UNSCENTED KALMAN INVERSION: EFFICIENT GAUSSIAN APPROXIMATION TO THE POSTERIOR DISTRIBUTION

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Abstract. The unscented Kalman inversion (UKI) method presented in [1] is a general derivative-free approach for the inverse problem. UKI is particularly suitable for inverse problems where the forward model is given as a black box and may not be differentiable. The regularization strategies, convergence property, and speed-up strategies [1, 2] of the UKI are thoroughly studied, and the method is capable of handling noisy observation data and solving chaotic inverse problems. In this paper, we study the uncertainty quantification capability of the UKI. We propose a modified UKI, which allows to well approximate the mean and covariance of the posterior distribution with an uninformative prior for identifiable (well-posed) inverse problems. Theoretical guarantees for both linear and nonlinear inverse problems are presented. Numerical results, including learning of permeability parameters in subsurface flow and of the Navier-Stokes initial condition from solution data at positive times are presented. The results obtained by the UKI require only $O(10)$ iterations, and match well with the expected results obtained by the Markov Chain Monte Carlo method.

Key words. Inverse Problem, Uncertainty Quantification, Kalman Filter, Bayesian Inference, Unscented Kalman Inversion

AMS subject classifications. 60G35, 62F15, 62M20, 65N21

1. Introduction. Inverse problems are ubiquitous in engineering and science applications. These include, to name only a few, global climate model calibration [3, 4, 5], material constitutive relation calibration [6, 7, 8], seismic inversion in geophysics [9, 10], and medical tomography [11, 12]. These problems may feature multiple scales and may include chaotic and turbulent phenomena, and hence the forward models are very expensive to evaluate. Moreover, the observation data are noisy and uncertainty quantification is important.

Inverse problems can be formulated as recovering unknown parameters $\theta \in \mathbb{R}^N$ from the noisy observation $y \in \mathbb{R}^N$, as following

\begin{equation}
    y = \mathcal{G}(\theta) + \eta,
\end{equation}

where $\mathcal{G}$ denotes a forward operator mapping parameters to observations, and $\eta$ denotes the observational error, which might depend on $\theta$ or $y$. An estimated distribution of $\eta \sim \mathcal{N}(0, \Sigma_\eta)$ is given.

From optimization viewpoint, the inverse problem can be formulated to the following nonlinear least-square optimization problem [13]:

\begin{align}
    \Phi_R(\theta, y) &:= \Phi(\theta, y) + \frac{1}{2} \| \Sigma_0^{-\frac{1}{2}} (\theta - r_0) \|^2, \\
    \Phi(\theta, y) &:= \frac{1}{2} \| \Sigma_\eta^{-\frac{1}{2}} (y - \mathcal{G}(\theta)) \|^2,
\end{align}

where $\Phi_R$ and $\Phi$ are regularized and non-regularized objective functions, respectively. $\Sigma_0 > 0$ is strictly positive-definite and normalizes the model-data misfit. $r_0$ and $\Sigma_\eta > 0$ encode prior mean and covariance information about $\theta$. From Bayesian viewpoint, $\theta$ and $y$ are treated as random variables, and the inverse problem can be formulated as posterior distribution approximation problem [14, 15]:

\begin{equation}
    \mu(d\theta) = \frac{1}{Z(y)} e^{-\Phi(\theta, y)} \mu_0(d\theta),
\end{equation}

where $\mu_0(d\theta)$ is the prior and $Z(y)$ is the normalization constant:

\begin{equation}
    Z(y) = \int e^{-\Phi(\theta, y)} \mu_0(d\theta).
\end{equation}

The optimization viewpoint and the Bayesian viewpoint are linked via the fact that the minimizer of the nonlinear least-square optimization problem $\Phi(\theta, y)$ coincides with the maximum a posterior (MAP) estimator of (1.3) with an uninformative prior, and the minimizer of the regularized nonlinear least-square optimization problem $\Phi_R(\theta, y)$ coincides with the MAP estimator of (1.3).

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Kalman inversion methods, which take advantage of Kalman filtering \cite{16, 17, 18, 19, 20}, a powerful state estimation technique, are able to unify both optimization and Bayesian viewpoints. This methodology, including but not limited to unscented (UKI) and ensemble (EKI) Kalman inversions, used as a non-intrusive optimization method for parameter estimation, originates in the papers \cite{21, 22, 23, 24, 25, 26}. For inverse problems in general, they are attractive because they are derivative-free, and hence introduce a significant flexibility in the forward solver design. Therefore, Kalman inversions are suitable for complex multiphysics problems requiring coupling of different solvers \cite{27, 28, 29, 30, 31} and methods containing discontinuities (i.e., immersed/embedded boundary method \cite{32, 33, 34, 35} and adaptive mesh refinement \cite{36, 37}). However, as for Bayesian inference, due to the Gaussian ansatz in Kalman filtering, the capability of Kalman inversions to quantify uncertainties or approximate posterior distribution remains unclarified. This work focuses on understanding and improving the capability of Kalman inversions, specifically the UKI, to provide accurate Gaussian approximations to the posterior distribution.

1.1. Literature Review. The Kalman filter \cite{16} and its variants, including but not limit to extended Kalman filter \cite{17}, ensemble Kalman filter \cite{18}, unscented Kalman filter \cite{19, 23}, and cubature Kalman filter \cite{20} are developed to sequentially update the probability distribution of states in partially observed dynamics. Kalman filtering is a two-step procedure: the prediction step, where the state is computed forward in time; the analysis step, where the state and its uncertainty are corrected to take into account the observation. In the analysis step, Kalman filters use Gaussian ansatz to formulate Kalman gain to assimilate the observation and update the distribution, which is valid only for linear state estimation problems, where the probability distribution of states remains Gaussian given Gaussian priors. Therefore, Kalman filters do not produce correct estimate of posterior distribution for non-Gaussian problems \cite{38}. However, numerous applications of Kalman filters, including weather forecasts \cite{18, 39, 40} and guidance, navigation, and control of vehicles \cite{17, 19, 20} demonstrate empirically that Kalman filters can not only calibrate the model prediction, but also provides uncertainty information for nonlinear state estimation problems, specifically the mean and covariance estimation. To get better posterior estimation, particle filters \cite{41} are needed, where the distribution is represented by a large number of random samples. Most of particle filters consist of prediction step and analysis step. In the analysis step, these samples and their associated weights are corrected with the information provided by the observation. The standard particle filter corrects the weights of each sample following Bayes’ theorem. Different correction methods are proposed, which lead to the random maximum likelihood method \cite{42, 43}, the nonparametric ensemble transform method \cite{44}, and etc.

Filter methods can also be used to estimate the parameters, where the filters are recursively applied to an artificial stochastic dynamical system generally with identity state transition matrix. This leads to different inversion methods, to name only a few, sequential Monte Carlo sampler (SMC) \cite{45, 46, 47}, random maximum likelihood method \cite{43, 24}, ensemble Kalman inversion \cite{48, 49, 25}, unscented Kalman inversion \cite{23, 1, 2}. Besides estimating the parameters by minimizing the nonlinear least square problems \eqref{1.2}, these inversion methods are derived in the Bayesian framework, and therefore, have the potential to deliver sensitivity and uncertainty information.

This paper mainly focuses on Kalman inversion methodology, which is a general derivative-free approach to solving the inverse problem. So far, the Kalman inversions have mainly been used for parameter estimation \cite{25, 50, 51, 52, 53, 54} rather than for Bayesian inference for quantifying uncertainty. Due to the Gaussian ansatz and the iterative nature, Kalman inversions generally do not converge to the posterior distribution. Specifically, the mean converges but not the covariance in the nonlinear case. Negative numerical evidences are reported in \cite{55, 56}. In the present work, we improve the UKI by modifying the stochastic dynamical system through iteratively updating the artificial evolution error covariance matrix. And we demonstrate both theoretically and numerically that equipping with the modified stochastic dynamical system, the Kalman inversion, specifically the UKI, is able to provide good Gaussian approximations to the posterior distribution with an uninformative prior for both linear and nonlinear inverse problems under certain regularity assumptions.

1.2. Our Contributions. Our main contribution is the development of theoretical and numerical understanding about UKI for Bayesian inference for quantifying uncertainty.

- We modify the stochastic dynamical system of Kalman inversions proposed in \cite{1, 2} by iteratively updating the artificial evolution covariance matrix, which enables better approximating the posterior covariance matrix.
• With this modification, for linear inverse problems, we prove the exponential convergence of the UKI. The mean converges to a minimizer of $\Phi$ and the precision matrix converges to the posterior precision matrix with an uninformative prior.

• With this modification, for nonlinear inverse problems, we prove the UKI approximates well with the mean and covariance of the posterior distribution with an uninformative prior, when the forward operator $G$ is bijective and satisfies certain regularity conditions.

• We demonstrate on model problems with 1 to 32 parameters that the UKI delivers similar mean and covariance comparing to Markov Chain Monte Carlo method. We believe the UKI can be used for large-scale Bayesian inference for quantifying uncertainty.

The remainder of the paper is organized as follows. In section 2, an overview of Kalman inversion algorithm and the modified UKI are presented. In section 3, theoretical results for the modified UKI are presented. Numerical applications are provided in section 4, that empirically confirm the theories and demonstrate the effectiveness of the UKI for Bayesian inference for quantifying uncertainty.

