Reducing the Variance of Gaussian Process Hyperparameter Optimization with Preconditioning

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Abstract

Gaussian processes remain popular as a flexible and expressive model class, but the computational cost of kernel hyperparameter optimization stands as a major limiting factor to their scaling and broader adoption. Recent work has made great strides combining stochastic estimation with iterative numerical techniques, essentially boiling down GP inference to the cost of (many) matrix-vector multiplies. Preconditioning – a highly effective step for any iterative method involving matrix-vector multiplication – can be used to accelerate convergence and thus reduce bias in hyperparameter optimization. Here, we prove that preconditioning has an additional benefit that has been previously unexplored. It not only reduces the bias of the log-marginal likelihood estimator and its derivatives, but it also simultaneously can reduce variance at essentially negligible cost. We leverage this result to derive sample-efficient algorithms for GP hyperparameter optimization requiring as few as \(O\left(\log(\epsilon^{-1})\right)\) instead of \(O(\epsilon^{-2})\) samples to achieve error \(\epsilon\). Our theoretical results enable provably efficient and scalable optimization of kernel hyperparameters, which we validate empirically on a set of large-scale benchmark problems. There, variance reduction via preconditioning results in an order of magnitude speedup in hyperparameter optimization of exact GPs.

1 Introduction

Gaussian processes (GPs) [1] are a theoretically well-founded and powerful probabilistic model. However, inference for exact GPs requires the inversion of the kernel matrix, which can prove prohibitive for large datasets. This bottleneck to scaling becomes more severe when performing model selection, for example via gradient-based optimization of kernel hyperparameters. This requires repeated evaluation of the log-marginal likelihood (MLL) and its derivative for different choices of hyperparameters, where each evaluation has cubic cost in the number of data points \(n\).

Recently, Krylov methods [2–5] based on matrix-vector multiplication with the kernel matrix have become popular for GP inference [6, 7]. The method of conjugate gradients (CG) reduces the complexity of kernel matrix solves to \(O(kn^2)\) for \(k \ll n\) iterations. This can be improved if the matrix is structured or sparse [8]. Iterative methods also make effective use of modern hardware and parallelization [7, 9] and their convergence can be accelerated using preconditioning [2, 4, 5]. For GP hyperparameter optimization one additionally needs to compute a log-determinant and matrix trace. This can be done efficiently by combining another Krylov method, namely the Lanczos process [5, 10], with stochastic trace estimation [11–16] and quadrature [17, 18]. One advantage of this approach being that it fundamentally only relies on matrix-vector products with the kernel matrix.

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Bias and variance reduction via preconditioning.

While the source of this variance is in itself unbiased (assuming sufficient Krylov iterations), it can prevent the use of higher order optimizers like L-BFGS. Reducing variance in this context either requires further approximation at the cost of more bias [22], or more random vectors which only reduces variance at a rate of $O(\ell^{-1/2})$. As Figure 1 illustrates, we demonstrate how preconditioning can be used to reduce variance which in turn accelerates hyperparameter optimization.

**Contribution** In this paper, we demonstrate theoretically and empirically that preconditioning can solve both the bias and variance issues associated with iterative methods and stochastic trace estimation for GP hyperparameter optimization. Our contributions are as follows.

- We show that preconditioning can reduce variance in stochastic trace estimation with only a slight modification to the algorithm. Asymptotically, the number of random vectors required to achieve error $\varepsilon$ shrinks from $\ell \in O(\varepsilon^{-2})$ to as few as $O(\log(\varepsilon^{-1}))$ depending on the preconditioner and kernel matrix spectrum.
- Based on this result, we propose variance-reduced stochastic approximations to the log-determinant, log-marginal likelihood and its derivative.
- This variance reduction allows us to prove asymptotically better theoretical guarantees for the forward pass than previously known [18] and a novel error bound for the backward pass.
- We empirically validate our results on large-scale benchmark problems with up to $n \approx 350,000$ datapoints, where our approach reduces training times by an order of magnitude.

**2 Background**

Suppose we want to infer a latent map $h : \mathcal{X} \rightarrow \mathcal{Y}$ from an input space $\mathcal{X} \subset \mathbb{R}^d$ to an output space $\mathcal{Y} \subset \mathbb{R}$, given a dataset $X \in \mathbb{R}^{n \times d}$ of $n$ training inputs $x_i \in \mathbb{R}^d$ and corresponding outputs $y \in \mathbb{R}^n$.

**Gaussian Processes** A stochastic process $f \sim \mathcal{GP}(\mu, k_\theta)$ with mean function $\mu$, kernel $k_\theta$ and hyperparameters $\theta$ is a Gaussian process if $f = [f(x_1), \ldots, f(x_n)]^T \sim \mathcal{N}(\mu, k_\theta(X, X))$ is jointly Gaussian with mean $\mu_i = \mu(x_i)$ and covariance $k_\theta(X, X)_{ij} = k_\theta(x_i, x_j)$. Assuming $y \mid f \sim$ 

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*Figure 1: Efficient hyperparameter optimization via preconditioned iterative methods. We estimate the log-marginal likelihood and its derivative by combining stochastic trace estimation (a) and Krylov subspace methods (b) with preconditioning (c). Preconditioning reduces not only bias, but also variance of these estimators (d). This enables efficient hyperparameter optimization for exact GPs.*
which is no restriction for Rademacher or unit vectors and equivalent in expectation for Gaussian

Table 1: Properties of Hutchinson’s estimator for different random vectors. Variance of \( \tau_i \) and number of random vectors to achieve (relative) error \( \varepsilon \) with probability \( 1 - \delta \) for different random vectors \( z_i \).

| Type            | Random vectors \( z_i \) | Variance \( \text{Var}(\tau_i) \) | Number of random vectors \( \ell \) | Ref.       |
|-----------------|--------------------------|----------------------------------|----------------------------------|------------|
| Rademacher      | Radem(1/2)               | \( \frac{2}{n}(\|A\|_F^2 - \sum_i \|A_{ii}\|^2) \) | \( 6e^{-2} \log(2\delta^{-1}) \) | [13, 14]  |
| unit vectors    | \( \sqrt{n} \varepsilon_i, j \sim U([n]) \) | \( \frac{1}{n} \sum_i \|A_{ii}\|^2 - \text{tr}(A)^2 \) | \( \frac{(n \max_i \|A_{ii}\|)^2}{2 \text{tr}(A)^2} e^{-2} \log(2\delta^{-1}) \) | [13]      |
| Gaussian        | \( N(0, I) \)            | \( \frac{2}{n} \|A\|_F^2 \) | \( 8e^{-2} \log(2\delta^{-1}) \) | [13, 14]  |
| sub-Gaussian    | subG(\( \sigma^2 \))     | -                                | \( O(e^{-2} \log(\delta^{-1})) \) | [16]      |

\( \mathcal{N}(f, \sigma^2 I) \), the posterior distribution for test points \( x_* \) is again Gaussian with

\[
\mathbb{E}[f_*] = \mu(x_*) + k_\theta(x_*, X)(k_\theta(X, X) + \sigma^2 I)^{-1} y, \\
\text{Cov}(f_*) = k_\theta(x_*, x_*) - k_\theta(x_*, X)(k_\theta(X, X) + \sigma^2 I)^{-1} k_\theta(X, x_*).
\]

For brevity, we write \( K = k_\theta(X, X) + \sigma^2 I \) omitting the explicit dependence on the hyperparameters.

Hyperparameter Optimization The computational bottleneck when optimizing kernel hyperparameters \( \theta \) is the repeated evaluation of the log-marginal likelihood (1) and its derivative (2)

\[
\log p(y | X, \theta) = -\frac{1}{2} (y^T K^{-1} y + \log(\det(K))) + n \log(2\pi), \\
\frac{\partial}{\partial \theta} \log p(y | X, \theta) = \frac{1}{2} (y^T K^{-1} \frac{\partial K}{\partial \theta} K^{-1} y - \text{tr}(K^{-1} \frac{\partial K}{\partial \theta})).
\]

Computing (1) and (2) naively, e.g. via Cholesky decomposition, has complexity \( O(n^3) \). However, they can be approximated more efficiently using any number of scalable methods [8, 23–26].

Numerical Methods for GP Inference

In this paper, we focus on a certain scalable method for exact GPs, which relies on stochastic trace estimation in combination with Krylov subspace methods, as pioneered by [6, 18, 20, 27, 28]. We will show that preconditioning can be used for variance reduction, allowing us to derive better stochastic numerical approximations to (1) and (2), for which we prove new theoretical guarantees in Section 3.

Stochastic Trace Estimation Consider a matrix \( A \in \mathbb{R}^{n \times n} \) and \( \ell \) independent, zero-mean random vectors \( z_i \in \mathbb{R}^n \) with unit-variance entries. Hutchinson’s estimator [11] is defined by

\[
\tau_i(A) = \frac{1}{\ell} \sum_{\ell=1}^{\ell} z_i^T A z_i \approx \text{tr}(A).
\]

Following Ubaru et al. [18], we assume normalized random vectors of the form \( z_i = \sqrt{n} \tilde{z}_i / \|\tilde{z}_i\|_2 \), which is no restriction for Rademacher or unit vectors and equivalent in expectation for Gaussian random vectors \( z \sim \mathcal{N}(0, I) \) due to rotation invariance. Hutchinson’s method is particularly viable if \( A \) is expensive to instantiate, but easily accessed through matrix-vector multiplication (e.g. if \( A \) is a polynomial of some other matrix \( B \)). In practice, it is important to know how many random vectors \( \ell \) are needed to achieve a desired error \( \varepsilon \in (0, 1] \) with probability \( 1 - \delta \in [1/2, 1] \). It holds that:

**Theorem 1** (Error Bound for Hutchinson’s Estimator [13–16])

*If the number of random vectors for Hutchinson’s estimator (3) satisfies \( \ell \geq c_1 \varepsilon^{-2} \log(\delta^{-1}) \), then*

\[
\mathbb{P}(|\tau_i(A) - \text{tr}(A)| \leq \varepsilon \|A\|_F) \geq 1 - \delta.
\]

Note, if \( A \) is positive semi-definite, this gives a relative error bound since then \( \|A\|_F \leq \text{tr}(A) \). This general result mainly relies on the Hanson-Wright inequality [29], a tail bound for quadratic forms of sub-Gaussian random variables.\(^2\) Depending on the choice of distribution of the random vectors, the constant \( c_1 \) in Theorem 1 differs as was previously shown [13–16] and is summarized in Table 1.

For hyperparameter optimization computing (1) and (2) requires the trace of \( A = \log(K) \), since \( \log(\det(K)) = \text{tr}(\log(K)) \), and \( A = K^{-1} \frac{\partial K}{\partial \theta} \). To use Hutchinson’s estimator, we need to efficiently compute quadratic terms \( z_i^T A z_i \) without explicitly instantiating \( A \). We use Krylov methods, namely the Lanczos process for the log as was suggested previously [17, 18] and CG for the linear solves.

\(^1\)This is necessary for the approximation of the quadratic form via Lanczos quadrature in (4).

\(^2\)Details on sub-Gaussian random variables can be found in Section S1.3 of the supplementary.
Krylov Subspace Methods    Recognizing that $f(K) = Vf(Λ)V^T$, for an eigendecomposition $K = VΛV^T$, one can approximate the $z^T\log(K)z$ terms by rewriting them as an integral

$$z^T\log(K)z = z^TV\log(Λ)V^Tz = \sum_{i=1}^n \log(λ_i)μ_i^2 = \int_{μ_i}^λ \log(t) \, dμ(t)$$  \hspace{1cm} (4)

where $μ_i = (V^Tz)_i$. This integral can then be approximated using quadrature, where the nodes and weights of the quadrature rule are computed efficiently via the Lanczos process. This approach, known as stochastic Lanczos quadrature (SLQ) [17, 18], relies primarily on repeated matrix-vector multiplication with $K$. Gardner et al. [6] show that these nodes and weights can also be derived from byproducts of the method of conjugate gradients (CG) [30, 31] when solving $K^{-1}z$. We also use CG to compute the linear system solve $K^{-1}y$ needed for both (1) and (2), where the solution is similarly realized through iterative matrix-vector products. Both CG and Lanczos converge in $\ll n$ iterations for well-conditioned matrices, especially if these have fast-decreasing or structured spectra [44].

