Approximate Solution of Large-scale Linear Inverse Problems with Monte Carlo Simulation

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Introduction & Motivation
- Inverse problems

The New Framework for Large-Scale Problems
- Approximation – Simulation – Regularization
- Everything but the simulation

Simulated Matrix Algebra
- Design of sampling distributions

Results & Conclusions

Ill-posed Inverse Problems

Input $\rightarrow$ [Model(p)] $\rightarrow$ 'Observation'

- From indirect observations infer model parameters.
- Models are linear/nonlinear in differential/integral form.
- Impact of noise on solution existence, uniqueness, stability.
- Applied in geosciences, biomedical imaging, industrial NDT.
- Bayesian inference: Find the posterior density of the unknown conditioned on the observations. MC Simulation/Integration

Integral equations of the first kind

- Classical ill-posed problem: Fredholm integral equation of the first kind. (Books by P.C. Hansen, G.M. Wing & J. D. Zahrt, C.W. Groetsch ,...)

- In continuum,

$$b(t) = \int_0^1 \mathrm{d}s \, A(s,t)x(s) + \epsilon,$$

  with integral operator compact.

- In discrete, approximated on a uniform 1d grid of resolution $n^{-1} \to 0$

$$b = Ax + \epsilon.$$

  $A \in \Re^{n \times n}$ dense, ill-conditioned, of smooth structure.

Main phases of methodology

- Initial hd problem

$$x^* = \arg\min_x \{ \|Ax - b\|^2 \}$$

- Approximate unknown in ld subspace

$$x \approx \Phi r$$

- Use simulation to estimate $G = \Phi' A' A \Phi$ and $c = \Phi' A' b$ in

$$\hat{c} = \hat{G}\ r + \text{simul. error} + \text{approx. error} + \epsilon$$

- Final ld regularization problem (MAP – Gaussian model assumption)

$$r^* = \arg\min_r \{ \|\hat{G} r - \hat{c}\|^2_{\Sigma^{-1}} + \|r - \bar{r}\|^2_{\Sigma_r^{-1}} \}$$

What to expect: Probing the solution error

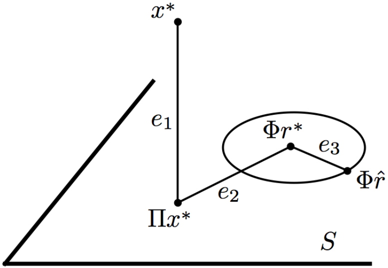


Figure: The approximation (e_1), simulation (e_2) and numerical (e_3) errors affecting the solution. Π is the projection mapping from $\Re^n$ to S, and $r^*(G, c)$ is the calculated and $\hat{r}(\hat{G}, \hat{c})$ the simulation-based ld solution.

The target of simulation

- Notice that the elements of the symmetric G and the vector c are 3d sums

$$G_{k,w} = \phi_k' A' A \phi_w = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} A_{i,j} \Phi_{j,k} \right) \left(\sum_{\bar{j}=1}^{n} A_{i,\bar{j}} \Phi_{\bar{j},w} \right),$$

$$c_k = \phi_k' A' b = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} A_{i,j} \Phi_{j,k} \right) b_i$$

needing n^3 and n^2 additions respectively. If $n \sim O(10^9)$???

- Proposed simulation-based algorithm has numerical complexity independent of n!

Simulation instead of Calculation

- Suppose $\hat{G}$ and $\hat{c}$ are estimators of G and c respectively, simulated element-by-element independently,
- Let $v_{G_{kw}} = \mathrm{var}(\hat{G}_{kw})$ and $v_{c_k} = \mathrm{var}(\hat{c}_k)$ sample-based, then

$$\Sigma(r) = \mathrm{diag}(v_G\, r^2) + \mathrm{diag}(v_c)$$

- For large sample numbers, CLT implies the error $\hat{G}r^* - \hat{c}$ approaches zero mean Gaussian with covariance $\Sigma(r) > 0$.
- Case is suitable for Bayesian inference under Gaussian model and data uncertainty.

Ill-posed integral eqs. have smooth kernels

Implication: Matrix A has smooth structure.

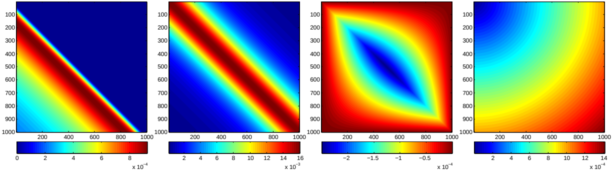


Figure: The kernels of some classical Fredholm integral eqs. of the first kind: heat, gravity, 2nd derivative and the Fox-Goodwin equation, discretized on a grid of dimension 1000.