2. The Algorithm. Kalman inversion methods pair the parameter-to-data map $G$ with a stochastic dynamical system for the parameter and then employ techniques from filtering to estimate the parameter given the data. Consider the following stochastic dynamical system,$^1$

\[
\begin{align*}
(2.1a) & \quad \text{evolution:} & \quad \theta_{n+1} &= \theta_n + \omega_{n+1}, & \quad \omega_{n+1} &\sim \mathcal{N}(0, \Sigma_\omega) \\
(2.1b) & \quad \text{observation:} & \quad y_{n+1} &= G(\theta_{n+1}) + \nu_{n+1}, & \quad \nu_{n+1} &\sim \mathcal{N}(0, \Sigma_\nu)
\end{align*}
\]

where $\theta_{n+1}$ is the unknown state vector, and $y_{n+1}$ the observation, the artificial evolution error $\omega_{n+1}$ and artificial observation error $\nu_{n+1}$ are mutually independent, zero-mean Gaussian sequences with covariances $\Sigma_\omega$ and $\Sigma_\nu$, respectively. Let denote $Y_{n+1} := \{y_1, y_2, \cdots, y_{n+1}\}$, the observation set at time $n+1$. Filtering techniques are employed to approximate $\mu_{n+1}$, the conditional distribution of $\theta_{n+1} | Y_{n+1}$. And the updating of $\{\mu_n\}$ is through the prediction and analysis steps $[57, 58]$: $\mu_n \mapsto \hat{\mu}_{n+1}$, and then $\hat{\mu}_{n+1} \mapsto \mu_{n+1}$, where $\hat{\mu}_{n+1}$ is the distribution of $\theta_{n+1} | Y_n$.

2.1. Gaussian Approximation. This conceptual algorithm maps Gaussians into Gaussians. In the prediction step, assume that $\mu_n \approx \mathcal{N}(m_n, C_n)$, then under (2.1a), $\hat{\mu}_{n+1} = \mathcal{N}(\hat{m}_{n+1}, \hat{C}_{n+1})$ is also Gaussian and satisfies

\[
\hat{m}_{n+1} = \mathbb{E}[\theta_{n+1} | Y_n] = m_n, \quad \hat{C}_{n+1} = \text{Cov}[\theta_{n+1} | Y_n] = C_n + \Sigma_\omega.
\]

In the analysis step, we assume that the joint distribution of $\{\theta_{n+1}, y_{n+1}\} | Y_n$ can be approximated by a Gaussian distribution

\[
\mathcal{N}\left( \begin{bmatrix} \hat{m}_{n+1} \\ \hat{y}_{n+1} \end{bmatrix}, \begin{bmatrix} \hat{C}_{n+1} & \hat{C}_{n+1}^{\text{pp}} \\ \hat{C}_{n+1}^{\text{dp}} & \hat{C}_{n+1}^{\text{pp}} \end{bmatrix} \right),
\]

where

\[
\begin{align*}
\hat{y}_{n+1} &= \mathbb{E}[y_{n+1} | Y_n] = \mathbb{E}[G(\theta_{n+1}) | Y_n], \\
\hat{C}_{n+1}^{\text{dp}} &= \text{Cov}[\theta_{n+1}, y_{n+1} | Y_n] = \text{Cov}[\theta_{n+1}, G(\theta_{n+1}) | Y_n], \\
\hat{C}_{n+1}^{\text{pp}} &= \text{Cov}[y_{n+1} | Y_n] = \text{Cov}[G(\theta_{n+1}) | Y_n] + \Sigma_\nu.
\end{align*}
\]

Conditioning the Gaussian in (2.3) to find $\theta_{n+1} | Y_n, y_{n+1} = \theta_{n+1} | y_{n+1}$, gives the following expressions for the mean $m_{n+1}$ and covariance $C_{n+1}$ of the approximation to $\mu_{n+1}$:

\[
\begin{align*}
m_{n+1} &= \hat{m}_{n+1} + \hat{C}_{n+1}^{\text{dp}} (\hat{C}_{n+1}^{\text{pp}})^{-1} (y_{n+1} - \hat{y}_{n+1}), \\
C_{n+1} &= \hat{C}_{n+1} - \hat{C}_{n+1}^{\text{dp}} (\hat{C}_{n+1}^{\text{pp}})^{-1} \hat{C}_{n+1}^{\text{dp}} T.
\end{align*}
\]

$^1$In the present study, we focus on the dynamics without regularization, which is equivalent to setting $\alpha = 1$ in [1, 2].
Remark 2.1. Assume $\mu_n = \mathcal{N}(m_n, C_n)$, for linear $\mathcal{G}$, the Gaussian approximation $\mathcal{N}(m_{n+1}, C_{n+1})$ in (2.5) is exact, namely $\mu_{n+1} = \mathcal{N}(m_{n+1}, C_{n+1})$; for nonlinear but close to linear $\mathcal{G}$, the Gaussian approximation $\mathcal{N}(m_{n+1}, C_{n+1})$ is a good approximation of the conditional distribution $\mu_{n+1}$, an upper bound of the Kullback–Leibler divergence between them is presented in Appendix A.

As a method for solving the inverse problem (1.1), it is implemented by assuming all observations $\{y_n\}$ are identical to $y$ ($Y_n = y$) and iterating in $n$. Equations (2.2)–(2.5) establish a conceptual algorithm for application of Gaussian approximation to solve the inverse problems. And the integrals appearing in (2.4) are approximated by the extended or unscented approach, which is detailed in the following subsections.

2.2. Extended Kalman Inversion (ExKI).

ExKI approximates integrals in (2.4) analytically by applying first-order Taylor expansion to $\mathcal{G}(\theta_{n+1})$ at the conditional expectation $\mathbb{E}[\theta_{n+1} \mid y] = \hat{m}_{n+1}$,

\begin{equation}
\mathcal{G}(\theta_{n+1}) \approx \mathcal{G}(\hat{m}_{n+1}) + d\mathcal{G}(\hat{m}_{n+1})(\theta_{n+1} - \hat{m}_{n+1}).
\end{equation}

And the iteration procedure of ExKI becomes:

- **Prediction step**:
  \begin{equation}
  \hat{m}_{n+1} = m_n \quad \hat{C}_{n+1} = C_n + \Sigma_w.
  \end{equation}

- **Analysis step**:
  \begin{equation}
  \begin{aligned}
  \hat{y}_{n+1} &= \mathcal{G}(\hat{m}_{n+1}), \\
  \hat{C}_{n+1}^\theta &= \hat{C}_{n+1} + d\mathcal{G}(\hat{m}_{n+1})^T, \\
  \hat{C}_{n+1}^{pp} &= d\mathcal{G}(\hat{m}_{n+1})\hat{C}_{n+1}^p d\mathcal{G}(\hat{m}_{n+1})^T + \Sigma_w, \\
  m_{n+1} &= \hat{m}_{n+1} + \hat{C}_{n+1}^\theta (\hat{y}_{n+1} - \hat{y}_{n+1}), \\
  C_{n+1} &= \hat{C}_{n+1} - \hat{C}_{n+1}^{pp} (\hat{C}_{n+1}^{pp})^{-1} \hat{C}_{n+1}^\theta.
  \end{aligned}
  \end{equation}

2.3. Unscented Kalman Inversion (UKI).

UKI approximates the integrals in (2.4) by means of deterministic quadrature rules. This is the idea of the unscented transform [19, 23] which we now define.

Definition 2.2 (Modified Unscented Transform [1]).

Let denote Gaussian random variable $\theta \sim \mathcal{N}(m, C) \in \mathbb{R}^{N_\theta}$, $2N_\theta + 1$ symmetric sigma points are chosen deterministically:

\begin{equation}
\theta^0 = m \quad \theta^j = m + c_j [\sqrt{C}]_{jj} \quad \theta^{j+N_\theta} = m - c_j [\sqrt{C}]_{jj} \quad (1 \leq j \leq N_\theta),
\end{equation}

where $[\sqrt{C}]_{jj}$ is the $j$th column of the Cholesky factor of $C$. The quadrature rule approximates the mean and covariance of the transformed variable $\mathcal{G}_i(\theta)$ as follows,

\begin{equation}
\mathbb{E}[\mathcal{G}_i(\theta)] \approx \mathcal{G}_i(\theta^0) \quad \text{Cov}[\mathcal{G}_1(\theta), \mathcal{G}_2(\theta)] \approx \sum_{j=1}^{2N_\theta} W_j^c (\mathcal{G}_1(\theta^j) - \mathbb{E}[\mathcal{G}_1(\theta)]) (\mathcal{G}_2(\theta^j) - \mathbb{E}[\mathcal{G}_2(\theta)])^T.
\end{equation}

Here these constant weights are

\begin{equation}
c_1 = c_2 \cdots = c_{N_\theta} = \sqrt{N_\theta + \lambda} \quad W_j^c = \frac{1}{2(N_\theta + \lambda)} \quad (j = 1, \cdots, 2N_\theta)
\end{equation}

\begin{equation}
\lambda = a^2(N_\theta + \kappa) - N_\theta \quad \kappa = 0 \quad a = \min\{\sqrt{\frac{4}{N_\theta + \kappa}} - 1\}.
\end{equation}