Preconditioning    Krylov subspace methods have convergence rates dependent on the number of iterations of the matrix. Therefore an equivalent preconditioned linear system with matrix $P^{-1}K$ is considered instead. The preconditioner inverse $P^{-1}$ can be thought of as an approximate inverse to $K$ such that $P^{-1}K \approx I$. To be useful, it should be cheap to obtain and allow efficient matrix-vector multiplication. A large class of preconditioners is based on low-rank approximations of the kernel matrix, such that

$$P_ℓ = L_ℓL_ℓ^T + σ^2I \approx K,$$

where $L_ℓ \in \mathbb{R}^{n×ℓ}$. This allows efficient linear solves in $O(nℓ^2)$ via the matrix inversion lemma. Typically, such preconditioners approximate matrices with fast decreasing spectra well. As an example, the optimal rank-ℓ approximation in Frobenius norm satisfies

$$\min_{\text{rank}(M)=ℓ} ∥K - M∥_F = ∥K - L_ℓL_ℓ^T∥_F = (\sum_{i=ℓ+1}^n λ_i^2)^{1/2} ≤ g(ℓ)∥K∥_F,$$

where $g(ℓ) = ℓ^{-1/2}$ [32]. This bound is tight if the spectrum of $K$ is uniform, but if the spectrum of $K$ decays quickly, the decay given by $g(ℓ)$ is much faster. However, computing $L_ℓ$ requires an eigendecomposition at cubic cost $O(n^3)$, rendering it infeasible as a preconditioner. Randomized approaches, such as randomized singular value decomposition [33, 34], or random Fourier features [35, 36], are a viable substitute that retain the same asymptotic dependence on the rank [37]. In this paper we will primarily explore partial matrix factorizations, such as the pivoted incomplete Cholesky decomposition [38], where $L_ℓ$ is a lower-triangular matrix approximating the Cholesky factor. This preconditioner has the desirable property that for a fast-decaying spectrum the residual decays at roughly the same rate as Lemma 1 shows. For this reason we use it for our experiments in Section 4.

Lemma 1 (Harbrecht et al. [38])

Let $k(x, y) = k(∥x - y∥)$ be a stationary kernel with associated kernel matrix $K \in \mathbb{R}^{n×n}$ and output scale $σ^2 = k(0) > 0$. Assume the kernel matrix spectrum decays at least exponentially, i.e. $λ_i \lesssim \exp(-bi)$ for some $b > \log(4)$. Then the rank-ℓ pivoted Cholesky decomposition satisfies

$$∥K - L_ℓL_ℓ^T∥_F ≤ \sqrt{n}σ^{-2} \exp(-bℓ)∥K∥_F.$$  \hspace{1cm} (5)

Lemma 1 holds for the RBF kernel, whose spectrum decays super-exponentially [6]. In practice one can observe fast rates of decay also for other kernels with quickly decreasing spectra (see Figure 2).

3 Variance-Reduced Hyperparameter Optimization via Preconditioning

Our goal is to reduce the variance of the stochastic estimates of $\text{tr}(\log(K))$ and its derivative in eqs. (1) and (2). Assume we are using Lanczos (and CG) and that we have access to a sufficiently good preconditioner $P \approx K$ improving convergence (and thus reducing bias) of these algorithms.

Similar to [16, 39], our variance reduction strategy is to separate $\text{tr}(\log(K))$ into a deterministic approximation of $\text{tr}(\log(K))$ and a residual term estimated via stochastic Lanczos quadrature. For many matrix functions of interest $f(P)$ also provides a cheap and accurate approximation of

While Lanczos and CG assume a symmetric positive-definite system matrix, both algorithms can be written in a way that only requires $P^{-1}$ instead of $P^{-1/2}KP^{-1/2}$, which is always symmetric positive definite. We therefore interchangeably write $P^{-1/2}KP^{-1/2}$ and $P^{-1}K$ for the preconditioned kernel matrix.
We now prove using a preconditioner as part of the decomposition in (6) indeed provides asymptotic variance reduction for both (1) and (2) and allows us to achieve arbitrarily good rates for the number of random vectors, it holds for $\tau = \text{tr}(A) + \tau_\ell(\Delta)$, that $\mathbb{P}(|\tau - \text{tr}(A)| \leq \mathbb{E}\|A\|_F) \leq \mathbb{N} - 1 - \delta$.

In comparison with Meyer et al. [16, Theorem 4], we do not assume $A$ to be positive semi-definite (allowing $A = \log(K)$, which is generally indefinite), nor do we assume $A$ to be a randomized low rank approximation with $g(\ell) = \ell^{-1/2}$ (allowing arbitrary preconditioners $A = P$). This enables variance reduction for both (1) and (2) and allows us to achieve arbitrarily good rates for the number of random vectors depending on the quality of the preconditioner given by $g(\ell)$. Note that if $P$ is a low-rank-plus-diagonal preconditioner, Theorem 2 defines a relationship between the rank of $P_{\ell}$ and $\ell$.

In Table 2 we depict how various residual decay rates $g(\ell)$ translate to the number of Hutchinson vectors $\ell$. We obtain the biggest improvements when the residual decay rate is exponential, a condition that can easily be met for certain kernels. As previously observed by Gardner et al. [6], by Lemma 1 the computationally efficient incomplete Cholesky preconditioner converges exponentially to RBF kernel matrices, and thus for these kernels we reduce $\ell$ from $\mathcal{O}(\varepsilon^{-2})$ to $\mathcal{O}(\log(\varepsilon^{-1}))$.

### 3.2 Log-Marginal Likelihood

If we combine the decomposition in (6) with Theorem 2 and Krylov iterations for $K^{-1}y$ and $z^\top \log(K)z$, we obtain a probabilistic error bound for the approximation of the log-marginal likelihood. We first analyze the error of the log-determinant estimate with our proposed variance reduction. Combining Theorem 2 with Lanczos quadrature analysis, the following holds.
Theorem 3 (Error Bound for the log-Determinant)
Let \( A = \log(K) \) and \( \Delta = \log(P^{-1}K) \) and assume we choose the number of random vectors \( \ell \) according to Theorem 2. If the number of Lanczos steps

\[
k \geq \frac{\sqrt{\pi}}{\delta} \sqrt{\kappa} \log(K_1 \varepsilon^{-1}) \tag{11}
\]

with \( K_1 = \frac{5\kappa \log(2(\kappa+1))}{\max_i \log[\lambda_i(K)]]} \sqrt{\kappa+1} \) and \( \kappa = \kappa(P^{-1}K) \), then for \( \tau = \log(\det(P)) + \tau_{1,\kappa}(\Delta) \),

\[
\mathbb{P}(|\tau - \log(\det(K))| \leq \varepsilon \|\log(K)\|_F) \geq 1 - \delta.
\]

Comparing this bound with Corollary 4.5 by Ubaru et al. [18], we note two major improvements. Firstly, the number of Lanczos steps now depends on the preconditioned system \( P^{-1}K \). This corresponds to the “standard” benefit of preconditioning, namely iteration / bias reduction. Secondly, and most importantly, we obtain the significantly lower number of random vectors required due to variance reduction via Theorem 2. We can now obtain a bound on the full log-marginal likelihood term by combining Theorem 3 with standard CG error analysis applied to \( K^{-1}y \):

Corollary 1 (Error Bound for the log-Marginal Likelihood)
Assume the conditions of Theorem 3 hold with \( K_1' = \frac{K_1}{2} \) and we solve \( Ku = y \) via preconditioned CG initialized at \( u_0 \) and terminated after

\[
k' \geq \frac{1}{2} \sqrt{\kappa} \log(K_2 \varepsilon^{-1}) \tag{12}
\]

iterations, where \( K_2 = \sqrt{\kappa} \|y\|_2 \|u_0 - u\|_2 \). Then for \( \eta = -\frac{1}{2}(y^Tu' + \tau + n \log(2\pi)) \),

\[
\mathbb{P}(|\eta - \log p(y | X, \theta)| \leq \varepsilon(1 + \|\log(K)\|_F)) \geq 1 - \delta.
\]

3.3 Derivative of the Log-Marginal Likelihood

We now propose a new variance reduction scheme for the backward pass. If we differentiate through the log-determinant decomposition in (6), we obtain

\[
\frac{\partial}{\partial \theta} \log(\det(PPP^{-1}K)) = \text{tr}(P^{-1}\frac{\partial P}{\partial \theta}) + \text{tr}(\Delta),
\]

where \( \Delta = K^{-1} \frac{\partial K}{\partial \theta} - P^{-1} \frac{\partial P}{\partial \theta} \). Note that this takes an analogous form to the variance reduction strategy for \( \text{tr}(\log(K)) \). Again, we estimate \( \Delta \) via stochastic trace estimation, which requires solves \( z^T K^{-1} \frac{\partial K}{\partial \theta} z \) and \( z^T P^{-1} \frac{\partial P}{\partial \theta} z \). The former can be efficiently computed with preconditioned CG, while the latter is simply a solve with the preconditioner. Note that the deterministic term \( \text{tr}(P^{-1} \frac{\partial P}{\partial \theta}) \) is efficient to calculate if \( P \) is a low-rank-plus-diagonal preconditioner (see Section S5.4). As for the forward pass, we obtain a novel probabilistic error bound for the derivative estimate.

Theorem 4 (Error Bound for the Derivative)
Let \( A = K^{-1} \frac{\partial K}{\partial \theta} \) and \( \Delta = K^{-1} \frac{\partial K}{\partial \theta} - P^{-1} \frac{\partial P}{\partial \theta} \) and assume we choose the number of random vectors \( \ell \) as in Theorem 2. If we use CG initialized at \( 0 \) or better to solve \( K^{-1} \frac{\partial K}{\partial \theta} \) and \( Ku = y \) with

\[
k \geq \frac{1}{2} \sqrt{\kappa} \log(2\sqrt{\kappa}n\varepsilon^{-1}), \quad \text{and} \quad \ell' \geq \frac{1}{2} \sqrt{\kappa} \log(K_4 \varepsilon^{-1}) \tag{14}
\]

We also note a slight difference in \( K_1 \) arising from formulation of the bounds using the Frobenius norm.
We connect variance reduction to preconditioning, we prove tighter probabilistic error bounds via Lanczos quadrature \cite{17, 18, 40}. Our work builds on recently proposed variance reduction.

Algorithm 1: log-Marginal Likelihood

\begin{algorithm}[H]
\begin{algorithmic}[1]
\Procedure{LogMargLik}{y, K, P, \ell, k, \ell'}
\State $u \leftarrow \text{LinSolve}(K, y, P, k')$
\State $\tau_0 \leftarrow \log(\det(P))$
\State $z_i \leftarrow z_i / \|z_i\|_2$ for $z_i \sim D$
\For{$i = 1, \ldots, \ell$}
\State $T \leftarrow \text{Lanczos}(P^{-1}K, z_i, k)$
\State $\omega_j \leftarrow (e_j^\top y_j)^2$ for $j = 0, \ldots, k$
\State $\gamma_i \leftarrow \sum_{j=0}^{k} \omega_j \log(\theta_j)$
\EndFor
\State $\tau \leftarrow \tau_0 + \frac{\pi}{\ell} \sum_{i=1}^{\ell} \gamma_i$
\State \Return $-\frac{1}{2} (y^\top u + \tau + n \log(2\pi))$
\EndProcedure
\end{algorithmic}
\end{algorithm}

Algorithm 2: Derivative

\begin{algorithm}[H]
\begin{algorithmic}[1]
\Procedure{Deriv}{y, K, \partial K, P, \partial P, \ell, k, \ell'}
\State $u \leftarrow \text{LinSolve}(K, y, P, k')$
\State $\tau_0 \leftarrow \text{tr}(P^{-1} \partial P)$
\State $z_i \leftarrow z_i / \|z_i\|_2$ for $z_i \sim D$
\For{$i = 1, \ldots, \ell$}
\State $w_i \leftarrow \text{LinSolve}(K, \partial K, z_i, P, k)$
\State $\hat{w}_i \leftarrow \text{LinSolve}(P, \partial P, z_i)$
\State $\gamma_i \leftarrow z_i^\top (w_i - \hat{w}_i)$
\EndFor
\State $\tau \leftarrow \tau_0 + \frac{\pi}{\ell} \sum_{i=1}^{\ell} \gamma_i$
\State \Return $\frac{1}{2} (u^\top \partial K \partial K u - \tau)$
\EndProcedure
\end{algorithmic}
\end{algorithm}

Computational Complexity  The cost of evaluating the log-marginal likelihood and its derivative is quadratic in the number of data points $n$. More precisely, Algorithm 1 has complexity $O(n^2(k^2 + k') + \text{Plogdet})$ and Algorithm 2 has complexity $O((n^2 k + \text{Psolve})\ell + \text{Ptrinv})$, where $k, k', \ll n$ and $\text{P}_{\cdot}$ denotes the cost of the corresponding operation with the preconditioner. Assuming a low-rank-plus-diagonal preconditioner, such as the incomplete Cholesky, the cost of a linear solve, log-determinant and trace of the inverse is $\text{Psolve} = \text{Plogdet} = \text{Ptrinv} = O(n\ell^2)$ via the matrix inversion lemma. Since Algorithms 1 and 2 primarily rely on matrix-vector multiplication with the kernel matrix, the more efficient $v \mapsto K'v$ is, the faster the MLL and its derivative(s) can be evaluated. This is the case for structured and sparse kernel matrices, for example. From a practical perspective, the loops over $\ell$ random vectors are embarrassingly parallelizable, allowing additional speedup.

