Efficient Krylov subspace methods for large-scale hierarchical Bayesian inverse problems

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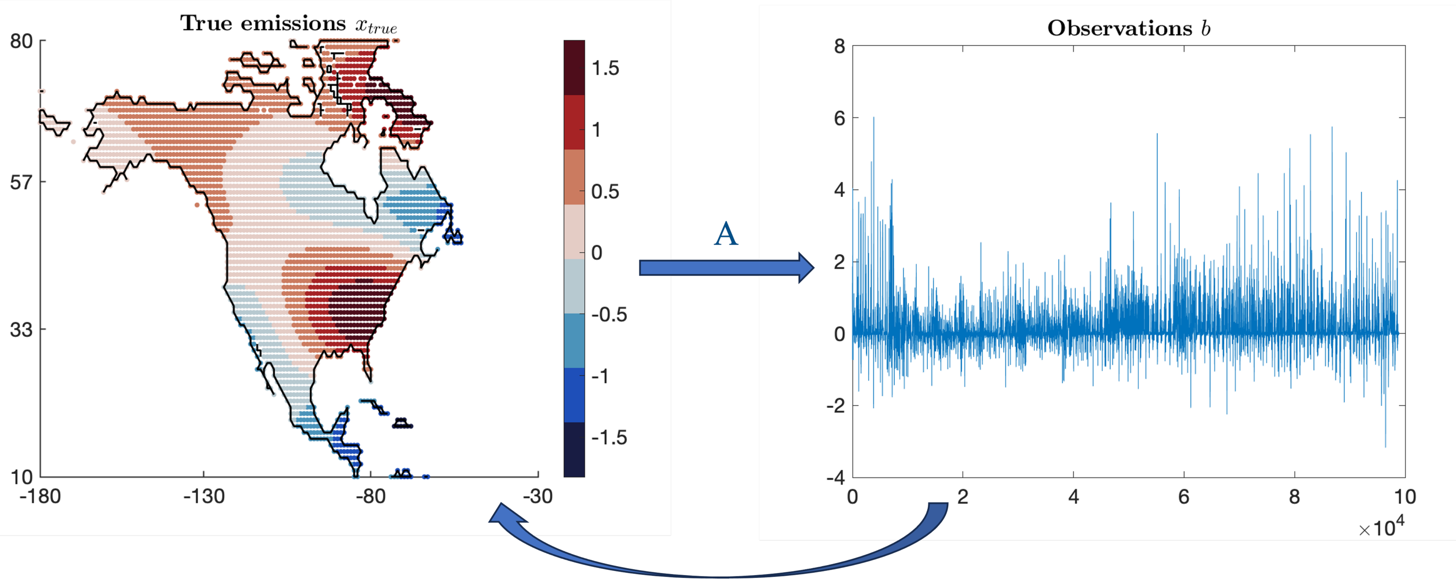
Motivation

- Inverse problems arise in many applications
  - Many unknown parameters
  - Dynamic problems have parameters that change over time
  - Example: Recovering CO_2 emissions from satellite data



$$\mathbf{b} = \mathbf{A}\mathbf{x}_{\text{true}} + \mathbf{e}$$

- $\mathbf{b} \in \mathbb{R}^m$ contains noisy observations
- $\mathbf{A} \in \mathbb{R}^{m \times n}$ represents the forward model
- $\mathbf{e} \in \mathbb{R}^m$ is noise
- $\mathbf{x}_{\text{true}} \in \mathbb{R}^n$ is the vectorized true image

- Uncertainty quantification (UQ) for large-scale problems is computationally challenging

Goal: Develop efficient sampling approaches that exploit generalized Golub-Kahan (genGK) methods

Hierarchical Bayesian Approach

Idea: Reformulate inverse problem as statistical inference where $\mathbf{x}$ and $\mathbf{e}$ are random variables:

$$\mathbf{x} \mid \delta \sim \mathcal{N}(\boldsymbol{\mu}, \delta^{-1}\mathbf{Q}) \qquad \mathbf{e} \mid \lambda \sim \mathcal{N}\left(\mathbf{0}, \lambda^{-1}\mathbf{R}\right)$$