Consider the Gaussian approximation algorithm defined by (2.2)–(2.5). By utilizing the aforementioned quadrature rule, the iteration procedure of the UKI becomes:

- **Prediction step**:
  \begin{equation}
  \hat{m}_{n+1} = m_n \quad \hat{C}_{n+1} = C_n + \Sigma_w.
  \end{equation}
under certain conditions. In the limit of large $G$ provides an accurate Gaussian approximation to the posterior distribution $\theta$. The approach is through the following updating relation

$$m_{n+1} = \widehat{m}_{n+1} = \widehat{m}_{n+1} + c_j \sqrt{\widehat{C}_{n+1}} \quad (1 \leq j \leq N_\theta),$$

$$\widehat{y}_{n+1} = \widehat{m}_{n+1} - c_j \sqrt{\widehat{C}_{n+1}}.$$  

• Analysis step:

$$\widehat{y}^i_{n+1} = G(\widehat{\theta}^i_{n+1}), \quad \widehat{y}_{n+1} = \widehat{y}^0_{n+1},$$

$$\widehat{C}_{n+1} = \sum_{j=1}^{2N_\nu} W^c_j (\widehat{\theta}^j_{n+1} - \widehat{m}_{n+1})(\widehat{y}^j_{n+1} - \widehat{y}_{n+1})^T,$$

$$m_{n+1} = \widehat{m}_{n+1} + \widehat{C}_{n+1}^{-1} (y - \widehat{y}_{n+1}),$$

$$C_{n+1} = \widehat{C}_{n+1} - \widehat{C}_{n+1}^{-1} \widehat{C}_{n+1}^T.$$

2.4. Choice of Hyperparameters. The hyperparameters $r$, $\Sigma_\omega$ and $\Sigma_\nu$ in the stochastic dynamical system (2.1) are chosen at the $n$-th iteration, as following

$$r = r_0, \quad \Sigma_\nu = 2\Sigma_\eta \quad \text{and} \quad \Sigma_\omega = C_n,$$

here $r_0$ is the prior mean. It is worth mentioning the artificial evolution error covariance $\Sigma_\omega$ is updated as the estimated covariance $C_n$. This choice of $\Sigma_\omega$ marks the key difference to the previous UKI discussed in [1, 2].

3. Theoretical Insights. The aforementioned Kalman inversion methodology recursively applies Gaussian approximation in each iteration to solve the inverse problem. A useful way to think of the iterative approach is through the following updating relation

$$\mu_{n+1}(d\theta) = \frac{1}{Z_n} \exp \left( -\Phi(\theta, y) \right) \mu_n(d\theta).$$

In the limit of large $n$, $\mu_n$ will tend to concentrate on minimizers of $\Phi$; this follows from the identity

$$\mu_n(d\theta) = \frac{1}{(\Pi_{t=0}^{n-1} Z_t)} \exp \left( -n\Phi(\theta, y) \right) \mu_0(d\theta).$$

The prior information fades away, and therefore, Kalman inversion methodology generally does not converge to the posterior distribution $\theta|y$.

However, in this section, we will show that Kalman inversion with the hyperparameters defined in (2.13) provides an accurate Gaussian approximation to the posterior distribution $\theta|y$ with an uninformative prior under certain conditions.

3.1. The Linear Setting. In this subsection, we study the UKI in the context of linear inverse problems, for which $G(\cdot) = G$. Thanks to the linearity, equations (2.4) are reduced to

$$\widehat{y}_{n+1} = Gm_n, \quad \widehat{C}_{n+1} = \widehat{C}_{n+1}^T G^T, \quad \text{and} \quad \widehat{C}_{n+1} = G\widehat{C}_{n+1}^T G^T + \Sigma_\nu.$$

The update equations (2.5) become

$$m_{n+1} = m_n + \widehat{C}_{n+1}^T (G\widehat{C}_{n+1} G^T + \Sigma_\nu)^{-1} (y - Gm_n),$$

$$C_{n+1} = \widehat{C}_{n+1} - \widehat{C}_{n+1}^T (G\widehat{C}_{n+1} G^T + \Sigma_\nu)^{-1} G\widehat{C}_{n+1},$$

with $\widehat{C}_{n+1} = C_n + \Sigma_\omega$. We have the following theorem about the convergence of the Kalman inversion:
Theorem 3.1. Assume the prior covariance matrix \( C_0 \succ 0 \) is strictly positive definite. The iteration for the conditional mean \( m_n \) and precision matrix \( C_n^{-1} \) characterizing the distribution of \( \theta_n | Y_n \) converges exponentially fast to limit \( m_\infty, C_\infty^{-1} \). Furthermore the limiting mean \( m_\infty \) is a minimizer of the unregularized least squares functional \( \Phi (1.2b) \); the limiting precision matrix \( C_\infty^{-1} = G^T \Sigma^{-1} G \), which is the posterior precision matrix with an uninformative prior.

Proof. The proof is in Appendix B.

Remark 3.2. When \( G \) has empty null space, which corresponds to an identifiable inverse problem, the posterior distribution with an uninformative prior exists. The covariance matrix \( \{ C_n \} \) converges to \( \left(G^T \Sigma^{-1} G\right)^{-1} \), which is the posterior covariance matrix with the uninformative prior.

Remark 3.3. When \( G \) has non-empty null space, namely \( G^T \Sigma^{-1} G \) is singular, and hence the posterior distribution with an uninformative prior does not exist. \( C_\infty^{-1} \) is singular and therefore, the covariance matrix \( \{ C_n \} \) diverges to \( \infty \). We have the following bound

\[
C_n \preceq 2^n C_0.
\]

3.2. The Nonlinear Setting. In this subsection, we study the UKI in the context of nonlinear identifiable (well-posed) inverse problems. The following pull-back distribution bridges the posterior distribution (1.3) and the stationary Gaussian distribution obtained by the Kalman inversion.

Definition 3.4 (Pull-back random variable). Assume \( \theta_0 = N_y \), given a bijective function \( \mathcal{G} : \mathbb{R}^{N_\theta} \mapsto \mathbb{R}^{N_y} \) and an arbitrary vector \( y \in \mathbb{R}^{N_y} \). For any random vector \( \xi \in \mathbb{R}^{N_\theta} \), the corresponding pull-back random variable is defined as

\[
\theta^\xi = \mathcal{G}^{-1}(y - \xi).
\]

We have the following theorem about the posterior distribution \( \theta | y \) with an uninformative prior defined in (1.3) and the pull-back distribution of \( \theta^\xi = \mathcal{G}^{-1}(y - \eta) \):

Theorem 3.5. Consider the posterior density function \( p(\theta | y) \) with an uninformative prior

\[
p(\theta | y) \sim \frac{1}{Z} e^{-\Phi(\theta, y)},
\]

and the pull-back density function \( p(\theta^\xi) \). We assume

1. the map \( \mathcal{G} \) is a bijection, hence, \( N_\theta = N_y \) and \( \mathcal{G}^{-1} \) exists,
2. \( \left| \det \frac{d \mathcal{G}^{-1}(\theta)}{d \theta} \right| \) has Lipschitz property:

\[
\left| \det \frac{d \mathcal{G}^{-1}(\theta_1)}{d \theta} - \det \frac{d \mathcal{G}^{-1}(\theta_2)}{d \theta} \right| \leq c_0 \| \theta_1 - \theta_2 \|^{c_1},
\]

3. \( \mathcal{G}^{-1}(\theta) \) does not grow too fast, and we have

\[
\frac{1}{\sqrt{(2\pi)^{N_\theta} \det \Sigma_\eta}} \int e^{-\frac{1}{2} (y - \hat{\theta})^T \Sigma_\eta^{-1} (y - \hat{\theta})} \left| \det \frac{d \mathcal{G}^{-1}(\theta)}{d \theta} \right|^{c_1} d \theta \leq c_2,
\]

4. The normalization constant

\[
Z = \int e^{-\Phi(\theta, y)} d \theta = \int e^{-\frac{1}{2} (y - \hat{\theta})^T \Sigma_\eta^{-1} (y - \hat{\theta})} \left| \det \frac{d \mathcal{G}^{-1}(\theta)}{d \theta} \right|^{c_1} d \theta' \text{ where } \theta' = \mathcal{G}(\theta)
\]

exists and has positive lower bound \( Z \geq c_3 > 0 \).

5. \( c_i \) and \( N_\theta \) are \( O(1) \) constants, and the spectral radius of \( \Sigma_\eta, \rho(\Sigma_\eta) \) is small enough.

Then \( p(\theta | y) \) and \( p(\theta^\xi) \) have close mean and covariance, which satisfy

\[
\| m - m^\xi \|_\infty = O(\rho(\Sigma_\eta)^{c_1} \sqrt{\det \Sigma_\eta}) \quad \text{and} \quad \| C - C^\xi \|_\infty = O(\rho(\Sigma_\eta)^{c_1} \sqrt{\det \Sigma_\eta}),
\]

here \( m \) and \( C \) and \( m^\xi \) and \( C^\xi \) are the mean and covariance of \( p(\theta | y) \) and \( p(\theta^\xi) \), respectively.
Proof. The proof is in Appendix C.