3.4 Algorithms

The above leads to Algorithms 1 and 2, which are fundamentally based on functions implementing matrix-vector products with $K$ and $P$, as well as their derivatives, instead of their full representations in memory. Our algorithms are similar to iterative-based GP algorithms presented in prior work \cite{6, 18, 20}, yet crucially they rely on \eqref{eq:6} and \eqref{eq:13} for reduced variance. \texttt{LinSolve}(A, b, P) denotes a linear system solve with preconditioner $P$, typically implemented with CG. For $k'$ random vectors, $k$ iterations of the Lanczos algorithm we obtain the following procedures.

3.5 Related Work

Krylov subspace methods \cite{3–5}, such as CG \cite{30} and the Lanczos process \cite{40}, in combination with preconditioning \cite{5} have been used for decades in numerical linear algebra for the solution of linear systems and eigenvalue estimation. While they have been applied to GP inference in the past \cite{41}, modern hardware and parallelization have made iterative methods increasingly popular \cite{6} and enabled exact GP inference on large-scale data \cite{7}. In turn, also specific preconditioners for kernel matrices have been studied \cite{20}. Iterative methods enable more efficient hyperparameter optimization \cite{22} and can be combined with stochastic approximation of the trace \cite{6, 28}. In this context, stochastic trace estimation \cite{11} has seen renewed interest in recent years \cite{12–14}, in particular in combination with Lanczos quadrature \cite{17, 18, 40}. Our work builds on recently proposed variance reduction techniques for Hutchinson’s estimator \cite{15, 16, 39}, but it differs in the following important ways. We connect variance reduction to preconditioning, we prove tighter probabilistic error bounds via improved asymptotic dependence on the number of random vectors and apply our findings to GP hyperparameter optimization. While Gardner et al. \cite{6} use a similar decomposition for the log-determinant in the forward pass, they did not consider its variance reducing properties. Additionally, we also propose a variance-reducing decomposition for the backward pass.
(b) Kernel spectra for $d \in \{1, 2, 3\}$.

Figure 3: Bias and variance decreases with preconditioner size and spectral decay. (a) Relative error and variance of the estimators for the log-marginal likelihood and its derivatives decrease substantially faster with the number of random samples using preconditioning. (b) The decrease is determined by the approximation quality of the preconditioner and in turn by the spectral decay of the kernel matrix. This decay generally slows down with dimension $d$ of the data.

4 Experiments

We validate our theoretical findings empirically by performing GP regression on synthetic and benchmark datasets with and without preconditioning for hyperparameter optimization. We find that:

- Preconditioning reduces bias and variance in the forward and backward pass.
- Preconditioner quality and the kernel spectrum determine the degree of variance reduction.
- Variance reduction lowers the number of model and gradient evaluations performed by the optimizer’s line search, which reduces training times by an order of magnitude.

Experimental Setup We consider a synthetic dataset of $n = 10,000$ iid standard normal samples, as well as a range of UCI datasets [42] with training set sizes ranging from $n = 12,449$ to 326,155 (see Table 3). All experiments were performed on single NVIDIA GPUs, a GeForce RTX 2080 and Titan RTX, respectively. We perform GP regression using an RBF and Matérn($\frac{3}{2}$) kernel with output scale $o$, lengthscale $\ell$ and noise $\sigma^2$. Hyperparameters were optimized with L-BFGS using an Armijo-Wolfe line search and early stopping via a validation set. We use an incomplete Cholesky preconditioner throughout. Our experiments and algorithms are implemented using GPyTorch [6].

Preconditioning reduces bias and variance in MLL and gradients. Figure 3(a) shows the relative error of the marginal log-likelihood and its derivatives on synthetic data. Already for $\ell \geq 16$ random samples bias and variance are reduced by several orders of magnitude. We observe exponential decay and then a return to the standard Hutchinson’s rate of $O(e^{-2})$. This is caused by dampening of the spectrum with the noise $\sigma^2 = 10^{-2}$, which invalidates the spectral decay assumption after a certain point. Similar observations hold for the Matérn and RatQuad kernel (see Table S1 and Figure S1). As predicted by Theorem 2 and illustrated by Figure 3, the variance reduction is determined by the preconditioner and therefore the spectral decay of the kernel matrix. For higher dimensions, the spectral decay slows, which in turn reduces the bias and variance reduction achieved by our method (see Table S1). However, on real datasets we still see strong variance reduction via our method, possibly since real data often lies on a low-dimensional manifold.

Variance reduction accelerates hyperparameter optimization. On datasets from the UCI repository, we find that preconditioning results in lower training loss ($-\text{MLL}$) on almost all datasets and essentially identical generalization error (see Table 3). However, variance reduction via preconditioning significantly lowers the number of model and gradient evaluations performed for the line searches during optimization (see Figure 4(b)). This reduces training times by an order of magnitude, as Figure 4(c) shows. Since the cost of computing and applying the preconditioner amortizes with increasing $n$, the larger the dataset, the larger the speedup. Finally, the noise in the loss and gradients caused by stochastic trace estimation previously necessitated the use of slower converging, but more robust optimizers [7], such as Adam [43]. As our experiments show, our variance-reduced estimators make the use of L-BFGS possible, which significantly outperforms Adam (c.f. Table 3 and Table S2).
Figure 4: **Variance reduction accelerates hyperparameter optimization.** Variance reduction improves optimization via better search directions and fewer evaluations of the loss and gradient per line search, resulting in lower training times. (a) Variance reduction for the MLL and its derivatives on the “Elevators” dataset. (b) Training loss and MLL evaluations for line search decrease with preconditioner size, as shown for the “Protein” dataset. (c) The reduction in loss and gradient evaluations per optimization step results in an order of magnitude speedup on UCI datasets.

Table 3: **Hyperparameter optimization on UCI datasets.** GP regression using a Matérn\((\frac{3}{2})\) kernel and incomplete Cholesky preconditioner of size 500 with \(\ell = 50\) random samples. Hyperparameters were optimized with L-BFGS for at most 20 steps using early stopping via a validation set. All results, but “3DRoad”, are averaged over 10 runs. Averages differing by at least one standard deviation in bold.

| Dataset    | n     | d     | \(-\text{MLL}_{\text{train}}\)\downarrow | \(-\text{MLL}_{\text{test}}\)\downarrow | RMSE\downarrow | Runtime (s) |
|------------|-------|-------|------------------|------------------|---------------|-------------|
|            | \(d\) |       | Standard Precond. | Precond. Standard Precond. | Standard Precond. |             |
| Elevators  | 12,449| 18    | 0.4647            | \textbf{0.4377} | 0.4021        | 0.4022       |
| Bike       | 13,034| 17    | \textbf{-0.9976} | -0.9905          | 0.0416        | 0.0415       |
| Kin40k     | 30,000| 8     | -0.3339           | \textbf{-0.4332} | -0.3141       | \textbf{0.0929} |
| Protein    | 34,297| 9     | 0.9963            | \textbf{0.9273} | 0.8869        | 0.8835       |
| KEGGdir    | 36,620| 20    | -0.9501           | \textbf{-1.0043} | -0.9459       | \textbf{0.5577} |
| 3DRoad     | 326,155| 3    | 0.7733            | \textbf{0.1284} | 1.4360        | \textbf{1.1690} |

5 Conclusion

We introduced a method using preconditioners not only to reduce bias of iterative methods but also to reduce variance of stochastic trace estimation. In particular, we constructed variance-reduced stochastic estimators for the \(\log\)-determinant, \(\log\)-marginal likelihood, and its derivative, primarily relying on matrix-vector multiplication. We proved probabilistic error bounds for these estimators and showed that asymptotically fewer random samples are needed than previously known, assuming a sufficiently good preconditioner. We empirically validated our theoretical findings by training exact GPs on a set of large-scale benchmark datasets, where our method substantially lowered the number of model evaluations of the optimizer, resulting in an order of magnitude faster training.

The degree of variance reduction depends on the approximation quality of the preconditioner and therefore typically on the spectral decay of the kernel matrix. It is worth noting that the accuracy of low-rank kernel matrix approximations decays with dimensionality [44, 45]. Therefore, assuming we use low-rank preconditioners, our theory suggests that our method is most viable for problems with lower dimensionality and many observations, e.g. from geostatistics or astrophysics. Nevertheless, in practice we observe meaningful variance reduction and speedups on up to 20-dimensional datasets.

We empirically observed that variance reduction works well, even for kernels for which the approximation quality of the incomplete Cholesky preconditioner is not known theoretically. Other scientific fields invest substantial research effort into design and theoretical analysis of preconditioners, e.g. for PDEs [3]. Our and previous work [6, 7, 20] suggest that developing specialized preconditioners for certain families or compositions of kernels is a promising research direction for scalable GPs.
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Supplementary Material:
Reducing the Variance of Gaussian Process Hyperparameter Optimization with Preconditioning

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This supplementary material contains background material and proofs for all theoretical results. Throughout we occasionally restate results from the literature to provide a clearer exposition to the reader. References referring to sections, equations or theorem-type environments within the supplement are prefixed with ‘S’, while references to, or results from, the main paper are stated as is.

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\noindent \textbf{Preliminaries and Notation} \ Let \( X \in \mathbb{R}^{n \times d} \) and \( y \in \mathbb{R}^n \) be a training dataset of \( n \) data points of dimension \( d \). Let \( K = k_\theta(X, X) + \sigma^2 I \in \mathbb{R}^{n \times n} \) denote a symmetric positive definite kernel matrix for kernel \( k_\theta \) with hyperparameters \( \theta \) and observation noise scale \( \sigma^2 \), and let \( P \in \mathbb{R}^{n \times n} \) be a symmetric positive definite preconditioner. For the probabilistic error bounds, define a desired (relative) error \( \varepsilon \in (0, 1) \) achieved with probability \( 1 - \delta \in [1/2, 1) \) and let \( \kappa = \kappa(P^{-1} K) \) be the condition number of the preconditioned kernel matrix. Throughout the following constants are used as follows: \( \ell \) denotes the number of random probe vectors and where appropriate the size of the preconditioner; \( k \) denotes the number of Lanczos iterations and \( k' \) the number of CG iterations.
S1 Mathematical Background

S1.1 Matrix Norms

We use the following matrix norms and basic properties throughout the paper. Proofs can be found in most standard textbooks on (numerical) linear algebra.

Let \( \| \cdot \| \) be a norm on \( \mathbb{R}^n \) and \( A : \mathbb{R}^n \to \mathbb{R}^m \) a linear operator. The induced matrix norm on \( \mathbb{R}^{m \times n} \) is defined by the operator norm

\[
\| A \| = \sup \{ \| Ax \| : x \in \mathbb{R}^n, \| x \| = 1 \}.
\]

It holds for the Euclidean norm that

\[
\| A \|_2 = \sqrt{\lambda_{\text{max}}(A^*A)} = \sigma_{\text{max}}(A).
\]

Alternatively one can define a norm on \( \mathbb{R}^n \) via \( \| x \|_p \) for any \( p \geq 1 \), then for any two matrix norms \( \| \cdot \|_p \) and \( \| \cdot \|_q \) such that

\[
\| A \|_p \leq \| A \|_q \leq c \| A \|_p
\]

In particular, we have for \( \text{rank}(A) = r \) that

\[
\| A \|_2 \leq \| A \|_F \leq \sqrt{r} \| A \|_2.
\]

Note, that the Frobenius norm is not an operator norm. The Frobenius norm satisfies:

\[
\| AB \|_F \leq \| A \|_F \| B \|_F \quad \text{Submultiplicativity (S15)}
\]

\[
\| Ax \|_2 \leq \| A \|_F \| x \|_2 \quad \text{(S16)}
\]

\[
\| A \|_F = \| AU \|_F = \| UA \|_F \quad \text{Unitary Invariance (S17)}
\]

**Proposition S1 (Equivalence of Norms)**

*Let \( A \in \mathbb{R}^{m \times n} \), then for any two matrix norms \( \| \cdot \|_\alpha \), \( \| \cdot \|_\beta \) there exist constants \( c, C > 0 \) such that

\[
c \| A \|_\alpha \leq \| A \|_\beta \leq C \| A \|_\alpha.
\]

In particular, we have for \( \text{rank}(A) = r \) that

\[
\| A \|_2 \leq \| A \|_F \leq \sqrt{r} \| A \|_2.
\]

S1.2 Functions of Matrices

**Lemma S2 (Lipschitz Continuity)**

*Let \( A, B \in \mathbb{R}^{n \times n} \) be symmetric. Assume \( f : \Omega \to \mathbb{R} \) is globally Lipschitz continuous with Lipschitz constant \( L > 0 \) on the combined spectrum \( \Omega = \lambda(A) \cup \lambda(B) \subset \mathbb{R} \), then there exists \( c_p > 0 \) such that

\[
\| f(A) - f(B) \|_p \leq c_p L \| A - B \|_p,
\]

where \( \| \cdot \|_p \) denotes any matrix norm. In particular \( c_2 = 1 \) and \( c_F = \sqrt{n} \).

