QUANTIFYING UNCERTAINTIES IN LARGE-SCALE BAYESIAN LINEAR INVERSE PROBLEMS USING KRYLOV SUBSPACE METHODS

ARVIND K. SAIBABA†, JULIANNE CHUNG‡, AND KATRINA PETROSKE §

Abstract. For linear inverse problems with a large number of unknown parameters, uncertainty quantification remains a challenging task. In this work, we use Krylov subspace methods to approximate the posterior covariance matrix and describe efficient methods for exploring the posterior distribution. Assuming that Krylov methods (e.g., based on the generalized Golub-Kahan bidiagonalization) have been used to compute an estimate of the solution, we get an approximation of the posterior covariance matrix for “free.” We provide theoretical results that quantify the accuracy of the approximation and of the resulting posterior distribution. Then, we describe efficient methods that use the approximation to compute measures of uncertainty, including the Kullback-Liebler divergence. We present two methods that use preconditioned Lanczos methods to efficiently generate samples from the posterior distribution. Numerical examples from tomography demonstrate the effectiveness of the described approaches.

Keywords: generalized Golub-Kahan, Bayesian inverse problems, uncertainty measures, Krylov subspace samplers.

AMS subject classifications. 65F22, 65F30, 15A29, 62F15

1. Introduction. Inverse problems arise in various scientific applications, and a significant amount of effort has focused on developing efficient and robust methods to compute approximate solutions. However, as these numerical solutions are increasingly being used for data analysis and to aid in decision-making, there is a critical need to be able to obtain valuable uncertainty information (e.g., solution variances, samples, and credible intervals) to assess the reliability of computed solutions. Tools for inverse uncertainty quantification (UQ) often build upon the Bayesian framework from statistical inverse problems. Great overviews and introductions can be found in, e.g., [8, 37, 38, 23, 12].

Unfortunately, for very large inverse problems, UQ using the Bayesian approach is prohibitively expensive from a computational standpoint. This is partly because the posterior covariance matrices are so large that constructing, storing, and working with them directly are not computationally feasible. For these scenarios, a hybrid generalized Golub-Kahan based method was proposed in [15] to compute Tikhonov regularized solutions efficiently and to select a regularization parameter simultaneously and automatically. In this work, we go beyond computing reconstructions (e.g., maximum a posteriori (MAP) estimates) and develop efficient methods for inverse UQ. We focus on methods that use the approximate posterior distribution to compute measures of uncertainty and develop preconditioned iterative solvers to efficiently sample from the posterior distribution by exploiting various tools from numerical linear algebra.

*Submitted to the editors August 29, 2018.

Funding: This work was partially supported by NSF DMS 1720398 (A. Saibaba and K. Petroske), NSF DMS 1654175 (J. Chung), and NSF DMS 1723005 (J. Chung).

†Department of Mathematics, North Carolina State University, Raleigh, NC (asaibab@ncsu.edu, http://www4.ncsu.edu/~asaibab/)

‡Department of Mathematics, Computational Modeling and Data Analytics Division, Academy of Integrated Science, Virginia Tech, Blacksburg, VA (jmchung@vt.edu, http://www.math.vt.edu/people/jmchung/).

§Department of Mathematics, North Carolina State University, Raleigh, NC (kepetros@ncsu.edu)
For concreteness, we consider linear inverse problems of the form

\[(1.1) \quad d = As + \delta,\]

where the goal is to reconstruct the desired parameters \(s \in \mathbb{R}^n\), given matrix \(A \in \mathbb{R}^{m \times n}\) and the observed data \(d \in \mathbb{R}^m\). Typically, \(A\) is an ill-conditioned matrix that models the forward process, and we assume that it is known exactly. We adopt a Bayesian approach where we assume that the measurement errors \(\delta\) and the unknowns \(s\) are mutually independent Gaussian variables, i.e., \(\delta \sim \mathcal{N}(0, R)\) and \(s \sim \mathcal{N}(\mu, \lambda^{-2}Q)\) where \(R\) and \(Q\) are positive definite matrices, \(\mu \in \mathbb{R}^n\), and \(\lambda\) is a scaling parameter also known as the regularization parameter. For the problems of interest, computing the inverse and square root of \(R\) are inexpensive, but explicit computation of \(Q\) (or its inverse or square root) may not be possible. However, we assume that matrix-vector multiplications (mat-vecs) involving \(A\), \(A^\top\), and \(Q\) can be done efficiently.

Recall Bayes’ theorem of inverse problems, which states that the posterior probability distribution function is given by

\[
\pi_{\text{post}} = \pi(s|d) = \frac{\pi(d|s)\pi(s)}{\pi(d)}. 
\]

Under our assumptions, the posterior distribution has the following representation,

\[
\pi_{\text{post}} \propto \exp \left( -\frac{1}{2} \|As - d\|^2_{R^{-1}} - \frac{\lambda^2}{2} \|s - \mu\|^2_{Q^{-1}} \right),
\]

where \(\|x\|_M = \sqrt{x^\top M x}\) is a vector norm for any symmetric positive definite matrix \(M\). Thus, the posterior distribution is Gaussian \(\pi_{\text{post}} = \mathcal{N}(s_{\text{post}}, \Gamma_{\text{post}})\) where the posterior covariance and mean are given as

\[
\Gamma_{\text{post}} \equiv (\lambda^2Q^{-1} + A^\top R^{-1} A)^{-1} \quad \text{and} \quad s_{\text{post}} = \Gamma_{\text{post}}(A^\top R^{-1} d + \lambda^2 Q^{-1} \mu)
\]

respectively [12]. In the Bayesian framework, the solution to the inverse problem is the posterior distribution. However, for practical interpretation and data analysis, it is necessary to describe various characteristics of the posterior distribution [37].

For our problem an explicit expression for the posterior distribution is known, but exploring the distribution and computing measures of uncertainty are computationally prohibitive. The reason is that \(\Gamma_{\text{post}}\) is large and dense, in general, and storing and computing this matrix is impossible unless an efficient representation is used. Prior work includes efficient approximations based on a low-rank perturbation to the prior covariance matrix [16, 10, 11, 35]. To explain this approach, first rewrite the posterior covariance matrix as

\[
\Gamma_{\text{post}} = \lambda^{-2} Q^{1/2}(I + \lambda^{-2} Q^{1/2} A^\top R^{-1} A Q^{1/2})^{-1} Q^{1/2}.
\]

The prevalent approach computes a low-rank approximation \(Q^{1/2} A^\top R^{-1} A Q^{1/2} \approx V_k \Lambda_k V_k^\top\) using, for example, the singular value decomposition (SVD) and uses this to develop an efficient representation of \(\Gamma_{\text{post}}\) as

\[
\Gamma_{\text{post}} \approx \lambda^{-2}(Q - Q^{1/2} V_k D_k V_k^\top Q^{1/2}) \quad \text{where} \quad D_k = \Lambda_k (\Lambda_k + \lambda^2 I)^{-1}.
\]

The computation of the SVD is expensive, so the authors in [10, 31] use a randomized approach to efficiently compute a low-rank approximation. In this paper, we pursue a different approach that is based on Krylov subspace methods.
Overview of main contributions. The main point of this paper is to compute uncertainty measures involving the posterior distribution by storing bases for the Krylov subspaces during the computation of the MAP estimate and reusing the information contained in these subspaces for inverse UQ. The main contributions are as follows:

- We propose an approximation to the posterior covariance matrix using the generalized Golub-Kahan approach that has an efficient representation (low-rank perturbation of the prior covariance matrix). We develop error bounds for the approximate posterior covariance matrix.
- We develop bounds for monitoring the accuracy of the posterior covariance matrix using the information from the Krylov subspaces. We then relate the error in the approximate posterior covariance matrix to the error in the approximate posterior distribution. We also show how to compute measures of uncertainty such as the Kullback-Leibler divergence between the posterior and the prior distributions.
- We develop efficient iterative methods for generating samples from the posterior distribution that exploit preconditioned Lanczos methods in two different ways.

The paper is organized as follows. In section 2, we provide a brief overview of the generalized Golub-Kahan bidiagonalization and preconditioning for Krylov methods. Then, in section 3, we use elements from the generalized Golub-Kahan bidiagonalization to approximate the posterior covariance matrix and provide theoretical bounds for the approximation. Not only are these bounds of interest for subsequent analysis and sampling, but they can also be used to determine a good stopping criterion for the iterative methods. In section 4 we describe efficient Krylov subspace samplers for sampling from the posterior distribution. Numerical results for large inverse problems from image processing are provided in section 5, and conclusions and future work are provided in section 6.

2. Background. In this section, we provide a brief background on two core topics that will be heavily used in the development of efficient methods to explore the posterior. In subsection 2.1, we review an iterative hybrid method based on the generalized Golub-Kahan bidiagonalization that can be used to approximate the MAP estimate, which amounts to minimizing the negative log likelihood of the posterior probability distribution function, i.e.

\[
(2.1) \quad s_{\text{post}} = \arg\min_{s \in \mathbb{R}^n} -\log \pi(s|d) = \arg\min_{s \in \mathbb{R}^n} \frac{1}{2} \|As - d\|_R^{-1}^2 + \frac{\lambda^2}{2} \|s - \mu\|_Q^{-1}^2.
\]

Notice that with a change of variables, \( s_{\text{post}} = \mu + Qx \) where \( x \) is the solution to

\[
(2.2) \quad \min_{x \in \mathbb{R}^n} \frac{1}{2} \|AQx - b\|_R^{-1}^2 + \frac{\lambda^2}{2} \|x\|_Q^2.
\]

where \( b = d - A\mu \). For readers familiar with hybrid Krylov iterative methods, subsection 2.1 can be skipped. Then in subsection 2.2, we review preconditioned Krylov subspace solvers for generating samples from normal distributions.

2.1. Generalized hybrid iterative methods. Here, we provide an overview of the hybrid method based on the generalized Golub-Kahan (gen-GK) bidiagonalization, but refer the interested reader to \([15, 2]\) for more details.

The basic idea behind the generalized hybrid methods is first to generate a basis \( V_k \) for the Krylov subspace

\[
(2.3) \quad S_k \equiv \text{Span}\{V_k\} = \mathcal{K}_k(A^T R^{-1} A, A^T R^{-1} b)
\]
where \( \mathcal{K}_k(M, g) = \text{Span}\{g, Mg, \ldots, M^{k-1}g\} \), and second to solve (2.2) in this subspace. A basis for \( S_k \) can be generated using the gen-GK bidiagonalization process\(^1\) summarized in Algorithm 2.1, where at the end of \( k \) steps, we have the matrices

\[
U_{k+1} \equiv [u_1, \ldots, u_{k+1}], \quad V_k \equiv [v_1, \ldots, v_k], \quad \text{and} \quad B_k \equiv \begin{bmatrix} \alpha_1 \\ \beta_2 \\ \vdots \\ \alpha_k \\ \beta_{k+1} \end{bmatrix}
\]

that in exact arithmetic satisfy

\[
AQ_k = U_{k+1}B_k, \quad A^\top R^{-1}U_{k+1} = V_kB_k^\top + \alpha_{k+1}v_{k+1}e_{k+1}^\top
\]

and

\[
U_k^\top R^{-1}U_{k+1} = I_{k+1}, \quad V_k^\top QV_k = I_k.
\]

Vector \( e_{k+1} \) corresponds to the \((k+1)\)st standard unit vector.

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**Algorithm 2.1 gen-GK bidiagonalization**

**Result:** \([U_k, V_k, B_k] = \text{gen-GK}(A, R, Q, b, k)\)

1. \( \beta_1u_1 = b \), where \( \beta_1 = \|b\|_{R^{-1}} \)
2. \( \alpha_1v_1 = A^\top R^{-1}u_1 \), where \( \alpha_1 = \|A^\top R^{-1}u_1\|_Q \)
3. for \( i = 1, \ldots, k \) do
4. \( \beta_{i+1}u_{i+1} = AQv_i - \alpha_iu_i \), where \( \beta_{i+1} = \|AQv_i - \alpha_iu_i\|_{R^{-1}} \)
5. \( \alpha_{i+1}v_{i+1} = A^\top R^{-1}u_{i+1} - \beta_{i+1}v_i \), where \( \alpha_{i+1} = \|A^\top R^{-1}u_{i+1} - \beta v_i\|_Q \)
6. end for

Then, we seek an approximate solution to (2.2) of the form \( x_k = V_kz_k \), so that \( x_k \in S_k \), where the coefficients \( z_k \) can be determined by solving the following problem

\[
\min_{x_k \in S_k} \frac{1}{2} \|AQx_k - b\|_{R^{-1}}^2 + \frac{\lambda^2}{2} \|x_k\|_Q^2 \quad \Leftrightarrow \quad \min_{z_k \in \mathbb{R}^n} \frac{1}{2} \|B_kz_k - \beta_1e_1\|_2^2 + \frac{\lambda^2}{2} \|z_k\|_2^2
\]

where the equivalency uses the relations in (2.5) and (2.6). For fixed \( \lambda \), an approximate MAP estimate can be recovered by undoing the change of variables,

\[
s_k = \mu + Qx_k = \mu + QV_k(B_k^\top B_k + \lambda^2I)^{-1}B_k^\top \beta_1 e_1,
\]

where, now, \( s_k \in \mu + QS_k \). If \( \lambda \) is not known a priori, a hybrid approach can be used where sophisticated SVD based methods are applied to the right equation in (2.7). In this work, we use the hybrid implementation described in [15] called genHyBR.

**2.2. Sampling from a Gaussian distribution.** Let \( \tilde{\nu} \in \mathbb{R}^n \) and let \( \Gamma \in \mathbb{R}^{n \times n} \) be any symmetric positive definite matrix. Suppose the goal is to obtain samples from the Gaussian distribution \( \mathcal{N}(\tilde{\nu}, \Gamma) \). Throughout this paper, let \( \epsilon \sim \mathcal{N}(0, I) \). If we have or are able to obtain a factorization of the form \( \Gamma = SS^\top \), then

\[
\nu = \tilde{\nu} + S\epsilon
\]

---

\(^1\)Generalized Golub-Kahan methods were first proposed by Benbow [6] for generalized least squares problems, and used in several applications, see e.g. [3, 2, 26]. However, the specific form of the bidiagonalization was developed in [15].
is a sample from $\mathcal{N}(\nu, \Gamma)$, since $E[\nu] = \bar{\nu}$ and

$$\text{Cov}(\nu) = E[(\nu - \bar{\nu})(\nu - \bar{\nu})^\top] = E[S\epsilon\epsilon^\top] = \Gamma.$$  

Note that any matrix $S$ that satisfies $SS^\top = \Gamma$ can be used to generate samples. In this section, we show how Krylov subspace solvers, in particular preconditioned versions, can be used to efficiently generate approximate samples from $\mathcal{N}(0, \Gamma)$ and $\mathcal{N}(0, \Gamma^{-1})$. These approaches will be extended for sampling from the posterior in section 4.

Given $\Gamma$ and starting guess $\epsilon$, then after $k$ steps of the symmetric Lanczos process, we have matrix $W_k = [w_1, \ldots, w_k] \in \mathbb{R}^{n \times k}$ that contains orthonormal columns and tridiagonal matrix $T_k = \begin{bmatrix} \gamma_1 & \delta_2 & & & \\ \delta_2 & \gamma_2 & \delta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \delta_{k-1} & \gamma_{k-1} & \delta_k \\ & & & \delta_k & \gamma_k \end{bmatrix} \in \mathbb{R}^{k \times k}$ such that in exact arithmetic we have the following relation,

$$\Gamma W_k = W_k T_k + \delta_{k+1} w_{k+1} \epsilon_1^\top.$$  

The Lanczos process is summarized in Algorithm 2.2. Computed matrices $W_k$ and $T_k$ can then be used to obtain approximate draws from $\mathcal{N}(0, \Gamma)$ and $\mathcal{N}(0, \Gamma^{-1})$ as

$$(2.9) \quad \xi_k = W_k T_k^{1/2} \delta_1 \epsilon_1 \quad \text{and} \quad \zeta_k = W_k T_k^{-1/2} \delta_1 \epsilon_1$$
respectively.

**Algorithm 2.2** Lanczos tridiagonalization

**Result:** $[W_k, T_k] = \text{Lanczos}(\Gamma, \epsilon, k)$

1. $\delta_0 = 1, w_0 = 0, \delta_1 = \|\epsilon\|_2, w_1 = \epsilon / \delta_1$
2. for $i = 1, \ldots, k$ do
3. $\gamma_i = w_i^\top \Gamma w_i,$
4. $r = \Gamma w_i - \gamma_i w_i - \delta_{i-1} w_{i-1},$
5. $w_{i+1} = r / \delta_i,$ where $\delta_i = \|r\|_2$
6. end for

**Convergence.** The approximation will improve as $k$ increases, and we expect typical convergence behavior for the Lanczos process whereby convergence to extremal (i.e., largest and smallest) eigenvalues will be fast. The following result [34, Theorem 3.3] sheds light into the convergence of the Krylov subspace method for sampling. The error in the sample $\zeta_k$ is given by

$$\|\Gamma^{-1/2} \epsilon - \zeta_k\|_2 \leq \sqrt{\lambda_{\min}(\Gamma)} \|r_k\|_2,$$

where $\lambda_{\min}(\Gamma)$ is the smallest eigenvalue of $\Gamma$ and $r_k$ is the residual vector at the $k$-th iteration of the conjugate gradient method. The residual vector $\|r_k\|_2$ can be bounded using standard techniques in Krylov subspace methods [30]. To use this as a
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stopping criterion, we note that \( \|r_k\|_2 = \delta_1 |e_k^T T_k^{-1} e_1| \) and by the Cauchy interlacing theorem \( \lambda_{\min}(\Gamma) \leq \lambda_{\min}(T_k) \). Combining the two bounds we have

\[
\|\Gamma^{-1/2} - \zeta_k\|_2 \leq \sqrt{\lambda_{\min}(T_k)} \delta_1 |e_k^T T_k^{-1} e_1|.
\]

However, in numerical experiments we found that the bound was too pessimistic and instead adopted the approach in [13]. Suppose we define the relative error norm as

\[
e_k = \frac{\|\zeta_k - \Gamma^{-1/2} \epsilon\|_2}{\|\Gamma^{-1/2} \epsilon\|_2}.
\]

In practice, this quantity cannot be computed, but can be estimated by using the successive iterates as

\[
\hat{e}_k = \frac{\|\zeta_k - \zeta_{k+1}\|_2}{\|\zeta_{k+1}\|_2}.
\]

When the convergence is fast, in numerical experiments we found this bound to be more representative of the true error. The downside is that computing this is expensive since it costs \( O(nk^2) \) flops. However, this cost can be avoided by first writing

\[
\zeta_k = W_k \tilde{\zeta}_k, \quad \text{where} \quad \tilde{\zeta}_k = \delta_1 T_k^{-1/2} e_1.
\]

Since the columns of \( W_k \) are orthonormal, then

\[
(2.10) \quad \hat{e}_k = \frac{\|\zeta_k' - \zeta_{k+1}\|_2}{\|\tilde{\zeta}_{k+1}\|_2} \quad \zeta_k' = \begin{bmatrix} \tilde{\zeta}_k \\ 0 \end{bmatrix}.
\]

Therefore, \( \hat{e}_k \) can be computed in \( O(k^3) \) operations rather than \( O(nk^2) \) operations. A similar approach can be used to monitor the convergence of \( \xi_k \) to \( \Gamma^{1/2} \epsilon \).

**Preconditioning.** It is well known that convergence of Krylov subspace methods for solving linear systems can be accelerated, if we have an appropriate preconditioner. Assume that we have a preconditioner \( G \) which satisfies \( \Gamma^{-1} \approx GG^T \). Then, the same preconditioner can be used to accelerate the convergence of the Krylov subspace methods for generating samples, as we now show. Let

\[
S = G^{-1}(GG^T)^{1/2} \quad \text{and} \quad T = G^T(GG^T)^{-1/2},
\]

then it is easy to see that

\[
SS^T = G^{-1}(GG^T)^{1/2}(GG^T)^{1/2}G^{-T} = \Gamma
\]

and similarly \( TT^T = \Gamma^{-1} \). The Lanczos process is then applied to \( GFG^T \) and approximate samples from \( N(0, \Gamma) \) and \( N(0, \Gamma^{-1}) \) can be obtained by computing

\[
(2.11) \quad \xi_k = G^{-1} W_k T_k^{1/2} \delta_1 e_1 \quad \zeta_k = G^T W_k T_k^{-1/2} \delta_1 e_1.
\]

If \( G \) is a good preconditioner, in the sense that \( GFG^T \approx I \), then the Krylov subspace method is expected to converge rapidly. The choice of preconditioner depends on the specific problem; we comment on the choice of preconditioners in the numerical experiments in section 5.
3. Approximating the posterior distribution using the gen-GK bidiagonalization. The basic goal of this work is to enable exploration of the posterior distribution for large-scale inverse problems by exploiting approximations that are generated from Krylov methods. In particular, we use elements and relationships from the gen-GK bidiagonalization (c.f., equations (2.4)–(2.6)) to approximate the posterior covariance matrix $\Gamma_{\text{post}}$.