We have the following theorem about the pull back distribution of $\theta^0$ and the ExKI,

**Theorem 3.6.** Assume $N_\theta = N_y$ and $G$ is a bijection. Any stationery mean and covariance $m_\ast, C_\ast$ obtained by the ExKI, which satisfy that both $dG(m_\ast)$ and $C_\ast$ are non-singular, then

$$m_\ast = G^{-1}(y) \quad \text{and} \quad C_\ast^{-1} = dG(m_\ast)^T \Sigma^{-1}_\eta dG(m_\ast).$$

And they are the mean and covariance estimation of the pull-back random variable $\theta^0$ obtained by the extended Kalman filter.

Proof. The proof is in Appendix D.

Combining Theorems 3.5 and 3.6, we have, in the presence of small observation error, the ExKI is able to well approximate the mean and covariance of the posterior distribution with an uninformative prior under certain conditions on the operator $G$. The UKI [1] further applies averaging on the inverse function $G$ and its gradient $dG$, which leads to $F_{\eta}G$ and $F_{\eta}dG$. By the analogy to the ExKI, the UKI is also able to approximate the mean and covariance of the posterior distribution with an uninformative prior under similar conditions.

**Remark 3.7.** Numerical studies presented in subsections 4.3 and 4.4 indicate the UKI delivers good Gaussian approximation to the posterior distribution also for over-determined inverse problems.

**Remark 3.8.** Numerical studies presented in subsection 4.1 indicate the injection and the Lipschitz continuity of $G$ are necessary for accurate posterior mean and covariance approximation.

4. Applications. In this section, we present numerical study of the UKI equipping with the stochastic dynamics (2.13) for approximating the posterior distribution. To be concrete, we initialize UKI with $\theta_0 \sim N(m_0, C_0)$, where $m_0 = r_0$. It is worth mentioning $r_0$ is the prior mean but $C_0$ is generally not the prior covariance. Specific choices of $r_0$ and $C_0$ will differ between examples and will be spelled out in each example. For comparison, we also apply the Markov Chain Monte Carlo method (MCMC), specifically the random walk Metropolis algorithm, and the Sequential Monte Carlo method [45, 46, 47] (SMC).

- Nonlinear 1-parameter model problems: the behavior of the UKI is studied on different forward maps, including discontinuous functions, non-injective functions, and etc.
- Nonlinear 2-parameter model problem: this is counterexample against the ensemble Kalman filter [55, 56]. This problem demonstrates the effectiveness of the modified stochastic dynamical system, which enables the UKI to obtain accurate posterior approximation.
- Nonlinear high dimensional model problem: this is a well-studied Darcy flow inverse problem. The comparison between UKI and MCMC is presented, good agreement in terms of mean and covariance estimations is achieved.
- Navier-Stokes problem: this is a model data assimilation problem in oceanography and meteorology, where the initial condition is recovered from noisy observations of the vorticity field at later times.

The code is accessible online: [https://github.com/Zhengyu-Huang/InverseProblems.jl](https://github.com/Zhengyu-Huang/InverseProblems.jl)

4.1. Nonlinear 1-Parameter Model Problem. The performance of the UKI is studied numerically on the following nonlinear 1-parameter problems:

- Exponential problem:
  $$y = G(\theta) + \eta \quad G(\theta) = \exp \left( \frac{\theta}{10} \right).$$

- Quadratic multimodal problem:
  $$y = G(\theta) + \eta \quad G(\theta) = \theta^2.$$

- Cubic problem:
  $$y = G(\theta) + \eta \quad G(\theta) = \theta^3.$$
- Sign discontinuous problem:
  \[ y = G(\theta) + \eta \quad G(\theta) = \text{sign}(\theta) + \theta^3. \]

- Hyperbola discontinuous problem:
  \[ y = G(\theta) + \eta \quad G(\theta) = \frac{1}{\theta}. \]

We assume the observation is generated as \( y = G(\theta_{\text{ref}}) \), where the reference solution \( \theta_{\text{ref}} = 2 \). And the observation error is \( \eta \sim \mathcal{N}(0, 0.1^2) \). For Bayesian inverse problems, we assume the prior distribution is \( \mathcal{N}(-1, 10^5) \), where the prior mean \(-1\) is on a different branch for these discontinuous problems. It is worth noticing, for these inverse problems, the observation error is small, and the prior is almost uninformative. However, \( G \) is not injective for the quadratic multimodal problem, and the Lipschitz property does not hold for these discontinuous problems.

The reference posterior distribution is approximated by the MCMC method with a step size 1.0 and \( 5 \times 10^6 \) samples (with a \( 10^6 \) sample burn-in period). The SMC method with 10\(^3\) particles and 10\(^2\) uniform steps is also applied for comparison. As for the UKI, 2 initial conditions are considered, which are \( \theta_0 \sim \mathcal{N}(-1, 0.5^2) \) and \( \theta_0 \sim \mathcal{N}(1, 0.5^2) \). We find that only the hyperbola discontinuous problem is sensitive to the initial covariance for the UKI.

The approximated posterior distributions are presented in Figure 1. Here the UKI results are from the 20th iteration. For the quadratic multimodal problem, the posterior distribution is a multimodal distribution, therefore, the UKI can only capture one modal, that is close to the initial condition \( \theta_0 \). For the hyperbola discontinuous problem, the UKI initialized on the different branch from \( \theta_{\text{ref}} \) diverges to \(-\infty\); but the UKI initialized on the same branch from \( \theta_{\text{ref}} \) converges to \( \theta_{\text{ref}} \) with good covariance estimation. This reveals the gradient-based nature of UKI, in contrast to the sampling-based nature of MCMC or SMC. For other cases, the distributions obtained by the UKI match well with the distributions delivered by the MCMC. It is worth mentioning, the UKI requires only 20 iterations (60 forward solver evaluations), which is much cheaper than MCMC and SMC methods.

4.2. Nonlinear 2-Parameter Model Problem. The numerical experiment considered here is a counterexample against the ensemble Kalman filter, which is proposed in [55] and further used in [59, 56]. Consider the one-dimensional elliptic boundary-value problem

\[
(4.1) \quad - \frac{d}{dx} \left( \exp(\theta_{(1)}) \frac{d}{dx} p(x) \right) = 1, \quad x \in [0, 1]
\]

with boundary conditions \( p(0) = 0 \) and \( p(1) = \theta_{(2)} \). The solution for this problem is given by

\[
p(x) = \theta_{(2)} x + \exp(-\theta_{(1)}) \left( - \frac{x^2}{2} + \frac{x}{2} \right).
\]

The inverse problem is to solve for \( \theta = (\theta_{(1)}, \theta_{(2)})^T \) with the observations \( y = (p(x_1), p(x_2))^T \) at \( x_1 = 0.25 \) and \( x_2 = 0.75 \). The Bayesian inverse problem is formulated as

\[
y = G(\theta) + \eta \quad \text{and} \quad G(\theta) = \begin{bmatrix} p(x_1, \theta) \\ p(x_2, \theta) \end{bmatrix},
\]

here \( G(\theta) \) is the forward model operator. The observation is \( y = (27.5, 79.7)^T \) with observation error \( \eta \sim \mathcal{N}(0, 0.1^2) \). And the prior is \( \mathcal{N}(0, 10^2) \), which is almost uninformative.

The reference posterior distribution is approximated by the MCMC method with a step size 1.0 and \( 5 \times 10^6 \) samples (with a \( 10^6 \) sample burn-in period). For the UKI, the initial condition is \( \theta_0 \sim \mathcal{N}(0, \text{diag} \{1, 10^2\}) \). The posterior distributions obtained by the UKI at the 5th, 10th, and 15th iterations are depicted in Figure 2. The mean converges efficiently to the true value \( \theta_{\text{ref}} \) and the covariance obtained by the UKI matches well with that obtained by MCMC.
Fig. 1: Estimated posterior distributions by different approaches for different nonlinear 1-parameter model problems.

Fig. 2: Contour plot: posterior distributions obtained by UKI at 5th, 10th, and 15th iterations (from left to right); blue dots: reference posterior distribution obtained by MCMC for the 2-parameter model problem. x-axis is for $\theta_{(1)}$ and y-axis is for $\theta_{(2)}$.

4.3. Nonlinear High-Dimensional Model Problem. A similar one-dimensional elliptic boundary-value problem but with high-dimensional parameters is considered in this section. The equation describes
the pressure field \( p(x) \) in a porous medium defined by a positive random permeability field \( a(x, \theta) \):

\[
- \frac{d}{dx} \left( a(x, \theta) \frac{d}{dx} p(x) \right) = f(x), \quad x \in [0, 1].
\]

Here Dirichlet boundary conditions on the pressure are applied with \( p(0) = 0 \) and \( p(1) = 0 \), and \( f \) defines the source of the fluid:

\[
f(x) = \begin{cases} 
1000 & 0 \leq x \leq \frac{1}{2} \\
2000 & \frac{1}{2} < x \leq 1 
\end{cases}.
\]

The random log-permeability field \( \log a(x, \theta) \), depending on parameters \( \theta \in \mathbb{R}^{N_\theta} \), is modeled as a log-Gaussian field with covariance operator

\[
C = (-\Delta + \tau^2)^{-d},
\]

where \(-\Delta\) denotes the Laplacian on \( D \) subject to homogeneous Neumann boundary conditions on the space of spatial-mean zero functions, \( \tau > 0 \) denotes the inverse length scale of the random field and \( d > 0 \) determines its regularity (\( \tau = 3 \) and \( d = 1 \) in the present study\(^2\)).