**Proof.** Since \( A, B \) are symmetric, they are normal. By Kittaneh [46], it holds that

\[
\| f(A) - f(B) \|_2 \leq L \| A - B \|_2.
\]

The result now follows by equivalence of norms on finite dimensional spaces. For the Frobenius norm we have \( \frac{1}{\sqrt{n}} \| M \|_F \leq \| M \|_2 \leq \| M \|_F \), and therefore \( c_F = \sqrt{n} \).

\[\square\]

**Lemma S3**

*Let \( K \in \mathbb{R}^{n \times n} \) be symmetric positive definite and assume \( f \) is analytic in a domain containing the spectrum \( \lambda(K) \). Then it holds that

\[
\| K \|_F \leq \| K \|_F \sum_{i=1}^{\nu} \left| f(\lambda_i(K)) \right|,
\]

where \( c_{f(\lambda)} = \max \{ \min_i \left| f(\lambda_i(K)) \right|, \frac{\max_i |f(\lambda_i(K))|}{\sqrt{n}} \} \).
Proof. It holds that
\[ \| f(K) \|_F = \sqrt{\sum_{i=1}^{n} f(\lambda_i)^2} \geq \sqrt{n \min_i f(\lambda_i)} \]
and therefore \( \| f(K) \|_F \geq \sqrt{n} c_{f(\lambda)}. \) Now we have
\[ \| K \|_F = \frac{\| K \|_F}{\| f(K) \|_F} \leq \frac{\| K \|_F}{\sqrt{n} c_{f(\lambda)}}, \]
\[ \| f(K) \|_F \leq \| K \|_F. \]
\[ \square \]

Proposition S2
Let \( K, P \in \mathbb{R}^{n \times n} \) be symmetric positive definite and assume \( f \) is analytic in a domain containing the spectrum \( \lambda(K) \). Suppose it holds for the preconditioner \( P \) that
\[ \| K - P \|_F \leq \gamma \| K \|_F. \] (S20)
Then we have
\[ \| f(K) - f(P) \|_F \leq \frac{L \| K \|_F}{c_{f(\lambda)}} \| f(K) \|_F \] (S21)
where \( L > 0 \) is the Lipschitz constant of \( f \) and \( c_{f(\lambda)} = \max \{ \min_i | f(\lambda_i(K)) |, \max_i | f(\lambda_i(K)) | \}. \)

Proof. It holds that
\[ \| f(K) - f(P) \|_F \leq L \sqrt{n} \| K - P \|_F \]
Lemma S2
\[ \leq \frac{L \| K \|_F}{c_{f(\lambda)}} \| f(K) \|_F \]
Preconditioner quality (S20)
\[ \leq \frac{L \| K \|_F}{c_{f(\lambda)}} \| f(K) \|_F \]
Lemma S3
\[ \square \]

Corollary S2
Given the assumptions of Proposition S2 and \( \lambda_{\min}(P, K) = \lambda_{\min}(K) \), we have
\[ \| \log(K) - \log(P) \|_F \leq \frac{\sqrt{n}}{\max_i | \log(\lambda_i(K)) |} \| K \|_F \gamma \| \log(K) \|_F \] (S22)
\[ \leq \frac{n \kappa(K)}{\lambda_{\min}(K)} \| K \|_F \gamma \| \log(K) \|_F, \] (S23)
\[ \| K^{-1} - P^{-1} \|_F \leq \frac{\sqrt{n}}{\lambda_{\min}(K)} \| K \|_F \gamma \| K^{-1} \|_F \] (S24)
\[ \leq n \kappa(K) \| K \|_F \gamma \| K^{-1} \|_F. \] (S25)

Proof. Define \( \Omega = [\lambda_{\min}, \lambda_{\max}] \subset (0, \infty) \) to be the interval containing the spectra of \( K, P \). Since \( K, P \) are positive definite, the logarithm and inverse function have bounded derivative on \( \Omega \) and are therefore Lipschitz continuous on \( \Omega \) with Lipschitz constant \( L_\log = \sup_{\xi \in \Omega} | g'(\xi) | \). We have \( L_{\log} = \lambda_{\min}^{-1} \) and \( L_{\text{inv}} = \lambda_{\min}^{-2} \). By Lemma S2, it holds that
\[ \| \log(K) - \log(P) \|_F \leq \frac{\sqrt{n}}{\lambda_{\min}} \| K - P \|_F \]
\[ \| K^{-1} - P^{-1} \|_F \leq \frac{\sqrt{n}}{\lambda_{\min}^2} \| K - P \|_F, \]
If \( P^{-1} \) and \( K \) commute, then \( \log(P^{-1} K) = \log(P^{-1}) + \log(K) \). Now applying Proposition S2, with the choices
\[ c_{\log(\lambda)} = \frac{1}{\sqrt{n}} \max_i | \log(\lambda_i(K)) | \]
\[ c_{\text{inv}(\lambda)} = \frac{1}{\sqrt{n}} \max_i | \lambda_i(K)^{-1} | = \frac{1}{\sqrt{n} \lambda_{\min}(K)} \]
proves the statement. \[ \square \]
S1.3 Sub-Gaussian Concentration

**Definition S1**
A centered random variable \( x : \Omega \to \mathbb{R} \) is sub-Gaussian with variance proxy \( \sigma^2 > 0 \), if any of the following equivalent conditions holds:

- **Laplace transform**
  \[ \forall t \in \mathbb{R} : \mathbb{E}[\exp(tx)] \leq \exp\left(\frac{\sigma^2 t^2}{2}\right) \quad (S26) \]

- **Tail bound**
  \[ \forall t > 0 : \mathbb{P}(|x| \geq t) \leq 2 \exp\left(\frac{-t^2}{2\sigma^2}\right) \quad (S27) \]

- **Moment condition**
  \[ \forall q \in \mathbb{N} : \mathbb{E}[x^{2q}] \leq q!(4\sigma^2)^q \quad (S28) \]

- **Orlicz condition**
  \[ \mathbb{E}[\exp\left(\frac{x^2}{8\sigma^2}\right)] \leq 2 \quad (S29) \]

Proofs of equivalency between the definitions can be found for example in [47, 48]. Clearly by definition zero-mean Gaussian random variables are sub-Gaussian. Similar to Gaussians the above definition can be extended to the multi-variate case.

**Definition S2**
A centered random vector \( x \in \mathbb{R}^n \) is sub-Gaussian with variance proxy \( \sigma^2 > 0 \) if for any \( u \in \mathbb{R}^n \), such that \( \|u\|_2 = 1 \), the random-variable \( u^\top x \) is sub-Gaussian with variance proxy \( \sigma^2 \). We write \( x \sim \text{subG}(\sigma^2) \).

**Proposition S3**
Let \( x \sim \text{subG}(\sigma^2) \) be a sub-Gaussian random variable, then \( \mathbb{E}[x] = 0 \) and \( \text{Var}(x) \leq \sigma^2 \).

One might wonder what random variables are in fact sub-Gaussian. Hoeffding’s lemma provides an answer for bounded random variables.

**Lemma S4** (Hoeffding’s Lemma [49])
Let \( x \in \mathbb{R} \) be a centered random variable such that \( a \leq x \leq b \) almost surely, then
\[ \mathbb{E}[\exp(tx)] \leq \exp\left(\frac{(b-a)^2}{8}t^2\right), \]
i.e. \( x \) is sub-Gaussian with variance proxy \( \sigma^2 = \frac{(b-a)^2}{4} \).

This shows that any almost surely bounded random variables, in particular \( \text{Radem}(\frac{1}{2}) \) (also called a symmetric Bernoulli distribution) and \( U[-a,a] \) distributed random variables are sub-Gaussian.

**Corollary S3**
Let \( x \in \mathbb{R}^n \) be a zero-mean, bounded random-variable, such that \( \|x\|_2 \leq b \), then \( x \sim \text{subG}(b^2) \).

**Proof.** Let \( u \in \mathbb{R}^n \), such that \( \|u\|_2 = 1 \). Then it holds that
\[ |u^\top x| \leq \|u\|_2 \|x\|_2 \leq b \]
By Lemma S4, it holds that \( u^\top x \sim \text{subG}(\sigma^2) \) with \( \sigma^2 = \frac{(b-(-b))^2}{4} = b^2 \). Therefore by Definition S2, \( x \) is sub-Gaussian with variance proxy \( b^2 \).

**Theorem S5** (Hanson-Wright Inequality [29])
Let \( A \in \mathbb{R}^{n \times n} \) and \( x \sim \text{subG}(\sigma^2) \) with independent components \( x_i \). Then for all \( t \leq 0 \), it holds that
\[ \mathbb{P}(|x^\top Ax - \mathbb{E}[x^\top Ax]| > t) \leq 2 \exp\left(-c \min\left(\frac{t^2}{\|A\|_F^2}, \frac{t}{\|A\|_2}\right)\right) \quad (S31) \]
where \( c = c(\sigma^2) > 0 \) is a constant only dependent on the choice of sub-Gaussian distribution.
Proof. Substituting $K^2 = 8\sigma^2$ in the Orlicz condition (S29) and using Theorem 1.1 by Rudelson et al. [29] results in

$$P(|x^\top A x - E[x^\top A x]| > t) \leq 2 \exp \left(-c' \min \left(\frac{t^2}{(8\sigma^2)^2 \|A\|_{F}^2}, \frac{t}{8\sigma^2 \|A\|_2} \right)\right)$$

where $c' > 0$ is an absolute constant. Now it holds that

$$\min \left(\frac{t^2}{K^4 \|A\|_{F}^2}, \frac{t}{K^2 \|A\|_2} \right) \geq \frac{1}{K^4 \max(K^2, 1)}$$

Choosing $c = \frac{c'}{K^4 \max(K^2, 1)}$ concludes the proof. \qed

### S1.4 Technical Results

**Lemma S5**

Let $x \in \mathbb{R}$ such that $x > 1$, then $\log \left(\frac{x+1}{x-1}\right) \geq \frac{2}{x}$. 

**Proof.** Substituting $y = \frac{x+1}{x-1} - 1$ in the known bound $\frac{\log(y+1)}{y} \geq \frac{2}{2+y}$, which holds for $y > -1$ gives the desired result. \qed

### S2 Krylov Subspace Methods

Krylov subspace methods are algorithms which rely on repeated matrix-vector multiplication with an $n \times n$ matrix $A$. For a starting vector $b \in \mathbb{R}^n$, they (implicitly) generate an expanding subspace called the Krylov subspace defined by

$$K_r(A, b) = \text{span}\{b, Ab, A^2b, \ldots, A^{r-1}b\}.$$ 

#### S2.1 Lanczos Algorithm

The Lanczos algorithm [10] is a Krylov subspace method, which for a symmetric matrix $A \in \mathbb{R}^{n \times n}$ iteratively builds an approximate tridiagonalization

$$A \approx \hat{Q} \hat{T} \hat{Q}^\top$$

where $\hat{Q} \in \mathbb{R}^{n \times r}$ orthonormal and $\hat{T} \in \mathbb{R}^{r \times r}$ tridiagonal. For an initial probe vector $b \in \mathbb{R}^n$, Gram-Schmidt orthogonalization is applied to the Krylov subspace basis. The orthogonalized vectors form $\hat{Q}$, while the Gram-Schmidt coefficients form $\hat{T}$. This low-rank approximation becomes an exact tridiagonalization $A = QTQ^\top$ for $r = n$. The Lanczos process is often used to compute (approximate) eigenvalues and eigenvectors, which is done by computing an eigendecomposition of the tridiagonal matrix $\hat{T}$ at cost $O(r^2)$.

The tridiagonal matrix $\hat{T}$ can also be formed by running the method of conjugate gradients on the linear system $Ax = b$ and by collecting the step lengths $\alpha_i$ and conjugacy corrections $\beta_i$ used in the solution and search direction updates [3, Section 6.7.3].

#### S2.2 Conjugate Gradient Method

The conjugate gradient method (CG) is an iterative method to solve linear systems

$$Ax = b$$

with symmetric positive definite system matrix $A \in \mathbb{R}^{n \times n}$ and right hand side $b \in \mathbb{R}^n$. It primarily relies on matrix-vector multiplication and has favorable convergence properties.

**Theorem S6** (Convergence Rate of Preconditioned CG [4])

Let $A \in \mathbb{R}^{n \times n}$ be symmetric positive definite with non-singular preconditioner $P = P^{\frac{1}{2}}(P^{\frac{1}{2}})^\top$. The error of the preconditioned conjugate gradient method after $k \in \mathbb{N}$ steps is given by

$$\|x_k - x\|_A \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^k \|x_0 - x\|_A$$

where $\kappa = \kappa(P^{-\frac{1}{2}}A(P^{-\frac{1}{2}})^\top)$ is the condition number of the preconditioned system matrix.
Proof. Preconditioned CG is equivalent to running CG on the transformed problem
\[ \tilde{A}\tilde{x} = P^{-\frac{1}{2}}A(P^{-\frac{1}{2}})^\top \tilde{x} = P^{-\frac{1}{2}}b \]
with the substitution \( \tilde{x} = (P^{\frac{1}{2}})^\top x \). By Nocedal and Wright [4], the convergence rate of CG on the problem is given by
\[ \| \tilde{x}_k - \tilde{x} \|_A \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \| \tilde{x}_0 - \tilde{x} \|_A \]
The result now follows by Lemma S5 with the choice \( \hat{x} \). This is a direct consequence of Theorem S6 and the Courant-Fischer-Weyl min-max principle, which asserts that
\[ \lambda_{\min}(A)\|x_k - x\|_2 \leq \|\tilde{x}_k - \hat{x}\|_A \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|x_0 - x\|_A \]
\[ \leq \lambda_{\max}(A) \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|x_0 - x\|_2. \]

Corollary S4
Let \( \varepsilon \in (0, 1) \), then (preconditioned) CG has relative error \( \|x_k - x\|_A \leq \varepsilon \|x_0 - x\|_A \) after
\[ k \leq \frac{\sqrt{\kappa}}{2} \log(2\varepsilon^{-1}) \]
iterations, where \( \kappa \) is the condition number of the (preconditioned) system matrix. In euclidean norm \( \|\cdot\|_2 \) relative error \( \varepsilon \) is achieved after \( k \leq \frac{\sqrt{\kappa}}{2} \log(2\sqrt{\kappa}\varepsilon^{-1}) \) iterations.

Proof. With Theorem S6 and \( \rho = \frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \) we obtain
\[ 2\rho^{-k} \leq \varepsilon \iff \rho^k \leq \frac{2}{\varepsilon} \iff k \log(\rho) \leq \log(2\varepsilon^{-1}) \]
The result now follows by Lemma S5 with the choice \( x = \sqrt{\kappa} \), giving \( k \log(\rho) \geq \frac{2k}{\sqrt{\kappa}}. \)

For \( \|\cdot\|_2 \), the same argument holds, except that the error bound is given by
\[ \lambda_{\min}(\tilde{A})\|x_k - x\|_2 \leq \|\tilde{x}_k - \hat{x}\|_A \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|x_0 - x\|_A \]
\[ \leq \lambda_{\max}(\tilde{A}) \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|x_0 - x\|_2. \]
This is a direct consequence of Theorem S6 and the Courant-Fischer-Weyl min-max principle, which asserts that
\[ \lambda_{\min}(M)\|z\|_2 \leq \|z\|_M \leq \lambda_{\max}(M)\|z\|_2 \]
for symmetric positive definite \( M \).

S2.3 Preconditioning

Pivoted Cholesky Decomposition The (incomplete) pivoted Cholesky decomposition [3, 38, 50, 51] is a (partial) matrix factorization of a symmetric positive semi-definite matrix
\[ A = LL^\top \approx L\ell L^\top \in \mathbb{R}^{n \times n}. \]
It can be computed recursively via the recursion relations
\[ L_{ii} = \left( A_{ii} - \sum_{k=1}^{i-1} L_{ik}^2 \right)^{\frac{1}{2}} \]
\[ L_{ji} = \frac{1}{L_{ii}} \left( A_{ji} - \sum_{k=1}^{i-1} L_{jk} L_{ik} \right)^{\frac{1}{2}} \]
where \( j \in \{i + 1, i + 2, \ldots, n\} \) and pivoting is used to ensure positivity of \( A_{ii} \). Sometimes it is desirable to preserve a certain sparsity pattern for memory efficiency (e.g. the sparsity pattern of \( A \) itself), which is done by simply setting the corresponding entries of \( L \) to zero. One can compute a low-rank approximation to \( A \) by stopping the Cholesky factorization early after computing \( \ell \) columns giving \( L\ell \), which has cost \( O(\ell^2 n) \). For matrices with fast-decaying spectra, this gives a good approximation after just a few iterations.
Proposition S4 (Harbrecht et al. [38])
Assume the eigenvalues of a positive definite matrix $A \in \mathbb{R}^{n \times n}$ satisfy $\lambda_i \leq \exp(-b)$ for some $b > \log(4)$, then the rank-$\ell$ pivoted Cholesky decomposition satisfies
\[
\|A - L_\ell L_\ell^\top\|_F \leq \text{tr}(A - L_\ell L_\ell^\top) \leq n \exp(-b\ell) \quad (S32)
\]

Proof. The assumption $\lambda_i \leq \exp(-b)$ is equivalent to $4^\ell \lambda_i \leq \exp(-b')$ for $b' > 0$. Applying Theorem 3.2 by Harbrecht et al. [38] results in $\text{tr}(A - L_\ell L_\ell^\top) \leq n \exp(-b\ell)$. Using $\|M\|_F \leq \text{tr}(M)$ for positive semi-definite $M$ we obtain the desired result.

Lemma 1 (Harbrecht et al. [38])
Let $k(x, y) = k(||x - y||)$ be a stationary kernel with associated kernel matrix $K \in \mathbb{R}^{n \times n}$ and output scale $\sigma^2 = k(0) > 0$. Assume the kernel matrix spectrum decays at least exponentially, i.e. $\lambda_i \leq \exp(-b)$ for some $b > \log(4)$. Then the rank-$\ell$ pivoted Cholesky decomposition satisfies
\[
\|K - L_\ell L_\ell^\top\|_F \leq \sqrt{n} \sigma^{-2} \exp(-b\ell) \|K\|_F. \quad (5)
\]

Proof. First note that since $k(\cdot, \cdot)$ is a positive definite kernel, the choice $\sigma^2 = k(0)$ is no restriction. By Proposition S4 it suffices to show that $n \leq \frac{\sqrt{n}}{o^2} \|K\|_F$. We have with $K_{ii} = \sigma^2$ that
\[
n = \sqrt{n} \left( \sum_{i=1}^{n} \frac{K_{ii}^2}{o^2} \right)^{\frac{1}{2}} \leq \frac{\sqrt{n}}{o^2} \left( \sum_{i,j=1}^{n} K_{ij}^2 \right)^{\frac{1}{2}} = \frac{\sqrt{n}}{o^2} \|K\|_F.
\]

S3 Stochastic Trace Estimation

Lemma S6
Let $A \in \mathbb{R}^{n \times n}$ and $g(\ell) \leq \ell^{-1/2}$ for $\ell \in \mathbb{N}$. There exists $c_H > 0$ such that if $\ell \geq c_H \log(\delta^{-1})$, then
\[
\mathbb{P}(|\tau_\ell(A) - \text{tr}(A)| \leq \sqrt{c_H \log(\delta^{-1})} g(\ell) \|A\|_F) \geq 1 - \delta.
\]

Proof. Consider $\ell$ independent, zero-mean random vectors $\tilde{z}_i \in \mathbb{R}^n$ such that $z_i = \tilde{z}_i/\|\tilde{z}_i\|_2$ has independent components. Define
\[
A' = \begin{pmatrix} A & 0 & \ldots & 0 \\
0 & A & \ddots & \\
\vdots & \ddots & \ddots & 0 \\
0 & \ldots & 0 & A \end{pmatrix} \in \mathbb{R}^{\ell n \times \ell n} \quad \text{and} \quad z' = \sqrt{n} \begin{pmatrix} z_1 \\
\vdots \\
z_{\ell} \end{pmatrix} \in \mathbb{R}^{\ell n}.
\]

Now since $z_i$ is bounded so is $z'$, which is therefore sub-Gaussian by Corollary S3. We assumed the $z_i$ to be independent and to have independent components and therefore the Hanson-Wright inequality (see Theorem S5) holds
\[
\mathbb{P}(|(z')^\top A' z' - \mathbb{E}[(z')^\top A' z']| > t) \leq 2 \exp \left( -c \cdot \min \left( \frac{t^2}{\|A'\|^2_2}, \frac{t}{\|A'\|_F} \right) \right). \quad (S33)
\]

Now, we have $(z')^\top A' z' = n \sum_{i=1}^{\ell} z_i^\top A z_i = \ell \tau_\ell(A)$ and
\[
\mathbb{E}[(z')^\top A' z'] = n \sum_{i=1}^{\ell} \mathbb{E}[z_i^\top A z_i] = \ell n \mathbb{E}[\text{tr}(z_i^\top A z_i)] = \ell n \mathbb{E}[\text{tr}(A z_i z_i^\top)]
\]
\[
= \ell n \mathbb{tr}(A \mathbb{E}[z_i z_i^\top]) = \ell n \mathbb{tr}(A n^{-1} \text{Cov}(\tilde{z})) = \ell \mathbb{tr}(A)
\]
as well as \( \|A\|_F = \ell \|A\|_F \) and \( \|A\|_2 = \|A\|_2 \). Therefore by setting \( t = \sqrt{\frac{\log(2\delta^{-1})}{c}} \sqrt{A} \|A\|_F \) and using \( g(\ell) \leq \ell^{-1/2} \), we obtain that

\[
P \left( |\tau_\ell(A) - \text{tr}(A)| > \sqrt{\frac{\log(2\delta^{-1})}{c}} g(\ell) \|A\|_F \right) \\
\leq 2 \exp \left( -c \cdot \min \left( \frac{\log(2\delta^{-1})}{c}, \frac{\log(2\delta^{-1})}{c} g(\ell) \frac{\|A\|_F}{\|A\|_2} \right) \right) \\
\leq 2 \exp \left( - \min \left( \frac{\log(2\delta^{-1})}{c}, \sqrt{c} \log(2\delta^{-1}) \frac{\|A\|_F}{\|A\|_2} \right) \right)
\]

Now assume \( \ell \geq \frac{1}{c} \log(2\delta^{-1}) \). Then since \( \|A\|_2 \leq \|A\|_F \), the minimum is given by

\[
\min \left( \frac{\log(2\delta^{-1})}{c}, \sqrt{c} \log(2\delta^{-1}) \frac{\|A\|_F}{\|A\|_2} \right) = \log(2\delta^{-1}).
\]

Further setting \( c_H = 2c^{-1} \), it holds that \( \ell \geq c_H \log(\delta^{-1}) = 2 \log(\delta^{-1}) c^{-1} \geq \log(2\delta^{-1}) c^{-1} \) since \( 0 < \delta \leq \frac{1}{2} \). Combining the above we obtain

\[
P \left( |\tau_\ell(A) - \text{tr}(A)| > \sqrt{c_H \log(\delta^{-1})} g(\ell) \|A\|_F \right) \\
\leq 2 \exp(- \log(2\delta^{-1})) = \delta
\]

This proves the statement. \( \square \)

**Theorem 1** (Error Bound for Hutchinson’s Estimator [13–16])

If the number of random vectors for Hutchinson’s estimator (3) satisfies \( \ell \geq c_H \varepsilon^{-2} \log(\delta^{-1}) \), then

\[
P(|\tau(A) - \text{tr}(A)| \leq \varepsilon \|A\|_F) \geq 1 - \delta.
\]

