Efficient Computation of the Posterior Covariance Matrix in Large-Scale Variational Data Assimilation Problems

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Data assimilation

- Numerical weather prediciton is an IVP: given initial conditions, forecast atmospheric evolution.
- Data assimilation is a technique for combining information such as observational and background data with numerical models to obtain the best estimate of state of a system (initial condition).
- Other application areas include hydrology, oceanography, environmental science etc.
- Variational assimilation is used to find the optimal analysis that minimises a specific cost function.

Motivation

Data assimilation problem

- Evolution process:

$$
\begin{aligned}
\frac{\partial \phi}{\partial t} &= F(\phi) + f, \qquad && t \in (0,T), \\
\phi\big|_{t=0} &= u, && \phi, u \in X,\ \phi \in Y
\end{aligned}
$$

true initial state	$\bar{u}$
true state evolution	$\bar{\phi}$
observation operator	$C_o : Y \to Y_o$
observations	$y = C_o \bar{\phi} + \xi_o$
background function	$u_b = \bar{u} + \xi_b$
background error	ξ_b
observation error	ξ_o

Discrete least-squares problem

- observations distributed within time interval (t_0, t_n)
- find $\mathbf{u}$ which minimises

$$
\begin{aligned}
J(\mathbf{u}) &= \frac{1}{2}(\mathbf{u}-\mathbf{u}_b)^T V_b^{-1}(\mathbf{u}-\mathbf{u}_b) \\
&+ \frac{1}{2}\sum_{i=0}^{N}(C_o(\mathbf{u}_i)-\mathbf{y}_i)^T V_o^{-1}(C_o(\mathbf{u}_i)-\mathbf{y}_i)
\end{aligned}
$$

subject to $\mathbf{u}_i$, $i = 1, \ldots, N$ satisfying

$$
\mathbf{u}_{i+1} = \mathcal{M}_{i,i+1}(\mathbf{u}_i), \qquad i = 0, \ldots, N-1.
$$

- discrete nonlinear evolution operator $\mathcal{M}_{i,i+1}$

Incremental 4D-Var

- Rewrite as an unconstrained minimisation problem using Lagrange's method.

- Incremental approach: linearise evolution operator and solve linearised problem iteratively.

- This involves a tangent linear model (TLM) and its adjoint.

- Each iteration requires one forward solution of the TLM equations and one backward solution of the adjoint equations.

Hessian matrix

- Linear system (Gauss-Newton method):

$$\mathcal{H}(\mathbf{u}_k)\delta\mathbf{u}_k = G(\mathbf{u}_k) \qquad (1)$$

Hessian of the cost function $\mathcal{H}$
gradient of the cost function $G(\mathbf{u}_k)$

- Solve (1) using PCG.
- Convergence depends on conditioning of the Hessian

$$\mathcal{H} = V_b^{-1} + R^T C_o^T V_o^{-1} C_o R.$$

- $\mathcal{H}$ is often too large to be stored in memory: all we need for PCG is $\mathcal{H}\mathbf{v}$.
- Evaluating $\mathcal{H}\mathbf{v}$ is very expensive, so we need a good preconditoner.

Approximating the inverse Hessian

- $\mathcal{H}^{-1}$ represents an approximation of the Posterior Covariance Matrix (PCM).
- The PCM can be used to find confidence intervals and carry out *a posteriori* error analysis.
- $\mathcal{H}^{-1/2}$ can be used in ensemble forecasting.
- $\mathcal{H}^{-1/2}$ can be used for preconditioning of the update equation (1).

- Our aim here is to construct a limited-memory approximation to $\mathcal{H}^{-1}$ using only matrix-vector multiplication.

First level preconditioning

- Use the background covariance matrix V_b.

- Projected Hessian:

$$H = (V_b^{1/2})^T \mathcal{H} V_b^{1/2} = I + (V_b^{1/2})^T R^T C_o^T V_o^{-1} C_o R V_b^{1/2}.$$

- Easy to recover $\mathcal{H}$ in the original space.

- Eigenvalues of H are usually clustered in a narrow band above one, with few eigenvalues distinct enough to contribute noticeably to the Hessian value.

- This makes $\mathcal{H}$ amenable to limited-memory approximation.

Limited-memory approximation

- Find n_e leading eigenvalues and orthonormal eigenvectors using the Lanczos method.