The log-Gaussian field is approximated by the following Karhunen-Loève (KL) expansion

\[
\log a(x, \theta) = \sum_{l=1}^{+\infty} \theta(l) \sqrt{\lambda_l} \psi_l(x),
\]

and the eigenpairs are of the form

\[
\psi_l(x) = \sqrt{2} \cos(\pi lx) \quad \text{and} \quad \lambda_l = (\pi^2 l^2 + \tau^2)^{-d},
\]

and \( \theta(l) \sim \mathcal{N}(0, 1) \) i.i.d. The forward problem is solved by the finite difference method with 512 grid points.

For the inverse problem, we generate a truth random field \( \log a(x, \theta_{ref}) \) with \( N_\theta = 32 \) and \( \theta_{ref} \sim \mathcal{N}(0, I_{32}) \), which consists of the first 32 KL modes (See Figure 3-left). The observation \( y_{ref} \) consists of pointwise measurements of the pressure value \( p(x) \) at 63 equidistant points in the domain (See Figure 3-right), with the observation error \( \eta \sim \mathcal{N}(0, 0.1^2 I) \). The prior is \( \mathcal{N}(0, 10^2 I) \), where the covariance is large, and therefore the prior is almost uninformative.

The reference posterior distribution is approximated by MCMC with \( 2 \times 10^8 \) samples (with a \( 10^8 \) sample burn-in period). In order to accelerate the convergence of MCMC, we initialize the sampling with \( \theta_{ref} \) and choose a step size \( 10^{-3} \). For the UKI, the initial condition is \( \theta_0 \sim \mathcal{N}(0, I) \).

\(^2d = 1\) ensures the eigenvalues do not decay too fast, and hence all parameters are effective.

Fig. 3: The reference log-permeability field \( \log a(x, \theta_{ref}) \) (left) and the pressure field with 63 equidistant pointwise measurements (right) of the Darcy flow problem.

The reference posterior distribution is approximated by MCMC with \( 2 \times 10^8 \) samples (with a \( 10^8 \) sample burn-in period). In order to accelerate the convergence of MCMC, we initialize the sampling with \( \theta_{ref} \) and choose a step size \( 10^{-3} \). For the UKI, the initial condition is \( \theta_0 \sim \mathcal{N}(0, I) \).
The estimated KL expansion parameters \( \{ \theta_{(i)} \} \) for the log-permeability field and the associated 3-\( \sigma \) confidence intervals obtained by the UKI at the 20th iteration and MCMC are depicted in Figure 4. Both UKI and MCMC converge to the true value \( \theta_{\text{ref}} \) (the relative \( L_2 \) error \( \frac{\| m_n - \theta_{\text{ref}} \|_2}{\| \theta_{\text{ref}} \|_2} \) obtained by UKI at the 20 iteration is about \( 10^{-2} \)), and the covariance estimations for each parameter match well with each other. The covariance for each pair \((\theta_{(i)}, \theta_{(j)})\) with \( i \leq j \) obtained by UKI and MCMC are depicted in Figure 5. These pairs are sorted in an ascent order by comparing the first element and then the second. The UKI and MCMC deliver very similar covariance estimations, which conforms to the theoretical results in subsection 3.2.

![Fig. 4: The estimated KL expansion parameters \( \theta_{(i)} \) and the associated 3-\( \sigma \) confidence intervals obtained by UKI and MCMC for the Darcy flow problem.](image1)

![Fig. 5: The estimated covariance for each parameter pair \((\theta_{(i)}, \theta_{(j)})\) obtained by UKI and MCMC for the Darcy flow problem.](image2)

4.4. Navier-Stokes Problem. Finally, we consider the 2D Navier-Stokes equation on a periodic domain \( D = [0, 2\pi] \times [0, 2\pi] \):

\[
\frac{\partial v}{\partial t} + (v \cdot \nabla)v + \nabla p - \nu \Delta v = 0, \\
\nabla \cdot v = 0, \\
\frac{1}{4\pi^2} \int v = v_b,
\]

where \( v \) is the velocity vector, \( p \) is the pressure, and \( \nu \) is the kinematic viscosity.
where $v$ and $p$ denote the velocity vector and the pressure, $\nu = 0.01$ denotes the dynamic viscosity, and $v_b = (2\pi, 2\pi)$ denotes the non-zero mean background velocity. The forward problem is rewritten in the vorticity-stream $(\omega - \psi)$ formulation:

$$
\frac{\partial \omega}{\partial t} - (v \cdot \nabla)\omega - \nu \Delta \omega = 0,
$$

$$\omega = -\nabla \psi + \frac{1}{4\pi^2} \int \psi = 0,
$$

$$v = \left( \frac{\partial \psi}{\partial x_2}, -\frac{\partial \psi}{\partial x_1} \right) + v_b,
$$

and solved by the pseudo-spectral method [60] on a $128 \times 128$ grid. To eliminating the aliasing error, the Orszag 2/3-Rule [61] is applied and, therefore there are $85^2$ Fourier modes (padding with zeros). The time-integrator is the Crank–Nicolson method with $\Delta T = 2.5 \times 10^{-4}$.

The random initial vorticity field $\omega_0(x, \theta)$, depending on parameters $\theta \in \mathbb{R}^{N\theta}$, is modeled as a Gaussian random field with covariance operator $C = \Delta^{-2}$, which subjects to periodic boundary conditions on the space of spatial-mean zero functions. The KL expansion of the initial vorticity field is given by

$$(4.4) \quad \omega_0(x, \theta) = \sum_{l \in K} \theta^{(c)}_l \sqrt{\lambda_l} \psi^c_l + \theta^{(s)}_l \sqrt{\lambda_l} \psi^s_l,$$

where $K = \{(k_x, k_y)|k_x + k_y > 0 \text{ or } (k_x + k_y = 0 \text{ and } k_x > 0)\}$, and the eigenpairs are of the form

$$\psi^c_l(x) = \cos(l \cdot x) \sqrt{\frac{2\pi}{2\pi}} \quad \psi^s_l(x) = \sin(l \cdot x) \sqrt{\frac{2\pi}{2\pi}} \quad \lambda_l = \frac{1}{|l|^2},$$

and $\theta^{(c)}_l, \theta^{(s)}_l \sim \mathcal{N}(0, 2\pi^2)$ i.i.d. The KL expansion (4.4) can be rewritten as a sum over $\mathbb{Z}^{0+}$ rather than a lattice:

$$(4.5) \quad \omega_0(x, \theta) = \sum_{k \in \mathbb{Z}^{0+}} \theta^{(k)}_k \sqrt{\lambda_k} \psi_k(x),$$

where the eigenvalues $\lambda_k$ are in descending order.

For the inverse problem, we recover the initial condition, specifically the initial vorticity field of the Navier-Stokes equation, given pointwise observations $y_{\text{ref}}$ of the vorticity field at 64 equidistant points ($N_y = 128$) at $T = 0.25$ and $T = 0.5$ (See Figure 6). And 5% Gaussian random noises are added to the observation, as follows,

$$y_{\text{obs}} = y_{\text{ref}} + 5\% y_{\text{ref}} \odot \mathcal{N}(0, 1),$$

here $\odot$ denotes element-wise multiplication. The observation error is $\eta \sim \mathcal{N}(0, 0.1^2 I)$, which corresponds to the noise level. The initial vorticity field is generated with 100 Fourier modes of (4.4), and the first 50 modes are recovered ($N_\theta = 100$), and hence the model is misspecified and model error exists. The UKI is initialized with $\theta_0 \sim \mathcal{N}(0, I)$.

The convergence of the initial vorticity field $\omega_0(x, m_n)$, the optimization errors, and the Frobenius norm of the covariance are depicted in Figure 7. Thanks to the linear (or superlinear) convergence rate of the LMA [1], the UKI converges efficiently.

The truth random initial vorticity field $\omega_0(x, \theta_{\text{ref}})$ and the initial vorticity field recovered by UKI at the 20th iteration are depicted in Figure 8. The UKI captures well main features of the truth random initial field and even small features, despite the irreversibility of the diffusion process ($\nu = 0.01$). The estimated parameters $\{\theta^{(c)}_l\}, \{\theta^{(s)}_l\}$, and the associated 3-$\sigma$ confidence intervals obtained by the UKI are depicted in Figure 9. Most of the reference values are in the confidence interval.

5. Conclusion. Unscented Kalman inversion is proposed as a derivative-free optimization method for inverse problems. In this paper, we further study the capability of UKI for Bayesian inference and uncertainty quantification. We focus on identifiable inverse problems, since a wide range of inverse problems belong to this category, especially with the availability of large and diverse data sets from experiments and direct
Fig. 6: The vorticity field of the Navier-Stokes problem and the 64 equidistant pointwise measurements (black dots) at two observation times ($T = 0.25$ and $T = 0.5$).

