Krylov Solvers for Shifted Systems with Applications to Solving Large Scale Inverse Problems

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Problem statement

Develop fast solvers for

$$(K + \sigma_j M)x_j = b \qquad j = 1, \ldots, N_\sigma$$

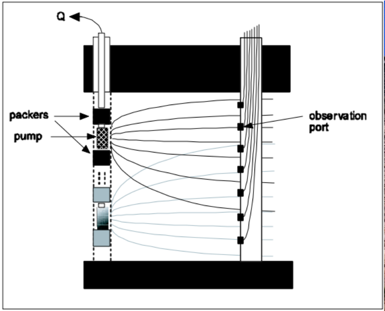
Assumptions:

- $\sigma_j \in \mathbb{C}$ is not close to eigenvalue of (K, M).
- K, M need not be symmetric.
- $N \sim \mathcal{O}(10^6)$ and $N_\sigma \sim \mathcal{O}(100)$

Big picture:

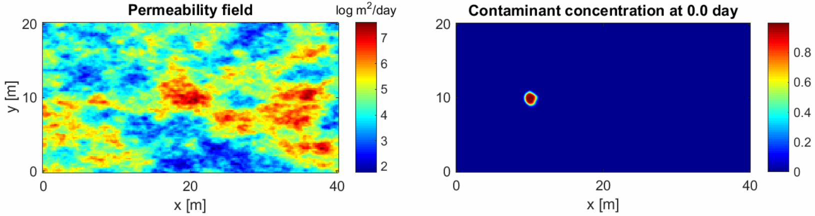
- Solve all the systems at nearly the cost of a single system.
  - Build a shift-invariant basis, and
  - Search within smaller subspace for optimal solution.

Hydraulic Tomography



- Collect pressure (head) measurements from pumping tests
- Recover aquifer properties such as conductivity, storage, etc.
- To better locate natural resources, treat pollution and manage underground sites.

Hydraulic Tomography



Modeling in frequency domain

The governing equations of groundwater flow are,

$$-\nabla \cdot K_{perm}(x)\nabla h(x,t) + S_s(x)\frac{\partial h(x,t)}{\partial t} \quad = \quad Q\delta(x - x_s)$$

Introducing a phasor $\phi(x,t) = \Re\left(h(x,t)e^{i\omega t}\right)$, the long-term solution is

$$-\nabla \cdot K_{perm}(x)\nabla \Phi(x) + i\omega S_s(x)\Phi(x) \quad = \quad Q_0\delta(x - x_s)$$

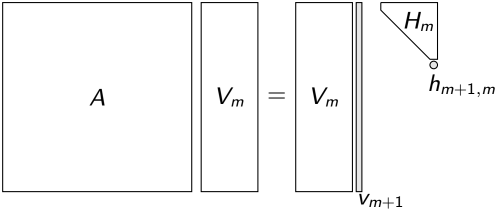
$$(\underbrace{K}_{\text{laplacian}} + \underbrace{i\omega}_{\text{complex shift}} \underbrace{M}_{\text{storage}})\underbrace{\Phi(\sigma)}_{phasor} = \underbrace{b}_{\text{forcing term}}$$

For large number of frequencies and sources, computationally expensive!

Review: Krylov subspace methods

Consider the Krylov subspace defined as

$$\mathcal{K}_m(A, b) = \text{Span}\{b, Ab, \ldots, A^{m-1}b\}$$



Krylov subspaces are shift invariant:

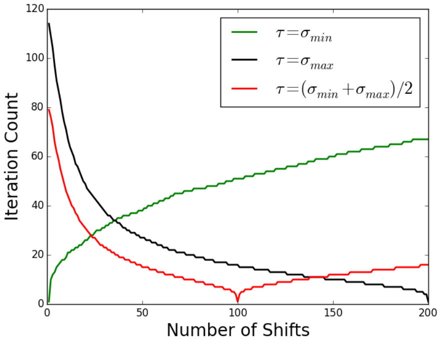
$$\mathcal{K}_m\{A, b\} = \mathcal{K}_m\{A + \sigma I, b\}$$

Preconditioners

Use shift-and-invert preconditioners of the form $(K + \tau M)^{-1}$

$$(K + \sigma M)(K + \tau M)^{-1} = I + (\sigma - \tau) \underbrace{M(K + \tau M)^{-1}}_{\overset{\text{def}}{=} A}$$

- Effective with σ near τ.



