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From Filtering to Inversion: Kalman-Based Methods for Nonlinear Parameter Estimation in Geotechnics

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Introduction

Consider inverse problem: find parameter θ given an observation y of the model

$$y = \mathcal{G}(\theta) + \eta \quad (1)$$

where $\mathcal{G} : \mathcal{R}^{N_\theta} \rightarrow \mathcal{R}^{N_y}$ is a forward map from the parameter to the observation space and $\eta \sim \mathcal{N}(\mathbf{0}, \Sigma_\eta)$ is the observational noise.

Optimization approach

From the optimization perspective, the optimal θ minimizes the loss function:

$$\Phi(\theta, y) = \frac{1}{2} \|\Sigma_{\eta}^{-\frac{1}{2}}(y - \mathcal{G}(\theta))\|^2 \quad (2)$$

When the problem is not well-posed regularization is required:

$$\Phi_R(\theta, y) = \Phi(\theta, y) + \frac{1}{2} \|\Sigma_0^{-\frac{1}{2}}(\theta - r_0)\|^2 \quad (3)$$

with r_0 and Σ_0 prior mean and prior covariance matrix, respectively.

Bayesian approach

From the Bayesian point of view, we seek the posterior distribution.

$$\rho(\theta|y) = \frac{\rho(y|\theta)\rho_0(\theta)}{\rho(y)} = \frac{1}{Z(y)} e^{-\Phi(\theta,y)} \rho_0(\theta), \text{ with } Z(y) = \int e^{-\Phi(\theta,y)} \rho_0(\theta) d\theta \quad (4)$$

For a flat prior $\rho_0(\theta)$

$$\rho(\theta|y) = \frac{1}{Z(y)} e^{-\Phi(\theta,y)} \propto e^{-\Phi(\theta,y)}$$

For a Gaussian prior $\rho_0(\theta)$

$$\rho(\theta|y) = \frac{1}{Z(y)} e^{-\Phi(\theta,y)} \rho_0(\theta) \propto e^{-\Phi_R(\theta,y)}$$

$$\hat{\theta}_{MAP} = \arg \max_{\theta} \rho(\theta|y) = \arg \min_{\theta} [\Phi(\theta,y) - \log \rho_0(\theta)]$$

Coupling Filters and Inversion

Consider the evolution of the state x_k and an observation y_k at time k :

$$\begin{aligned}x_{k+1} &= f(x_k) + \omega_{k+1}, \quad \omega_{k+1} \sim \mathcal{N}(0, \Sigma_\omega) \\y_{k+1} &= h(x_{k+1}) + \nu_{k+1}, \quad \nu_{k+1} \sim \mathcal{N}(0, \Sigma_\nu)\end{aligned}\tag{5}$$

Kalman Filter follows the probabilistic approach and can be viewed as a 2-step procedure leading to the recursive relation $\rho(x_k | Y_k) \rightarrow \rho(x_{k+1} | Y_{k+1})^{[1,2]}$.

1. Prediction step

Estimate $\hat{m}_{k+1}$, $\hat{C}_{k+1}$ of $\rho(x_{k+1}|Y_k)$ given $\rho(x_k|Y_k) \sim \mathcal{N}(m_k, C_k)$

$$\begin{aligned}\hat{m}_{k+1} &= \int f(x_k) \rho(x_k|Y_k) dx_k = \mathbb{E}[f(x_k)|Y_k] \\ \hat{C}_{k+1} &= \int [f(x_k)f(x_k)^T + \Sigma_\nu] \rho(x_k|Y_k) dx_k - \hat{m}_{k+1}\hat{m}_{k+1}^T = \text{Cov}[f(x_k)|Y_k] + \Sigma_\nu\end{aligned}\tag{6}$$

2. Analysis step

Kalman Filter

1. Prediction step

2. Analysis step

Obtain $\rho(x_{k+1}|Y_{k+1})$ via conditioning of the joint distribution $\rho(x_{k+1}, y_{k+1}|Y_k)$ approximated by Gaussian.

$$\begin{aligned}\hat{y}_{k+1} &= \mathbb{E}[h(x_{k+1})|Y_k] \\ \hat{C}_{k+1}^{xy} &= \text{Cov}[x_{k+1}, h(x_{k+1})|Y_k] \\ \hat{C}_{k+1}^{yy} &= \text{Cov}[h(x_{k+1})|Y_k] + \Sigma_\nu \\ m_{k+1} &= \hat{m}_{k+1} + \hat{C}_{k+1}^{xy}(\hat{C}_{k+1}^{yy})^{-1}(y_{k+1} - \hat{y}_{k+1}) \\ C_{k+1} &= \hat{C}_{k+1} - \hat{C}_{k+1}^{xy}(\hat{C}_{k+1}^{yy})^{-1}(\hat{C}_{k+1}^{xy})^T\end{aligned}$$

(7)

Nonlinear Kalman Filters

Different nonlinear Kalman filters are designed to approximate integrals in (7) under nonlinear transformations.

- **Extended Kalman Filter(ExKF)**

Makes use of Taylor approximations → requires explicit gradient computations.

- **Unscented Kalman Filter(UKF)**

Utilizes a deterministic quadrature rule → works with a deterministic set of transformed particles ([sigma points](#)).

- **Ensemble Kalman Filter(EKF)**

Utilizes Monte Carlo sampling → computes empirical mean and covariances over an ensemble of particles.

Coupling Filters and Inversion

If we couple an inverse problem (1) with a dynamical system for the parameter, we obtain a hidden Markov model with $\eta \sim \mathcal{N}(\mathbf{0}, \frac{1}{N}\Sigma_\eta)$:

$$\begin{aligned}\theta_{n+1} &= \theta_n \\ y_{n+1} &= \mathcal{G}(\theta_{n+1}) + \eta_{n+1}\end{aligned}\tag{8}$$

We can apply Kalman filters iteratively N times on (8) to approximate the posterior distribution.

$$\begin{aligned}\rho_0(\theta) &= \rho_{\text{prior}}(\theta) \\ \rho_n(\theta) &\rightarrow \rho_{n+1}(\theta) \propto \rho_n(\theta) e^{-\frac{1}{N}\Phi(\theta, y)}\end{aligned}\tag{9}$$

The process can be generalized by a meta algorithm, **the Gaussian Approximation Algorithm (GAA)**^[1,4]

Gaussian Approximation Algorithm

Consider the following stochastic dynamical system (**mean-field system**):

$$\begin{aligned}\theta_{n+1} &= \alpha\theta_n + (1 - \alpha)r_0 + \omega_{n+1} \\ y_{n+1} &= \mathcal{G}(\theta_{n+1}) + \nu_{n+1}\end{aligned}\tag{10}$$

where $\omega_{n+1} \sim \mathcal{N}(\mathbf{0}, \Sigma_\omega)$ and $\nu_{n+1} \sim \mathcal{N}(\mathbf{0}, \Sigma_\nu)$ are artificial evolution error in parameter and observation space, and α is a regularization parameter^[1,4].

Gaussian Approximation Algorithm

Prediction Step

- **Prediction step**

$$\begin{aligned}\hat{m}_{n+1} &= \mathbb{E}[\theta_{n+1}|Y_n] = \alpha\theta_n + (1 - \alpha)r_0 \\ \hat{C}_{n+1} &= \text{Cov}[\theta_{n+1}|Y_n] = \alpha^2 C_n + \Sigma_w\end{aligned}\tag{11}$$

$\rho_n(\theta) \rightarrow \hat{\rho}_{n+1}(\theta)$ with $\rho_n \sim \mathcal{N}(m_n, C_n)$