Sampling with Monte Carlo

- Instead of computing

$$G_{k,w} = \sum_{i=1}^{n} \Big(\sum_{j=1}^{n} A_{i,j} \Phi_{j,k} \Big) \Big(\sum_{\bar{j}=1}^{n} A_{i,\bar{j}} \Phi_{\bar{j},w} \Big),$$

  estimate

$$\hat{G}_{k,w} = \frac{1}{T} \sum_{t=1}^{T} \frac{A_{i_t,j_t} A_{i_t,\bar{j}_t} \Phi_{j_t,k} \Phi_{\bar{j}_t,w}}{n^{-1}}, k = 1, \dots, s \quad w = k, \dots, s$$

  and the variance statistic $v_{G_{kw}}$, where $(i_t, j_t, \bar{j}_t) \in \mathbb{N}^3$ are uniformly sampled indices from $[1, \dots, n]^3$.
- Repeat as appropriate for $\hat{c}_k$, $k = 1, \dots, s$.

Variance Reduction with Importance Sampling

- Instead design an optimal importance sampling distribution customized for $G_{k,w}$, or c_k,

- The optimal $\xi^* : \Re^n \times \Re^n \times \Re^n \rightarrow \Re_+$ is hd !

$$\xi^*_{G_{k,w}}(i,j,\bar{j}) \propto (\Phi_{j,k}\|A_j\|_1)(\Phi_{\bar{j},w}\|A_{\bar{j}}\|_1)\frac{A_{i,j}A_{i,\bar{j}}}{\|A_j\|_1\|A_{\bar{j}}\|_1}$$

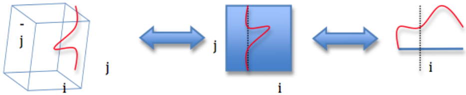
where A_j is the j'th column of A and $\|A_j\|_1 = \sum_{i=1}^n |A_{i,j}|$.

Variance Reduction with Importance Sampling

- How to sample a 3D distribution:

$$\xi^*(i,j,\bar{j}) = \xi(\bar{j}|i,j)\xi(i,j) = \xi(\bar{j}|i,j)\xi(j|i)\xi(i) \propto G_{w,k}(i,j,\bar{j})$$

where $\xi(i,j) = \sum_{\bar{j}=1}^{n} \xi(i,j,\bar{j})$, and $\xi(i) = \sum_{j=1}^{n} \xi(i,j)$.



- Evaluate $G_{w,k}(i,j,\bar{j})$ on a coarse grid in $[1,\ldots,n]^3$,
- Approximate $G_{w,k}$ over ld polynomial bases,
- Compute approximate sums analytically,
- Scale to make sampling distributions.

IS distribution approximation in pictures.

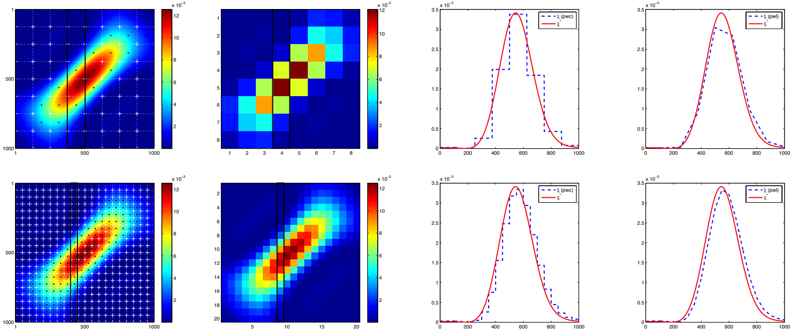


Figure: Top row an approximation of ξ^* in dimension 8, below at 20.

MC Vs IS scheme comparison: estimators.

10 samples 100 samples 1000 samples

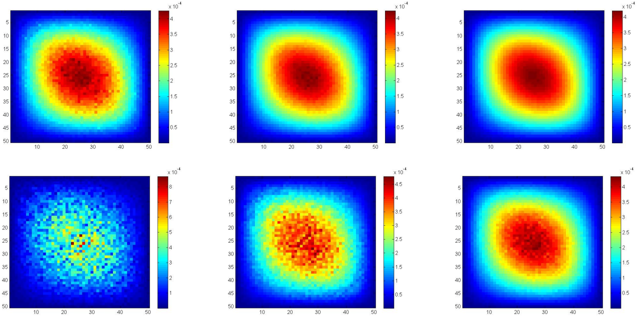


Figure: Estimators of $G = \Phi' A' A \Phi$ with $n = 10^6$, $s = 50$, and Φ piecewise constant basis functions. Top row results with IS and below MC. A is derived from the second derivative kernel.