Flexible Krylov Approach

- A single preconditioner is insufficient
- Can we use information from different preconditioners?

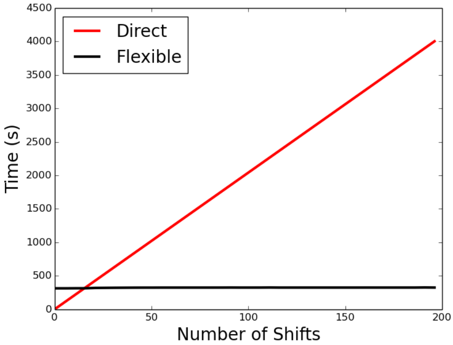
A Flexible approach[1]

- Use preconditioners $(K + \tau_k M)$ for $k = 1, \dots$
- Store another set of vectors Z_m

$$(K + \sigma M) Z_m = V_{m+1} \underbrace{\left(\begin{bmatrix} I \\ 0 \end{bmatrix} + \bar{H}_m (\sigma I - T_m) \right)}_{\stackrel{\text{def}}{=} \bar{H}_m(\sigma, T_m)}$$

[1] Saibaba, B., Kitanidis, A Flexible Krylov Solver for Shifted Systems with Application to Oscillatory Hydraulic Tomography, SISC 2013.
Gu et al. (2007) A flexible preconditioned Arnoldi method for shifted linear systems. JACM International Edition, 2007

Speedup using Flexible GMRES-Sh



- System size 501×501 with 200 shifts
- Stopping tolerance used for all systems $\|r_k(\sigma_j)\|_2/\|r_0\|_2 < 10^{-10}$

Quasi-linear geostatistical approach

Consider the measurement equation

$$y = h(s) + v \qquad v \sim \mathcal{N}(0, R)$$

where,

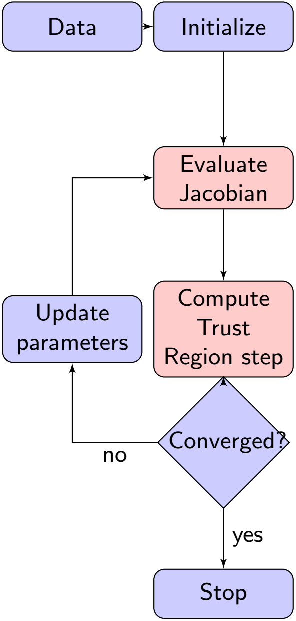
$$\begin{array}{lcl} y & := & \text{measurements.} \\ s & := & \text{model parameters} \\ h(s) & := & \text{measurement op.} \end{array}$$

Further, assume Gaussian prior

$$s \sim \mathcal{N}(X\beta, Q)$$

Maximum a posteriori estimate

$$\arg\min_{s,\beta} \underbrace{\frac{1}{2}\|y - h(s)\|^2_{R^{-1}}}_{Likelihood} + \underbrace{\frac{1}{2}\|s - X\beta\|^2_{Q^{-1}}}_{prior}$$

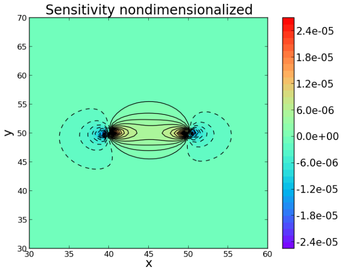


Sensitivity calculation

Adjoint approach: Solve same number of systems as number of measurements

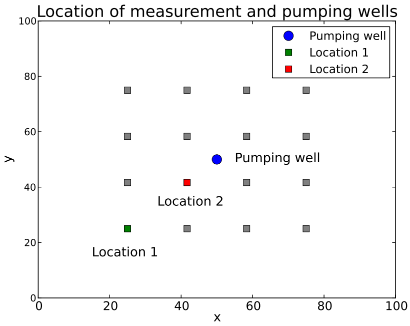
The adjoint field Ψ_i satisfies

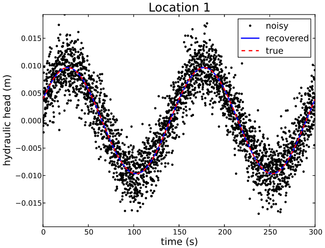
$$-\nabla \cdot (K_{perm} \nabla \Psi_i) + i\omega S_s \Psi_i = \quad -\delta(\mathbf{x} - \mathbf{x}_i), \qquad \mathbf{x} \in \Omega$$

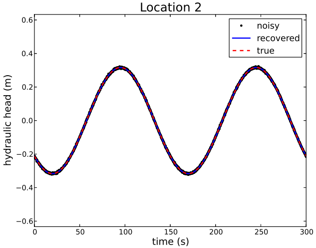


The adjoint calculation is also a multiple shift system.