- $\boldsymbol{\mu} \in \mathbb{R}^n$, $\mathbf{0} \in \mathbb{R}^m$ are the mean vectors, assume $\boldsymbol{\mu} = \mathbf{0}$
- $\mathbf{Q} \in \mathbb{R}^{n\times n}$, $\mathbf{R} \in \mathbb{R}^{m \times m}$ symmetric positive definite
- $\delta > 0$, $\lambda > 0$ hyper-parameters with gamma hyperpriors

$$\pi(\lambda) \propto \lambda^{\alpha_\lambda - 1}\exp(-\beta_\lambda \lambda) \qquad \pi(\delta) \propto \delta^{\alpha_\delta - 1}\exp(-\beta_\delta \delta)$$

By Bayes theorem, we get the posterior, which is the solution of the inverse problem

$$\boxed{\pi(\mathbf{x}, \lambda, \delta \mid \mathbf{b}) \propto \pi(\mathbf{b} \mid \mathbf{x}, \lambda)\, \pi(\mathbf{x} \mid \delta)\, \pi(\lambda)\, \pi(\delta)}$$

Challenges for large-scale UQ:

- Need efficient methods to explore the posterior
  - Maximum a Posteriori estimate: $\max_{\mathbf{x},\lambda,\delta} \pi(\mathbf{x}, \lambda, \delta \mid \mathbf{b})$
  - Estimating variances requires drawing samples, which can be expensive
- $\mathbf{A}$ and $\mathbf{Q}$ may only be accessible via matrix-vector multiplications
- Computing factorization $\mathbf{Q} = \mathbf{L}\mathbf{L}^\top$ is computationally infeasible

Hierarchical Gibbs Sampling:

- **Idea:** Sample from the conditional densities of $\mathbf{x}$, λ and δ:

$$\lambda \mid \mathbf{b}, \mathbf{x} \sim \Gamma\big(m/2 + \alpha_\lambda, \tfrac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2_{\mathbf{R}^{-1}} + \beta_\lambda\big)$$
$$\delta \mid \mathbf{b}, \mathbf{x} \sim \Gamma\big(n/2 + \alpha_\delta, \tfrac{1}{2}\|\mathbf{x} - \boldsymbol{\mu}\|^2_{\mathbf{Q}^{-1}} + \beta_\delta\big)$$
$$\mathbf{x} \mid \mathbf{b}, \lambda, \delta \sim \mathcal{N}\left((\lambda\mathbf{A}^\top\mathbf{R}^{-1}\mathbf{A} + \delta\mathbf{Q}^{-1})^{-1}\lambda\mathbf{A}^\top\mathbf{R}^{-1}\mathbf{b},\ (\lambda\mathbf{A}^\top\mathbf{R}^{-1}\mathbf{A} + \delta\mathbf{Q}^{-1})^{-1}\right)$$

where $\|\mathbf{x}\|_{\mathbf{M}} = \sqrt{\mathbf{x}^\top\mathbf{M}\mathbf{x}}$

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1: Initialize (λ^0, δ^0) and x̂^0 = (λ^0 A^T R^-1 A + δ^0 Q^-1)^-1 A^T R^-1 b, set J
2: for j = 1 : J
3:     Compute λ^j ~ Γ(m/2 + α_λ, 1/2 ||A x^{j-1} − b||^2_{R^-1} + β_λ)
4:     Compute δ^j ~ Γ(n/2 + α_δ, 1/2 ||x^{j-1} − μ||^2_{Q^-1} + β_δ)
5:     Compute x^j ~ N((λ^j A^T R^-1 A + δ^j Q^-1)^-1 λ^j A^T R^-1 b, (λ^j A^T R^-1 A + δ^j Q^-1)^-1)
6: end for
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Sampling from a Gaussian Distribution with genGK

Note in line 5 of the hierarchical Gibbs sampling algorithm:

- λ, δ fixed
- $\mathbf{x}|\mathbf{b}, \lambda, \delta \sim \mathcal{N}(\hat{\mathbf{x}}, \boldsymbol{\Gamma})$ with

$$\boldsymbol{\Gamma} = (\lambda\mathbf{A}^\top\mathbf{R}^{-1}\mathbf{A} + \delta\mathbf{Q}^{-1})^{-1} \quad \text{and} \quad \hat{\mathbf{x}} = \lambda\boldsymbol{\Gamma}\mathbf{A}^\top\mathbf{R}^{-1}\mathbf{b}$$

Compute samples, $\mathbf{x}^j$, as

$$\mathbf{x}^j = \hat{\mathbf{x}} + \boldsymbol{\Gamma}^{1/2}\boldsymbol{\xi}, \quad \text{with} \quad \boldsymbol{\xi} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

