A N-BODY SOLVER FOR FREE MESH INTERPOLATION *

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Abstract. Factorization of the Gaussian RBF kernel is developed for free-mesh interpolation in the flat, polynomial limit corresponding to Taylor expansion and the Vandermonde basis of geometric moments. With this spectral approximation, a top-down octree-scoping of an interpolant is found by recursively decomposing the residual, similar to the work of Driscoll and Heryudono (2007), except that in the current approach the grid is decoupled from the low rank approximation, allowing partial separation of sampling errors (the mesh) from representation errors (the polynomial order). Then, it is possible to demonstrate roughly 5 orders of magnitude improvement in free-mesh interpolation errors for the three-dimensional Franke function, relative to previous benchmarks. As in related work on N-body methods for factorization by square root iteration (Challacombe 2015), some emphasis is placed on resolution of the identity.

1. Introduction. A reproducing kernel Hilbert space (RKHS) $\mathcal{H}_d$ is associated with $d$-dimensional kernels $K_d$, mapping $\mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ via an inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ [51, 34, 49, 16]. Kernels of the RKHS are reproducing:

$$K(x', x) = \langle K(\cdot, x'), K(\cdot, x) \rangle,$$

with the ability to reconstruct all functions in the native space:

$$f(x) = \langle f(\cdot), K(\cdot, x) \rangle.$$

The natural bases for the RKHS are the kernel eigenfunctions $\varphi_i$:

$$K(x', x) = \sum_i \lambda_i \varphi_i(x') \varphi_i(x) = \langle \sqrt{\lambda} \varphi', \sqrt{\lambda} \varphi \rangle.$$

In many applications, the RKHS provides an extremely powerful framework for interpolation, reconstruction, convolutions & so on. Startling advances have been achieved for higher dimensional problems associated with inference and probability, through new formalisms that are asymptotically well behaved with respect to dimensionality [2, 31, 6, 54, 15, 17].

In practical applications, the pointwise function $f$ and the corresponding Kernel or Gramian matrix $K$ determine a function through the linear system $K \cdot \omega = f$:

$$f(x) = \sum_i \omega_i K(x, x_i).$$

Kernels like the Gaussian Radial Basis Function kernel,

$$\phi(\|x' - x\|) = e^{-\epsilon^2(x' - x)^2},$$

have many excellent properties, including translational invariance, a separable $d$-dimensional product form, analytic solutions to the kernel eigenfunctions [16] and

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super-spectral (exponential) convergence [20, 45, 46]. Another remarkable feature of the Gaussian RBF kernel is that towards the flat limit of the shape parameter, \( \varepsilon \to 0 \), interpolation tends towards approximations with early low-rank saturation but with severely ill-conditioned Gramian matrices, \( \phi \) [41, 13, 22, 20, 48, 18]. This is the RBF-direct problem, identical to the Gaussian LCAO problem faced in quantum chemistry [47, 36, 33].

Little appreciated, this ill-conditioning can be partially sidesteped through only low rank factorization in the case of kernels with rapid spectral decay [16, 18, 53]. Also, recent progress in analysis of the Gaussian kernel shows that in the flat limit, eigenfunctions of the Gaussian RBF kernel tend to moments of the Hermite polynomials with rank corresponding to the number of centers [16, 18, 53], \( \mathcal{L} = N_p \), equivalent to any other polynomial moments of the same rank, via \( e.g. \) orthogonality of the Vandermonde basis [9, 25, 43]. The transition from exponential (Gaussian RBF) to polynomial (Vandermonde) behavior in the flat regime gives Gaussian RBF error curves their characteristic \( \sqrt{-} \)-like dip [20, 45, 46, 53].

These spectral approximations may reach convergence much faster than a naively taken grid can establish an accurate fill distance [11, 45, 59]. Then low, \( \mathcal{L} \)-rank factorization can be much faster than the unisolvent case, \( \mathcal{O}(\mathcal{L}^2 N_p) \) vs. \( \mathcal{O}(N_p^2) \), allowing partial separation between complexity of the representation and of the grid. In just 1-dimension however, RBF expansions to numerical accuracy for challenging functions may require \( N_p \sim 20 - 30 \) centers [18], corresponding to rank \( \mathcal{L} \sim \mathcal{L}^4 \). In just three dimensions, factorization is \( \mathcal{O}(\mathcal{L}^6 N_p) \), already a formidable challenge for large (naive) grids. Notable attacks on this problem include statistical methods for very long and skinny matrix factorizations [32, 30, 38].