Consider computing the approximate eigenvalue decomposition of $H = A^\top R^{-1}A$. We define the Ritz pairs $(\theta, y)$ obtained as the solution of the following eigenvalue problem,

$$(HQV_k y - \theta V_k y) \perp Q \text{ Span } \{V_k\}.$$ 

Here the orthogonality condition $\perp Q$ is defined with respect to the weighted inner product $\langle \cdot, \cdot \rangle_Q$. From (2.6), the Ritz pairs can be obtained by the solution of the eigenvalue problem

$$B_k^\top B_k y_j = \theta_j y_j \quad j = 1, \ldots, k.$$ 

The Ritz pairs can be combined to express the eigenvalue decomposition in matrix form as,

$$B_k^\top B_k = Y_k \Theta_k Y_k^\top.$$ 

The accuracy of the Ritz pairs can be quantified by the residual, defined as

$$\|r_j\|_Q \equiv \|HQV_k y_j - \theta_j V_k y_j\|_Q = \alpha_k \beta_{k+1} |e_k^\top y_j| \quad j = 1, \ldots, k.$$ 

Furthermore, using arguments from [28, Theorem 11.4.2] it can be shown that $T_k \equiv B_k^\top B_k = \min_{\Delta \in \mathbb{R}^{k \times k}} \|HQV_k - V_k \Delta\|_Q$ is the best approximation over the subspace $S_k \equiv K_k(HQ, A^\top R^{-1}b)$, using which we can write $H \approx V_k T_k V_k^\top$ is the best low-rank approximation of $H$ over the space $S_k$. Here we define the matrix $\| \cdot \|_Q$ norm to be $\|M\|_Q = \max_{\|x\|_2=1} \|Mx\|_Q$.

An approximation of this kind has been previously explored in [31, 16, 10, 11]; however, the error estimates developed in the above references assume that the exact eigenpairs are available. If the Ritz pairs converge to the exact eigenpairs of the matrix $QH$, then furthermore, the optimality result in [35, Theorem 2.3] applies here as well.

For the rest of this paper, we use the following low-rank approximation to $H$ which is constructed using the gen-GK bidiagonalization

$$(3.1) \quad \hat{H} \equiv V_k T_k V_k^\top.$$ 

Using this low-rank approximation, we can define the approximate posterior distribution $\hat{\pi}_{\text{post}} = N(s_k, \hat{\Gamma}_{\text{post}})$, which is a Gaussian distribution with covariance matrix

$$(3.2) \quad \hat{\Gamma}_{\text{post}} \equiv (\lambda^2 Q^{-1} + \hat{H})^{-1}$$ 

and mean $s_k$ defined in (2.8). Using (3.2), we note that

$$(3.3) \quad s_k = \mu + \hat{\Gamma}_{\text{post}} A^\top R^{-1} b.$$ 

See Appendix A.1 for the derivation.
3.1. Posterior covariance approximation. First, we derive a way to monitor the accuracy of the low-rank approximation using the information available from the gen-GK bidiagonalization. This result is similar to [33, Proposition 3.3].

Proposition 1. Let \( H_Q = Q^{1/2}HQ^{1/2} \) and \( \hat{H}_Q = Q^{1/2}\hat{H}Q^{1/2} \). After running \( k \) steps of Algorithm 2.1, the error in the low-rank approximation \( \hat{H} \), measured as

\[
\omega_k = \|H_Q - \hat{H}_Q\|_F,
\]

satisfies the recurrence

\[
\omega_{k+1}^2 = \omega_k^2 - 2|\alpha_{k+1}\beta_{k+1}|^2 - |\alpha_{k+1}^2 + \beta_{k+2}|^2.
\]

Proof. See Appendix A.2.

This proposition shows that, in exact arithmetic, the error in the low-rank approximation \( \hat{H} \) to \( H \) decreases monotonically as the iterations progress. Estimates for \( \omega_k \) can be obtained in terms of the singular values of \( R^{-1/2}AQ^{1/2} \) following the approach in [33, Theorem 3.2] and [22, Theorem 2.7]. However, we do not pursue them here.

Given the low-rank approximation, we can define the approximate posterior covariance \( \hat{\Gamma}_{\text{post}} \) in (3.2). The recurrence relation in Proposition 1 can be used to derive the following error estimates for \( \Gamma_{\text{post}} \).

Theorem 3.1. The approximate posterior covariance matrix \( \hat{\Gamma}_{\text{post}} \) satisfies

\[
\|\Gamma_{\text{post}} - \hat{\Gamma}_{\text{post}}\|_F \leq \lambda^{-2} \min\left\{ \omega_k \lambda^{-2} \|Q\|_2, \frac{\omega_k \|Q\|_F}{\lambda^2 + \omega_k} \right\}
\]

Proof. See Appendix A.2.

The above theorem quantifies the error in the posterior covariance matrix in the Frobenius norm. However, the authors in [35] argue that the Frobenius norm is not the appropriate metric to measure the distance between covariance matrices. Instead, they advocate the Förstner distance since it respects the geometry of the cone of positive definite covariance metrics. We take a different approach and consider metrics between the approximate and the true posterior distributions.

3.2. Accuracy of posterior distribution. The Kullback-Leibler (KL) divergence is a measure of “distance” between two different probability distributions. The KL divergence is not a true metric on the set of probability measures, since it is not symmetric and does not satisfy the triangle inequality [36]. Despite these shortcomings, the KL divergence is widely used since it has many favorable properties. Both the true and the approximate posterior distributions are Gaussian, so the KL divergence between these distributions takes the form (using [36, Exercise 5.2]):

\[
D_{\text{KL}}(\hat{\pi}_{\text{post}} || \pi_{\text{post}}) = \frac{1}{2} \left[ \text{trace}(\Gamma_{\text{post}}^{-1}\hat{\Gamma}_{\text{post}}) + \|s_{\text{post}} - s_k\|^2_{\Gamma_{\text{post}}^{-1}} - n + \log \frac{\det \Gamma_{\text{post}}}{\det \hat{\Gamma}_{\text{post}}} \right].
\]

We first present a result that can be used to monitor the accuracy of the trace of \( H_Q \).

Proposition 3.2. Let \( \theta_k = \text{trace}(H_Q - \hat{H}_Q) \). Then \( \theta_k \) satisfies the recurrence relation

\[
\theta_{k+1} = \theta_k - (\alpha_{k+1}^2 + \beta_{k+2}^2).
\]

Proof. See Appendix A.4.
Note that the Cauchy interlacing theorem implies that $\theta_k$ is non-negative; therefore, as with Proposition 1, this result implies that $\theta_k$ is monotonically decreasing.

**Theorem 3.3.** At the end of $k$ iterations, the KL divergence between the true and the approximate posterior distributions satisfies

$$0 \leq D_{KL}(\hat{\pi}_{post} \parallel \pi_{post}) \leq \frac{\lambda^{-2}}{2} \left[ \theta_k + \frac{\omega_k^2}{\lambda^2 + \omega_k} \alpha_1^2 \beta_1^2 \right].$$

**Proof.** See Appendix A.4.

Both $\theta_k$ and $\omega_k$ are monotonically decreasing, implying that the accuracy of the estimator for the KL divergence improves as the iterations progress. This theorem can be useful in providing bounds for the error using other metrics.

For example, consider the Hellinger metric and Total Variation (TV) distance denoted by $d_H(\pi_{post}, \hat{\pi}_{post})$ and $d_{TV}(\pi_{post}, \hat{\pi}_{post})$ respectively. Combining Pinsker’s inequality [36, Theorem 5.4] and Kraft’s inequality [36, Theorem 5.10], we have the following relationship

$$(3.5) \quad d_H^2(\pi_{post}, \hat{\pi}_{post}) \leq d_{TV}(\pi_{post}, \hat{\pi}_{post}) \leq \sqrt{2D_{KL}(\hat{\pi}_{post} \parallel \pi_{post})}.$$  

Thus, Theorem 3.3 can be used to find upper bounds for the Hellinger metric and the TV distance between the true and approximate posterior distributions. Furthermore, if $\mu$ and $\nu$ are two probability measures on $\mathbb{R}^n$ and $f : (\mathbb{R}^n, \| \cdot \|_{\mathbb{R}^n}) \rightarrow (\mathbb{R}^d, \| \cdot \|_{\mathbb{R}^d})$ is a function with finite second moments with respect to both measures, then by [36, Proposition 5.12]

$$\| E_\mu[f] - E_\nu[f] \|_{\mathbb{R}^n} \leq 2 \sqrt{E_\mu[\| f \|_{\mathbb{R}^d}^2] + E_\nu[\| f \|_{\mathbb{R}^d}^2]} d_H(\mu, \nu).$$

This implies that the error in the expectation of a function computed using the approximate posterior instead of the true posterior can be bounded by combining (3.5) and Theorem 3.3.

**3.3. Computation of information-theoretic metrics.** In addition to providing a measure of distance between the true and approximate posterior distributions, the KL divergence can also be used to measure the information gain between the prior and the posterior distributions. Similar to the derivation in subsection 3.2 since both $\pi_{prior}$ and $\pi_{post}$ are Gaussian, the KL divergence takes the form

$$D_{KL}(\pi_{post} \parallel \pi_{prior}) = \frac{1}{2} \left[ \text{trace}(\lambda^2 Q^{-1} \Gamma_{post}) + \lambda^2 (s_{post} - \mu)^T Q^{-1} (s_{post} - \mu) 
- n - \log \det(\lambda^2 Q^{-1} \Gamma_{post}) \right]$$

$$= \frac{1}{2} \left[ \text{trace}(I + \lambda^{-2} H_Q)^{-1} + \lambda^2 (s_{post} - \mu)^T Q^{-1} (s_{post} - \mu) 
- n + \log \det(I + \lambda^{-2} H_Q) \right].$$

Then, using the approximations generated by the gen-GK bidiagonalization, we consider the approximation

$$D_{KL} \equiv D_{KL}(\pi_{post} \parallel \pi_{prior}) \approx D_{KL}(\hat{\pi}_{post} \parallel \pi_{prior}) \equiv \hat{D}_{KL}.$$
Using the fact that \( \log \det(I + \lambda^{-2} \hat{H}_Q) = \log \det(I + \lambda^{-2} T_k) \),
\[
\text{trace}(I + \lambda^{-2} \hat{H}_Q) = n - \text{trace}(T_k(T_k + \lambda^2 I)^{-1}),
\]
and
\[
\|s_k - \mu\|_Q^{-1} = \|QV_k(B_k^T B_k + \lambda^2 I)^{-1} B_k^T \beta_1 e_1\|_Q^{-1} = \|\alpha_1 \beta_1 (T_k + \lambda^2 I)^{-1} e_1\|_2^2,
\]
we get
\[
\hat{D}_{\text{KL}} = \frac{1}{2} \left[ -\text{trace}(T_k(T_k + \lambda^2 I)^{-1}) + \lambda^2 \|z_k\|_2^2 + \log \det(I + \lambda^{-2} T_k) \right]
\]
where \( z_k = \alpha_1 \beta_1 (T_k + \lambda^2 I)^{-1} e_1 \). Note that all of the terms only involve \( k \times k \) tridiagonal matrices and, therefore, \( \hat{D}_{\text{KL}} \) can be computed in \( \mathcal{O}(k^3) \), once the gen-GK bidiagonalization has been computed.

What can we say regarding the accuracy of the estimator for the KL divergence between the posterior and the prior? The following result quantifies the error.