- Estimate $\hat{\mathbf{x}}$ with genGK iterative methods

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}\in\mathbb{R}^n} -\log \pi(\mathbf{x}|\mathbf{b}, \lambda, \delta) = \arg\min_{\mathbf{x}\in\mathbb{R}^n} \frac{\lambda}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2_{\mathbf{R}^{-1}} + \frac{\delta}{2}\|\mathbf{x}\|^2_{\mathbf{Q}^{-1}}$$

1. Introduce a change in variables $\mathbf{s} = \mathbf{Q}^{-1}\mathbf{x}$

$$\min_{\mathbf{s}\in\mathbb{R}^n} \frac{\lambda}{2}\|\mathbf{A}\mathbf{Q}\mathbf{s} - \mathbf{b}\|^2_{\mathbf{R}^{-1}} + \frac{\delta}{2}\|\mathbf{s}\|^2_{\mathbf{Q}}$$

2. Project transformed problem onto a Krylov subspace of increasing dimension
3. Using genGK process to generate a basis $\mathbf{V}_k$ of subspace: Let $\gamma_1 = \|\mathbf{b}\|_{\mathbf{R}^{-1}}$

$$\mathbf{U}_{k+1}\gamma_1\mathbf{e}_1 = \mathbf{b}, \qquad \mathbf{A}\mathbf{Q}\mathbf{V}_k = \mathbf{U}_{k+1}\mathbf{B}_k, \quad \text{and} \quad \mathbf{A}^\top\mathbf{R}^{-1}\mathbf{U}_{k+1} = \mathbf{V}_k\mathbf{B}_k^\top + \alpha_{k+1}\mathbf{v}_{k+1}\mathbf{e}_{k+1}^\top$$

with

$$\mathbf{U}_{k+1}^\top\mathbf{R}^{-1}\mathbf{U}_{k+1} = \mathbf{I}_{k+1} \quad \text{and} \quad \mathbf{V}_k^\top\mathbf{Q}\mathbf{V}_k = \mathbf{I}_k$$

4. Let $\mathbf{s}_k = \mathbf{V}_k\mathbf{y}_k \implies$ projected problem

$$\min_{\mathbf{s}_k\in\mathcal{R}(\mathbf{V}_k)} \frac{\lambda}{2}\|\mathbf{A}\mathbf{Q}\mathbf{s}_k - \mathbf{b}\|^2_{\mathbf{R}^{-1}} + \frac{\delta}{2}\|\mathbf{s}_k\|^2_{\mathbf{Q}} \iff \min_{\mathbf{y}_k\in\mathbb{R}^k} \frac{\lambda}{2}\|\mathbf{B}_k\mathbf{y}_k - \gamma_1\mathbf{e}_1\|_2^2 + \frac{\delta}{2}\|\mathbf{y}_k\|_2^2$$

5. Project back: $\mathbf{x}_k = \mathbf{Q}\mathbf{s}_k = \mathbf{Q}\mathbf{V}_k\mathbf{y}_k \approx \hat{\mathbf{x}}$

- Estimate $\boldsymbol{\Gamma}^{1/2}$ using genGK

$$\begin{aligned}\boldsymbol{\Gamma}^{1/2} &= \delta^{-1/2}\mathbf{Q}^{1/2}\left(\mathbf{I} + \frac{\lambda}{\delta}\mathbf{Q}^{1/2}\mathbf{A}^\top\mathbf{R}^{-1}\mathbf{A}\mathbf{Q}^{1/2}\right)^{-1/2} \\ &\approx \delta^{-1/2}\mathbf{Q}^{1/2}(\mathbf{I} + \frac{\lambda}{\delta}\underbrace{\mathbf{Q}^{1/2}\mathbf{V}_k\mathbf{B}_k^\top\mathbf{B}_k\mathbf{V}_k^\top\mathbf{Q}^{1/2}}_{\mathbf{Z}_k\boldsymbol{\Theta}_k\mathbf{Z}_k^\top})^{-1/2} \\ &= \delta^{-1/2}\mathbf{Q}^{1/2}(\mathbf{I} - \mathbf{Z}_k\mathbf{D}_k\mathbf{Z}_k^\top)\end{aligned}$$