Fig. 7: Relative error $\|\omega(x,m_n) - \omega_{0,\text{ref}}\|^2$ (left), the optimization error $\frac{1}{2}||\Sigma_v^{-\frac{1}{2}}(y_{\text{obs}} - \hat{y}_n)||^2$ (middle), and the Frobenius norm of covariance $\|C_n\|_F$ for the Navier-Stokes initial inverse problem.

Simulations. Theoretical guarantees are presented, for linear inverse problems, the mean and covariance obtained by the UKI converge exponentially fast to the posterior mean and covariance; for nonlinear inverse problems, the error bounds of the mean and covariance are derived, in terms of the observation error. Numerical studies empirically confirm the theoretical results and demonstrate the effectiveness of UKI as an efficient Bayesian inference tool. For the Navier-Stokes problem, the model error exists. It is interesting to systematically quantify model-form error by using UKI in the future.

Acknowledgments. D.Z.H. is supported by the generosity of Eric and Wendy Schmidt by recommendation of the Schmidt Futures program. J.H. is supported by the Simons Foundation as a Junior Fellow at New York University.

Appendix A. Gaussian Approximation. For the Gaussian approximation in subsection 2.1, assume the distribution of $\theta_n|Y_n$ is $\mu_n = \mathcal{N}(m_n, C_n)$, then the distribution of $\theta_{n+1}|Y_n$ is $\hat{\mu}_{n+1} = \mathcal{N}(\hat{m}_{n+1}, \hat{C}_{n+1})$. The joint density function of $\{\theta_{n+1}, y_{n+1}\}|Y_n$ is $p(\theta, y)$:

\begin{equation}
 p(\theta_{n+1}, y_{n+1}|Y_n) = p(y_{n+1}|\theta_{n+1}, Y_n)p(\theta_{n+1}|Y_n) \propto e^{-\Phi(\theta_{n+1}, y_{n+1})} p_0(\theta_{n+1}),
\end{equation}
Fig. 8: Truth initial vorticity field $\omega_0(x, \theta_{ref})$ (left) and the Initial vorticity fields $\omega_0(x, m_n)$ recovered by the UKI (right) for the Navier-Stokes problem.

Fig. 9: The estimated Fourier expansion parameters $\{\theta^c_{(l)}\}, \{\theta^n_{(l)}\}$ and the associated 3-σ confidence intervals obtained by UKI for the Navier-Stokes problem.

where $p_0$ is the density function of $\theta_{n+1}|Y_n$. The Gaussian approximated joint density function is $p^G(\theta, y)$

$$p^G(\theta_{n+1}, y_{n+1}|Y_n) = \mathcal{N}\left(\begin{bmatrix} \hat{m}_{n+1} \\ \hat{y}_{n+1} \end{bmatrix}, \begin{bmatrix} \hat{C}^{\theta}_{n+1} & \hat{C}^{\theta y}_{n+1} \\ \hat{C}^{y\theta}_{n+1} & \hat{C}^{yy}_{n+1} \end{bmatrix}\right),$$

It is worth mentioning $p(\theta, y)$ and $p^G(\theta, y)$ have the same mean and covariance by the definition of $p^G$. To obtain an upper bound for the Kullback–Leibler divergence between the true distribution $\theta_{n+1}|Y_{n+1}$ and $\mathcal{N}(m_{n+1}, C_{n+1})$, we need the following theorem:

**Theorem A.1.** Let denote the joint density function of $x = (\theta; y)$

$$p(x) = \frac{1}{Z} e^{-Q(x) - \epsilon H(x)} \quad \text{with} \quad Q(x) = \frac{1}{2} (x - \hat{m})^{T} \hat{C}^{-1} (x - \hat{m}),$$

here $Q(x)$ represents the quadrature term, $\epsilon H(x)$ represents other terms and $Z$ is the normalization constant.

Let $\hat{m}^G$ and $\hat{C}^G$ denote the mean and covariance of $p(x)$, the approximated joint Gaussian density function is

$$p^G(x) = \frac{1}{Z^G} e^{-Q^G(x)} \quad \text{with} \quad Q^G(x) = \frac{1}{2} (x - \hat{m}^G)^{T} \hat{C}^{-1} (x - \hat{m}^G).$$
We assume
1. \( \exists \epsilon_0 > 0 \) and \( c_1 > 0 \), such that \( |H(x)| \leq c_0 x^T x + c_1 \), and \( \lambda_{\min}(\hat{C}^{-1}) > 2\epsilon c_0 \),
2. \( \exists \epsilon_2 > 0 \), such that \( \lambda_{\min}(\hat{C}) > c_2 \), \( \lambda_{\min}(\hat{C}^{-1}) > c_2 \), and \( \lambda_{\min}(\hat{C}^G) > c_2 \),
3. \( \dim(x) \), \( c_1 \), and each entry of \( y \), \( \hat{m} \), \( \hat{C} \), \( \hat{C}^{-1} \), \( \hat{m}^G \), \( \hat{C}^G \), \( \hat{C}^{-1} \) are \( O(1) \) constants, and \( \epsilon \) is small enough.

We have an upper bound for the Kullback–Leibler divergence between the conditional distributions:

\[
\mathcal{D}_{KL}(p^G(\theta|y) \parallel p(\theta|y)) = O(\epsilon).
\]

**Proof.** We first prove \( \dim(x) = 3 \).

\[
\exists \epsilon_1.
\]

\[
\|\hat{m}^G - \hat{m}\|_\infty = O(\epsilon) \quad \text{and} \quad \|\hat{C}^G - \hat{C}\|_\infty = O(\epsilon).
\]

We denote the Gaussian distribution \( p_0(x) \) with mean \( \hat{m} \) and covariance \( \hat{C} \), and its associated expectation \( \hat{E}[] \) as following,

\[
p_0(x) = \frac{1}{Z_0} e^{-Q(x)} \hat{E}[f] = \int f(x)p_0(x)dx.
\]

Since we consider only mean and covariance, we restrict \( f \) to be \( x \) and \( xx^T \) in the following discussion. The expectation with respect to the density function \( p(x) \) in (A.3) can be written as

\[
\int f(x)p(x)dx = \frac{\hat{E}[e^{-H(x)}]}{\hat{E}[e^{-H(x)}]}e^{-H(x)},
\]

which leads to

\[
\int f(x)p(x) - f(x)p_0(x)\,d\theta = \frac{\hat{E}[e^{-H(x)}]}{\hat{E}[e^{-H(x)}]} - \hat{E}[f(x)]
\]

\[
= \int_{0}^{\epsilon} \partial t \frac{\hat{E}[e^{-H(x)}]}{\hat{E}[e^{-H(x)}]}dt
\]

\[
= \int_{0}^{\epsilon} \hat{E}[-f(x)H(x)e^{-H(x)}] + \frac{\hat{E}[f(x)e^{-H(x)}]e^{-H(x)}[H(x)e^{-H(x)}]}{\hat{E}[e^{-H(x)}]}dt.
\]

Since \( \lambda_{\min}(\hat{C}^{-1}) > 2\epsilon c_0 \), \( p_0(x)e^{c_0 x^T x} \) decays exponentially. For \( t \in [0, \epsilon] \), we have

\[
\left| \frac{1}{\hat{E}[e^{-H(x)}]} \right| \leq \frac{1}{\hat{E}[e^{-\epsilon_1 x^T x + \epsilon c_1}]} = O(1),
\]

\[
\left| \hat{E}[f(x)e^{-tH(x)}] \right|_\infty \leq \hat{E}[\|x\|_\infty + N_0 x^T x + c_1 e^{\epsilon c_0 x^T x + \epsilon c_1}] = O(1),
\]

\[
\left| \hat{E}[H(x)e^{-tH(x)}] \right|_\infty \leq \hat{E}[c_0 x^T x + c_1 e^{\epsilon c_0 x^T x + \epsilon c_1}] = O(1),
\]

\[
\left| \hat{E}[f(x)H(x)e^{tH(x)}] \right|_\infty \leq \hat{E}[\|x\|_\infty + N_0 x^T x + c_1 e^{\epsilon c_0 x^T x + \epsilon c_1}] = O(1).
\]

Plugging (A.8) into (A.7) leads to

\[
\left| \int f(x)p(x) - f(x)p_0(x)dx \right|_\infty = O(\epsilon),
\]

which finishes the proof of (A.5).

Next, we define conditional distributions

\[
p(\theta|y) = \frac{p(x)}{p(x)dy} = \frac{1}{Z(y)} e^{-Q(\theta|y) + H(\theta, y)} \quad \text{and} \quad p^G(\theta|y) = \frac{p^G(x)}{p^G(x)dy} = \frac{1}{Z^G(y)} e^{-Q^G(\theta|y)},
\]

\[
\lambda_{\min}(A) \text{ denotes the smallest eigenvalue of matrix } A.
\]
where
\[ Q(\theta|y) = \frac{1}{2}(\theta - m)^T C^{-1}(\theta - m) \quad \text{and} \quad Q^G(\theta|y) = \frac{1}{2}(\theta - m^G)^T C^G G^{-1}(\theta - m^G). \]

The conditional normal distribution theorem leads to
\[ m = \hat{m}_1 + \hat{C}_{12} \hat{C}_{22}^{-1}(y - \hat{m}_2) \quad \text{and} \quad C = \hat{C}_{11} - \hat{C}_{12} \hat{C}_{22}^{-1} \hat{C}_{21}, \]
\[ m^G = \hat{m}_1 + \hat{C}_{12} \hat{C}_{22}^{-1}(y - \hat{m}_2) \quad \text{and} \quad C^G = \hat{C}_{11} - \hat{C}_{12} \hat{C}_{22}^{-1} \hat{C}_{21}, \]
here the subscripts 1 and 2 correspond to \( \theta \) and \( y \) components, respectively.