MC Vs IS scheme comparison: estimator variances

10 samples | 100 samples | 1000 samples

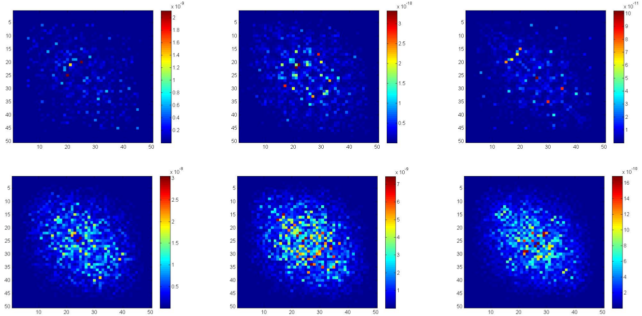


Figure: Variances of the elements of $G = \Phi' A' A \Phi$ with $n = 10^6$, $s = 50$, and Φ piecewise constant basis functions. Top row results with IS and below MC. A is derived from the second derivative kernel.

One test example: Inverse heat conduction

Starting from the familiar elliptic pde, for $u(y, t)$ the temperature at point y at time t.

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial y}, \quad y \geq 0, t \geq 0$$
$$u(y, 0) = 0, \quad u(0, t) = x(t)$$

using the Green's function method

$$b(t) = \int_0^T \mathrm{d}\tau A(\tau, t) x(\tau),$$

measured at point y_m away from the source $y = 0$, where

$$A(\tau, t) = \begin{cases} \frac{y_m/\alpha}{\sqrt{4\pi(\tau - t)^3}} \exp\left(-\frac{(y_m/\alpha)^2}{4(\tau - t)}\right) & \text{if } 0 \leq t < \tau \leq T, \\ 0 & \text{otherwise.} \end{cases}$$

One test example: Solution plot

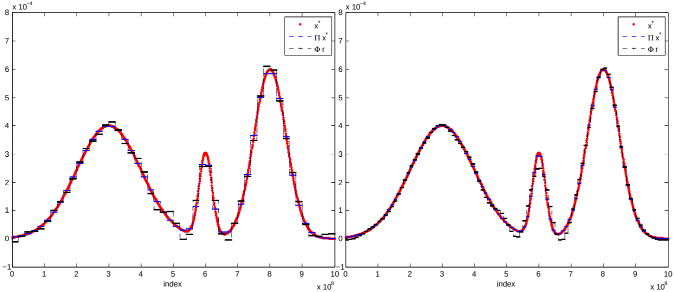


Figure: Results with 50 and 100 piecewise constant basis function. Large problem dimension is 10^9. The optimal ξ^* was approximated on a linear basis. Results with 5×10^4 samples per simulated entry, and zero additive noise!

One test example: Inverse heat conduction

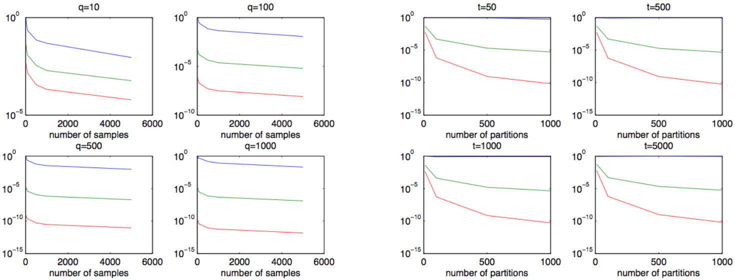


Figure: Simulation error metric: Trace of the covariance of $\hat{G}$ and $\hat{c}$. Results with different number of samples, matrix partitions and polynomial approximation of ξ^*. Tests with inverse heat problem at $n = 10^9$ and $s = 50$ piecewise constant Φ. MC, $\hat{\xi}$ in pwc basis, and $\hat{\xi}$ in pwl.

Conclusion

- Simulation timings: 50-80 μs per sample for pwc - pwq $\hat{\xi}$.
- Method robust for 'applied' ill-posed inverse problems
- Simulation scheme is suitable for multi-thread or parallel processing
- Can be utilized in the context of model reduction
- More analysis, error bounds and results at web.mit.edu/dimitrib/www/publ.html
- Thank you .- Questions?