**Theorem 3.4.** The error in the KL divergence, in exact arithmetic, is given by
\[
|D_{\text{KL}} - \hat{D}_{\text{KL}}| \leq \lambda^{-2} \left[ \frac{\theta_k}{\lambda^2} + \frac{\lambda^2 \omega_k}{\lambda^2 + \omega_k \sigma_1^2} \right],
\]
where \( \omega_k \) and \( \theta_k \) were defined in Proposition 1 and Proposition 3.2 respectively.

**Proof.** See Appendix A.4.

Notice that the bound is similar to Theorem 3.3.

Related to the KL divergence is the D-optimal criterion for optimal experimental design. This is defined as
\[
\phi_D \equiv \log \det(T_{\text{post}}) - \log \det(\lambda^{-2} Q) = \log \det(I + \lambda^{-2} H_Q).
\]
The D-optimal criterion can be seen as the expected KL divergence, with the expectation taken over the posterior distribution. A precise statement of this result was derived in [1, Theorem 1]. Similar to the KL divergence, we can estimate the D-optimal criterion as
\[
\hat{\phi}_D = \log \det(I + \lambda^{-2} T_k).
\]
From the proof of Theorem 3.4, it can be readily seen that a bound for the error in the D-optimal criterion is given by
\[
|\phi_D - \hat{\phi}_D| \leq \lambda^{-2} \theta_k.
\]

**4. Sampling from the posterior distribution.** Since the posterior distribution is very high-dimensional, visualizing this distribution is challenging. A popular method is to generate samples from the posterior distribution (also sometimes known as conditional realizations), which provides a family of solutions and can be used for quantifying the reconstruction uncertainty. For instance, to compute the expected value of a quantity of interest \( q(x) \), defined as
\[
Q \equiv \mathbb{E}[q(x) \mid d] = \int_{\mathbb{R}^n} q(x) \pi_{\text{post}}(x \mid d) dx.
\]
Suppose, we have samples \( \{ x^{(j)} \}_{j=1}^N \) then \( Q_N \equiv N^{-1} \sum_{j=1}^N q(x^{(j)}) \) is the Monte Carlo estimate of \( Q \).

Furthermore, the Monte Carlo estimate converges to the expected value of the quantity of interest, i.e., \( Q_N \to Q \) as \( N \to \infty \).

We now show how to draw samples from the posterior distribution \( N(s_{\text{post}}, \Sigma_{\text{post}}) \). As described in subsection 2.2, if \( \epsilon \sim N(0, I) \) and \( \mathbf{S} \mathbf{S}^\top = \Sigma_{\text{post}} \), then

\[
\mathbf{s} = \mathbf{s}_{\text{post}} + \mathbf{S} \epsilon
\]

is a sample from \( N(\mathbf{s}_{\text{post}}, \Sigma_{\text{post}}) \). However, computing the posterior covariance matrix \( \Sigma_{\text{post}} \) and its factorization \( \mathbf{S} \) is infeasible for reasons described before. We propose generating samples from the posterior distribution using preconditioned Krylov subspace methods. A direct application of the approach in subsection 2.2 to the posterior covariance matrix is expensive since it involves application of \( Q^{-1} \). To avoid this, we present several reformulations. The first approach we describe computes a low-rank approximation of \( \mathbf{H} \) using the gen-GK approach and then uses this low-rank approximation to generate samples from the approximate posterior distribution. Any low-rank approximation can be used, provided it is sufficiently accurate. On the other hand, the second approach generates approximate samples from the exact posterior distribution. Both methods use a preconditioner, albeit in different ways.

Before describing our proposed methods, we briefly review a few methods for sampling from high-dimensional Gaussian distributions. The idea of using Krylov subspace methods for sampling from Gaussian random processes seems to have originated from [32]. Variants of this idea have also been proposed in [27, 13]. It has also found applications in Bayesian inverse problems in [18, 34]. The use of a low-rank surrogate of \( \mathbf{H} \) has also been explored in [10, 11] and is similar to Method 1 (c.f., subsection 4.1) that we propose. Other approaches to sampling from the posterior distribution include Randomize-then-optimize (RTO) [5, 4] and Randomized MAP approach [39].

### 4.1. Method 1

Consider generating samples from \( N(\mathbf{0}, \Sigma_{\text{post}}) \), where \( \Sigma_{\text{post}} = (\lambda^2 Q^{-1} + \mathbf{H})^{-1} \) is the posterior covariance matrix. Given a preconditioner \( \mathbf{G} \), which we assume to be invertible, we can write

\[
Q^{-1} = \mathbf{G}^\top (\mathbf{GQG}^\top)^{-1} \mathbf{G}.
\]

We factorize \( \lambda^2 Q^{-1} = \mathbf{L}^\top \mathbf{L} \) where

\[
\mathbf{L} \equiv \lambda (\mathbf{GQG}^\top)^{-1/2} \mathbf{G}.
\]

Plugging this into the expression for the posterior covariance, we obtain

\[
\Sigma_{\text{post}} = (\mathbf{L}^\top \mathbf{L} + \mathbf{H})^{-1} = \mathbf{L}^{-1} (\mathbf{I} + \mathbf{L}^{-\top} \mathbf{H} \mathbf{L}^{-1})^{-1} \mathbf{L}^{-\top}.
\]

The low-rank approximation of \( \mathbf{H} \) in (3.1) can be used to derive an approximate factorization of the posterior covariance matrix

\[
\hat{\Sigma}_{\text{post}} = \hat{\mathbf{S}} \hat{\mathbf{S}}^\top \text{ where } \hat{\mathbf{S}} \equiv \mathbf{L}^{-1} (\mathbf{I} + \mathbf{L}^{-\top} \hat{\mathbf{H}} \mathbf{L}^{-1})^{-1/2}.
\]

To efficiently compute matvecs with \( \hat{\mathbf{S}} \), we first compute the low-rank representation

\[
\mathbf{L}^{-\top} \hat{\mathbf{H}} \mathbf{L}^{-1} = \mathbf{Z}_k \Theta_k \mathbf{Z}_k^\top.
\]
Algorithm 4.1 Low-rank representation $Z\Theta Z^\top = WW^\top$

Result: $[Z, \Theta] = \text{Lowrank}(W)$ for $W \in \mathbb{R}^{n \times k}$ with $k \leq n$

1: Compute thin-QR factorization $QR = W$
2: Compute eigenvalue decomposition $RR^\top = Y\Theta Y^\top$
3: Compute $Z = QY$

Computing the low-rank representation is accomplished using Algorithm 4.1.

Computing matvecs with $L$ (including its inverse and transpose) is done using the preconditioned Lanczos method described in subsection 2.2. We can compute the square root of the inverse of $I + Z_k\Theta_kZ_k^\top$ using a variation of the Woodbury identity

$$(I + Z_k\Theta_kZ_k^\top)^{-1/2} = I - Z_kD_kZ_k^\top$$

In summary, the procedure for computing samples $\xi^{(j)} \sim \mathcal{N}(0, \hat{\Gamma}_{\text{post}})$ is provided in Algorithm 4.2. The accuracy of the generated samples is discussed in subsection 4.3.

Algorithm 4.2 Method 1: Sampling from $\mathcal{N}(0, \hat{\Gamma}_{\text{post}})$

Result: $[\xi^{(1)}, \ldots, \xi^{(N)}] = \text{Method1}(A, R, Q, L, b, k)$

1: Compute $[U_k, V_k, B_k] = \text{gen-GK}(A, R, Q, b, k)$
2: Compute Cholesky factorization $M^\top M = B_k^\top B_k$
3: Apply $L^{-\top}$ to columns of $V_kM^\top$ to get $Y_k$ using approach in subsection 2.2
4: Compute $[Z_k, \Theta_k] = \text{Lowrank}(Y_k)$
5: Compute $D_k = I_k \pm (I_k + \Theta_k)^{-1/2}$
6: for $j = 1, \ldots, N$ do
7:   Draw sample $\epsilon^{(j)} \sim \mathcal{N}(0, I)$
8:   Compute $z = \epsilon^{(j)} - Z_kD_kZ_k^\top \epsilon^{(j)}$
9:   Compute $\xi^{(j)} = L^{-1}z$
10: end for

4.2. Method 2. The second approach we describe generates approximate samples from the exact posterior distribution. First, we rewrite the posterior covariance matrix as

$$\Gamma_{\text{post}} = (\lambda^2Q^{-1} + H)^{-1} = QF^{-1}Q \quad F \equiv \lambda^2Q + QHQ.$$

We compute the factorization

$$\Gamma_{\text{post}} = SF^\top S^\top \quad S \equiv QF^{-1/2}(QF^{-1/2})^\top.$$

In this method, computing a factorization of $\Gamma_{\text{post}}$ requires computing square-roots with $F$. Assume that we have a preconditioner $G$ satisfying $GG^\top \approx F^{-1}$. Armed with this preconditioner, we have the following factorization

$$\Gamma_{\text{post}} = SF^\top S^\top \quad S \equiv QG^\top(GFG^\top)^{-1/2}.$$

The application of the matrix $(GFG^\top)^{-1/2}$ to a randomly drawn vector can be accomplished by the Lanczos approach described in subsection 2.2.

As currently described, computing approximate samples from $\Gamma_{\text{post}}$ requires applying the matrix $A$ and its adjoint $A^\top$. However, this may be computationally
Algorithm 4.3 Method 2: Sampling from $\mathcal{N}(0, \Gamma_{\text{post}})$

Result: $[\xi] = \text{Method2}(A, R, Q, G, b, \epsilon, k)$

1: Draw sample $\epsilon \sim \mathcal{N}(0, I)$
2: Compute $z = G^\top (GFG^\top)^{-1/2} \epsilon$ using Lanczos approach in subsection 2.2
3: Compute $\xi = Qz$

expensive for several problems of interest. However, as with the previous approach, we can use a low-rank approximation to $H$. A variant of this method, not considered in this paper, follows by replacing the data-misfit part of the Hessian $H$ by its approximation $\hat{H}$, defined in (3.1). Define

$$\hat{F} = \lambda^2 Q + \hat{Q} \hat{H} Q.$$

Therefore, we compute the following factorization of the approximate posterior covariance

$$\hat{\Gamma}_{\text{post}} = \hat{S} \hat{F}\hat{S}^\top \quad \hat{S} = QG^\top (GFG^\top)^{-1/2}.$$

4.3. Discussion. We now compare the two proposed methods for generating approximate samples from the posterior. The first approach only uses the forward operator $A$ in the precomputation phase to generate the low-rank approximation, and subsequently uses the low-rank approximation as a surrogate. This can be computationally advantageous if the forward operator is very expensive or if many samples are desired. On the other hand, if accuracy is important or only a few samples are needed, then the second approach is recommended since it targets the full posterior distribution.

In Method 1, we generate samples from the approximate posterior distribution; the following result quantifies the error in the samples. Define $S = Q^{1/2}(\lambda^2 I + HQ)^{-1/2}$ such that $\Gamma_{\text{post}} = SS^\top$ and let $\epsilon$ be a random draw from $\mathcal{N}(0, I)$, then

$$s = s_{\text{post}} + S\epsilon \quad \text{and} \quad \hat{s} = s_k + \hat{S}\epsilon$$

are samples from $\pi_{\text{post}}$ and $\hat{\pi}_{\text{post}}$ respectively, where $\hat{S}$ is defined in (4.2).