- Construct approximation

$$H \approx I + \sum_{i=1}^{n_e} (\lambda_i - 1)\mathbf{u}_i \mathbf{u}_i^T$$

- Easy to evaluate matrix powers:

$$H^p \approx I + \sum_{i=1}^{n_e} (\lambda_i^p - 1)\mathbf{u}_i \mathbf{u}_i^T$$

Second level preconditioning

- Construct a multilevel approximation to H^{-1} based on coarser grids (where it is cheaper to use Lanczos).
- Discretise evolution equation on a grid with $m+1$ nodes (level 0).
- Grid level k contains $m_k = m/2^k + 1$ nodes.
- Grid transfer matrices using piecewise cubic splines:
  - Restriction matrix R_c^0 from $k=0$ to $k=c$.
  - Prolongation matrix P_0^c from $k=c$ to $k=0$.
- Identity matrix I_k on grid level k.
- Hessian H_0 available on finest grid level.

Grid transfers with "correction"

- Need grid transfer operators which minimise the loss of information between grid levels.
- Introduce specific operators which transfer a matrix between a course grid level c and a fine grid level f.

  - From coarse to fine:

$$M_{c \to f} = P_f^c (M_c - I_c) R_c^f + I_f$$

  - From fine to coarse:

$$M_{f \to c} = R_c^f (M_f - I_f) P_f^c + I_c$$

Outline of multilevel algorithm

- Represent H_0 at a given level (k, say):

$$H_{0\to k} = R_k^0 (H_0 - I_0) P_0^k + I_k$$

- Precondition to improve eigenvalue spectrum:

$$\tilde{H}_{0\to k} = (B_k^{k+1})^T H_{0\to k} B_k^{k+1}$$

- Find n_k eigenvalues/eigenvectors of $\tilde{H}_{0\to k}$ using the Lanczos method.

- Approximate $\tilde{H}^{-1}_{0\to k}$:

$$\tilde{H}^{-1/2}_{0\to k} \approx I_k + \sum_{i=1}^{n_k} \left(\frac{1}{\sqrt{\lambda_i}} - 1 \right) \mathbf{u}_i \mathbf{u}_i^T .$$

Preconditioners

- On coarsest grid, level $k+1$ does not exist so set $B_k^{k+1} = I_k$.

- For other levels, construct preconditioners recursively:

$$B_k^{k+1} = \left[B_{k+1}^{k+2} \tilde{H}_{0\to k+1}^{-1/2} \right]_{\to k}, \quad B_k^{k+1^T} = \left[\tilde{H}_{0\to k+1}^{-1/2} B_{k+1}^{k+2^T} \right]_{\to k}$$

- Square brackets represent projection to the correct grid level using "corrected" grid transfers, e.g.

$$[M_{k+1}]_{\to k} = R_k^{k+1}(M_{k+1} - I_{k+1})P_{k+1}^k + I_k$$

Finest level

- We already have H_0, so precondition to obtain

$$\tilde{H}_0 = {B_0^1}^T H_0 B_0^1$$

- Find n_0 eigenvalues/eigenvectors of $\tilde{H}_0$ using the Lanczos method.

- Approximate $\tilde{H}_0^{-1}$:

$$\tilde{H}_0^{-1} \approx I_k + \sum_{i=1}^{n_0} \left(\frac{1}{\lambda_i} - 1 \right) \mathbf{u}_i \mathbf{u}_i^T$$