In higher dimensions and for functions that are strongly cusped, the number of grid points naively taken to maintain an accurate fill distance \( h_p \sim N_p^{-1/d} \) may grow explosively [55, 11, 45, 59]. Then, factorization demands a scoping mechanism capable of culling-out low-dimensional sub-space representations from higher dimensional manifolds [2, 6, 54], including \( e.g. \) dimension-free shape parameter sequences [17, 15] and sparse grids [31, 26]. Similarly, finding low complexity sub-structures in Gramian factorizations is enabled by octree-scoping of the \( \text{SpAMM} \) bound in \( \alpha \)-body approaches to square root iteration [8].

For potential-like RBF kernels with also spectral convergence, such as the multi-quadratic, Taylor expansions converge rapidly only in the far-field limit. These kernels are enabled by well known methods, including the Barnes-Hut Tree-Code and the Fast-Multipole-Method (FMM), with octree scoping of the bi-polar expansion based on range criteria, and the upwards accumulation of long ranged, increasingly smooth potentials [56, 37, 39, 40]. Different from these FMM-like approaches, the focus of this work is instead on top-down expansion of the residual via low-rank factorization of the Gaussian kernel in the truncated polynomial limit, obtaining the largest and smoothest components of the interpolant first, resolving increasingly fine details with decreasing magnitudes. With large quasi-random grids, can low rank octree-scoping yield high accuracy?

This paper is organized as follows: In the next section, we develop polynomial interpolation through Taylor expansion of the Gaussian RBF kernel, and discuss equivalence with kernel eigenfunctions in the flat limit. Then, we show how the low rank approximation describes the three-dimensional Franke function, used to benchmark other methods for scattered data interpolation [5, 7, 10]. Finally, we show increasingly compact and accurate representation of the method with increasing
expansion order and grid size, through $N_p = 8^9$.

2. Taylor Expansions of Gaussian Kernels. In this section, the polynomial limit of the flat Gaussian RBF kernel is sketched in three-dimensions with emphasis on concepts and notation familiar to chemistry and materials science. To start, expansion of the Gaussian RBF kernel can be factored by polynomial order,

$$
\phi (\| \mathbf{x}' - \mathbf{x} \|) = \sum_{lmn} \varepsilon^{l+m+n} \frac{x_1^l x_2^m x_3^n}{l! m! n!} h_l (\varepsilon x_1) h_m (\varepsilon x_2) h_n (\varepsilon x_3)
$$

$$
= \sum_{L=0}^{L_{max}} \varepsilon^L \sum_{l_m=n}^{L_{max}} A_{lmn}(\mathbf{x}') \ h_l (\varepsilon x_1) h_m (\varepsilon x_2) h_n (\varepsilon x_3)
$$

where $h_i (x) = e^{-\varepsilon^2 x^2} H_i (x)$ are the Hermite functions, and

$$
\ell^3_i = i(i + 1)(i + 2)/6
$$

is the rank stride of the three dimensional multi-index $lmn$. Then, with the Taylor expansion

$$
h_{\alpha} (t) = \sum_{\beta} \frac{t^{\beta}}{\beta!} h_{\alpha+\beta} (0)
$$

the Gaussian RBF kernel is

$$
\phi (\| \mathbf{x}' - \mathbf{x} \|) = \sum_{L=0}^{L_{max}} \varepsilon^L \sum_{L'=0}^{L_{max}} \sum_{lmn=\ell^3_L}^{\ell^3_{L'}} \sum_{lmn'=\ell^3_{L'}} A_{lmn}(\mathbf{x}) A_{lmn'}(\mathbf{x}')
$$

$$
\times (-1)^{l+m+n} h_{l+m+n} (0) h_{m+m'} (0) h_{n+n'} (0) .
$$

So far, the unisolvent $L = N_p$ case has been implied. Now please consider a truncated expansion with $L \equiv L_{max} \ll N_p$. Then, the kernel expansion may be written:

$$
\phi_{N_p \times N_p} = A_{N_p \times \mathcal{L} \times \mathcal{L} \times \mathcal{L} \times \mathcal{L}} = T_{L \times \mathcal{L} \times \mathcal{L} \times \mathcal{L} \times \mathcal{L}} A_{L \times N_p}^T , \tag{2.1}
$$

where

$$
\varepsilon = \text{diag} \left[ \varepsilon^0, \varepsilon^1, \varepsilon^1, \varepsilon^2, \ldots, \varepsilon^{L_{max}} \right]_{\mathcal{L} \times \mathcal{L}} ,
$$

$$
T_{lmn,lmn'} = (-1)^{l+m+n} h_{l+m+n} (0) h_{m+m'} (0) h_{n+n'} (0) ,
$$

$$
h_{\alpha} (0) = \begin{cases} 0 & \alpha \text{ odd} \\ (-1)^{\frac{\alpha}{2} (\alpha - 1)!!} & \alpha \text{ even} \end{cases}
$$

are the Hermite numbers, and

$$
A_{lmn} (\mathbf{x}) = \frac{x_1^l x_2^m x_3^n}{l! m! n!}
$$
are the geometric moments \([35, 48, 43, 19]\), also known as the unabridged multipole moments in chemistry \([1]\).

QR factorization of the Vandermonde matrix of polynomial moments,

\[
\Lambda = Q_{N_p \times \ell} \cdot R_{\ell \times \ell},
\]

provides a representation-free basis, \(Q\), as shown by Fornberg and others \([24, 3, 21, 44, 18]\), and including the early work of Gene Golub \([28, 29]\).

Then,

\[
\phi_{N_p \times N_p} = Q_{N_p \times \ell} \cdot \Phi_{\ell \times \ell} \cdot \varphi_{\ell \times \ell}^{T} \cdot Q_{\ell \times N_p}^{T},
\]

where the auxiliary representation of the kernel is:

\[
\Phi = R \cdot \varepsilon \cdot V \cdot e \cdot V^{T} \cdot \varepsilon \cdot R^{T},
\]

with \(V\) and \(Q\) orthogonal, \(T = V \cdot e \cdot V^{T}\), and where \(e\) and \(\varepsilon\) are diagonal. By the properties of orthogonal matrices, the inverse is simply

\[
\phi^{-1} = Q \cdot [R^{-1}]^{T} \cdot \varepsilon^{-1} \cdot V \cdot e^{-1} \cdot V^{T} \cdot \varepsilon^{-1} \cdot R^{-1} \cdot Q^{T},
\]

and relative expressions involving poorly behaved powers of the shape parameter can be handled safely in a number of ways. So far, this is the RBF-QR analysis of Fornberg \([\ldots]\) and others \([\ldots]\) with analytically well conditioned solutions due to careful handling as \(\varepsilon \to 0\).

Sidestepping an elegant treatment of the shape-factor, consider now the problem of transforming a pointwise interpolant \(p\),

\[
f_{p} = \{ f(x_{i,1}, x_{i,2}, x_{i,3}) \mid i = 1, N_p \},
\]

sampled on a random grid,

\[
x_{p} = \{ [a, b, c]_{i} \mid [a, b, c] \in [-1, 1]^{3}, i = 1, N_p \}
\]

to another randomly chosen grid, \(x_{q} \neq x_{p}\). With \('\) denoting \(q\) dependent terms, the transformation between these free-mesh pointsets \(p \to q\) is:

\[
f'_{q} = \phi'_{N_q \times N_p} \cdot \lambda_{p}
\]
\[
= \phi'_{N_q \times N_p} \cdot \phi^{-1}_{N_p \times N_p} \cdot f_{p}
\]
\[
= Q'_{N_q \times \ell} \cdot \Phi_{\ell \times \ell}^{1/2} \cdot \Phi^{-1/2}_{\ell \times \ell} \cdot Q_{\ell \times N_p}^{T} \cdot f_{p}
\]
\[
= I'_{N_q \times N_p} \cdot f_{p},
\]

where

\[
I' = Q' \cdot [R']^{T} \cdot R^{-1} \cdot Q^{T}
\]

is the pointwise resolution of identity.

This somewhat surprising, shape-parameter-free result does not follow from a special handling of the shape parameter, but obtains simply from polynomial independence in the factored Taylor space, via orthogonality of the Vandermonde basis \([9, 25, 43]\).
Fig. 2.1. Unscop free-mesh interpolation of the three-dimensional Franke function, \( f_{3d} \), with low rank polynomial approximation corresponding to random, \( N_p = 8^6 \) grids in \([0, 1]^3\). Shown from left to right, top to bottom, are equispaced surfaces with values between \(-.10\) and \(.79\) (blue to red) for orders \( L_{\text{max}} = 6, 10 \) & 14, and in the lower rightmost panel, surfaces of the native function.

This result is similar to the RI method developed in quantum chemistry by Yu-Cheng Zheng and Jan Almlöf [57, 58], and related to random phase Vandermonde matrices with very interesting properties [52, 12], to the problem of statistical and sub-random grids [42, 27], and to the computation of weakly admissible meshes [4] and approximate Fette points [50].

In this contribution however, we are interested only in grid independence in the limit of small fill distances, assumed here to be \( h_p \sim N_p^{-1/3} \). Also, in practice there is no need to actually form \( \mathbf{I}' \), since

\[
\mathbf{f}'_q = \Lambda_{N_q \times L} \cdot \mathbf{R}^{-1}_{L \times L} \cdot \mathbf{Q}_{L \times N_p}^T \cdot \mathbf{f}_p
\]

\[
= \Lambda_{N_q \times L} \cdot \mathbf{F}_p
\]

where \( \mathbf{F}_p \) is the truncated Taylor representation of \( \mathbf{f}_p \). More generally,

\[
f(\mathbf{r}) = \Lambda(\mathbf{r}) \cdot \mathbf{F}_p
\]
3. Low Rank Approximation of the 3-D Franke Function. In three-dimensional studies of scattered mesh interpolation for smooth functions, the three-dimensional Franke function

\[
f_{\text{F3d}}(x, y, z) = \frac{3}{4} \left[ e^{-\frac{1}{4} \left[ (9x-2)^2 + (9y-2)^2 + (9z-2)^2 \right]} + e^{-\frac{1}{4} \left( 9x+1 \right)^2 + \frac{1}{5} (9y+1)^2 + \frac{1}{2} (9z+1)^2 } \right] + \frac{1}{2} e^{-\frac{1}{4} \left[ (9x-7)^2 + (9y-3)^2 + (9z-5)^2 \right]} - \frac{1}{5} e^{-\left( (9x-4)^2 - (9y-7)^2 - (9z-5)^2 \right)} , \tag{3.1}
\]

is perhaps the most common choice for benchmarking errors [23, 5, 7, 10]. In Fig. 2.1, interpolation surfaces of \( f_{\text{F3d}} \) are shown for orders \( L_{\text{max}} = 6, 10, \) and 14, corresponding to \( L = 84, 286, \) and 680. In this challenging example, the correct qualitative behavior (ability to resolve positive and negative lobes) is obtained only for \( L_{\text{max}} = 14. \)

**Algorithm 1** Recursive octree decomposition of the FMT residual.

1: procedure FMT_Mesh_to_Tree\((N, L, L, x_{(1:N,1:3)}, f_{(1:N)}, P)\)
2: \(x_{(1:N,1:3)} = (x_{(1:N,1:3)} - P_{C(1:3)}) \ast P_{\text{scale}}\)
3: FMT_Mesh_to_Moments\((N, L, L, x_{(1:N,1:3)}, f_{(1:N)}, P_{F(1:L)})\)
4: FMT_Ordered_by_Octant\((N, x_{(1:N,1:3)}, f_{(1:N)}, n_{(1:8)})\)
5: \(j \leftarrow 1\)
6: for \(o \leftarrow 1 \) to 8 do
7: \(k \leftarrow \sum_{i=0}^{n_0} n_i\)
8: \(E_{\text{RMS}} \leftarrow \sqrt{\sum_{i=j}^{k} f_i^2 / n_0}\)
9: if \(E_{\text{RMS}} > \tau \) and \(n_o \geq L\) then
10: \(j \leftarrow j + k\)