**Theorem 4.1.** Let $\hat{\Gamma}_{\text{post}}$ be the approximate posterior covariance matrix generated by running $k$ steps of the gen-GK algorithm. The error in the sample $\hat{s}$ satisfies

$$||s - \hat{s}||_{\lambda^2 Q^{-1}} \leq \lambda^{-1} \left( \frac{\omega_k \alpha \beta}{\lambda^2 + \omega_k} + \sqrt{\frac{\lambda^2 \omega_k}{\lambda^2 + \omega_k}} ||\epsilon||_2 \right).$$

**Proof.** See Appendix A.5.

Theorem 4.1 states that if $\omega_k$ is sufficiently small, then the accuracy of the samples is high. The samples, thus generated, can then be used as is in applications. Otherwise they can be used as candidate draws from a proposal distribution $\hat{\pi}_{\text{post}}$. This proposal distribution can be used inside an independence sampler, similar to the approach in [9].

5. Numerical results. In the first set of experiments, we investigate the accuracy of the low-rank approximation to $H$ and the subsequent bounds that were derived in section 3. Then, we demonstrate the efficiency of the preconditioned Lanczos approach proposed in section 4 for generating samples.
5.1. Bounds for the posterior covariance matrix. First, we investigate the accuracy of the bounds derived in section 3 using the heat example from the Regularization Toolbox [19]. Matrix $A$ was $256 \times 256$, and the observations were generated as (1.1), where $\delta$ models the observational error. In the experiments, we take $\delta$ to be 1% additive Gaussian white noise. We let $Q$ be a $256 \times 256$ covariance matrix that was generated using an exponential kernel $\kappa(r) = \exp(-r/\ell)$ where $r$ is the distance between two points and $\ell = 0.1$ is the correlation length. First, we use gen-HyBR to compute an approximate MAP estimate and simultaneously estimate a good regularization parameter. Using a weighted generalized cross validation (WGCV) method, the computed regularization parameter was $\lambda^2 \approx 5 \times 10^3$. The regularization parameter was then fixed for the remainder of the experiment.

![Graph](image)

**Fig. 5.1.** (left) In this plot, we provide the computed values of $\omega_k$: the error between the true and the approximate prior-preconditioned Hessian for the data-misfit, as a function of the iteration $k$. In the dotted line, we provide the values for $\omega_k$ as computed by the recurrence relationship presented in Proposition 1. (right) Here, we provide the errors for the posterior covariance matrix $\|\Gamma_{\text{post}} - \hat{\Gamma}_{\text{post}}\|_F$ as a function of the iteration, along with the two predicted bounds proposed in Theorem 3.1.

Figure 5.1 shows the performance of the derived bounds. In the left plot, we track the accuracy of the prior-preconditioned data-misfit Hessian $\omega_k = \|HQ - \hat{H}_Q\|_F$ as a function of the number of iterations. It is readily seen that the error decreases considerably and monotonically with increasing $k$, and that $\omega_k$ obtained by recursion is in close agreement with the actual error. This plot shows that, even in floating point arithmetic, the recursion relation for $\omega_k$ can be used to monitor the error of $H_Q$. The right plot in Figure 5.1 contains the errors in the posterior covariance matrix $\|\Gamma_{\text{post}} - \hat{\Gamma}_{\text{post}}\|_F$, which also decreases exponentially. We also provide both of the predicted bounds from Theorem 3.1. While both bounds are qualitatively good, the first bound is slightly better at later iterations, whereas the second bound is more informative at earlier iterations. This can be attributed to the difference in the behavior of $\omega_k$ in the first bound versus $\omega_k/(\lambda^2 + \omega_k)$ in the second bound. These plots provide evidence that the low-rank approximation $\hat{H}_Q$ constructed using available components from the gen-GK bidiagonalization are quite accurate, and the bounds describing their behavior are informative.

For the next illustration, we use the same problem setup, but we investigate a bound for the KL divergence between the prior and the posterior distribution. We found that the bound for the quadratic term $\lambda^2 (s_{\text{post}} - \mu)\top Q^{-1} (s_{\text{post}} - \mu)$ was too pessimistic, which in turn made the bound for the KL divergence in Theorem 3.4 too
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Fig. 5.2. This figure provides the computed error in the simplified KL divergence, along with the predicted bound, as a function of the iteration $k$.

pessimistic. For this reason, we simplified the expression for the KL divergence to

$$D_{KL} = \frac{1}{2} \left[ \text{trace}(Q^{-1}\Gamma_{post}) - n - \log \det(Q^{-1}\Gamma_{post}) \right],$$

and the corresponding approximation is

$$\hat{D}_{KL} = \frac{1}{2} \left[ -\text{trace}(T_k(T_k + \lambda^2 I)^{-1}) + \log \det(I + \lambda^{-2} T_k) \right].$$

Theorem 3.4 then simplifies to $|D_{KL} - \hat{D}_{KL}| \leq \lambda^{-2}\theta_k$, where $\theta_k$ is given in Proposition 3.2. The error in the KL divergence is plotted in Figure 5.2, along with the corresponding bound. We see that the bound captures the behavior of the KL divergence quite well. As for the quadratic term, we found empirically that the error decreases monotonically and is comparable to the simplified expression for the KL divergence. Even the pessimistic bound of Theorem 3.4 suggests that the error eventually decreases to zero with enough iterations. However, a more refined analysis is needed to develop informative bounds for the quadratic term and will be considered in future work.

5.2. Sampling. After discussing the choice of preconditioners, we investigate the performance of the preconditioned Lanczos approaches proposed in section 4.

5.2.1. Choice of preconditioners. In our first example, we explain the choice of preconditioners and show the performance of these preconditioners. We use preconditioners of the form $G = (-\Delta)^\gamma$ for parameters $\gamma \geq 1$, where $\Delta$ is the Laplacian operator discretized using the finite difference operator. This choice of preconditioners is inspired by [24], and exploits the fact that the inverse of integral operators based on the Matérn kernels have inverses which are fractional differential operators.

In this experiment, we pick three different covariance matrices corresponding to Matérn parameters $\nu = 1/2$, $3/2$, and $5/2$; this parameter controls the mean-squared differentiability of the underlying process. For a precise definition of the Matérn covariance function, see [24, Equation (1)]. We now briefly discuss the choice of the exponent $\gamma$. We choose $\gamma = 1/2$, 1, and 2 corresponding to $\nu = 1/2$, $3/2$, and $5/2$ respectively. The domain is taken to be $[0,1]^2$, and we choose a $300 \times 300$ grid of
Fig. 5.3. Convergence of the Lanczos based sampling approach described in subsection 2.2 applied to the prior covariance matrix $Q$. The relative error plotted here is $\tilde{e}_k$ computed as (2.10). Preconditioners are based on fractional powers of the Laplacian $(-\Delta)^\gamma$. The plots correspond to various choices of $\nu$ in the Matern covariance kernel and $\gamma$ in the preconditioner. (left) $\nu = 1/2$ and $\gamma = 1/2$, (middle) $\nu = 3/2$ and $\gamma = 1$, and (right) $\nu = 5/2$ and $\gamma = 2$.

evenly spaced points; thus, $Q$ is a $90,000 \times 90,000$ matrix. The correlation length $\ell$ was taken to be 0.25. In Figure 5.3, we provide the relative errors (computed as $\tilde{e}_k$ from (2.10)) per iteration of the preconditioned and unpreconditioned Lanczos approach for sampling from $N(0, Q)$. It is readily seen that for $\nu = 1/2$ and $3/2$, including the preconditioner can dramatically speed up the convergence. Some improvement is seen for the case of $\nu = 5/2$, but the unpreconditioned solver does not even converge within the maximum allotted number of iterations, which was set to 300. Also, the number of iterations that it takes to converge increases with increasing parameter $\nu$; this is because the systems become more and more ill-conditioned for a fixed grid size. In summary, we see that fractional powers of the Laplacian operator can be good preconditioners to use within the Lanczos methods described in subsection 2.2 for sampling. Next, we investigate the use of these preconditioners for sampling from the posterior distribution.

5.2.2. Sampling from the posterior distribution. In this experiment, we choose two different test problems from the IRTools toolbox [17, 20]. Specifically, we choose the PRspherical which models spherical means tomography such as in photoacoustic tomography, and PRtomo which models parallel X-ray tomography. For both applications, the true image $s$ and forward model matrix $A$ are provided. We use the default settings provided by the toolbox; see [17] for details. To simulate measurement error, we add 2% additive Gaussian noise.

For the PRspherical problem, we first compute the MAP estimate for a grid size of $128 \times 128$ and for $Q$ representing a Matern kernel with $\nu = 1/2$. The reconstruction was computed using gen-HyBR and is provided in the left panel of Figure 5.4. The relative reconstruction error in the 2-norm was 0.0168, and the regularization parameter determined using WGCV was $\lambda^2 \approx 19.48$. The regularization parameter was fixed for the remainder of this experiment. In Figure 5.4, we also show a random draw from the prior distribution $N(0, \lambda^{-2}Q)$ in the middle panel and a random draw from the posterior distribution (computed using Method 2 in subsection 4.2) in the
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Fig. 5.4. For the PRspherical problem, we provide the computed MAP estimate (left), a random draw from the prior distribution (middle), and a random draw from the posterior distribution (right).

In the next experiment, we demonstrate the performance of the preconditioned Lanczos solver proposed in subsection 4.2 for both applications. We vary the grid sizes from $16 \times 16$ to $256 \times 256$, and fix all other parameters ($\nu = 1/2$, 2\% additive Gaussian noise) except the regularization parameter, which was determined for each problem using WGCV. The choice of preconditioners was described in subsection 5.2.1. In Table 5.1 we report the number of iterations for the Lanczos solver to converge (i.e., achieving a residual tolerance of $10^{-6}$) with and without a preconditioner.