- Recover projected inverse Hessian using

$$H_0^{-1} = B_0^1 \tilde{H}_0^{-1} {B_0^1}^T$$

Summary

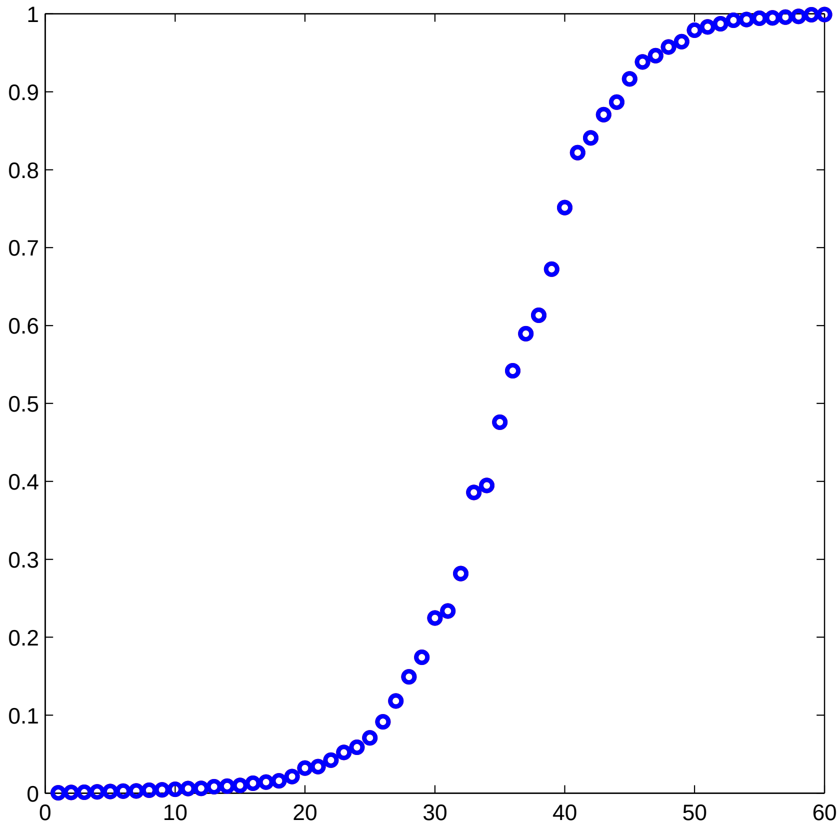
- At each level:
  - represent H_0 on this level;
  - find its eigenvalues/vectors using the Lanczos method;
  - use these to approximate H_0^{-1} in this level;
  - use preconditioners based on these local approximations to accumulate the key eigenvalue structure from every grid level.

Example

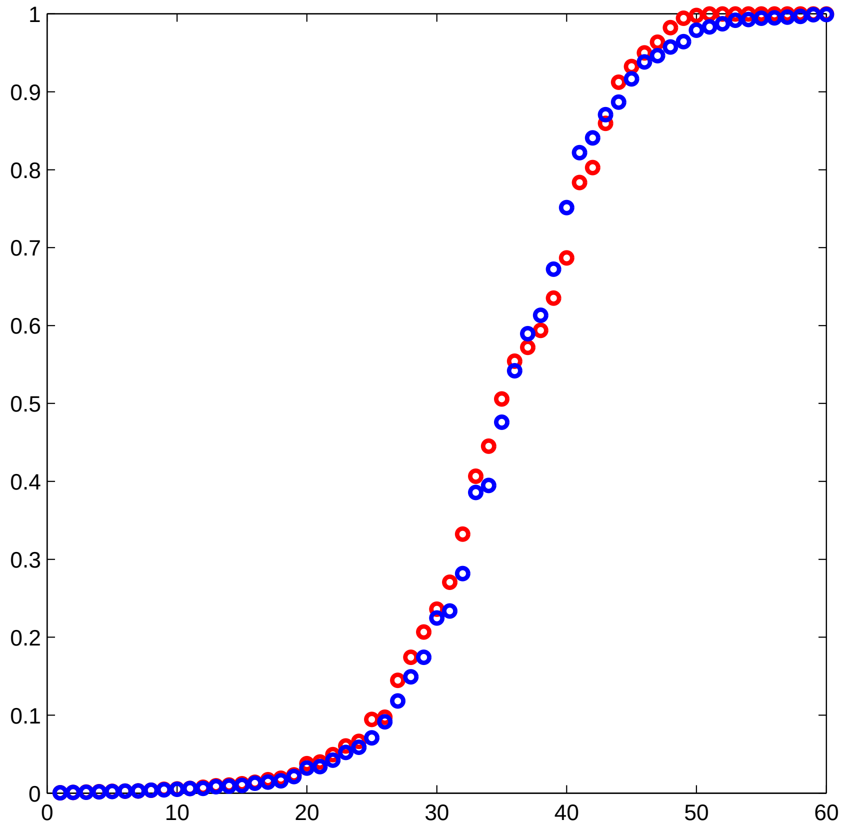
- Test using 1D Burgers' equation.
- 1D uniform grid with 5 sensors.
- Multilevel preconditioning with four grid levels: $k = 0, 1, 2, 3$ with 401, 201, 101 and 51 grid points, respectively.
- Vary number of eigenvalues chosen on each grid level (n_0, n_1, n_2, n_3).
- Compare eigenvalues of exact and computed projected inverse Hessian on the finest grid level $k = 0$.