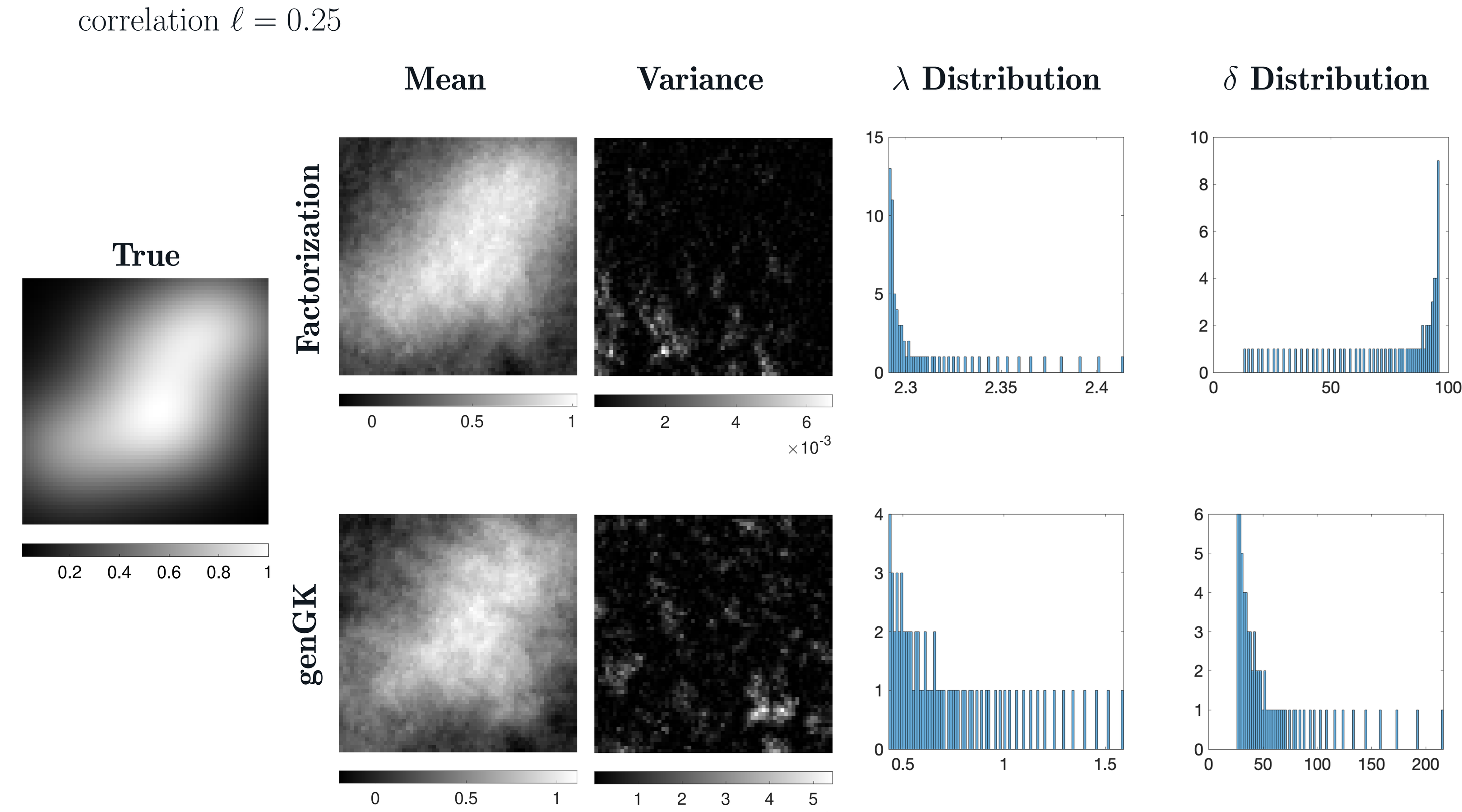
where $\mathbf{D}_k \equiv \mathbf{I}_k - (\mathbf{I}_k + \frac{\lambda}{\delta}\boldsymbol{\Theta}_k)^{-1/2}$

- Draw the sample

$$\mathbf{x}^j = \mathbf{x}_k + \delta^{-1/2}\mathbf{Q}^{1/2}(\mathbf{I} - \mathbf{Z}_k\mathbf{D}_k\mathbf{Z}_k^\top)\boldsymbol{\xi}$$

Seismic Tomography Results

- $\mathbf{x}_{\text{true}}$ represents a vectorized 64×64 image of the Earth's interior
- observations $\mathbf{b} \in \mathbb{R}^{3200}$ contains simulated measurements with 2% noise
- compare to hierarchical Gibbs with full factorization of $\mathbf{Q}$: Matérn Kernel with smoothness $\nu = 0.5$ and correlation $\ell = 0.25$