- **Analysis step**

Gaussian Approximation Algorithm

Analysis Step

- **Prediction step**
- **Analysis step**

We have the following joint Gaussian distribution $\{\theta_{n+1}, y_{n+1}\} | Y_n$:

$$\mathcal{N}\left(\begin{bmatrix} \hat{m}_{n+1} \\ \hat{y}_{n+1} \end{bmatrix}, \begin{bmatrix} \hat{C}_{n+1} & \hat{C}_{n+1}^{\theta y} \\ (\hat{C}_{n+1}^{\theta y})^T & \hat{C}_{n+1}^{yy} \end{bmatrix}\right) \quad (12)$$

$\hat{\rho}_{n+1}(\theta) \rightarrow \rho_{n+1}(\theta)$ for $\theta_{n+1} | Y_n$ with $\rho_{n+1} \sim \mathcal{N}(m_{n+1}, C_{n+1})$

Gaussian Approximation Algorithm

Analysis Step

1. Projecting the joint distribution:

$$\begin{aligned}\hat{y}_{n+1} &= \mathbb{E}[\mathcal{G}(\theta_{n+1})|Y_n] \\ \hat{C}_{n+1}^{\theta y} &= \text{Cov}[\theta_{n+1}, \mathcal{G}(\theta_{n+1})|Y_n] \\ \hat{C}_{n+1}^{yy} &= \text{Cov}[\mathcal{G}(\theta_{n+1})|Y_n] + \Sigma_\nu\end{aligned}\tag{13}$$

2. Conditioning the Gaussian to find $\theta_{n+1}|\{Y_n, y_{n+1}\} = \theta_{n+1}|Y_{n+1}$

$$\begin{aligned}m_{n+1} &= \hat{m}_{n+1} + \hat{C}_{n+1}^{\theta y}(\hat{C}_{n+1}^{yy})^{-1}(y_{n+1} - \hat{y}_{n+1}) \\ C_{n+1} &= \hat{C}_{n+1} - \hat{C}_{n+1}^{\theta y}(\hat{C}_{n+1}^{yy})^{-1}\hat{C}_{n+1}^{\theta y T}\end{aligned}\tag{14}$$

In case of nonlinear $\mathcal{G}$, integrals appear in (13).

Unscented Kalman Inversion

If we apply the Unscented Kalman Filter on the system (10) the GAA looks as follows [1]:

1. Prediction step

$$\begin{aligned}\hat{m}_{n+1} &= \alpha m_n + (1 - \alpha)r_0 \\ \hat{C}_{n+1} &= \alpha^2 C_n + \Sigma_\omega\end{aligned}\tag{15}$$

2. Generate sigma points

3. Analysis step

Unscented Kalman Inversion

The UKI ensemble is deterministic and has the size $J = 2N_\theta + 1$.

1. **Prediction step**
2. **Generate sigma points**

$$\begin{aligned}\hat{\theta}_{n+1}^0 &= \hat{m}_{n+1} \\ \hat{\theta}_{n+1}^j &= \hat{m}_{n+1} + c[\sqrt{\hat{C}_{n+1}}]_j \quad (1 \leq j \leq N_\theta) \\ \hat{\theta}_{n+1}^{j+N_\theta} &= \hat{m}_{n+1} - c[\sqrt{\hat{C}_{n+1}}]_j \quad (1 \leq j \leq N_\theta)\end{aligned}\tag{16}$$

With $a = \min(\sqrt{\frac{4}{N_\theta}}, 1)$, weights $c = a\sqrt{N_\theta}$, $[\sqrt{\hat{C}_{n+1}}]_j$ is column j of Cholesky Factor of $\hat{C}_{n+1}$.

3. **Analysis step**

The integrals appearing in the analysis step for a nonlinear $\mathcal{G}$ are approximated by the deterministic quadrature rule.