### Table 5.1

For various examples from the PRspherical and PRtomo applications, we compare the performance of Method 2 described in Algorithm 4.3. We report the number of unknown parameters and measurements for each problem. Then, we provide the number of iterations (averaged over 10 different runs) required for convergence in the preconditioned and unpreconditioned cases.

| PRspherical application | # unknowns | # measurements | Preconditioner | No preconditioner |
|-------------------------|------------|----------------|----------------|-------------------|
| $16 \times 16$          | 368        | 22.0           | 40.5           |
| $32 \times 32$          | 1,440      | 31.4           | 69.5           |
| $64 \times 64$          | 5,824      | 44.0           | 120.9          |
| $128 \times 128$        | 23,168     | 61.5           | 210.1          |
| $256 \times 256$        | 92,672     | 85.6           | 366            |

| PRtomo application      | # unknowns | # measurements | Preconditioner | No preconditioner |
|-------------------------|------------|----------------|----------------|-------------------|
| $16 \times 16$          | 4,140      | 40.3           | 56.9           |
| $32 \times 32$          | 8,100      | 56.8           | 96.3           |
| $64 \times 64$          | 16,380     | 84.8           | 168.1          |
| $128 \times 128$        | 32,580     | 124.5          | 291.8          |
| $256 \times 256$        | 65,160     | 180.6          | 500+           |

Several observations can be made. First, for both applications the number of iterations required to achieve a desired tolerance increases with increasing problem size. This is to be expected since the number of measurements is also increasing with increasing problem size, and the iterative solver has to work harder to process the additional “information content.” Second, for the same grid size, more iterations are required for the PRtomo application compared to the PRspherical application, which can also be attributed to the additional “information content” brought in by additional measurements. Third, in both applications, the use of a preconditioner cuts the
number of iterations roughly in half. For the largest PRtomo problem we considered, the unpreconditioned iterative solver did not converge within the maximum number of iterations taken to be 500. Since each iteration involves one forward and adjoint matvec involving $A$, each iteration can be quite expensive; the use of a preconditioner is beneficial in this case. Finally, another important observation is that although the preconditioners proposed in subsection 5.2.1 were designed for the prior covariance matrix $Q$, here they were used for the matrix $F$ instead; nevertheless, the results in Table 5.1 demonstrate that the preconditioners were similarly effective.

5.3. Sampling from the approximate posterior distribution. In the next experiment, we investigate the performance of Method 1 described in Algorithm 4.2 for generating samples from the approximate posterior distribution $\hat{\pi}_{\text{post}}$. The problem setup is the same as the previous experiment. We first use the gen-HyBR method to obtain the MAP estimate, the regularization parameter $\lambda^2$, and the low-rank approximation $H_Q$. In the third column of Table 5.2, we report the number of genHyBR iterations; see [15, 14] for details on stopping criteria. Then, we use Algorithm 4.2 to generate samples. Notice that step 3 of Algorithm 4.2 requires the application of $L^{-1}$ to the low-rank approximation; this is accomplished by using the approach described in subsection 2.2, coupled with the choice of preconditioner described in subsection 5.2.1. The number of Lanczos iterations required for Step 3 is reported in the fourth column of Table 5.2. Then, for each sample, step 9 of Algorithm 4.2 requires the application of $L^{-1}$, which is also done using a Lanczos iterative process; the number of iterations for this step, averaged over 10 samples, is listed in the final column of Table 5.2.

| PRspherical application | # unknowns | # measurements | $k$ | Precomputation | Sampling |
|-------------------------|------------|----------------|-----|----------------|----------|
| 16 $\times$ 16          | 368        | 32             | 761 | 14.7           |
| 32 $\times$ 32          | 1,440      | 32             | 653 | 21.1           |
| 64 $\times$ 64          | 5,824      | 27             | 749 | 29.6           |
| 128 $\times$ 128        | 23,168     | 37             | 1433| 42.2           |
| 256 $\times$ 256        | 92,672     | 63             | 3310| 60.2           |

| PRtomo application      | # unknowns | # measurements | $k$ | Precomputation | Sampling |
|-------------------------|------------|----------------|-----|----------------|----------|
| 16 $\times$ 16          | 4,140      | 93             | 1334| 14.0           |
| 32 $\times$ 32          | 8,100      | 51             | 1047| 21.0           |
| 64 $\times$ 64          | 16,380     | 32             | 886 | 29.4           |
| 128 $\times$ 128        | 32,580     | 37             | 1425| 42.0           |
| 256 $\times$ 256        | 65,160     | 51             | 2665| 61.0           |

We make a few remarks about the results. First, the precomputation step to generate the low-rank approximation requires a considerable number of matvecs involving $Q$ but far fewer involving $A$. Next, the number of iterations required for generating
the samples is, on average, smaller than those reported in Table 5.1 for a comparable problem size. The reason for this is that the preconditioner is designed for $Q$ rather than $F$. Finally, the numbers of iterations show similar trends as those in Table 5.1.

6. Conclusions. This paper considers the challenging problem of providing an efficient representation for the posterior covariance matrix arising in high-dimensional inverse problems. To this end, we propose an approximation to the posterior covariance matrix as a low-rank perturbation of the prior covariance matrix. The approximation is computed using information from the Krylov subspaces generated while computing the MAP estimate. As a result, we obtain an approximate and efficient representation for “free.” Several results are presented to quantify the accuracy of this representation and of the resulting posterior distribution. We also show how to efficiently measure uncertainties involving the posterior distribution. Then we present two variants that utilize a preconditioned Lanczos solver to efficiently generate samples from the posterior distribution. The first approach generates samples from an approximate posterior distribution, whereas the second approach generates samples from the exact posterior distribution. The approximate samples can be used as is or as candidate draws from a proposal distribution that closely approximates the exact posterior distribution.

There are several avenues for further research. The first important question is: Can we replace the bounds in the Frobenius norm by the spectral norm? The reason we employed the Frobenius norm is because of the recurrence relation in Proposition 1. Another issue worth exploring is if we can give bounds for the error in the low-rank approximation $\omega_k$ explicitly in terms of the eigenvalues of $H_Q$. This can be beneficial for deciding a priori the number of iterations required for an accurate low-rank approximation when the rate of decay of eigenvalues of $H_Q$ is known. Finally, we are interested in exploring the use of the approximate posterior distribution as a surrogate for the exact posterior distribution inside a Markov Chain Monte Carlo (MCMC) sampler. This is of particular interest for nonlinear problems where the posterior distribution is non-Gaussian. MCMC methods rely heavily on the availability of a good proposal distribution. One approach is to linearize the forward operator about the MAP estimate (the so-called Laplace’s approximation) resulting in a Gaussian distribution with similar structure to $\pi_{\text{post}}$. This approximation to the true posterior distribution can be used as a proposal distribution, see for e.g. [25, 29].

7. Acknowledgements. The authors would like to thank Silvia Gazzola, Per Christian Hansen, and James Nagy for generously sharing an advanced copy of their preprint [17] and code that we used in our numerical experiments.

Appendix A. Proofs.

A.1. Derivation of (3.3). First, we plug in $\hat{\mathbf{\Gamma}}_{\text{post}} = (\lambda^2 \mathbf{Q}^{-1} + \hat{\mathbf{H}})^{-1}$ and rearrange to get

$$\hat{\mathbf{\Gamma}}_{\text{post}} \mathbf{A}^\top \mathbf{R}^{-1} \mathbf{b} = (\lambda^2 \mathbf{Q}^{-1} + \mathbf{V}_k \mathbf{T}_k \mathbf{V}_k^\top)^{-1} \mathbf{A}^\top \mathbf{R}^{-1} \mathbf{b}$$

$$= (\lambda^2 \mathbf{I} + \mathbf{Q} \mathbf{V}_k \mathbf{T}_k \mathbf{V}_k^\top)^{-1} \mathbf{Q} \mathbf{A}^\top \mathbf{R}^{-1} \mathbf{b}.$$  

Then, using the gen-GK relationships, we note that

$$\mathbf{A}^\top \mathbf{R}^{-1} \mathbf{b} = \mathbf{A}^\top \mathbf{R}^{-1} \mathbf{U}_{k+1} \beta_1 e_1 = \mathbf{V}_k \mathbf{B}_k^\top \beta_1 e_1.$$  

Furthermore, using the Woodbury formula, we have

$$(\lambda^2 \mathbf{I} + \mathbf{Q} \mathbf{V}_k \mathbf{T}_k \mathbf{V}_k^\top)^{-1} = \lambda^{-2} \mathbf{I} - \lambda^{-4} \mathbf{Q} \mathbf{V}_k (\mathbf{T}_k^{-1} + \lambda^{-2} \mathbf{I})^{-1} \mathbf{V}_k^\top.$$
Thus, we get
\[ \hat{\Gamma}_{\text{post}} A^T R^{-1} b = (\lambda^{-2} I - \lambda^{-4} Q V_k (T_k^{-1} + \lambda^{-2} I)^{-1} V_k^T) Q V_k B_k^T \beta_1 e_1 \]
\[ = Q V_k (\lambda^{-2} I - \lambda^{-4} (T_k^{-1} + \lambda^{-2} I)^{-1}) B_k^T \beta_1 e_1 \]
\[ = Q V_k (T_k + \lambda^2 I)^{-1} B_k^T \beta_1 e_1, \]
where the last equality uses the fact that \((T_k^{-1} + \lambda^{-2} I)^{-1} = \lambda^2 I - \lambda^4 (T_k + \lambda^2 I)^{-1}. \)
Since \( T_k = B_k^T B_k \), we have the desired result.

**A.2. Proofs for subsection 3.1.**

**Proposition 1.** First, we recognize that \( \hat{H} = V_k T_k V_k^T \), where \( T_k = V_k^T Q H Q V_k \) is a tridiagonal matrix of the form
\[ T_k = \begin{bmatrix}
\mu_1 & \nu_2 & \nu_3 & & \\
\nu_2 & \mu_2 & \nu_3 & \ddots & \\
& \ddots & \ddots & \ddots & \\
& & \nu_{k-1} & \mu_{k-1} & \nu_k \\
& & & \nu_k & \mu_k
\end{bmatrix}, \]
where \( \mu_j = \alpha_j^2 + \beta_{j+1}^2 \) and \( \nu_j = \alpha_j \beta_j \) for \( j = 1, \ldots, k. \)

For simplicity denote \( \hat{V}_k = Q^{1/2} V_k \) and note that the columns of \( \hat{V}_k \) are orthonormal. Then write
\[ H_Q - \hat{H}_Q = (I - \hat{V}_k \hat{V}_k^T) H_Q + \hat{V}_k \hat{V}_k^T H_Q (I - \hat{V}_k \hat{V}_k^T). \]

The observation that \((I - \hat{V}_k \hat{V}_k^T) H_Q \perp \hat{V}_k \hat{V}_k^T H_Q (I - \hat{V}_k \hat{V}_k^T)\) with respect to the trace inner product means we can apply Pythagoras’ theorem to obtain
\[ \omega_k^2 = ||(I - \hat{V}_k \hat{V}_k^T) H_Q||_F^2 + ||\hat{V}_k \hat{V}_k^T H_Q (I - \hat{V}_k \hat{V}_k^T)||_F^2. \]

The second term is easy since using the gen-GK relationships, we have
\[ \hat{V}_k \hat{V}_k^T H_Q (I - \hat{V}_k \hat{V}_k^T) = \alpha_{k+1} \beta_{k+1} \hat{V}_k \hat{V}_k^T, \]
and thus \( ||\alpha_{k+1} \beta_{k+1} \hat{V}_k \hat{V}_k^T||_F^2 = ||\alpha_{k+1} \beta_{k+1}|^2. \) For the first term, denote \( \eta_k = ||(I - \hat{V}_k \hat{V}_k^T) H_Q||_F, \) so that
\[ (A.1) \]
\[ \omega_k^2 = \eta_k^2 + ||\alpha_{k+1} \beta_{k+1}|^2. \]