**Proof.** Let \( c_H > 0 \) such that \( \ell \geq c_H \varepsilon^{-2} \log(\delta^{-1}) \). Since \( \varepsilon \leq 1 \), it holds that \( \ell \geq c_H \log(\delta^{-1}) \). Therefore choosing \( g(\ell) = \ell^{-1/2} \) in Lemma S6, we have with probability \( 1 - \delta \), that

\[
|\tau_\ell(A) - \text{tr}(A)| \leq \sqrt{c_H \log(\delta^{-1}) \ell^{-1}} \|A\|_F \leq \varepsilon \|A\|_F.
\]

Now, if \( A \) is positive semi-definite, then \( \|A\|_F \leq \text{tr}(A) \). This proves the statement. \( \square \)

**Theorem 2** (Variance-reduced Stochastic Trace Estimation)

Let \( A, \Delta \in \mathbb{R}^{n \times n} \). Assume \( \text{tr}(A) = \text{tr}(A) + \text{tr}(\Delta) \) and assume there exists \( c_\Delta > 0 \) and strictly monotonic \( g : [0, \infty) \to [0, \infty) \) with \( g(\ell) \leq \ell^{-1/2} \), such that

\[
\|\Delta\|_F \leq c_\Delta g(\ell) \|A\|_F. \tag{9}
\]

If we use

\[
\ell \geq \max \left( g^{-1} \left( \varepsilon \sqrt{c_\Delta \log(\delta^{-1})} \right)^{\frac{1}{2}}, \frac{1}{c_H \log(\delta^{-1})} \right) \tag{10}
\]

random vectors, it holds for \( \tau = \text{tr}(\hat{A}) + \tau_\ell(\Delta) \), that \( P(|\tau - \text{tr}(A)| \leq \varepsilon \|A\|_F) \geq 1 - \delta \).

**Proof.** By assumption \(|\tau - \text{tr}(A)| = |\tau_\ell(\Delta) - \text{tr}(\Delta)| \). By Lemma S6 it holds with probability \( \geq 1 - \delta \), that

\[
|\tau_\ell(\Delta) - \text{tr}(\Delta)| \leq \sqrt{c_H \log(\delta^{-1})} g(\ell) \|\Delta\|_F \\
\leq \sqrt{c_H \log(\delta^{-1})} c_\Delta g(\ell)^2 \|A\|_F \\
\leq \sqrt{c_H \log(\delta^{-1})} c_\Delta \frac{\varepsilon}{c_\Delta \sqrt{c_H \log(\delta^{-1})}} \frac{\varepsilon \|A\|_F}{\|A\|_2} \text{ Bound in (10) and } g(\ell) \text{ monotonic.} \\
\leq \varepsilon \|A\|_F \text{ If } A \text{ positive semi-definite.}
\]

This concludes the proof. \( \square \)
S4 Lanczos Quadrature

For an eigendecomposition of \( K = V \Lambda V^T \) it holds that \( f(K) = V f(\Lambda) V^T \). Using this fact, one can formulate the quadratic terms arising in Hutchinson’s estimator for \( f(K) \) as an integral

\[
z^T f(K) z = z^T V f(\Lambda) V^T z = \sum_{i=1}^{n} f(\lambda_i) \mu_i^2 = \int_{\lambda_1}^{\lambda_n} f(t) \, d\mu(t) \tag{S34}
\]

where \( \mu_i = (V^T z)_i \) and the measure \( \mu \) is defined by

\[
\mu(t) = \begin{cases} 
0 & t < \lambda_1 \\
\sum_{j=1}^{i-1} \mu_j^2 & \lambda_{i-1} \leq t \leq \lambda_i \\
\sum_{j=1}^{n} \mu_j^2 & t \geq \lambda_n
\end{cases}
\tag{S35}
\]

This integral can be efficiently approximated using Lanczos quadrature [17]

\[
\int_{\lambda_1}^{\lambda_n} f(t) \, d\mu(t) \approx \sum_{j=0}^{k} \omega_j f(\theta_j) =: I_k.
\]

For a starting vector \( z \), Lanczos generates an orthonormal basis \( Q_k \) for the Krylov subspace \( \mathcal{K}_k(A, z) \), such that \( Q_k^T A Q_k = T_k \in \mathbb{R}^{k \times k} \) is tridiagonal. Now the associated Lanczos polynomials \( p_j \), recursively defined via columns \( u_j = p_{j-1}(A) u_0 \) of \( Q_k \), are orthogonal with respect to \( \mu \) [17]. The eigenvalues of \( T_k \) define the nodes \( \theta_j \) and the squared first elements of the normalized eigenvectors of \( T_k \) define the weights \( \omega_j \) of Lanczos quadrature.

We want to establish an error bound for the stochastic trace estimator

\[
\tau_{\ell,k} = \frac{n}{\ell} \sum_{i=1}^{\ell} f^{(i)}(k) \approx \tau_{\ell}(f(K)) \approx \text{tr}(f(K)) \tag{S36}
\]

which combines a variance-reduced Hutchinson’s estimator with Lanczos quadrature. In order to do so, we recall a result by Ubaru et al. [18] on the error of Lanczos quadrature.

Definition S3 (Bernstein Ellipse)
Let \( \rho > 1 \) and \( C(0, \rho) \subset \mathbb{C} \) be the circle with radius \( \rho \) in the complex plane. We call

\[
E_\rho = \left\{ \frac{1}{2} (z + z^{-1}) \mid z \in C(0, \rho) \right\}
\]

a Bernstein ellipse with focii \( -1, 1 \) and major semiaxis \( \frac{1}{2} (\rho + \rho^{-1}) \).

Lemma S7 (Lemma 4.4 of Ubaru et al. [18])
Let \( A \in \mathbb{R}^{n\times n} \) be symmetric positive definite with condition number \( \kappa = \lambda_{\text{max}}/\lambda_{\text{min}} \) and let \( f \) be an analytic function in \( [\lambda_{\text{min}}, \lambda_{\text{max}}] \) and analytically continuable inside a Bernstein ellipse \( E_\rho \) encompassing the interval such that \( |f(z)| \leq M_\rho \) for all \( z \in \mathbb{C} \) inside \( E_\rho \). Then it holds for \( \tau_{\ell,k} \) as in (S36) that

\[
|\tau_{\ell}(f(A)) - \tau_{\ell,k}(f(A))| \leq \frac{nC_\rho}{\rho^{2k}} \tag{S37}
\]

where \( \rho = \frac{\sqrt{2}+1}{\sqrt{\kappa}-1} > 1 \) and \( C_\rho = 2M_\rho \frac{\lambda_{\text{max}}-\lambda_{\text{min}}}{\rho^{2k-1}} = (\lambda_{\text{max}} - \lambda_{\text{min}})(\sqrt{\kappa} - 1)^2 M_\rho/2\sqrt{\kappa} \).

Lemma S7 is only applicable to functions \( f \) which are uniformly bounded inside the choice of Bernstein ellipse. This is not generally the case for the logarithm. However, we can obtain a similar error bound with a different choice of ellipse.

Corollary S5 (Section 4.3 of Ubaru et al. [18])
Let \( A \in \mathbb{R}^{n\times n} \) be symmetric positive definite with condition number \( \kappa \). Then it holds that

\[
|\tau_{\ell}(\log(A)) - \tau_{\ell,k}(\log(A))| \leq \frac{C_\rho}{\rho^{2k}} \tag{S38}
\]

where \( \rho = \frac{\sqrt{2\kappa+1}}{\sqrt{2\kappa-1}-1} > 1 \) and \( C_\rho = \frac{5\kappa \log(2\kappa+1)}{2\sqrt{2\kappa+1}} \).

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S5  Main Theoretical Results and Proofs

S5.1  General Error Bound using Preconditioning

Theorem S7
Let $K \in \mathbb{R}^{n \times n}$ be symmetric positive definite and $P \in \mathbb{R}^{n \times n}$ a positive definite preconditioner, such that $B = P^{-1}K$ is symmetric positive definite and has eigenvalues in $\lambda = [\lambda_{\min}, \lambda_{\max}]$. Let $f$ be an analytic function in $J$ and be either positive or negative (i.e. does not cross zero). Assume that $f$ is analytically continuable inside a Bernstein ellipse $E_\rho$, with $\rho = (\sqrt{\kappa(B)} + 1) / (\sqrt{\kappa(B)} - 1)$, such that $|f(z)| \leq M_\rho$ for all $z \in \mathbb{C}$ inside $E_\rho$ and let $m_f = \min_{z \in J} |f(z)|$. Now assume that

\[ tr(f(K)) = tr(f(B)) + tr(f(B)), \quad \|f(B)\|_F \leq c_\Delta \ell^{-\frac{1}{2}} \|f(K)\|_F, \quad \|f(B)\|_F \leq c_\Delta \ell^{-\frac{1}{2}} \|f(K)\|_F. \quad (S39) \]

There exists a constant $c' = \sqrt{2\pi}\epsilon_\Delta > 0$ such that if

\[ \ell \geq 2c' \epsilon^{-1} \sqrt{\log(\delta^{-1})} \text{ random vectors}, \quad k \geq \frac{1}{4} \sqrt{\kappa(B)} \log(K \epsilon^{-1}) \text{ number of Lanczos steps}, \quad (S41) \]

where $K = \sqrt{n} (\lambda_{\max} - \lambda_{\min}) (\sqrt{\kappa(B)} - 1)^2 M_\rho / m_f$. It holds for $\tau = tr(f(B)) + \tau_{\ell,k}(f(B))$, that

\[ \mathbb{P} \left[ \left| \tau - tr(f(K)) \right| \leq \epsilon \|f(K)\|_F \right] \geq 1 - \delta. \]

Proof. Let $\kappa = \kappa(B)$. It holds for the number of Lanczos steps $k$ (S42) that

\[ \log(K \epsilon^{-1}) \leq \frac{4k}{\sqrt{\kappa}} \leq 2k \log \left( \frac{\sqrt{n} + 1}{\sqrt{n} - 1} \right) \quad \text{Lemma S5 with the choice } x = \sqrt{n}. \]

\[ = \log(\rho^{2k}) \]

Therefore $K \epsilon^{-1} \leq \rho^{2k}$. Now, we have by Lemma S7 that

\[ \left| \tau_{\ell}(f(B)) - \tau_{\ell,k}(f(B)) \right| \leq \frac{nC_\rho \epsilon}{\rho^{2k}} \leq \frac{nC_\rho \epsilon}{K} \frac{\sqrt{n} \epsilon \sqrt{\ell}}{2c_\Delta m_f} \leq \frac{\epsilon \sqrt{\ell}}{2c_\Delta} \min_{i} \lambda_i(f(B))) \leq \frac{\epsilon \sqrt{\ell}}{2c_\Delta} \|f(B)\|_F. \quad (S43) \]

where we made use of the fact that $B$ symmetric positive definite and therefore $\lambda(f(B)) = \{f(\lambda_1), \ldots, f(\lambda_n)\}$.

Now by assumption (S39), we obtain

\[ \left| \tau - tr(f(K)) \right| = \left| tr(f(B)) - \tau_{\ell,k}(f(B)) \right| \leq \left| tr(f(B)) - \tau_{\ell}(f(B)) \right| + \left| \tau_{\ell}(f(B)) - \tau_{\ell,k}(f(B)) \right| \]

By Theorem 2 and (S43), we have with probability $\geq 1 - \delta$, that

\[ \leq \frac{\epsilon}{2} \|f(K)\|_F + \frac{\epsilon \sqrt{\ell}}{2c_\Delta} \|f(B)\|_F, \quad \leq \frac{\epsilon}{2} \|f(K)\|_F + \frac{\epsilon \sqrt{\ell}}{2c_\Delta} \|f(B)\|_F, \quad \leq \frac{\epsilon}{2} \|f(K)\|_F \]

Assumption (S40).