Unscented Kalman Inversion

1. **Prediction step**
2. **Generate sigma points**
3. **Prediction step**

$$\begin{aligned}\hat{y}_{n+1}^j &= \mathcal{G}(\hat{\theta}_{n+1}^j) ; \hat{y}_{n+1} = \hat{y}_{n+1}^0 \\ \hat{C}_{n+1}^{\theta y} &= \sum_{j=1}^{2N_\theta} \frac{1}{2a^2N_\theta} (\hat{\theta}_{n+1}^j - \hat{m}_{n+1})(\hat{y}_{n+1}^j - \hat{y}_{n+1})^T \\ \hat{C}_{n+1}^{yy} &= \sum_{j=1}^{2N_\theta} \frac{1}{2a^2N_\theta} (\hat{y}_{n+1}^j - \hat{y}_{n+1})(\hat{y}_{n+1}^j - \hat{y}_{n+1})^T + \Sigma_\nu \\ m_{n+1} &= \hat{m}_{n+1} + \hat{C}_{n+1}^{\theta y} (\hat{C}_{n+1}^{yy})^{-1} (y - \hat{y}_{n+1}) \\ C_{n+1} &= \hat{C}_{n+1} - \hat{C}_{n+1}^{\theta y} (\hat{C}_{n+1}^{yy})^{-1} (\hat{C}_{n+1}^{\theta y})^T\end{aligned}\tag{17}$$

Ensemble Kalman Inversion

If we apply the Ensemble Kalman Filter on the system (10) the GAA looks as follows^[1,2]:

1. Prediction step

$$\begin{aligned}\hat{\theta}_{n+1}^j &= \alpha \theta_n^j + (1 - \alpha) r_0 + \omega_{n+1}^j \\ \hat{m}_{n+1} &= \frac{1}{J} \sum_{j=1}^J \hat{\theta}_{n+1}^j\end{aligned}\tag{18}$$

2. Analysis step

EKI works with a set of particles whose dynamics is predicted by (10) and then used to predict empirical approximations of covariances.

For large J the updates in the analysis step match to those of the GAA.

Ensemble Kalman Inversion

1. **Prediction step**
2. **Analysis step**

$$\begin{aligned}\hat{y}_{n+1}^j &= \mathcal{G}(\theta_{n+1}^j) ; \quad \hat{y}_{n+1} = \frac{1}{J} \sum_{j=1}^J \mathcal{G}(\theta_{n+1}^j) \\ \hat{C}_{n+1}^{\theta y} &= \frac{1}{J-1} \sum_{j=1}^J (\theta_{n+1}^j - \hat{m}_{n+1})(\hat{y}_{n+1}^j - \hat{y}_{n+1})^T \\ \hat{C}_{n+1}^{yy} &= \frac{1}{J-1} \sum_{j=1}^J (\hat{y}_{n+1}^j - \hat{y}_{n+1})(\hat{y}_{n+1}^j - \hat{y}_{n+1})^T + \Sigma_\nu \\ \theta_{n+1}^j &= \hat{\theta}_{n+1}^j + \hat{C}_{n+1}^{\theta y} (\hat{C}_{n+1}^{yy})^{-1} (y - \hat{y}_{n+1}^j - \nu_{n+1}^j)\end{aligned}$$

(19)

Comparison

Feature	EKI	UKI
Ensemble type	Stochastic	Deterministic
Ensemble collapse	Yes	No
Low-rank approximation	Yes	No

When to use

- **EKI**: High-dimensional problems, covariance estimate is of a lesser interest.
- **UKI**: Low- to moderate-dimensional problems, we assume that the Gaussian-like uncertainty is plausible.

The choice of the inversion method is a tradeoff.

Inverse Problems in Geotechnical Engineering

Stiffness Inversion

The forward model $\mathcal{G}$ computes the surface uplift u (scaled for cm) for a vertical slice of a homogeneous rock layer split into n cells given stiffness E , porosity μ , bulk weight γ_w , discretization step Δz .

$$Y = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_i \\ \vdots \\ u_n \end{pmatrix} = (1 - \mu)\gamma_w \Delta z^2 \begin{pmatrix} \frac{1}{2} & 0 & 0 & \cdots & 0 \\ 1 & \frac{1}{2} & 0 & \cdots & 0 \\ 1 & 1 & \frac{1}{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{E_1} \\ \frac{1}{E_2} \\ \vdots \\ \frac{1}{E_n} \end{pmatrix} \quad (20)$$

We have noisy uplift observations with the noise $\eta \sim \mathcal{N}(0, \gamma I_{N_y})$, $\gamma = 1 \text{ mm}^2$, and assume $\theta = \log E$ is normally distributed.

