FAST LARGE-SCALE INVERSION FOR DEEP AQUIFER CHARACTERIZATION

Jonghyun Harry Lee Amalia Kokkinaki Judith Yue Li Peter K. Kitanidis

Department of Civil and Environmental Engineering, Stanford University

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- Error in y and h leads to uncertainty in estimation s
- $\bullet\,$ Therefore, s is characterized in a statistical framework
- requires \$\mathcal{O}\$ (min(n_{obs}, n_{unknowns})) TOUGH2 runs (or more)

Consider the measurement equation

$$\mathbf{y} = \mathbf{h}(\mathbf{s}) + \mathbf{v} \qquad \mathbf{v} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma}_{\text{noise}})$$

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where,

у	:=	<i>n</i> _{obs} measurements, e.g., pressure or temperature
$\mathbf{h}(\cdot)$:=	TOUGH2, e.g., TOUGH2-MP EOS1
s	:=	nunknowns model parameters, e.g., permeability
v	:=	measurement and model error

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$$p(\mathbf{s}) \sim \exp\left(\underbrace{-\frac{1}{2}(\mathbf{y} - \mathbf{h}(\mathbf{s}))^{\top} \mathbf{\Gamma}_{\text{prior}}^{-1}(\mathbf{y} - \mathbf{h}(\mathbf{s}))}_{\textit{likelihood}} \underbrace{-\frac{1}{2}(\mathbf{s} - \mathbf{s}_{\textit{prior}})^{\top} \mathbf{\Gamma}_{\text{prior}}^{-1}(\mathbf{s} - \mathbf{s}_{\textit{prior}})}_{\textit{prior}}\right)$$

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and the best estimate is given by

$$\hat{\mathbf{s}} = \mathbf{s}_{prior} + \mathbf{\Gamma}_{prior} \mathbf{J}^{\top} \boldsymbol{\xi}$$

where J is Jacobian (sensitivity) matrix

$$\mathsf{J}=rac{\partial \mathsf{h}}{\partial \mathsf{s}}_{\mathsf{s}=\hat{\mathsf{s}}}$$

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With advances in sensor technology and computational power (e.g.,min(n_{obs} , $n_{unknowns}$) $\geq 10^6$), we need a scalable approach!





images adapted from USGS, http://cs.txstate.edu/~xc10 and CERN

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In geostatistical approach (as well as other approaches), computational costs from

- Jacobian-Covariance products (e.g., prior cross-covariance) $J\Gamma_{\text{prior}}$
- $\mathcal{O}(\min(n_{obs}, n_{unknowns}))$ forward model runs for **J**
- $\mathcal{O}(n_{unknowns}^2)$ storage for $\mathbf{\Gamma}_{prior}$
- $\mathcal{O}(n_{unknowns}^2 n_{obs})$ multiplication for **JF**_{prior}

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$$\begin{split} \mathbf{\Gamma}_{prior} &= \mathbf{U} \mathbf{\Sigma} \mathbf{U}^{T} \approx \mathbf{U}_{1:K} \mathbf{\Sigma}_{1:K} \mathbf{U}_{1:K}^{T} = \sum_{i=1}^{K} \zeta_{i} \zeta_{i}^{T} \\ \mathbf{J} \mathbf{\Gamma}_{prior} &\approx \mathbf{J} \sum_{i=1}^{K} \zeta_{i} \zeta_{i}^{T} = \sum_{i=1}^{K} (\mathbf{J} \zeta_{i}) \zeta_{i}^{T} \end{split}$$

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$$\boldsymbol{\mathsf{J}}\boldsymbol{\zeta}_{i} = \frac{h(\boldsymbol{\mathsf{s}} + \delta\boldsymbol{\zeta}_{i}) - h(\boldsymbol{\mathsf{s}})}{\delta} + O(\delta)$$

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To avoid explicit construction of J and Γ , we use a Jacobian-free algorithm:

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- only K + 1 TOUGH2 executions in each iteration; total runs $\sim O(100)$ in most cases
- use TOUGH2 as a black-box; easy to implement without code modification!
- easily parallelizable
- previously applied to 3-D hydraulic tomography ($n_{unknown} \sim 3$ mil.), MRI-imaged tracer data inversion ($n_{obs} \sim 6$ mil.), arsenic-bearing mineral characterization (flow - transport - multi-species reaction) and so on

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FAST LARGE-SCALE INVERSION



- 120 m \times 120 m \times 20 m permeability field estimation
- 640 m \times 640 m \times 20 m model domain
- 5 pumping & 8 monitoring wells
- "True" field from TPROGS [Carle and Fogg, 1996], *n*unknowns = 24,040
- pressure and heat tracer data generated from TOUGH2-MP EOS1

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- $\bullet\,$ total inversion $\sim\,400$ TOUGH2 runs for each test
- On a 16-core workstation, it took 8 hours.
- Estimation uncertainty is reduced with additional temperature data

Conclusion

Contributions

- use of TOUGH2-MP as a black box to perform joint inversion
- total $\sim \mathcal{O}(100)$ TOUGH2-MP executions for complex inverse problems
- Potential benefits using temperature tracer data to improve the inversion in CO2 leakage monitoring network

References

- Lee and Kitanidis, Large-Scale Hydraulic Tomography and Joint Inversion of Head and Tracer Data using the Principal Component Geostatistical Approach (PCGA), *WRR*, 2014
- Kitanidis and Lee, Principal Component Geostatistical Approach for Large-Dimensional Inverse Problem, WRR, 2014
- Kitanidis, Quasi-linear Geostatistical Theory for Inversing, WRR, 1995
- Carles and Fogg, Transition Probability-based Indicator Geostatistics, Math. Geology, 1996

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