This concludes the proof. \qed
S5.2 Approximation of the Log-Determinant

Lemma S8
Let \( K, P \in \mathbb{R}^{n \times n} \) be positive definite and define \( \Delta \in \mathbb{R}^{n \times n} \) such that
\[
\text{tr}(\Delta) = \text{tr}(\log(K) - \log(P)) \quad \text{or equivalently} \quad \text{tr}(\Delta) = \text{tr}\left(\left(P^{-\frac{1}{2}}\right)KP^{-\frac{1}{2}}\right) \tag{S44}
\]
where \( P^{\frac{1}{2}} \) is \( P \)'s principal square root. Then it holds that
\[
\log(\text{det}(K)) = \text{tr}(\log(K)) \tag{S45}
\]
\[
= \log(\text{det}(P)) + \text{tr}(\Delta) \tag{S46}
\]
\[
= \text{tr}(\log(P)) + \text{tr}(\Delta) \tag{S47}
\]
If additionally \( P \) and \( K \) commute or \( P^{-1}K \) is positive definite, then
\[
\text{tr}(\Delta) = \text{tr}(\log(P^{-1}K)). \tag{S48}
\]

Proof. We begin by proving equivalence in (S44). Since \( P \) is positive definite so is \( P^{-1} \), which therefore has unique positive definite square root \( P^{-\frac{1}{2}} \). It holds that
\[
\text{tr}(\Delta) = \text{tr}(\log(K) - \log(P)) = \text{tr}\left(\left(P^{-\frac{1}{2}}\right)KP^{-\frac{1}{2}}\right) \text{ P square.}
\]

now, we have
\[
\text{tr}(\log(K)) = \log(\text{det}(K)) \rightarrow \text{K positive definite.}
\]
\[
\text{tr}(\log(P)) + \text{tr}(\Delta) \text{ K, P square matrices.}
\]
\[
\text{tr}(\log(P)) + \text{tr}(\log(P^{-1})) + \text{tr}(\log(K)) \rightarrow \text{K, P positive definite.}
\]
Finally, if \( K \) and \( P^{-1} \) commute, then
\[
\Delta = \log(P^{-1}) + \log(K) = \log(P^{-1}K).
\]
If instead \( P^{-1}K \) is positive definite, then
\[
\text{tr}(\Delta) = \log(\text{det}(P^{-1}K)) = \text{tr}(\log(P^{-1}K)).
\]
This concludes the proof. \( \square \)

Theorem 3 (Error Bound for the Log-Determinant)
Let \( A = \log(K) \) and \( \Delta = \log(P^{-1}K) \) and assume we choose the number of random vectors \( \ell \) according to Theorem 2. If the number of Lanczos steps
\[
k \geq \frac{\sqrt{2\kappa + 1} + 1}{\sqrt{2\kappa + 1}} \sqrt{\log(K_1 \varepsilon^{-1})}, \tag{11}
\]
with \( K_1 = \frac{5\kappa \log(2(\kappa + 1))}{\max_i \log(\lambda_i(K))} \sqrt{2\kappa + 1} \) and \( \kappa = \kappa(P^{-1}K) \), then for \( \tau = \log(\text{det}(P)) + \gamma_{l,k}(\Delta) \),
\[
\mathbb{P}(|\tau - \log(\text{det}(K))| \leq \varepsilon \log(K_1)) \geq 1 - \delta.
\]

Proof. Define \( \rho = \frac{\sqrt{2\kappa + 1} + 1}{\sqrt{2\kappa + 1}} \). We have by (11), that
\[
\log(K_1 \varepsilon^{-1}) \leq \frac{4k}{\sqrt{3\kappa}} \leq \frac{4k}{\sqrt{2\kappa + 1}} \quad \kappa \geq 1
\]
\[
\leq 2k \log(\rho) \quad \text{Lemma S5 with the choice } x = \sqrt{2\kappa + 1}
\]
\[
= \log(\rho^{2k})
\]
23
Using Corollary S5 and recognizing that \( C_{\rho} = \frac{\max_i |\log(\lambda_i(K))|}{2} K_1 \), we obtain

\[
|\tau_{\ell}(\Delta) - \tau_{\ell,k}(\Delta)| \leq \frac{C_{\rho}^2}{\rho2K} \leq \frac{C_{\rho}^2}{K_1} = \frac{\max_i |\log(\lambda_i(K))|}{2} \varepsilon
\]  
(S49)

And therefore, by Lemma S8, we have

\[
|\tau - \log(\det(K))| = |\tau_{\ell}(\Delta) - \tau_{\ell,k}(\Delta)|
\leq |\tau_{\ell}(\Delta)| + |\tau_{\ell,k}(\Delta)|
\]

By using Theorem 2 and eq. (S49), we have with probability \( \geq 1 - \delta \), that

\[
\leq \frac{\varepsilon}{2} \|\log(K)\|_F + \frac{\varepsilon}{2} \max_i |\log(\lambda_i(K))| + \varepsilon \|\log(K)\|_F
\]

This concludes the proof.

\[\square\]

S5.3 Approximation of the Log-Marginal Likelihood

**Corollary 1** (Error Bound for the log-Marginal Likelihood)

Assume the conditions of Theorem 3 hold with \( K_1 = \frac{K}{2} \) and we solve \( Ku = y \) via preconditioned CG initialized at \( u_0 \) and terminated after

\[
k' \geq \frac{1}{2} \sqrt{n} \log(K_2 \varepsilon^{-1})
\]  
(12)

iterations, where \( K_2 = \sqrt{n} \|y\|_2 \|u_0 - u\|_2 \). Then for \( \eta = -\frac{1}{2}(y^T u_{k'} + \tau + n \log(2\pi)), \)

\[
\mathbb{P} \left( |\eta - \log p(y \mid X, \theta)| \leq \varepsilon(1 + \|\log(K)\|_F) \right) \geq 1 - \delta.
\]

**Proof.** It holds that

\[
|y^T u_{k'} - y^T u| \leq \|y\|_2 \|u_{k'} - u\|_2
\]

\[
\leq \|y\|_2 2\sqrt{n} \varepsilon \|u_0 - u\|_2
\]

CG convergence Corollary S4.

\[
= 2\varepsilon
\]

It holds by assumption that

\[
|\eta - \log p(y \mid X, \theta)| = \frac{1}{2} |y^T u_{k'} - y^T u + \tau - \log(\det(K))|
\]

\[
\leq \frac{1}{2} \left( |y^T u_{k'} - y^T u| + |\tau - \log(\det(K))| \right)
\]

\[
\leq \frac{1}{2} (2\varepsilon + |\tau - \log(\det(K))|)
\]

Now applying Theorem 3 we have with probability \( 1 - \delta \) that

\[
\leq \frac{1}{2} \varepsilon (2 + 2\|\log(K)\|_F) = \varepsilon (1 + \|\log(K)\|_F)
\]

This proves the statement.

\[\square\]

S5.4 Approximation of the Derivative

**Computation of** \( \text{tr}(P^{-1} \frac{\partial P}{\partial \theta}) \)

Algorithm 1 and Algorithm 2 primarily rely on matrix-vector multiplication, except for computation of \( \tau_0 = \text{tr}(P^{-1} \frac{\partial P}{\partial \theta}) \). Efficient computation of this term depends on the structure of \( P^{-1} \). If \( P \) is the pivoted-Cholesky preconditioner, or any other low-rank-plus-diagonal preconditioner \( L_\ell L_\ell^\top + \sigma^2 I \), we can rewrite this term using the matrix inversion lemma

\[
\text{tr} \left( P^{-1} \frac{\partial P}{\partial \theta} \right) = \sigma^{-2} \text{tr} \left( \frac{\partial P}{\partial \theta} \right) - \sigma^{-2} \text{tr} \left( L_\ell \left( \sigma^2 I + L_\ell^\top L_\ell \right)^{-1} L_\ell^\top \frac{\partial P}{\partial \theta} \right)
\]

\[
= \sigma^{-2} \sum_{i=1}^n \frac{\partial P_{ii}}{\partial \theta} - \sigma^{-2} \left( L_\ell \left( \sigma^2 I + L_\ell^\top L_\ell \right)^{-1} \circ \left( \frac{\partial P}{\partial \theta} L_\ell \right) \right) 1,
\]  
(S50)
where $\circ$ denotes elementwise multiplication. The second term requires $\ell$ matrix-vector multiplies with $\partial P / \partial \theta$ and $O(n\ell^2)$ additional work. The first term is simply the derivative of the kernel diagonal which will take $O(n)$ time. We note that similar efficient procedures exists for other types of preconditioners, such as when $P^{-1}$ has banded structure.

**Proposition S5** (Error Bound for the Trace of the Inverse)

Let $A = K^{-1} \frac{\partial K}{\partial \theta}$ and $\Delta = K^{-1} \frac{\partial K}{\partial \theta} - P^{-1} \frac{\partial P}{\partial \theta}$ and assume we choose the number of random vectors $\ell$ as in Theorem 2. If we use CG initialized at 0 or better to solve $K^{-1} \frac{\partial K}{\partial \theta}$ with

$$k \geq \frac{1}{2} \sqrt{\kappa} \log(2\sqrt{\kappa}n\varepsilon^{-1})$$

(iterations, where $\kappa = \kappa(P^{-1}K)$, then for $\tau = \text{tr}(P^{-1} \frac{\partial P}{\partial \theta} + \tau_{\ell,k}(\Delta))$, it holds that

$$P \left( |\tau - \text{tr}(K^{-1} \frac{\partial K}{\partial \theta})| \leq 2\varepsilon \|K^{-1} \frac{\partial K}{\partial \theta}\|_F \right) \geq 1 - \delta$$

**Proof.** By assumption it holds that

$$|\tau - \text{tr}(K^{-1} \frac{\partial K}{\partial \theta})| = |\tau - \text{tr}(P^{-1} \frac{\partial P}{\partial \theta} + \Delta)|$$

Definition of $\Delta$.

$$|\tau_{\ell,k}(\Delta) - \text{tr}(\Delta)| \leq |\tau_{\ell,k}(\Delta) - \text{tr}(\Delta) - \tau_{\ell,k}(\Delta)|$$

The first term is bounded with probability $1 - \delta$ by Theorem 2. Therefore

$$|\tau_{\ell}(\Delta) - \text{tr}(\Delta)| \leq \text{tr}(P^{-1} \frac{\partial P}{\partial \theta} + \tau_{\ell}(\Delta)) - \text{tr}(K^{-1} \frac{\partial K}{\partial \theta}) \leq \varepsilon \|K^{-1} \frac{\partial K}{\partial \theta}\|_F.$$  

Now for the second term. Let $w_{k,i}$ be the solution computed by preconditioned CG of the linear system $Kw = \frac{\partial K}{\partial \theta}z_i$ with preconditioner $P^{-1}$. Let $\hat{w}_i = P^{-1} \frac{\partial P}{\partial \theta}z_i$, then

$$|\tau_{\ell,k}(\Delta) - \tau_{\ell}(\Delta)| = \left| \sum_{i=1}^{\ell} \left( w_{k,i} - \hat{w}_i - (w_i - \hat{w}_i) \right) \right|$$

$\hat{w}_i$ computed with negligible error.

$$\leq \frac{\varepsilon}{n} \sum_{i=1}^{\ell} \|w_{0,i} - w_i\|_2$$

CG convergence Corollary S4 with $\varepsilon' = \frac{\varepsilon}{n}$.

$$\leq \frac{\varepsilon}{\ell} \sum_{i=1}^{\ell} \|w_i\|_2$$

CG initialized at 0 or better.