We then prove
\[ \|m^G - m\|_\infty = O(\epsilon) \quad \text{and} \quad \|C^G - C\|_\infty = O(\epsilon). \]

Since \( \lambda_{\min}(\hat{C}) > 2c_2 \), we have
\[ \lambda_{\min}(\hat{C}_{22}) = \min_{y^T y = 1} y^T \hat{C}_{22} y = \min_{y^T y = 1, \theta = 0} (\theta; y)^T \hat{C}(\theta; y) \geq \min_{x^T x = 1} x^T \hat{C} x = \lambda_{\min}(\hat{C}) > c_2, \]
and
\[ \lambda_{\min}(\hat{C}_{22}^G) = \min_{y^T y = 1} y^T \hat{C}_{22}^G y = \min_{y^T y = 1, \theta = 0} (\theta; y)^T \hat{C}^G(\theta; y) \geq \min_{x^T x = 1} x^T \hat{C}^G x = \lambda_{\min}(\hat{C}^G) > c_2. \]

Bringing (A.5), (A.12), and (A.13) into (A.10) leads to (A.11).

Moreover, since the Schur complement \( C \) in (A.10) satisfies
\[ \lambda_{\max}(\hat{C}) = \lambda_{\max}\left( \begin{bmatrix} C & 0 \\ \hat{C}_{12} \hat{C}_{22}^{-1/2} & \hat{C}_{22}^{-1/2} \hat{C}_{21} \hat{C}_{22}^{-1/2} \end{bmatrix} \right) \geq \lambda_{\max}(C), \]
we have
\[ \lambda_{\min}(\hat{C}^{-1}) \geq \lambda_{\min}(\hat{C}^{-1}) > 2\epsilon c_0 \quad \lambda_{\min}(C^{-1}) \geq \lambda_{\min}(\hat{C}^{-1}) > c_2. \]

Finally, the Kullback–Leibler divergence can be written as
\[ \int p^G(\theta|y) \log \left( \frac{p^G(\theta|y)}{p(\theta|y)} \right) d\theta = \int p^G(\theta|y) \left( Q(\theta|y) + \epsilon H(\theta, y) - Q^G(\theta|y) + \log Z - \log Z^G \right) d\theta. \]
The first part of (A.16) can be written as
\[ \int p^G(\theta|y) \left( Q(\theta|y) + \epsilon H(\theta, y) - Q^G(\theta|y) \right) d\theta \]
\[ = \int p^G(\theta|y) \epsilon H(\theta, y) d\theta + \int p^G(\theta|y) \left( Q(\theta|y) - Q^G(\theta|y) \right) d\theta \]
\[ = \int p^G(\theta|y) \epsilon H(\theta, y) d\theta + \frac{1}{2} \text{tr}(C^{-1} C^G) + \frac{1}{2} (m^G - m)^T C^{-1} (m^G - m) - \frac{1}{2} \text{tr}(C^{-1} C^G) \]
\[ = \int p^G(\theta|y) \epsilon H(\theta, y) d\theta + \frac{1}{2} \text{tr} \left( C^{-1} (C^G - C) \right) + \frac{1}{2} (m^G - m)^T C^{-1} (m^G - m) \]
\[ = O(\epsilon). \]

For the second part of (A.16), let denote \( Z_0 = \int e^{-Q(\theta|y)} d\theta \) and the expectation \( \mathbb{E}[\cdot] \) with respect to the Gaussian distribution
\[ p_0(\theta|y) = \frac{1}{Z_0(y)} e^{-Q(\theta|y)}. \]
Combining (A.15) and (A.8) leads to
\begin{equation}
\log Z - \log Z_0 = \log \mathbb{E}[e^{-tH(\theta,y)}] = \int_0^\epsilon \partial_t \log \mathbb{E}[e^{-tH(\theta,y)}] dt = \int_0^\epsilon \mathbb{E}\left[ -H(\theta,y)e^{-tH(\theta,y)} \right] \frac{dt}{\mathbb{E}[e^{-tH(\theta,y)}]} = \mathcal{O}(\epsilon),
\end{equation}
(A.18)

\begin{equation}
\log Z_0 - \log Z^G = \frac{1}{2} \left( \log \det C^G - \log \det C \right) = \mathcal{O}(\epsilon).
\end{equation}
(B.3)

Bringing (A.18) into the second part of (A.16) leads to
\begin{equation}
\int p^G(\theta|y) \left( \log Z - \log Z^G \right) d\theta = (\log Z - \log Z_0) + (\log Z_0 - \log Z^G) = \mathcal{O}(\epsilon). \quad \Box
\end{equation}

Combining (A.17) and (A.19) leads to the upper bound of the Kullback–Leibler divergence.

Following Theorem A.1, we assume $\Phi$ can be decomposed into the quadratic part $Q^\Phi(\theta,y)$ and the high order part $\epsilon H(\theta,y)$, as following
\[ \Phi(\theta,y) = Q^\Phi(\theta,y) + \epsilon H(\theta,y), \]
which is true when $G(\theta)$ is close to a linear function. We further define
\[ Q(\theta,y) = Q^\Phi(\theta,y) + \frac{1}{2} (\theta - \bar{m}_{n+1})^T \bar{C}^{-1}_{n+1} (\theta - \bar{m}_{n+1}). \]

When $Q$ and $H$ satisfy the conditions in Theorem A.1, the conditional distribution $\mathcal{N}(m_{n+1}, C_{n+1})$ well approximates the true distribution $\theta_{n+1}|Y_{n+1}$.

Remark A.2. When $G$ is linear, namely $\Phi(\theta,y)$ is quadratic and $\epsilon = 0$, $\mathcal{N}(m_{n+1}, C_{n+1})$ is the exact distribution of $\theta_{n+1}|Y_{n+1}$.

Appendix B. Proof of Theorem 3.1.

Proof. With the hyperparameters defined in (2.13), the update equation of $\{C_n\}$ in (3.1) can be rewritten as
\begin{equation}
C_{n+1}^{-1} = G^T \Sigma_{\nu}^{-1} G + (C_n + \Sigma_{\omega})^{-1} = \frac{1}{2} G^T \Sigma_{\eta}^{-1} G + (2C_n)^{-1},
\end{equation}
(B.1)

We have a close formula for $C_n^{-1}$:
\begin{equation}
C_n^{-1} = \left[ 1 - \frac{1}{2n} \right] G^T \Sigma_{\eta}^{-1} G + \frac{1}{2n} C_0^{-1}.
\end{equation}
(B.2)

This leads to the exponential convergence $\lim_{n \to \infty} C_n^{-1} = G^T \Sigma_{\eta}^{-1} G$.

The convergence proof of $m_n$ basically follows [1]. Equations (B.1) and (B.2) lead to
\begin{equation}
\frac{1}{2} G^T \Sigma_{\nu}^{-1} G = G^T \Sigma_{\nu}^{-1} G \preceq C_{n+1}^{-1} \preceq G^T \Sigma_{\nu}^{-1} G + \Sigma_+ \quad \text{where} \quad \Sigma_+ = G^T \Sigma_{\nu}^{-1} G + C_0^{-1}.
\end{equation}
(B.3)

The update equation of $m_n$ in (3.1) can be rewritten as
\begin{equation}
m_{n+1} = m_n + C_{n+1} G^T \Sigma_{\nu}^{-1} (y - Gm_n).
\end{equation}
(B.4)