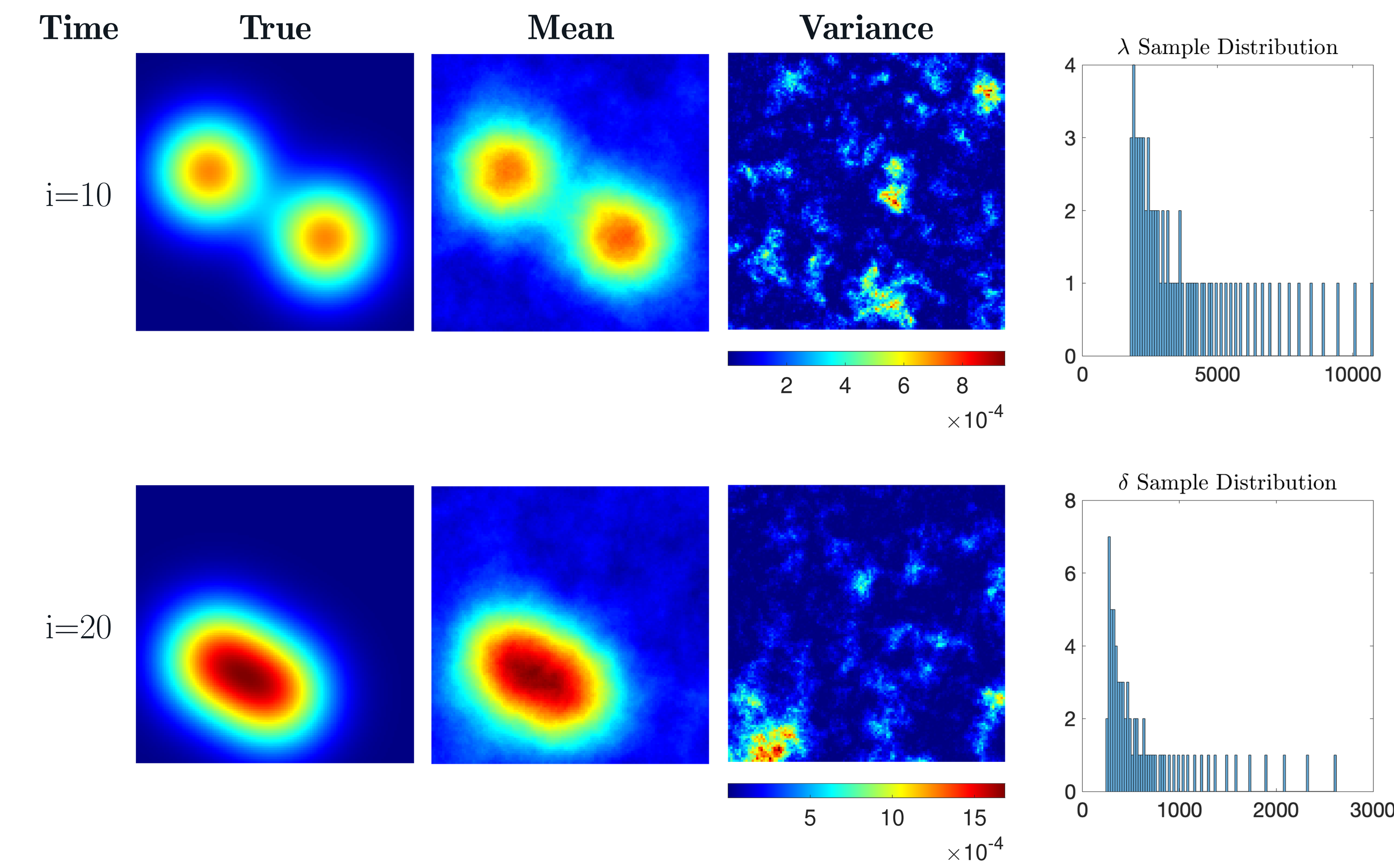


Dynamic Photoacoustic Tomography Results

- $\mathbf{x}^{(i)} \in \mathbb{R}^{16,384}$ is a vectorized 128×128 image
- forward model $\mathbf{A} \in \mathbb{R}^{65,160 \times 327,680}$ is spherical projection with 18 angles
- observations $\mathbf{b} \in \mathbb{R}^{65,160}$ contain projection data with 2% noise