Now combining the two bounds we obtain with probability $1 - \delta$

$$|\tau - \text{tr}(K^{-1} \frac{\partial K}{\partial \theta})| \leq |\tau_{\ell}(\Delta) - \text{tr}(\Delta)| + |\tau_{\ell,k}(\Delta) - \tau_{\ell}(\Delta)| \leq 2\varepsilon \|K^{-1} \frac{\partial K}{\partial \theta}\|_F.$$  

**Theorem 4** (Error Bound for the Derivative)

Let $A = K^{-1} \frac{\partial K}{\partial \theta}$ and $\Delta = K^{-1} \frac{\partial K}{\partial \theta} - P^{-1} \frac{\partial P}{\partial \theta}$ and assume we choose the number of random vectors $\ell$ as in Theorem 2. If we use CG initialized at 0 or better to solve $K^{-1} \frac{\partial K}{\partial \theta}$ and $Ku = y$ with

$$k \geq \frac{1}{2} \sqrt{\kappa} \log(2\sqrt{\kappa}n\varepsilon^{-1}), \quad k' \geq \frac{1}{2} \sqrt{\kappa} \log(K_4\varepsilon^{-1})$$

(14)
We provide some additional experimental results and ablation experiments in this section. All
it holds for \( \phi = \frac{1}{2}(u_k^t \frac{\partial K}{\partial \theta} u_k - \tau) \) that
\[
P \left( |\phi - \frac{\theta}{\tau} \log p(y \mid X, \theta)| \leq \varepsilon (1 + \|K^{-1} \frac{\partial K}{\partial \theta}\|_F) \right) \geq 1 - \delta.
\]

**Proof.** Define \( z(t) = \max(t, t^2) \). We have
\[
\left| u^t \frac{\partial K}{\partial \theta} u - u_k^t \frac{\partial K}{\partial \theta} u_k \right| = \left| \|u_k' - u + u_k'\|_2^2 - \|u_k'\|_2^2 \right|
\leq \left( \|u_k' - u\|_2^2 + \|u_k'\|_2^2 \right) - \|u_k'\|_2^2
\leq \left( \|u_k' - u\|_2^2 + 2\|u_k' - u\|_2 \right)
\leq \left( \|u_k' - u\|_2 \right)(1 + 2\|u_k\|_2).
\]

Applying Corollary S4 and using monotonicity of \( z \) as well as \( \frac{2}{\kappa_4} < 1 \) we obtain
\[
z(\|u_k' - u\|_2) \leq z(\sqrt{\kappa} \frac{2}{\kappa_4} \|u_0 - u\|_2 \varepsilon) \leq \frac{4\kappa}{\kappa_4} z(\|u_0 - u\|_2 \varepsilon).
\]

Assuming initialization of CG at \( u_0 = 0 \) or better, we obtain
\[
\|u_0 - u\|_2 \leq \|u\|_2 = \|K^{-1} y\|_2 \leq \|K^{-1}\|_2 \|y\|_2 = \sqrt{\lambda_{\min}(K)} \|y\|_2
\]
Plugging this back into the above and using the definition of \( K_4 \) we have
\[
\left| u^t \frac{\partial K}{\partial \theta} u - u_k^t \frac{\partial K}{\partial \theta} u_k \right| \leq \frac{4\kappa}{\kappa_4} \left( 1 + 2\|u\|_2 \right) z(\|u_0 - u\|_2 \varepsilon)
\leq \frac{12\kappa}{\kappa_4} \left( 1 + 2\sqrt{\lambda_{\min}(K)} \|y\|_2 \right) z(\sqrt{\lambda_{\min}(K)} \|y\|_2 \varepsilon)
\leq 2\varepsilon
\]
where we made use of the fact that \((1 + 2\alpha) \max(\alpha, \alpha^2) \leq 3 \max(\alpha, \alpha^3) = 3h(\alpha)\). Now, we have
with the definition of \( \phi \) that
\[
\left| \phi - \frac{\partial}{\partial \theta} \log p(y \mid X, \theta) \right| \leq \frac{1}{2} \left| u^t \frac{\partial K}{\partial \theta} u - u_k^t \frac{\partial K}{\partial \theta} u_k \right| + \frac{1}{2} \tau - \text{tr} \left( K^{-1} \frac{\partial K}{\partial \theta} \right)
\leq \varepsilon + \frac{1}{2} \tau - \text{tr} \left( K^{-1} \frac{\partial K}{\partial \theta} \right)
\]
Using Proposition S5 we have with probability \( 1 - \delta \) that
\[
\leq \varepsilon + \frac{1}{2} \|K^{-1} \frac{\partial K}{\partial \theta}\|_F
\]
This proves the statement.

**S6 Additional Experimental Results**

We provide some additional experimental results and ablation experiments in this section. All experiments were performed as described in Section 4.
Table S1: Bias and variance reduction for different kernels. Bias and variance of the stochastic estimators for the log-marginal likelihood and its derivative(s) computed for synthetic data \((n = 10,000, \sigma^2 = 10^{-2})\) with 25 repetitions.

| Kernel          | d | Prec. | MLL Bias | Var. | \(\partial/\partial o\) Bias | Var. | \(\partial/\partial \ell\) Bias | Var. | \(\partial/\partial \sigma\) Bias | Var. |
|-----------------|---|--------|----------|------|--------------------------|------|-------------------------------|------|---------------------------------|------|
| Matérn\((3/2)\) | 1 | 0      | 3e-4     | 3e-8 | 9e-4                     | 1e-9 | 2e-3                          | 8e-9 | 2e-3                            | 2e-9 |
|                 | 128 |        | 9e-6     | 4e-11| 4e-6                     | 8e-12| 1e-5                          | 7e-11| 7e-6                            | 2e-11|
|                 | 2 | 0      | 3e-1     | 3e-3 | 4e-1                     | 4e-3 | 1                             | 3e-2 | 9e-1                            | 3e-2 |
|                 | 128 |        | 3e-4     | 5e-8 | 7e-5                     | 3e-9 | 2e-4                          | 3e-8 | 1e-4                            | 7e-9 |
|                 | 3 | 0      | 3e-1     | 6e-4 | 4e-1                     | 7e-4 | 1                             | 6e-3 | 8e-1                            | 4e-3 |
|                 | 128 |        | 7e-3     | 7e-7 | 2e-2                     | 3e-8 | 5e-2                          | 4e-7 | 3e-2                            | 8e-8 |
| RBF             | 1 | 0      | 1e-4     | 1e-8 | 1e-5                     | 4e-11| 1e-4                          | 3e-9 | 2e-5                            | 1e-10|
|                 | 128 |        | 5e-8     | 1e-15| 3e-8                     | 4e-16| 7e-7                          | 2e-13| 4e-8                            | 1e-15|
|                 | 2 | 0      | 3e-3     | 7e-8 | 5e-3                     | 2e-9 | 8e-2                          | 1e-7 | 1e-2                            | 2e-9 |
|                 | 128 |        | 1e-6     | 1e-12| 5e-7                     | 2e-13| 1e-5                          | 1e-10| 8e-7                            | 5e-13|
|                 | 3 | 0      | 1e-1     | 2e-7 | 2e-1                     | 4e-8 | 2                             | 9e-7 | 4e-1                            | 8e-9 |
|                 | 128 |        | 3e-4     | 5e-8 | 5e-5                     | 2e-9 | 7e-4                          | 3e-7 | 8e-5                            | 4e-9 |
| RatQuad         | 1 | 0      | 1e-4     | 1e-8 | 1e-5                     | 1e-10| 1e-4                          | 5e-9 | 2e-5                            | 3e-10|
|                 | 128 |        | 3e-7     | 6e-14| 2e-7                     | 2e-14| 2e-6                          | 4e-12| 2e-7                            | 4e-14|
|                 | 2 | 0      | 3e-2     | 2e-7 | 4e-2                     | 3e-8 | 3e-1                          | 2e-1 | 1e-1                            | 7e-9 |
|                 | 128 |        | 8e-5     | 3e-9 | 2e-5                     | 2e-10| 2e-4                          | 1e-8 | 3e-5                            | 5e-10|
|                 | 3 | 0      | 2e-1     | 2e-4 | 3e-1                     | 3e-4 | 2                             | 1e-2 | 8e-1                            | 2e-3 |
|                 | 128 |        | 4e-4     | 1e-7 | 2e-4                     | 1e-8 | 4e-3                          | 4e-7 | 4e-4                            | 4e-8 |

S6.1 Synthetic Data

We report bias and variance of the stochastic estimators for the log-marginal likelihood and its derivatives for the exponentiated quadratic, Matérn\((\frac{3}{2})\) and rational quadratic kernel on a synthetic dataset of size \(n = 10,000\) with varying dimensionality \(d \in \{1, 2, 3\}\) in Table S1. Using \(\ell = 128\) random samples with a preconditioner of the same size bias and variance are reduced by several orders of magnitude across different kernels. Note, that the variance reduction tends to decline with dimensionality, even though this is not necessarily universal across kernels. We show the bias and variance reduction for increasing number of random samples, respectively preconditioner size in Figure S1.

S6.2 UCI Datasets

For the experiments we conducted on UCI datasets, we report the full experimental results with their deviation across 10 runs in Table S3. Test errors with and without preconditioning did not differ by more than two standard deviations. However, model evaluations of the optimizer were significantly reduced when using a preconditioner of size 500, leading to substantial speedup. Note, that the experiment on the “3DRoad” dataset was only carried out once due to the prohibitive runtime without preconditioning.

We used the L-BFGS optimizer in our experiments due to its favorable convergence properties. As an ablation experiment we compared to the Adam optimizer as sometimes used for its robustness to noise, when using stochastic approximations of the log-marginal likelihood \([6, 7]\). We find that with preconditioning optimization with L-BFGS significantly outperformed optimization with Adam, both in terms of training and test error, except for the “KEGGdir” dataset (cf. Table 3 and Table S2). Additionally, L-BFGS converged faster across all experiments. This shows that variance reduction via preconditioning makes the use of second-order optimizers not only possible, but preferred for GP hyperparameter optimization when using stochastic approximations.
Figure S1: Bias and variance decrease on synthetic datasets for different kernels. Relative error and variance of the stochastic estimators of the log-marginal likelihood and its derivative for increasing number of random vectors, equivalently preconditioner size. Hyperparameter optimization was performed for different kernels on a synthetic dataset of size \( n = 10,000 \) with dimension \( d \in \{1, 2, 3\} \). Plots show mean and 95% confidence intervals for the relative error computed over 25 repetitions.
Table S2: Hyperparameter optimization using Adam. GP regression using a Matérn($\frac{3}{2}$) kernel and incomplete Cholesky preconditioner of size 500 with $\ell = 50$ random samples. Hyperparameters were optimized with Adam for at most 20 steps using early stopping via a validation set.

| Dataset | $n$  | $d$  | Prec. Size | $-\text{MLL}_{\text{train}}$ | $-\text{MLL}_{\text{test}}$ | RMSE | Runtime (s) |
|---------|-----|-----|------------|-----------------------------|-----------------------------|------|-------------|
| Elevators | 12,449 | 18 | 500 | 0.4803 | 0.4593 | 0.3684 | 109 |
| Bike    | 13,034 | 17 | 500 | 0.2265 | 0.3473 | 0.2300 | 64  |
| Kin40k  | 30,000 | 8  | 500 | 0.4392 | -0.1200 | 0.0982 | 159 |
| Protein | 34,297 | 9  | 500 | 0.9438 | 0.9319 | 0.5681 | 92  |
| KEGGdir | 36,620 | 20 | 500 | -1.0070 | -1.0390 | 0.0810 | 239 |
Table S3: Hyperparameter optimization on UCI datasets. GP regression using a Matérn($\frac{3}{2}$) kernel and incomplete Cholesky preconditioner of size 500 with $\ell = 50$ random samples. Hyperparameters were optimized with L-BFGS for at most 20 steps using early stopping via a validation set. All results, but "3DRoad", are averaged over 10 runs.

| Dataset   | n    | d    | Prec. | Size | Optim. Steps | Model evals. | Runtime (s) | Speedup | -MLL$_{\text{train}}$ | -MLL$_{\text{test}}$ | RMSE  |
|-----------|------|------|-------|------|---------------|--------------|-------------|---------|----------------------|----------------------|-------|
|           |      |      | mean  | std  | mean          | mean         | mean        | std      | mean                 | mean                |       |
| Elevators | 12,449 | 18   | 0     | 19   | 42.2           | 53.0         | 1.0         | 0.0      | 0.4647               | 0.4021               | 0.3484 |
|           | 500  |      |       |      |               |              |             |          | 0.0035               | 0.0102               | 0.0052 |
| Bike      | 13,034| 17   | 0     | 19   | 32.3           | 30.6         | 1.0         | 0.0      | −0.9976              | −0.9934              | 0.0446 |
|           | 500  |      |       |      |               |              |             |          | 0.0114               | 0.0137               | 0.0040 |
| Kin40k    | 30,000 | 8    | 0     | 19   | 19.0           | 186.5        | 1.0         | 0.0      | −0.3339              | −0.3141              | 0.0929 |
|           | 500  |      |       |      |               |              |             |          | 0.0018               | 0.0016               | 0.0014 |
| Protein   | 34,297| 9    | 0     | 15   | 124.2          | 892.6        | 1.0         | 0.0      | 0.9963               | 0.8869               | 0.5722 |
|           | 500  |      |       |      |               |              |             |          | 0.0031               | 0.0081               | 0.0065 |
| KEGGdir   | 36,620| 20   | 0     | 19   | 55.8           | 1450.3       | 1.0         | 0.0      | −0.9501              | −0.9459              | 0.0861 |
|           | 500  |      |       |      |               |              |             |          | 0.0087               | 0.0343               | 0.0043 |
| 3DRoad    | 326,155 | 3    | 0     | 9    | 68.0           | 82,200.0     | 1.0         | 0.0      | 0.7733               | 1.4360               | 0.2982 |
|           | 500  |      |       |      |               |              |             |          | 0.0128               | 1.1690               | 0.1265 |