Hence, $\mathcal{G}(\phi(\theta))$, with a nonlinear transformation $\phi(\theta) = \exp(\theta)$.

Figure 1: Estimated stiffness E .

Figure 2: Coverage probability.

Inversion of Gas Cavern Parameters

We use the following model for modelling a subsidence induced by multiple caverns of a cylindrical shape^[3].

$$s_{total}(r, t) = \sum_{i=0}^N s_i(r, t) = \sum_{i=0}^N s_i^{max}(t) \exp\left[-\pi \frac{r(x, y)_i^2}{R_i^2}\right]$$
$$R_i = \frac{\sqrt{H_i^f \cdot H_i^r}}{\tan \beta_i} ; s_i^{max}(t) = \frac{\Delta k(t)_i V_i^0}{R_i^2}$$
(21)

The goal is to estimate individual influence angles β_i and current convergence ratio $k(t)$ for each period given noisy yearly subsidence observations $\mathbf{s}$ with the noise $\eta \sim \mathcal{N}(0, \gamma I_{N_y})$, $\gamma = 1 \text{ cm}^2$, initial cavern volumes V_i^0 , geometric parameters.

Inversion of Gas Cavern Parameters

The inverse problem is solved for 3 caverns having 63 parameters in total: 3 influence angles β_i and 60 convergence volumes for observation period t of 20 years.

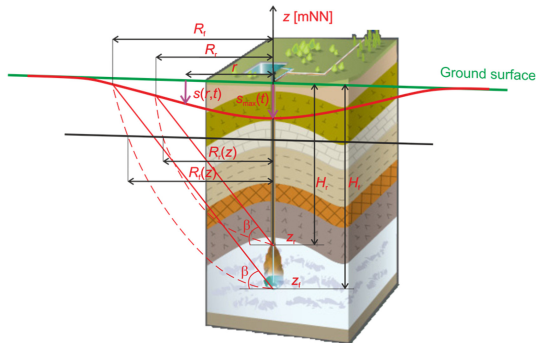


Figure 3: Gas caverns and observed subsidence.

Inversion of Gas Cavern Parameters

Figure 4: EKI estimates for β s and k s

Inversion of Gas Cavern Parameters

Figure 5: UKI estimates for β s and k s.

Inversion of Gas Cavern Parameters

Figure 6: $\mathcal{G}(\phi(\beta^*, k^*))_{EKI}$ compared to noise-free subsidence.

Inversion of Gas Cavern Parameters

Figure 7: $\mathcal{G}(\phi(\beta^*, k^*))_{UKI}$ compared to noise-free subsidence.

- Both UKI and EKI provide good parameter estimates for the presented nonlinear inverse problems.
- Both UKI and EKI provide gaussian-like uncertainty, which is valid under particular assumptions for parameter distributions and inverse problem.
- The quality of the obtained confidence intervals is questionable. EKI tends to underestimate the uncertainty due to ensemble collapse, whereas UKI yields a conservative estimate (too wide intervals).
- The choice of the inversion method depends on the dimensionality of the parameter space and assumptions about the parameter distribution.

Thank you for your attention!