Consider the Range($G^T$) $\otimes$ Ker($G$) decomposition of $m_n = m_n^\parallel + m_n^\perp$ with projections $P_{G^\parallel}$ and $P_{G^\perp}$, we have
\begin{equation}
m_{n+1}^\parallel = m_n^\parallel + P_{G^\parallel} C_{n+1} G^T \Sigma_{\nu}^{-1} (y - Gm_n^\parallel),
\end{equation}
(B.5a)
\begin{equation}
m_{n+1}^\perp = m_n^\perp + P_{G^\perp} C_{n+1} G^T \Sigma_{\nu}^{-1} (y - Gm_n^\perp).
\end{equation}
(B.5b)
Constraining on \( \text{Range}(G^T) \), we have the fact that \( B := G^T \Sigma^{-1}_\nu G \) is symmetric and \( B \succ 0 \). From this, it follows that \( \mathbb{I} - C_{n+1} B \) has the same spectrum as \( \mathbb{I} - B \tilde{C}_{n+1} B^\perp \). Using the bounds on \( C_{n+1} \) appearing in (B.3), the spectral radius of the update matrix in (B.5a) satisfies

\[
\rho(P_{G^n} - P_{G^n} C_{n+1} G^T \Sigma^{-1}_\nu G) \leq \rho(P_{G^n}) \rho\left( \mathbb{I} - \sqrt{G^T \Sigma^{-1}_\nu G C_{n+1} \sqrt{G^T \Sigma^{-1}_\nu G}} \right) \\
\leq 1 - \rho\left( \sqrt{G^T \Sigma^{-1}_\nu G (G^T \Sigma^{-1}_\nu G + \Sigma_+)^{-1} \sqrt{G^T \Sigma^{-1}_\nu G}} \right) \\
= 1 - \epsilon_0,
\]

where \( \epsilon_0 \in (0, 1) \). Hence, we have \( \{m_n^\parallel\} \) converges exponentially to \( m_\infty^\parallel \), which satisfies \( G^T \Sigma^{-1}_\nu (y - G m_\infty^\parallel) = 0 \). The update equation (B.5b) of \( m_n^\perp \) can be written as

\[
m_{n+1}^\perp = m_n^\perp + P_{G^n} C_{n+1} G^T \Sigma^{-1}_\nu G (m_\infty^\parallel - m_n^\parallel).
\]

Since \( \rho(P_{G^n} C_{n+1} G^T \Sigma^{-1}_\nu G) \leq \rho(P_{G^n}) \leq 1 \) and \( \lim_{n \to \infty} m_n^\parallel - m_\infty^\parallel = 0 \) converges exponentially fast, we have the exponential convergence of \( \{m_n^\parallel\} \) to \( m_\infty^\parallel \). Therefore, the converged vector \( m_\infty = m_\infty^\parallel + m_\infty^\perp \) satisfies \( G^T \Sigma^{-1}_\nu (y - G m_\infty) = 0 \), which is a minimizer of \( \Phi \).

**Appendix C. Proof of Theorem 3.5.**

**Proof.** Since we consider only mean and covariance, we consider function \( f(\theta) = \theta \) or \( \theta \theta^T \). The expectation with respect to the posterior distribution \( p(\theta|y) \) is

\[
\mathbb{E}[f(\theta)|y] = \int_\mathbb{R} e^{-\mathcal{F}(\theta, y)} f(\theta) d\theta \\
= \frac{1}{Z} \int_\mathbb{R} e^{-\frac{1}{2} (y - G(\theta))^T \Sigma^{-1}_\nu (y - G(\theta))} f(\theta) d\theta \\
= \frac{1}{Z} \int_\mathbb{R} e^{-\frac{1}{2} (y - \theta')^T \Sigma^{-1}_\nu (y - \theta')} f(G^{-1}(\theta')) \left| \det \frac{dG^{-1}(\theta')}{d\theta} \right| d\theta' \text{ where } \theta' = G(\theta).
\]

The expectation with respect to the pull-back distribution is

\[
\mathbb{E}[f(\theta^\eta)] = \frac{1}{Z_\eta} \int f(G^{-1}(y - \eta)) e^{-\frac{1}{2} \eta^T \Sigma^{-1}_\eta \eta} d\eta \\
= \frac{1}{Z_\eta} \int f(G^{-1}(\theta')) e^{-\frac{1}{2} (y - \theta')^T \Sigma^{-1}_\eta (y - \theta')} d\theta' \text{ where } \theta' = y - \eta.
\]

here \( Z_\eta = \sqrt{(2\pi)^N \det \Sigma_\eta} \). Let denote \( \mathbb{E}_\theta[\cdot] \) the expectation with respect to the Gaussian density function \( \mathcal{N}(y, \Sigma_\eta) \):

\[
\mathbb{E}_\theta[f] = \frac{1}{Z_\eta} \int e^{-\frac{1}{2} (y - \theta)^T \Sigma^{-1}_\eta (y - \theta)} f(\theta) d\theta.
\]

The difference between these two expectations (C.1) and (C.2) becomes

\[
\mathbb{E}[f(\theta)|y] - \mathbb{E}[f(\theta^\eta)] = \frac{1}{Z_\eta} \int e^{-\frac{1}{2} (y - \theta')^T \Sigma^{-1}_\eta (y - \theta')} f(G^{-1}(\theta')) \left| \frac{\det \frac{dG^{-1}(\theta')}{d\theta}}{Z_\eta} \right| - 1 \right| d\theta' \\
= \mathbb{E}_\theta\left[f(G^{-1}(\theta')) \left| \frac{\det \frac{dG^{-1}(\theta')}{d\theta}}{\mathbb{E}_\theta[\det \frac{dG^{-1}(\theta)}{d\theta}]} - 1 \right| \right].
\]

Here we use

\[
\frac{Z}{Z_\eta} = \mathbb{E}_\theta\left| \frac{dG^{-1}(\theta)}{d\theta} \right|.
\]
Since we have the Lipschitz property, this leads to
\[
\left| \frac{\det dG^{-1}(\theta')}{\det dG^{-1}(\theta)} \right| - 1 = \frac{\left| \frac{\det dG^{-1}(\theta')}{\det dG^{-1}(\theta)} \right| - 1}{\frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')}} \leq \frac{\left| \frac{\det dG^{-1}(\theta')}{\det dG^{-1}(\theta)} \right| - 1}{\frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')}} + \frac{\left| \frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')} \right| - 1}{\frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')}}
\]

\[
(C.5)
\]
\[
= \frac{\left| \frac{\det dG^{-1}(\theta')}{\det dG^{-1}(\theta)} \right| - 1}{\frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')}}.
\]

Bringing (C.5) into (C.4) leads to
\[
\left\| \frac{\det dG^{-1}(\theta')}{\det dG^{-1}(\theta)} - 1 \right\|_\infty \leq c_0 \left( E_{\theta'} \left[ \left| \frac{\det dG^{-1}(\theta')}{\det dG^{-1}(\theta)} \right| ^2 \right] \right)^{1/2} + c_0 E_{\theta'} \left[ \left| \frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')} \right| ^2 \right]^{1/2} \leq \frac{c_0 (E_{\theta'} \left[ \left| \frac{\det dG^{-1}(\theta')}{\det dG^{-1}(\theta)} \right| ^2 \right] \left\| \frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')} \right\|_\infty}{c_3/Z_\eta} \left( E_{\theta'} \left[ \left| \frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')} \right| ^2 \right] \left\| \frac{\det dG^{-1}(\theta)}{\det dG^{-1}(\theta')} \right\|_\infty \right)^{1/2} \leq \frac{2c_0 (c_2 + N_\nu)}{c_3} \mathcal{O} \left( \rho(\Sigma_\eta)^{\nu_1} \sqrt{\det \Sigma_\eta} \right).
\]

This leads to the bounds (3.5).

\[
\text{Appendix D. Proof of Theorem 3.6.}
\]

Proof. The update equations of the ExKI in (2.7) and (2.8) can be written as
\[
\begin{align*}
m_{n+1} &= m_n + \hat{C}_{n+1} dG(m_n)^T \left( dG(m_n) \hat{C}_{n+1} dG(m_n)^T + \Sigma_\nu \right)^{-1} (y - \hat{G}(m_n)), \\
C_{n+1} &= \hat{C}_{n+1} - \hat{C}_{n+1} dG(m_n)^T \left( dG(m_n) \hat{C}_{n+1} dG(m_n)^T + \Sigma_\nu \right)^{-1} dG(m_n) \hat{C}_{n+1},
\end{align*}
\]

(D.1)

where \( \hat{C}_{n+1} = C_n + \Sigma_\omega = 2C_n \). By applying Sherman–Morrison–Woodbury formula, the ExKI update equations (D.1) can be rewritten as
\[
\begin{align*}
m_{n+1} &= m_n + C_{n+1} dG(m_n)^T \Sigma_\nu^{-1} (y - G(m_n)), \\
C_{n+1}^{-1} &= \frac{1}{2} C_n^{-1} + dG(m_n)^T \Sigma_\nu^{-1} dG(m_n).
\end{align*}
\]

(D.2)

The stationery mean and covariance \( m_*, C_* \) of (D.2) satisfy
\[
\begin{align*}
0 &= C_* dG(m_*)^T \Sigma_\nu^{-1} (y - G(m_*)), \\
C_*^{-1} &= \frac{1}{2} C_*^{-1} + dG(m_*)^T \Sigma_\nu^{-1} dG(m_*).
\end{align*}
\]

(D.3)
Since $C_\ast$ and $dG(m_\ast)$ are non-singular, they are uniquely determined as following,

$$m_\ast = G^{-1}(y) \quad \text{and} \quad C_\ast^{-1} = dG(m_\ast)^T \Sigma^{-1} dG(m_\ast).$$

When the extended Kalman filter is applied to estimate the mean and covariance of the pull-back random variable $\theta^\ast = G^{-1}(y - \eta)$, we have

$$\mathbb{E}[\theta^\ast] := G^{-1}(y - \mathbb{E}[\eta]) = G^{-1}(y) = m_\ast,$$

$$\text{Cov}[\theta^\ast] := dG^{-1}(y) \text{Cov}[\eta] dG^{-T}(y) = dG^{-1}(y) \Sigma_g dG^{-T}(y) = C_\ast.$$

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