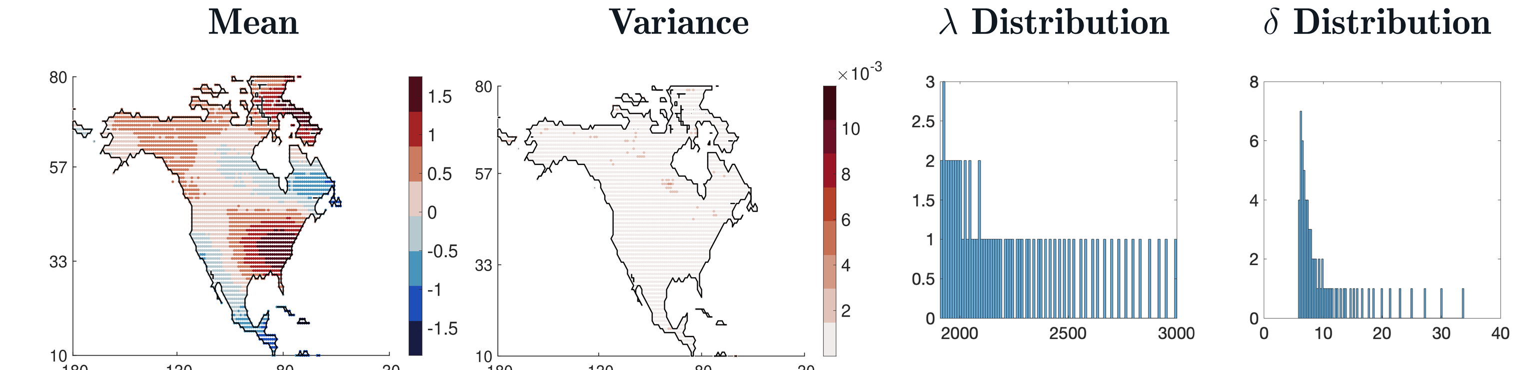
$$\mathbf{x}_{\text{true}} = \begin{bmatrix}\mathbf{x}^{(1)} \\ \vdots \\ \mathbf{x}^{(20)}\end{bmatrix}, \ \mathbf{b} = \begin{bmatrix}\mathbf{b}^{(1)} \\ \vdots \\ \mathbf{b}^{(20)}\end{bmatrix}, \ \mathbf{A} = \begin{bmatrix}\mathbf{A}^{(1)} & & \\ & \ddots & \\ & & \mathbf{A}^{(20)}\end{bmatrix}, \ \mathbf{Q} = \mathbf{Q}_t \otimes \mathbf{Q}_s$$

- $\mathbf{Q}_s, \mathbf{Q}_t$ Matérn Kernel with smoothness $\nu = 0.5, \nu = 2.5$ and correlations $\ell = 0.25, \ell = 0.1$



Atmospheric Inverse Modeling Results

- Solution $\mathbf{x} \in \mathbb{R}^{11,900}$ is vectorized 2D image of average CO_2 emissions over North America
- observations $\mathbf{b} \in \mathbb{R}^{98,880}$ contains satellite data with 4% noise
- $\mathbf{Q}$: Matérn Kernel with smoothness $\nu = 2.5$ and correlation $\ell = 0.05$



Conclusions

- UQ for large-scale inverse problems can be challenging
- For Gaussian posterior distributions, generalized Krylov methods can be used to efficiently
  - compute point estimates
  - perform UQ (e.g., draw samples)
- For non-Gaussian posterior distributions, hierarchical Bayesian approaches are needed
  - Sampling can be computationally infeasible and slow
  - Generalized Krylov methods can be exploited within hierarchical Bayesian approaches

References

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[1] Julianne Chung and Arvind K. Saibaba. "Generalized Hybrid Iterative Methods for Large-Scale Bayesian Inverse Problems". In: *SIAM Journal on Scientific Computing* 39.5 (2017), S24–S46.

[2] Silvia Gazzola, Per Christian Hansen, and James G Nagy. "IR Tools: a MATLAB package of iterative regularization methods and large-scale test problems". In: *Numerical Algorithms* 81.3 (2019), pp. 773–811.

[3] Arvind Saibaba, Julianne Chung, and Katrina Petroske. "Efficient Krylov subspace methods for uncertainty quantification in large Bayesian linear inverse problems". In: *Numerical Linear Algebra with Applications* 27 (Aug. 2020).