**Algorithm 2**

1: procedure FMT_Mesh_to_Moments\((N, L, L, x_{(1:N,1:3)}, f_{(1:N)}, P_{F(1:L)})\)
2: for \(l \leftarrow 0, \) \(L\) do
3: \(f_l \leftarrow 0, \) \(L - l\) do
4: for \(n \leftarrow 0, \) \(L - l - m\) do
5: \(\Lambda_{(1:N,lmn[l,m,n])} \leftarrow x_{(1:N,1)} x_{(1:N,2)} x_{(1:N,3)} / l!m!n!\)
6: \(\{Q, R\} \leftarrow \text{FMT_DGEOQRF_DGOR}\(N, L, \Lambda_{(1:N,L)}\)\)
7: \(P_{F(1:L)} \leftarrow R_{(L,L)}^{-1} Q^T_{(L,1:N)} \cdot f_{(1:N)}\)
8: \(f_{(1:N)} \leftarrow f_{(1:N)} - P_{F(1:L)}\)

4. Free Mesh Transform. The free-mesh transform (FMT), shown in Algorithm 1, is simpler than other fast methods with octree-scoping, with only downward recursion to accumulate local polynomial representation of the residual. This approach is similar to the adaptive residual sub-sampling method of Driscoll and Hryundono [14], except that in the current approach, the grid is decoupled from the low rank approximation, allowing partial separation of sampling errors (the mesh) from representation errors (the Taylor order \( L \)).

Starting at the top level, the interpolant and grid, \(\{f_{N_p}, x_{(1:N_p,1:3)}\}\), together with the octree \(P\), are recursively subdivided, constructing approximations to residuals in
A N-Body Solver for Free Mesh Interpolation

Fig. 3.1. Convergence of the $\epsilon_{\text{rms}}$ and $\epsilon_\infty$ errors for Fast Field Transform of $F^1$, Eq. 3.1, on random grid $p$ ($p \in [0, 1]^3$) to random grid $q$ ($q \in [0, 1]^3$). Shown are errors for expansion order $L = 6 \& 10$ with respect to the number of nodes, corresponding to random grids of size $N_p = N_q = \{8^4, 8^5, 8^6, 8^7\}$.

Sub-octants through coordinate translations and dilations that smooth and re-center the interpolant within $[-1, 1]^3$. At some depth, the number of points in a new octant, $n_o$, will approach the most effective resolution possible; Algorithm 1 looks ahead, terminating recursion for any octants obeying $n_o < L$. Recursion also terminates when the local RMS error meets the convergence criteria $E_{\text{RMS}} < \tau$, determined by ability of the polynomial representation to completely annihilate local residuals.

In Figures 3.1-3.3, scoping experiments with $L_{\text{max}} = 4, 8, \& 12$ are carried out with thresholds $\tau = \{10^{-6}, 10^{-8}, 10^{-10}, 10^{-12}\}$ and separate grids with $N_q = N_p = \{8^4, 8^5, 8^6, 8^7, 8^8, 8^9\}$. Shown are the total RMS error:

$$E_{\text{rms}} = \sqrt{\frac{\sum_i \{[f_q]_i - f(x_i, y_i, z_i)\]^2}{N_q}}$$

and the max error:

$$E_\infty = \max_i \|[f_q]_i - f(x_i, y_i, z_i)\|,$$

with respect to the total number of octree-nodes. These results show saturation of the representation, set by $L_{\text{max}}$, with respect to given RMS error threshold, $\tau$, and with respect to an increasing mesh, $N_q = N_p$. Notably, with increasing order, $L_{\text{max}}$, behavior of the scoping error in terms of octree-complexity becomes noticeably more tree like; $O(N) \to O(\log N)$.

Related benchmarks for $f_{F3d}$ by Bozzini, Mira and Rossini found $E_{\text{rms}} = 4 \times 10^{-4}$ and $E_\infty = 8 \times 10^{-3}$ using $N_p = 3375$ [5], while Cavoretto, Rossi and Perracchione [7]
Fig. 3.2. Convergence of the $\epsilon_{\text{rms}}$ and $\epsilon_{\infty}$ errors for Fast Field Transform of $F_2$, Eq. 37, on random grid $p (p \in [0,1]^3)$ to random grid $q (q \in [0,1]^3)$. Shown are errors for expansion order $L = 6$ to 10 with respect to the number of nodes, corresponding to random grids of size $N_p = N_q = \{8^4, 8^5, 8^6, 8^7\}$.

found $E_{\text{rms}} = 6 \times 10^{-5}$ and $E_{\infty} = 6 \times 10^{-3}$ with $N_p = 41665$. In this study, it was possible to achieve compact support with fewer than $10^3$ octree nodes, $E_{\text{rms}} < 10^{-11}$ and $E_{\infty} < 10^{-8}$; a roughly 5 order of magnitude improvement.

5. Conclusions. In this contribution, a free-mesh interpolation was developed based on factorization of the Gaussian-RBF kernel in the flat polynomial limit, corresponding to Taylor expansion and the Vandermonde basis of geometric moments. A top-down octree-scoping based on low-rank polynomial approximation was developed and demonstrated, achieving roughly 5 orders of magnitude improvement in free-mesh interpolation errors for the three-dimensional Franke function, relative to previous benchmarks. A small advantage of the current implementation over the continuous Gaussian RBF interpolation is the ease of implementation, and the potential for a simplified downward propagation of smooth components, e.g. in implementations with a scoping grid.

This contribution also highlighted interesting forms of the identity, viz Eq.(2.3), obtaining also from the flat limit of the continuous case [51, 16]:

$$I_H = \left\langle \sqrt{\lambda} \varphi \right\rangle \langle \varphi / \sqrt{\lambda} \rangle .$$

Interpolation in this case achieves super-spectral rates of convergence [20, 16], enabling many additional orders of precision to be obtained in the tuned shape-parameter “dip” [20, 16].

Recently, we developed an $n$-body method for ill-conditioned Gramian factorization through octree-scoping on the sub-space metric of the product manifold of the matrix-
matrix multiply, achieving multiple order of magnitude compression through strongly contractive identity iteration [8]. In that effort, a nested product form of the factor and its inverse was advocated; these factored forms are certainly compatible with low-rank factors alternatively found through QR factorization, via methods motivated by this and related work. Hybrid formulations of these two fast approaches are an interesting possibility, with the potential for extreme kernel factorizations.