Then write \( I - \hat{V}_k \hat{V}_k^T = I - \hat{V}_{k+1} \hat{V}_{k+1}^T + \hat{V}_{k+1} \hat{V}_{k+1}^T \) and again apply Pythagoras’ theorem to get
\[ \eta_k^2 = \eta_{k+1}^2 + ||\hat{V}_{k+1} \hat{V}_{k+1}^T H_Q||_F^2. \]

From the gen-GK relations, it can be verified that
\[ (A.2) \]
\[ H_Q \hat{V}_{k+1} \hat{V}_{k+1}^T = \alpha_{k+1} \beta_{k+1} \hat{V}_{k+1} \hat{V}_{k+1}^T + (\alpha_{k+1}^2 + \beta_{k+2}^2) \hat{V}_{k+1} \hat{V}_{k+1}^T + \alpha_{k+2} \beta_{k+2} \hat{V}_{k+2} \hat{V}_{k+2}^T. \]

Since each term is mutually orthogonal, this implies
\[ \eta_k^2 = \eta_{k+1}^2 + ||\alpha_{k+1} \beta_{k+1}|^2 + ||\alpha_{k+1}^2 + \beta_{k+2}^2|^2 + ||\alpha_{k+2} \beta_{k+2}|^2. \]
Together with (A.1), we get the desired recurrence. □
**Theorem 3.1.** We now consider the error in the posterior covariance matrix. For the first bound, using

\[ \Gamma_{\text{post}} = Q^{1/2}(\lambda^2 I + H_Q)^{-1}Q^{1/2}, \]

we have

\[
\begin{align*}
\|\Gamma_{\text{post}} - \tilde{\Gamma}_{\text{post}}\|_F & \leq \|Q\|_2 \|(\lambda^2 I + H_Q)^{-1} - (\lambda^2 I + \tilde{H}_Q)^{-1}\|_F \\
& = \lambda^{-2}\|Q\|_2 \|(I + \lambda^{-2}H_Q)^{-1} - (I + \lambda^{-2}\tilde{H}_Q)^{-1}\|_F.
\end{align*}
\]

With \( f(x) = x/(1 + x) \), it is verifiable that

\[
(I + \lambda^{-2}H_Q)^{-1} - (I + \lambda^{-2}\tilde{H}_Q)^{-1} = f(\lambda^{-2}\tilde{H}_Q) - f(\lambda^{-2}H_Q).
\]

The function \( f \) is operator monotone \cite[Proposition V.1.6]{Ho} and satisfies \( f(0) = 0 \). Since both \( \lambda^{-2}H_Q \) and \( \lambda^{-2}\tilde{H}_Q \) are positive semi-definite, using \cite[Theorem X.1.3]{Ho}, we obtain

\[
\|(I + \lambda^{-2}H_Q)^{-1} - (I + \lambda^{-2}\tilde{H}_Q)^{-1}\|_F \leq \|E(I + |E|)^{-1}\|_F,
\]

where we let \( E = \lambda^{-2}(H_Q - \tilde{H}_Q) \), and \( |E| = (E^*E)^{1/2} \). Note that both \(|E|\) and \( E \) have the same singular values, so \( \|E\|_F = \|E\|_F \). Since \( |E| \) is positive semi-definite, the singular values of \((I + |E|)^{-1}\) are at most 1. By submultiplicativity inequality and \( \|E\|_F = \|E\|_F \), we have

\[
\|(\lambda^2 I + H_Q)^{-1} - (\lambda^2 I + \tilde{H}_Q)^{-1}\|_F \leq \|\lambda^{-2}(H_Q - \tilde{H}_Q)\|_F = \lambda^{-2}\omega_k
\]

and hence the desired result:

\[
\|\Gamma_{\text{post}} - \tilde{\Gamma}_{\text{post}}\|_F \leq \lambda^{-2}\|Q\|_2 \lambda^{-2}\|H_Q - \tilde{H}_Q\|_F = \lambda^{-4}\omega_k\|Q\|_2.
\]

For the second bound, we reserve the use of spectral and Frobenius norms

\[
\|\Gamma_{\text{post}} - \tilde{\Gamma}_{\text{post}}\|_F \leq \lambda^{-2}\|Q\|_2 \|(I + \lambda^{-2}H_Q)^{-1} - (I + \lambda^{-2}\tilde{H}_Q)^{-1}\|_2.
\]

Again, let \( E = \lambda^{-2}(H_Q - \tilde{H}_Q) \), and use \cite[Theorem X.1.1]{Ho} with \( f(x) = x/(1 + x) \), to obtain

\[
\|(I + \lambda^{-2}H_Q)^{-1} - (I + \lambda^{-2}\tilde{H}_Q)^{-1}\|_2 \leq \frac{\|E\|_2}{1 + \|E\|_2}.
\]

It is readily verified that if \( 0 \leq a \leq b \), then \( a(1 + a)^{-1} \leq b(1 + b)^{-1} \), and so

\[
\|(I + \lambda^{-2}H_Q)^{-1} - (I + \lambda^{-2}\tilde{H}_Q)^{-1}\|_2 \leq \frac{\|E\|_2}{1 + \|E\|_2} \leq \frac{\|E\|_F}{1 + \|E\|_F} = \frac{\omega_k}{\lambda^2 + \omega_k}.
\]

The recognition that \( \|E\|_F = \lambda^{-2}\omega_k \) completes the proof. \( \square \)

**A.3. Lemma of independent interest.** We will need the following lemma to prove Theorems 3.3 and 3.4. This may be of independent interest beyond this paper.

**Lemma A.1.** Let \( A \in \mathbb{R}^{n \times n} \) be symmetric positive semi-definite and let \( P \in \mathbb{R}^{n \times n} \) be an orthogonal projection matrix. Then the following results hold

\[
\begin{align*}
\text{(A.8)} & \quad |\text{trace}(I + A)^{-1} - \text{trace}(I + PAP)^{-1}| \leq \text{trace}(A - PAP), \\
\text{(A.9)} & \quad \text{trace}[(I + A)(I + PAP)^{-1}] \leq n + \text{trace}(A - PAP), \\
\text{(A.10)} & \quad 0 \leq \log \text{det}(I + A) - \log \text{det}(I + PAP) \leq \text{trace}(A - PAP).
\end{align*}
\]
Proof. Let \( \{\lambda_i\}_{i=1}^n \) and \( \{\mu_i\}_{i=1}^n \) denote the eigenvalues of \( A \) and \( PAP \). Since both matrices are positive semidefinite, their eigenvalues are non-negative. Since \( P \) is a projection matrix, its singular values are at most 1. The multiplicative singular value inequalities [7, Problem III.6.2] say \( \sigma_i(PA^{1/2}) \leq \sigma_i(A^{1/2}) \), so \( \lambda_i \geq \mu_i \) for \( i = 1, \ldots, n \), and therefore, \( \text{trace}(A) \geq \text{trace}(PAP) \). Then for the first inequality

\[
|\text{trace}(I + PAP)^{-1} - \text{trace}(I + A)^{-1}| = \left| \sum_{i=1}^{n} \frac{\lambda_i - \mu_i}{(1 + \mu_i)(1 + \lambda_i)} \right| \\
\leq \sum_{i=1}^{n} |\lambda_i - \mu_i| = |\text{trace}(A - PAP)|.
\]

The inequalities follow since \( \lambda_i, \mu_i \) are nonegative. The absolute value disappears since \( \text{trace}(A) \geq \text{trace}(PAP) \).

For the second inequality, write

\[
(I + A)(I + PAP)^{-1} = A(I + PAP)^{-1} - PAP(I + PAP)^{-1} + I.
\]

Both \( A \) and \( (I + PAP)^{-1} \) are positive semidefinite (the second matrix is definite), so the trace of their product is nonnegative [21, Exercise 7.2.26]. Then a straightforward application of the von Neumann trace theorem [21, Theorem 7.4.1.1] leads to

\[
\text{trace}(A(I + PAP)^{-1}) \leq \sum_{i=1}^{n} \frac{\lambda_i}{1 + \mu_i}.
\]

By utilizing its eigendecomposition, it is readily seen that \( \text{trace}[PAP(I + PAP)^{-1}] = \sum_{i=1}^{n} \frac{\mu_i}{1 + \mu_i} \). Putting it together, we get

\[
\text{trace}[(I + A)(I + PAP)^{-1}] \leq n + \sum_{i=1}^{n} \left( \frac{\lambda_i}{1 + \mu_i} - \frac{\mu_i}{1 + \mu_i} \right) \\
\leq n + \sum_{i=1}^{n} \frac{\lambda_i - \mu_i}{1 + \mu_i} \leq n + \sum_{i=1}^{n} (\lambda_i - \mu_i).
\]

Connecting the sum of the eigenvalues with the trace delivers the desired result.

For the third inequality, use Sylvester’s determinant lemma to write

\[
\log \det(I + PAP) = \log \det(I + A^{1/2}PA^{1/2}).
\]

Denote \( B = A^{1/2}PA^{1/2} \). Since \( P \leq I \), it follows that \( B \leq A \). Then apply [1, Lemma 9], to obtain

\[
0 \leq \log \det(I + A) - \log \det(I + B) \leq \log \det(I + A - B).
\]

Finally since \( \log(1 + x) \leq x \) for \( x \geq 0 \), \( \log \det(I + A - B) \leq \text{trace}(A - B) \). The proof is completed by observing that \( \text{trace}(B) = \text{trace}(PAP) \) by the cyclic property of trace.

A.4. Proofs of subsection 3.2 and subsection 3.3.