Eigenvalues of the inverse Hessian

- Exact (blue circles), approximated (red circles)



(400,0,0,0)



(4,8,16,32)

Eigenvalues of the inverse Hessian

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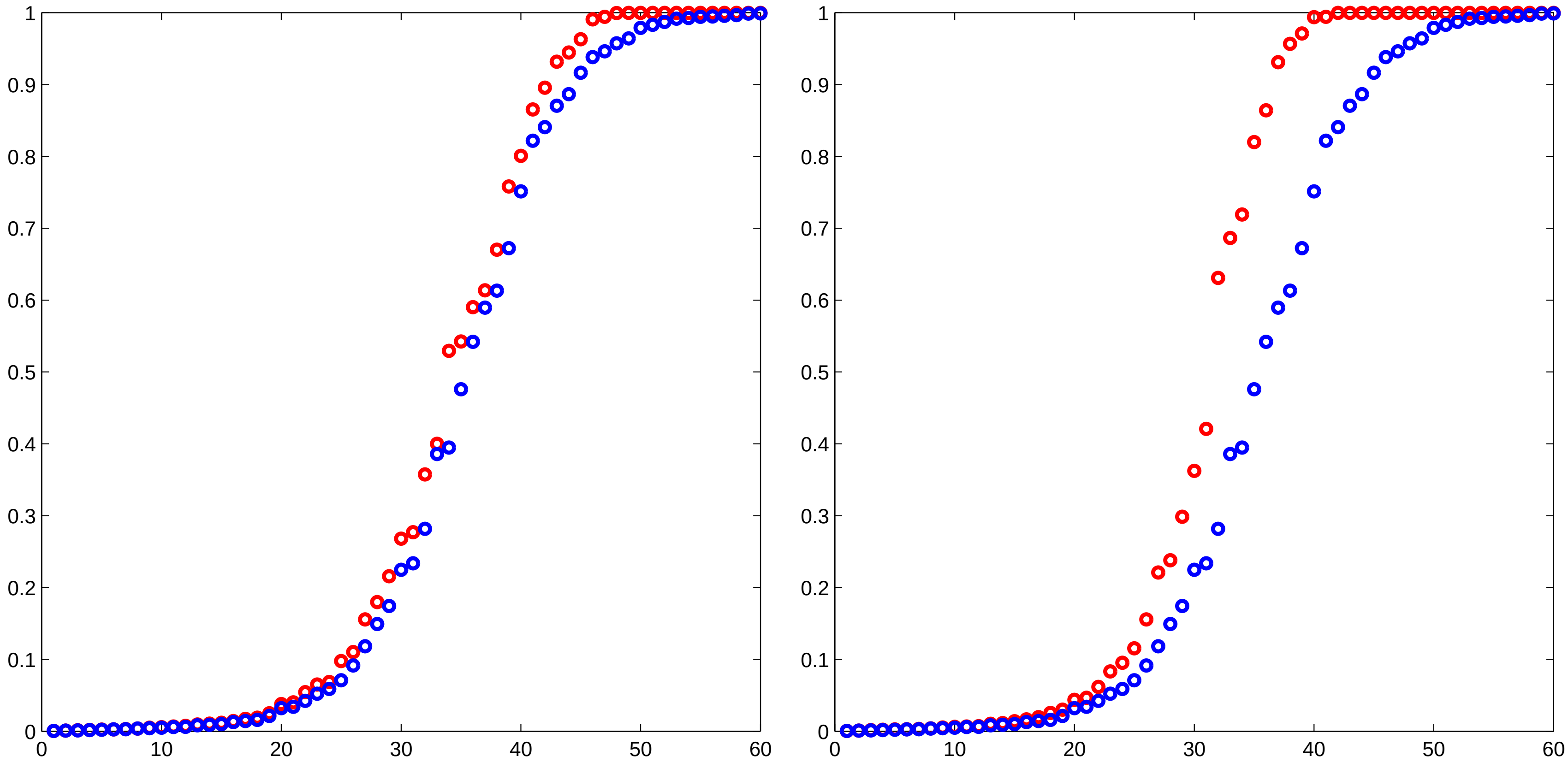

(0,8,16,32) (0,0,16,32)

PCG iteration for Newton step

- measurement units:
  - memory: length of vector on finest grid L
  - cost: cost of MVM on finest grid M

Preconditioner	# CG iterations	storage	cost
none	57	0L	57M
MG(400,0,0,0)	1	400L	402M
MG(4,8,16,32)	4	16L	34M
MG(0,8,16,32)	5	12L	14M
MG(0,0,16,32)	8	8L	10M

Conclusions and next steps

- Although this is only one test problem, multilevel preconditioning looks promising for constructing a good limited-memory approximation to H^{-1}.
- The balance between restrictions on memory/cost limitations may vary between particular applications.
- Identifying globally appropriate values for $(n_0, n_1, n_2, .n_3)$ is tricky.

- Future investigations will include

- constructing local Hessians based on sensor domains of influence;
- applying Lanczos locally at sensor level.

It is sometimes nice in Scotland. . .