REFERENCES

[1] J. Applequist, Fundamental relationships in the theory of electric multipole moments and multipole polarizabilities in static fields (Chemical Physics 85 (1984) 279290), Chem. Phys., 190 (1995), pp. 153–154.
[2] M. Belkin and P. Niyogi, Laplacian Eigenmaps and Spectral Techniques for Embedding and Clustering, Science (80-. )., 1 (2002), pp. 585–591.
[3] A. Björck, The calculation of linear least squares problems, Acta Numerica, 13 (2004), pp. 1–53.
[4] L. Bos, A. Sommariva, and M. Vianello, Least-squares polynomial approximation on weakly admissible meshes: disk and triangle, Journal of computational and applied mathematics, 235 (2010), pp. 660–668.
[5] M. Bozzini and M. Rossini, Testing methods for 3d scattered data interpolation, Multivariate Approximation and Interpolation with Applications, 20 (2002).
[6] C. J. Burges, Dimension reduction: A guided tour, Machine Learning, 2 (2009), pp. 275–365.
[7] R. Cavoretto, A. de Rossi, and E. Perracchione, Partition of unity interpolation on multivariate convex domains, International Journal of Modeling, Simulation, and Scientific Computing, 0 (0), p. 1550034.
[8] M. Challacombe, T. Haut, and N. Bock, A N-body solver for square root iteration, CoRR, abs/1508.05856 (2015).
[9] C. De Boor, What is the inverse of a basis?, 2001.
[10] S. De Marchi, M. Marchioro, and A. Sommariva, Polynomial approximation and cubature at approximate fekete and leja points of the cylinder, Applied Mathematics and Computation, 218 (2012), pp. 10617–10629.
[11] S. De Marchi and R. Schaback, Stability of kernel-based interpolation, Adv. Comput. Math., 32 (2010), pp. 155–161.
[12] M. Debbah et al., Convolution operations arising from vandermonde matrices, Information Theory, IEEE Transactions on, 57 (2011), pp. 4647–4659.
[13] T. A. Driscoll and B. Fornberg, Interpolation in the limit of increasingly flat radial basis functions, Computers & Mathematics with Applications, 43 (2002), pp. 413–422.
[14] T. A. Driscoll and A. R. Heryudono, Adaptive residual subsampling methods for radial basis function interpolation and collocation problems, Computers & Mathematics with Applications, 53 (2007), pp. 927–939.
[15] G. Fasshauer, F. J. Hickernell, and H. Woźniakowski, Average case approximation: convergence and tractability of gaussian kernels, in Monte Carlo and Quasi-Monte Carlo Methods 2010, Springer, 2012, pp. 329–344.
[16] G. E. Fasshauer, Positive definite kernels: past, present and future.
[17] G. E. Fasshauer, F. J. Hickernell, and H. Woźniakowski, On dimension-independent rates of convergence for function approximation with gaussian kernels, SIAM Journal on Numerical Analysis, 50 (2012), pp. 247–271.
[18] G. E. Fasshauer and M. J. McCourt, Stable Evaluation of Gaussian RBF Interpolants, SIAM J. Sci. Comput., 34 (2012), pp. 737–762.
[19] J. Flusser, T. Suk, and B. Zitov, Moments and Moment Invariants in Pattern Recognition, John Wiley & Sons Ltd, Chichester, UK, oct 2009.
[20] B. Fornberg and N. Flyer, Accuracy of radial basis function interpolation and derivative approximations on 1-d infinite grids, Advances in Computational Mathematics, 23 (2005), pp. 5–20.
[21] B. Fornberg and C. Piret, A stable algorithm for flat radial basis functions on a sphere, SIAM Journal on Scientific Computing, 30 (2007), pp. 60–80.
[22] B. Fornberg, G. Wright, and E. Larsson, Some observations regarding interpolants in the limit of flat radial basis functions, Computers & Mathematics with Applications, 47 (2004), pp. 37–55.
[23] R. Franke, A critical comparison of some methods for interpolation of scattered data, tech. rep., DTIC Document, 1979.
[24] W. Gander, Algorithms for the qr decomposition, (1980).
[25] ———, Change of basis in polynomial interpolation, Numerical linear algebra with applications, 12 (2005), pp. 769–778.
[26] J. Garcke, Sparse grids in a nutshell, Lect. Notes Comput. Sci. Eng., 88 (2013), pp. 57–80.
[27] Z. Gha¨hr¨aman and C. E. Rasmussen, Bayesian monte carlo, in Advances in neural information processing systems, 2002, pp. 489–496.
[28] G. Golub, Numerical methods for solving linear least squares problems, Numerische Mathematik, 7 (1965), pp. 206–216.
[29] G. Golub and W. Kahan, Calculating the singular values and pseudo-inverse of a matrix, Journal of the Society for Industrial & Applied Mathematics, Series B: Numerical Analysis, 2 (1965), pp. 205–224.
[30] L. Grasedyck, D. Kressner, and C. Tobler, A literature survey of low-rank tensor approximation techniques, arXiv preprint arXiv:1302.7121, (2013).
[31] M. Griebel, Sparse grids and related approximation schemes for higher dimensional problems.
[32] N. Halko, P.-G. Martinsson, and J. A. Tropp, Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions, SIAM review, 53 (2011), pp. 217–288.
[33] T. Helgaker, P. Jørgensen, and J. Olsen, Molecular Electronic-structure Theory, Wiley, 2008.
[34] T. Hofmann, B. Schölkopf, and A. J. Smola, Kernel methods in machine learning, The annals of statistics, (2008), pp. 1171–1220.
[35] M.-K. Hu, Visual pattern recognition by moment invariants, Information Theory, IRE Transactions on, 8 (1962), pp. 179–187.
[36] B. Jans´ık, S. Host, P. Jørgensen, J. Olsen, and T. Helgaker, Linear-scaling symmetric square-root decomposition of the overlap matrix., J. Chem. Phys., 126 (2007), p. 124104.
[37] R. Krasny and L. Wang, Fast evaluation of multiquadric rbf sums by a cartesian treecode, SIAM Journal on Scientific Computing, 33 (2011), pp. 2341–2355.
[38] M. W. Mahoney, Randomized algorithms for matrices and data, Foundations and Trends® in
[39] W. B. March, B. Xiao, and G. Biros, Askit: Approximate skeletonization kernel-independent treecode in high dimensions, SIAM Journal on Scientific Computing, 37 (2015), pp. A1089–A1110.