1. D. Z. Huang, T. Schneider, and A. M. Stuart, 2022. Iterated Kalman Methodology For Inverse Problems / Unscented Kalman Inversion, Journal of Computational Physics 463 (2022) 111262
2. M. A. Iglesias, K. J H Law and A. M. Stuart, 2013. Ensemble Kalman methods for inverse problems, Inverse Problems. 29 (4) (2013) 045001.
3. R. Misa, A. Sroka et al, 2023. Determination of convergence of underground gas storage caverns using non-invasive methodology based on land surface subsidence measurement, Journal of Rock Mechanics and Geotechnical Engineering V. 15, 8, 1944-1950.
4. InverseProblems.jl <https://github.com/PKU-CMEGroup/InverseProblems.jl/tree/master>

Supplementary slides

Supplementary slides

Modified Unscented Transform^(1,4)

Let $\mathcal{G}_i, i = 1, 2$ denote any pair of real vector-valued functions on $\mathbb{R}^{N_\theta}$, $\theta^0 = m$

If $\theta \sim \mathcal{N}(m, C)$ then

$$\mathbb{E}\mathcal{G}_i(\theta) = \mathcal{G}_i(\theta^0) + \mathcal{O}(\|C\|)$$

$$\text{Cov}(\mathcal{G}_1(\theta), \mathcal{G}_1(\theta)) = \sum_{j=1}^{2N_\theta} W_j^c (\mathcal{G}_1(\theta^j) - \mathbb{E}\mathcal{G}_1(\theta^j))(\mathcal{G}_2(\theta^j) - \mathbb{E}\mathcal{G}_2(\theta^j))^T + \mathcal{O}(\|C\|^2) \quad (22)$$

thus the modified unscented transform is first and second order accurate in approximating means and covariances of $\mathcal{G}_1(\theta)$ and $\mathcal{G}_2(\theta)$ with respect to small $(\|C\|)$. Furthermore, if $\mathcal{G}_1$ and $\mathcal{G}_2$ are linear then the modified unscented transform is exact for these quantities.

Supplementary slides

Stiffness Inversion

- The layer is split into $d = 80$ cells with stiffness E_i , bulk weight γ_w , porosity μ . We want to solve an inverse problem for stiffness E_i given noisy observations for uplift $y_i = u_i + \eta$, where $\eta \sim \mathcal{N}(0, \gamma l_d)$, with $\gamma = 1$ mm.
- We assume that $\log(E)$ is normally distributed with $m_0 = \ln(\text{range}(10\text{MPa}, ..80\text{MPa}))_d$ and $C_0 = \sigma^2 \exp(-2 \frac{\|d_i - d_j\|}{\lambda})_{d \times d}$ with $\sigma = 0.2$ and $\lambda = 1.8$.
- For EKI we initialize an ensemble of particles $J = 800$ drawn from $\mathcal{N}(m_0, C_0)$.
- For UKI we set prior mean m_0 and prior covariance C_0 , $J = 161$.
- The forward map is updated as follows $\mathcal{G}(\phi(\theta)) = \mathcal{G}(\exp(\theta))$.

Supplementary slides

Stiffness Inversion

Figure 8: RMSE for E^* .

Supplementary slides

Stiffness Inversion

Figure 9: Observed Uplift vs $\mathcal{G}(\exp(\log E^*))$.

Supplementary slides

Inversion of Gas Cavern Parameters

- We assume observational noise $\eta \sim \mathcal{N}(0, \gamma l_{gs^2 \times t})$ with $\gamma = 1 \text{ cm}$, $gs = 10$, $t = 20$ years.
- The prior for β_i s assumed to be multivariate $U(a, b)$ with $a = 25^\circ$, and $b = 50^\circ$, and for converged volumes k_i s we set multivariate $\mathcal{N}(0.2_{60}, 0.1 l_{60})$.
- The prior is $U(25, 50) \otimes \mathcal{N}(0.2_{60}, 0.1 l_{60})$.
- The ensemble sizes are $J = 189$ and $J = 127$ for EKI and UKI, respectively.

Supplementary slides

Inversion of Gas Cavern Parameters

Figure 10: Coverage probability for β .

Supplementary slides

Inversion of Gas Cavern Parameters

Figure 11: RMSE for β and k for EKI.

Supplementary slides

Inversion of Gas Cavern Parameters

Figure 12: RMSE for β and k for UKI.