Proposition 3.2. The linearity and cyclic property of trace estimator implies

\[
\theta_k = \text{trace}((I - \hat{V}_k\hat{V}_k^\top)H_Q).
\]
As in the proof of Proposition 1, write $\mathbf{I} - \tilde{\mathbf{V}}_k \tilde{\mathbf{V}}_k^\top = \mathbf{I} - \tilde{\mathbf{V}}_{k+1} \tilde{\mathbf{V}}_{k+1}^\top + \tilde{\mathbf{v}}_{k+1} \tilde{\mathbf{v}}_{k+1}^\top$, so that

$$\theta_k = \theta_{k+1} + \text{trace}(\tilde{\mathbf{v}}_{k+1} \tilde{\mathbf{v}}_{k+1}^\top \mathbf{H}_Q).$$

The proof is finished if we apply the trace to the right hand side of \eqref{eq:loss}. \hfill \Box

**Theorem 3.3.** The lower bound follows from the property of the KL divergence and the fact that the distributions are not degenerate. The proof for the upper bound begins by providing an alternate expression for the error in the KL divergence.

$$D_{KL}(\hat{\pi}_{\text{post}}\|\pi_{\text{post}}) = \frac{1}{2} [\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3],$$

where $\mathcal{E}_1 = \text{trace}(\hat{\mathbf{\Gamma}}_{\text{post}} \mathbf{\Gamma}_{\text{post}}^{-1}) - n$

$$\mathcal{E}_2 = \log \det(\mathbf{\Gamma}_{\text{post}}) - \log \det(\hat{\mathbf{\Gamma}}_{\text{post}}) \quad \mathcal{E}_3 = \|\mathbf{s}_{\text{post}} - \mathbf{s}_k\|^2_{\mathbf{\Gamma}_{\text{post}}^{-1}}.$$

We tackle each term individually. The second term $\mathcal{E}_2$ simplifies since

$$\log \det(\mathbf{\Gamma}_{\text{post}}) - \log \det(\hat{\mathbf{\Gamma}}_{\text{post}}) = \log \det(\mathbf{I} + \lambda^{-2} \hat{\mathbf{H}}_Q) - \log \det(\mathbf{I} + \lambda^{-2} \mathbf{H}_Q).$$

Let $\mathbf{M} = \lambda^{-2}(\mathbf{H}_Q)$, then with $\mathbf{P} = \tilde{\mathbf{V}}_k \tilde{\mathbf{V}}_k^\top$ we have $\lambda^{-2} \hat{\mathbf{H}}_Q = \mathbf{PMP}$. Apply the third inequality in Lemma A.1 to conclude $\mathcal{E}_2 \leq 0$. For the first term $\mathcal{E}_1$, apply the second part of Lemma A.1 to obtain

$$\text{trace}(\hat{\mathbf{\Gamma}}_{\text{post}} \mathbf{\Gamma}_{\text{post}}^{-1}) = \text{trace}((\mathbf{I} + \lambda^{-2} \hat{\mathbf{H}}_Q)^{-1} (\mathbf{I} + \lambda^{-2} \hat{\mathbf{H}}_Q)^{-1}) \leq n + \lambda^{-2} \text{trace}(\mathbf{H}_Q - \hat{\mathbf{H}}_Q).$$

Therefore, $\mathcal{E}_1 \leq \lambda^{-2} \theta_k$. For the third term, notice that

$$\mathbf{\Gamma}_{\text{post}} - \hat{\mathbf{\Gamma}}_{\text{post}} = \lambda^{-2} Q^{1/2} \left( (\mathbf{I} + \lambda^{-2} \mathbf{H}_Q)^{-1} - (\mathbf{I} + \lambda^{-2} \hat{\mathbf{H}}_Q)^{-1} \right) Q^{1/2}$$

and let $\mathbf{D} = (\mathbf{I} + \lambda^{-2} \mathbf{H}_Q)^{-1} - (\mathbf{I} + \lambda^{-2} \hat{\mathbf{H}}_Q)^{-1}$. Then

$$\|\mathbf{s}_{\text{post}} - \mathbf{s}_k\|^2_{\mathbf{\Gamma}_{\text{post}}^{-1}} = \mathbf{b}^\top \mathbf{D} (\mathbf{I} + \lambda^{-2} \mathbf{H}_Q) \mathbf{D} \mathbf{b} \leq \|\mathbf{D} \mathbf{b}\|_2 \|\mathbf{D}\|_2 \|\mathbf{I} + \lambda^{-2} \mathbf{H}_Q\| \|\mathbf{D} \mathbf{b}\|_2,$$

where $\mathbf{b} = Q^{1/2} \mathbf{A}^\top \mathbf{R}^{-1} \mathbf{b}$. The inequality is due to Cauchy-Schwartz. Using \eqref{eq:bound2}, we can bound

$$\|\mathbf{D} \mathbf{b}\|_2 \leq \frac{\omega_k \|\mathbf{D}\|_2 \|\mathbf{b}\|_2}{\lambda^2 + \omega_k}.$$

Next, with $\mathbf{E} = \lambda^{-2} (\mathbf{H}_Q - \hat{\mathbf{H}}_Q)$, consider the simplification

$$(\mathbf{I} + \lambda^{-2} \mathbf{H}_Q) \mathbf{D} = -\mathbf{E} (\mathbf{I} + \lambda^{-2} \hat{\mathbf{H}}_Q)^{-1},$$

so that $\|\mathbf{I} + \lambda^{-2} \mathbf{H}_Q\| \|\mathbf{D} \mathbf{b}\|_2 \leq \lambda^{-2} \omega_k \|\mathbf{b}\|_2$. Here, we have used submultiplicativity and the fact that singular values of $(\mathbf{I} + \lambda^{-2} \hat{\mathbf{H}}_Q)^{-1}$ are at most 1. We also see that $\|\mathbf{b}\|_2 = \alpha_1 \beta_1$. Putting everything together, we see

$$\mathcal{E}_3 \leq \frac{\lambda^{-2} \omega_k^2 \alpha_1^2 \beta_1^2}{\lambda^2 + \omega_k}.$$

Gathering the bounds for $\mathcal{E}_1$, $\mathcal{E}_2$ and $\mathcal{E}_3$ we have the desired result. \hfill \Box
Theorem 3.4. The error in the KL-divergence satisfies

\[ |D_{\text{KL}} - \tilde{D}_{\text{KL}}| \leq \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3, \]

where

\[ \mathcal{E}_1 = \frac{1}{2} \left| \text{trace}(I + \lambda^{-2}H_Q)^{-1} - \text{trace}(I + \lambda^{-2}\hat{H}_Q)^{-1} \right| \]
\[ \mathcal{E}_2 = \frac{1}{2} \left| \log \det(I + \lambda^{-2}H_Q) - \log \det(I + \lambda^{-2}\hat{H}_Q) \right| \]
\[ \mathcal{E}_3 = \frac{1}{2} \lambda^2 |(s_{\text{post}} - \mu)^\top Q^{-1}(s_{\text{post}} - \mu) - (s_k - \mu)^\top Q^{-1}(s_k - \mu)|. \]

We tackle the first two terms together. As in the proof of Theorem 3.3, let \( M = \lambda^{-2}(H_Q) \), then with \( P = \tilde{V}_k \tilde{V}_k^\top \) we have \( \lambda^{-2}\hat{H}_Q = PMP \). Apply the first and the third parts of Lemma A.1 to obtain

\[ \mathcal{E}_1 \leq \frac{\lambda^{-2}}{2} \text{trace}(H_Q - \hat{H}_Q) \quad \mathcal{E}_2 \leq \frac{\lambda^{-2}}{2} \text{trace}(H_Q - \hat{H}_Q). \]

For the third term, let \( s_{\text{post}} = s_k + e \), then

\[ \mathcal{E}_3 = \frac{1}{2} \lambda^2 |(s_{\text{post}} - s_k)^\top Q^{-1}(s_{\text{post}} - \mu) + (s_k - \mu)^\top Q^{-1}e|. \]

Notice that \( e = s_{\text{post}} - s_k = (\Gamma_{\text{post}} - \tilde{\Gamma}_{\text{post}})A^\top R^{-1}b \). Let

\[ \tilde{b} = Q^{1/2}A^\top R^{-1}b = \alpha_1 \beta_1 Q^{1/2}v_1, \]

and write

\[ Q^{-1/2}e = \left( (\lambda^2 I + H_Q)^{-1} - (\lambda^2 I + \hat{H}_Q)^{-1} \right) \tilde{b}. \]

So, the submultiplicative inequality and (A.7) implies

\[ \|Q^{-1/2}e\|_2 \leq \lambda^{-2} \| (I + \lambda^{-2}\hat{H}_Q)^{-1} - (I + \lambda^{-2}H_Q)^{-1} \|_2 \| \tilde{b} \|_2 \leq \lambda^{-2} \frac{\omega_k}{\lambda^2 + \omega_k} \alpha_1 \beta_1 , \]

where we have used (A.5). Next, applying the Cauchy-Schwartz inequality

\[ |x^\top Q^{-1}(s_{\text{post}} - \mu)| \leq \|Q^{-1/2}e\|_2 \|Q^{-1/2}(s_{\text{post}} - \mu)\|_2. \]

Then, rewriting \( s_{\text{post}} = \mu + \Gamma_{\text{post}}A^\top R^{-1}b \), we have

\[ \|Q^{-1/2}(s_{\text{post}} - \mu)\|_2 = \| (I + \lambda^{-2}H_Q)^{-1} \tilde{b} \|_2 \leq \| \tilde{b} \|_2 = \alpha_1 \beta_1 , \]

since the singular values of \( (I + \lambda^{-2}\hat{H}_Q)^{-1} \) are less than 1. The other term is bounded in the same way. So, we have

\[ \mathcal{E}_3 \leq \frac{\omega_k}{\lambda^2 + \omega_k} \alpha_1^2 \beta_1^2. \]

Putting everything together along with \( \mathcal{E}_1 + \mathcal{E}_2 \leq \lambda^{-2} \theta_k \) gives the desired result. \( \square \)
A.5. Proofs of section 4.

Theorem 4.1. By the triangle inequality, we have
\[ \|s - \hat{s}\|_{\lambda^2 Q^{-1}} \leq \|s_{\text{post}} - s_k\|_{\lambda^2 Q^{-1}} + \|S\epsilon - \hat{S}\epsilon\|_{\lambda^2 Q^{-1}}. \]
Similar to previous proofs, we use \( s_{\text{post}} - s_k = (\Gamma_{\text{post}} - \hat{\Gamma}_{\text{post}})A^\top R^{-1}b = \lambda^{-2}Q^{1/2}Db \), where \( D = (I + \lambda^{-2}H_Q)^{-1} - (I + \lambda^{-2}\hat{H}_Q)^{-1} \) to get
\[ \|s_{\text{post}} - s_k\|_{\lambda^2 Q^{-1}} = \hat{b}^\top DQ^{1/2}\lambda^{-2}(\lambda^2 Q^{-1})\lambda^{-2}Q^{1/2}Db = \lambda^{-2}\|Db\|_2^2. \]
Thus,
\[ \|s_{\text{post}} - s_k\|_{\lambda^2 Q^{-1}} = \lambda^{-1}\|Db\|_2 \leq \lambda^{-1} \frac{\omega_k\alpha_1\beta_1}{\lambda^2 + \omega_k}. \]
For the second term, we write
\[ \lambda Q^{-1/2}(S - \hat{S})\epsilon = \left[ (I + \lambda^{-2}H_Q)^{-1/2} - (I + \lambda^{-2}\hat{H}_Q)^{-1/2} \right] \epsilon. \]
Then, applying submultiplicativity
\[ \|S\epsilon - \hat{S}\epsilon\|_{\lambda^2 Q^{-1}} = \|\lambda Q^{-1/2}(S - \hat{S})\epsilon\|_2 \leq \|(I + \lambda^{-2}\hat{H}_Q)^{-1/2} - (I + \lambda^{-2}H_Q)^{-1/2}\|_2 \|\epsilon\|_2. \]
When we apply [7, Theorem X.1.1 and (X.2)], we have
\[ \|(I + \lambda^{-2}\hat{H}_Q)^{-1/2} - (I + \lambda^{-2}H_Q)^{-1/2}\|_2 \leq \|D\|_2^{1/2}. \]
From (A.7), \( \|D\|_2 \leq \omega_k/(\lambda^2 + \omega_k) \). Plugging this in gives the desired result. \( \square \)

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