[40] W. B. March, B. Xiao, S. Tharakan, C. D. Yu, and G. Biros, Robust treecode approximation for kernel machines, in Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, ACM, 2015, pp. 775–784.

[41] V. Maz’ya and G. Schmidt, On approximate approximations using gaussian kernels, IMA Journal of Numerical Analysis, 16 (1996), pp. 13–29.

[42] W. J. Morokoff and R. E. Caflisch, Quasi-random sequences and their discrepancies, SIAM Journal on Scientific Computing, 15 (1994), pp. 1251–1279.

[43] P. O’Leary and M. Harker, Discrete polynomial moments for real-time geometric surface inspection, Journal of Electronic Imaging, 18 (2009), pp. 013015–013015.

[44] M. Pazouki and R. Schaback, Bases for kernel-based spaces, J. Comput. Appl. Math., 236 (2011), pp. 575–588.

[45] R. B. Platte, How fast do radial basis function interpolants of analytic functions converge?, IMA journal of numerical analysis, (2011), p. drq020.

[46] R. B. Platte, L. N. Trefethen, and A. B. Kuijlaars, Impossibility of fast stable approximation of analytic functions from equispaced samples, SIAM review, 53 (2011), pp. 308–318.

[47] U. Röthlisberger, M. Sprik, and J. Hutter, Time and length scales in ab initio molecular dynamics, in Bridging Time Scales: Molecular Simulations for the Next Decade, P. Nielaba, M. Mareschal, and G. Cicotti, eds., vol. 605 of Lecture Notes in Physics, Springer Berlin Heidelberg, 2002, pp. 413–442.

[48] R. Schaback, Multivariate interpolation by polynomials and radial basis functions, Constructive Approximation, 21 (2005), pp. 293–317.

[49] R. Schaback and S. De Marchi, Nonstandard kernels and their applications, (2009).

[50] A. Sommariva and M. Vianello, Computing approximate fekete points by qr factorizations of vandermonde matrices, Computers & Mathematics with Applications, 57 (2009), pp. 1324–1336.

[51] I. Steinwart, D. Hush, and C. Scovel, An explicit description of the reproducing kernel hilbert spaces of gaussian rbf kernels, Information Theory, IEEE Transactions on, 52 (2006), pp. 4635–4643.

[52] G. H. Tucci, P. Whiting, et al., Eigenvalue results for large scale random vandermonde matrices with unit complex entries, Information Theory, IEEE Transactions on, 57 (2011), pp. 3938–3954.

[53] A. J. Wathen and S. Zhu, On spectral distribution of kernel matrices related to radial basis functions, Numerical Algorithms, pp. 1–18.

[54] K. Q. Weinberger, F. Sha, and L. K. Saul, Learning a kernel matrix for nonlinear dimensionality reduction, in Proceedings of the twenty-first international conference on Machine learning, ACM, 2004, p. 106.

[55] H. Wendland, Scattered data approximation, (2004).

[56] R. Yokota, L. A. Barba, and M. G. Knepley, Petrbfa parallel o (n) algorithm for radial basis function interpolation with gaussians, Computer Methods in Applied Mechanics and Engineering, 199 (2010), pp. 1793–1804.

[57] Y. C. Zheng and J. Almlöf, Density functionals without meshes and grids, Chemical Physics Letters, 214 (1993), pp. 397–401.

[58] Y. C. Zheng and J. E. Almlöf, A grid-free dft implementation of non-local functionals and analytical energy derivatives, Journal of Molecular Structure: THEOCHEM, 388 (1996), pp. 277–284.

[59] B. Zwicknagl and R. Schaback, Interpolation and approximation in taylor spaces, Journal of Approximation Theory, 171 (2015), pp. 65–83.