Example Problem







Time to compute Jacobian

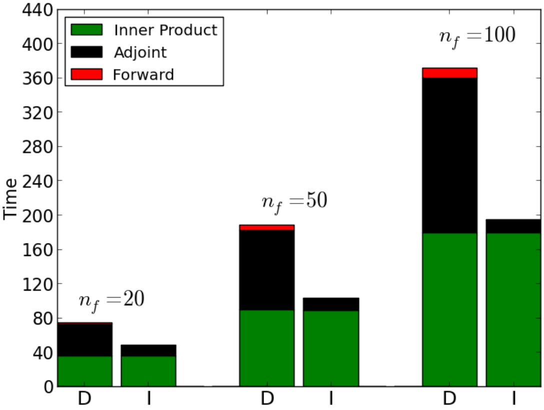


Figure 1 : Comparison of time taken for different components in the Jacobian. Forward refers to solving the forward problem for multiple frequencies. Adjoint refers to solving the adjoint field for multiple frequency at each measurement location. Inner prod. refer to forming the inner product to form the rows of the Jacobian.

Multi Preconditioned GMRES[2]

Joint work with Daniel Szyld and Scott Ladenheim from Temple University

[2] Greif, Rees, and Szyld, MPGMRES: a generalized minimum residual method with multiple preconditioners, Research Report 11-12-23, Department of Mathematics, Temple University

MPGMRES-Sh

Recall: Krylov subspace

$$x_k \quad \in \quad \text{Span}\{b, (AP^{-1})b, \ldots, (AP^{-1})^{k-1}b\}$$

Consider 2 preconditioners P_1, P_2

$$\begin{aligned}
x_1 \quad &\in \quad \text{Span}\{b\} \\
x_2 \quad &\in \quad \text{Span}\{b, AP_1^{-1}b, AP_2^{-1}b\} \\
x_3 \quad &\in \quad \text{Span}\Big\{b, AP_1^{-1}b, AP_2^{-1}b, \\
&\quad (AP_1^{-1})^2 b, AP_1^{-1}AP_2^{-1}b, AP_2^{-1}AP_1^{-1}b, (AP_2^{-1})^2 b\Big\}
\end{aligned}$$

In general:

$$\begin{aligned}
x_k \quad &\in \quad \mathcal{S}_k^{P_1,\ldots,P_t}(A, b) \\
\mathcal{S}_k^{P_1,\ldots,P_t}(A, b) \quad &\stackrel{\text{def}}{=} \quad \{p(AP_1^{-1}, \ldots, AP_t^{-1})b \quad | \quad \in \mathbb{P}_{k-1}[X_1, \ldots, X_t]\}
\end{aligned}$$

Problem Setup

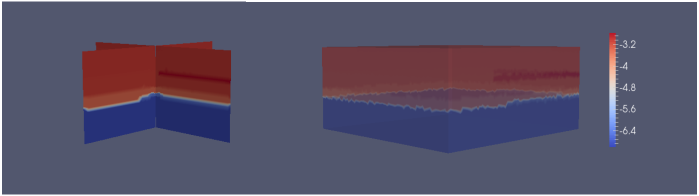


Figure 2 : Log conductivity field of the synthetic example. The pumping well is located at the center of the domain.

The system is of size $132,089 \times 132,089$ with approximately 1.9 million nonzero entries. The number of shifts chosen is 100 with the periods evenly spaced in range from 10 seconds to 15 minutes.

Results

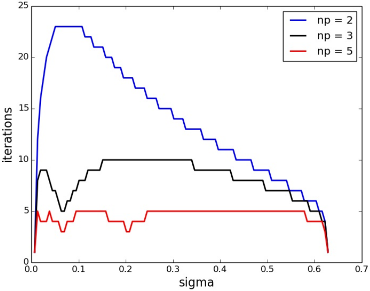


Figure 3 : Iteration count for using different number of preconditioners. System size is $132,089$. The preconditioners are chosen on a log scale.

# Precs	FGMRES-Sh		MPGMRES-Sh	
	Iter.	CPU Time [s]	Iter.	CPU Time [s]
2	81	110	46	101.3
3	61	85.3	30	58.7

Thank you! Any questions?

Some field pictures: