature formulas (Fong and Darve, 2009) which require the evaluation of the covariance function at arbitrary points. Another possibility is to use rank-revealing LU decompositions (Miranian and Gu, 2003), rank-revealing QR decomposition (Gu and Eisenstat, 1996) or adaptive cross-approximation (Bebendorf and Rjasanow, 2003), which is very similar to rank-revealing LU decomposition. Quadrature-based methods usually rely on access to evaluations of the covariance at arbitrary points. Although methods based on rank-revealing factorisations only need to read a subset of the entries of the matrix, they are nonlinear and the required entries depend on the covariance matrix. For our method, in contrast, the relevant entries are known based only on the geometry of the measurement locations. This might be advantageous in settings where the covariance matrix is estimated from a large number of realisations of the Gaussian process. In this case, to avoid having to store those realisations, one might resort to using the empirical covariance of the data. If this matrix is large as well, our method allows to discard all but near-linearly many entries which are known a-priori. Instead, a rank-revealing LU decomposition would need to see the covariance matrix before being able to decide, which entries need to be kept and which can be discarded.
5.2 Conclusion and outlook

To summarise, we have shown that the Green’s matrices of elliptic boundary value problems have exponentially localised Cholesky factorisations when represented in a multiresolution basis. Based on this result, we have shown that we can obtain a sparse approximation of this Cholesky factorisation, with the approximation error decaying exponentially in the size of the sparsity set. The computation of this decomposition can be equivalently expressed as a zero fill-in incomplete Cholesky factorisation of the truncated kernel matrix restricted to a sparsity set and can, for approximately equally spaced measurement locations and an approximation accuracy $\epsilon$, be computed in complexity $O(N \log^2(N) \log^{2d}(N/\epsilon))$ in time and $O(N \log(N) \log^d(N/\epsilon))$ in space. In particular, only $O(N \log(N) \log^d(N/\epsilon))$ entries of the kernel matrix expressed in the multiresolution basis need to be known for a reconstruction up to an error of size $\epsilon$. This appears to be a new type of rigidity result for the inverses of sparse matrices. In the case where $s > d/2$, i.e. when the solution space of the PDE contains continuous functions, we prove that a simple hierarchical ordering of the original matrix can be used as a multiresolution basis. Therefore, this hierarchical ordering, by avoiding the need for aggregation in the multiresolution transform, enables the exact change of basis in linear time and further strengthens our rigidity result (by implying that kernel matrices of this type are determined, up to an exponentially small errors, by near-linearly many of their entries, which in turn can be determined only based on the measurement locations).

Surprisingly, as a byproduct of our algorithm, we also obtain a sparse approximate principal component analysis in near-linear complexity, thereby opening the complexity bottleneck of this widely popular statistical procedure. Finally, as a corollary of our results, we obtain the existence of sparse approximations of the Cholesky factorisation of the inverse of the kernel matrix. More generally, we also observe a form of duality in the sense that for an ordering that leads to a sparse factorisation of the dense Green’s matrix, the reverse ordering leads to a sparse factorisation of the associated stiffness matrix, which naturally leads to a fast direct solver for elliptic partial differential equations with rough coefficients.

The motivation for our sparse Cholesky decomposition has been the obvious, yet rarely used equivalence between the conditioning of gaussian vectors and the Cholesky factorisation of their covariance matrix. We suspect that this link between one of the most fundamental operations in computational mathematics (i.e. Gaussian elimination) and one of the most fundamental operations in statistics and probability (i.e. the conditioning of random variables) has not yet given up all of its fruits.

This article naturally omits a number of aspects that we deem interesting targets of future investigation:
(i) We plan to provide a software package based on the results in this article. As part of this project, it will be interesting to compare different approaches for generating sparsifying orderings. Furthermore, it will be interesting to exploit the parallelism permitted by the locality of the factorisation.
(ii) In the article we have been dealing with point clouds in low-dimensional space. Since our algorithm only needs a notion of distance between points, it might be applicable to point clouds in high-dimensional space that have low intrinsic dimension, e.g. lying on a low-dimensional manifold or having low doubling dimension. Section 4.3.4 provides preliminary results of this kind.
(iii) Somewhat related to the above point, we hope to be able to establish analogues of our method on graphs. The robustness of our algorithm and its independence from any notion of polynomials appears to suggest that it might be better suited for this purpose than other PDE-based methods.
(iv) Some analytical questions might merit further investigation. These include the rigorous analysis of the case where $2s$ is odd and the case where $s$ is fractional. Furthermore, it is also of interest to examine to what extent subsampling is still feasible in the case $s < d/2$.
(v) In the wavelet literature (Gines et al., 1998), by using the so-called non-standard form, the complexity of the Cholesky decomposition for a fixed bandwidth can be reduced from $O(N \log^2 N)$ in time and $O(N \log(N))$ in space to $O(N \log(N))$ in time and space. We believe that an analogous use of non-standard form can reduce the complexity of our algorithm by a factor of $\log^2 N$ (resp. $\log N$).
(vi) In the statistical literature, banded approximations of the Cholesky factors of the covariance matrix or its inverse have been used for the purpose of the estimation of covariance matrices (Bickel and Levina, 2008; Rothman et al., 2010; Fan et al., 2016). In this work we show that a large class of covariance matrices corresponding to smooth random fields can be very accurately approximated by their truncated Cholesky factors. Therefore, it seems promising to investigate whether truncated Cholesky factors (with the ordering and truncation pattern chosen as suggested in this work) can be useful as models for the estimation of covariance matrices.
Acknowledgements

FS and HO gratefully acknowledge support by the Air Force Office of Scientific Research and the DARPA EQUiPS Program under award number FA9550-16-1-0054 (Computational Information Games). TJS is supported by the Free University of Berlin within the Excellence Initiative of the German Research Foundation (DFG). This article is based upon work partially supported by the National Science Foundation (NSF) under Grant DMS-1127914 to the Statistical and Applied Mathematical Sciences Institute (SAMSI). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the NSF or SAMSI. We would like to thank Chris Oates and Peter Schröder for helpful discussions.

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