A multilevel preconditioner for data assimilation with 4D-Var

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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, data analytics, sensor networks. . .

- Variational assimilation is used to find the optimal analysis that minimises a specific cost function.

Motivation


JST SERVICES

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

- Hessian of the cost function:

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

- Discrete tangent linear operator R and its adjoint.
- $\mathcal{H}$ is often too large to be stored in memory.
- Action of applying $\mathcal{H}$ to a vector is available, but expensive:
  - involves both forward and backward solves with the linearised evolution operator and its adjoint.

Approximating the inverse Hessian

Why approximate $\mathcal{H}^{-1}$?

- $\mathcal{H}^{-1}$ 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.
- $\mathcal{H}^{-1}$, $\mathcal{H}^{-1/2}$ can be used for preconditioning in a Gauss-Newton method (focus of this talk).

AIM: construct a limited-memory approximation to $\mathcal{H}^{-1}$ using only matrix-vector multiplication.

Return to 4D-Var

- Linear system (within a Gauss-Newton method):

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

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

- Solve using Preconditioned Conjugate Gradient iteration (needs only $\mathcal{H}\mathbf{v}$).

- Convergence depends on eigenvalues of the Hessian

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

- Evaluating $\mathcal{H}\mathbf{v}$ is very expensive, so we need a good preconditoner.

First level preconditioning

- Use the background covariance matrix V_b.

- Projected Hessian:

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

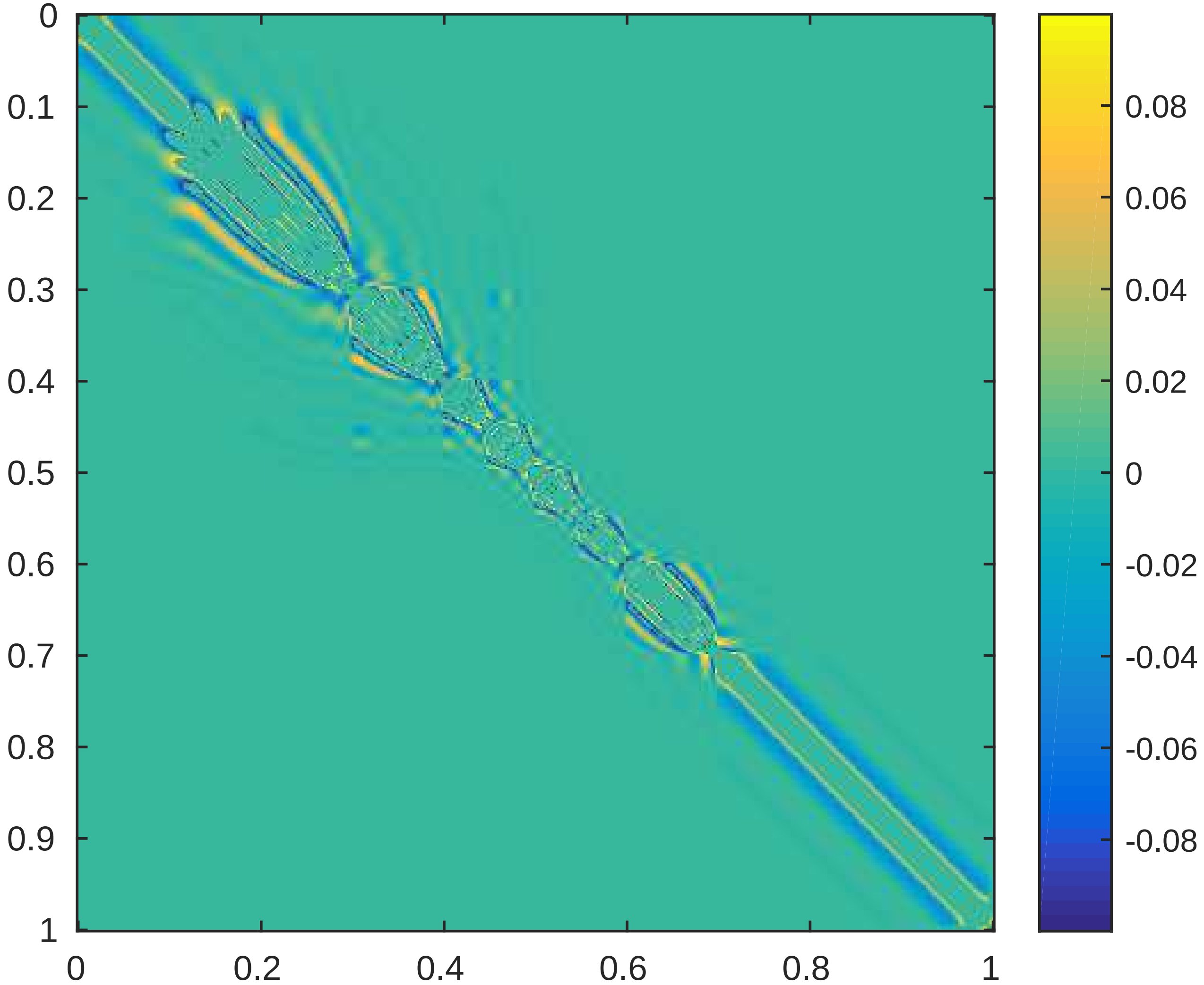
- Easy to recover $\mathcal{H}$ in the original space.

- 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.

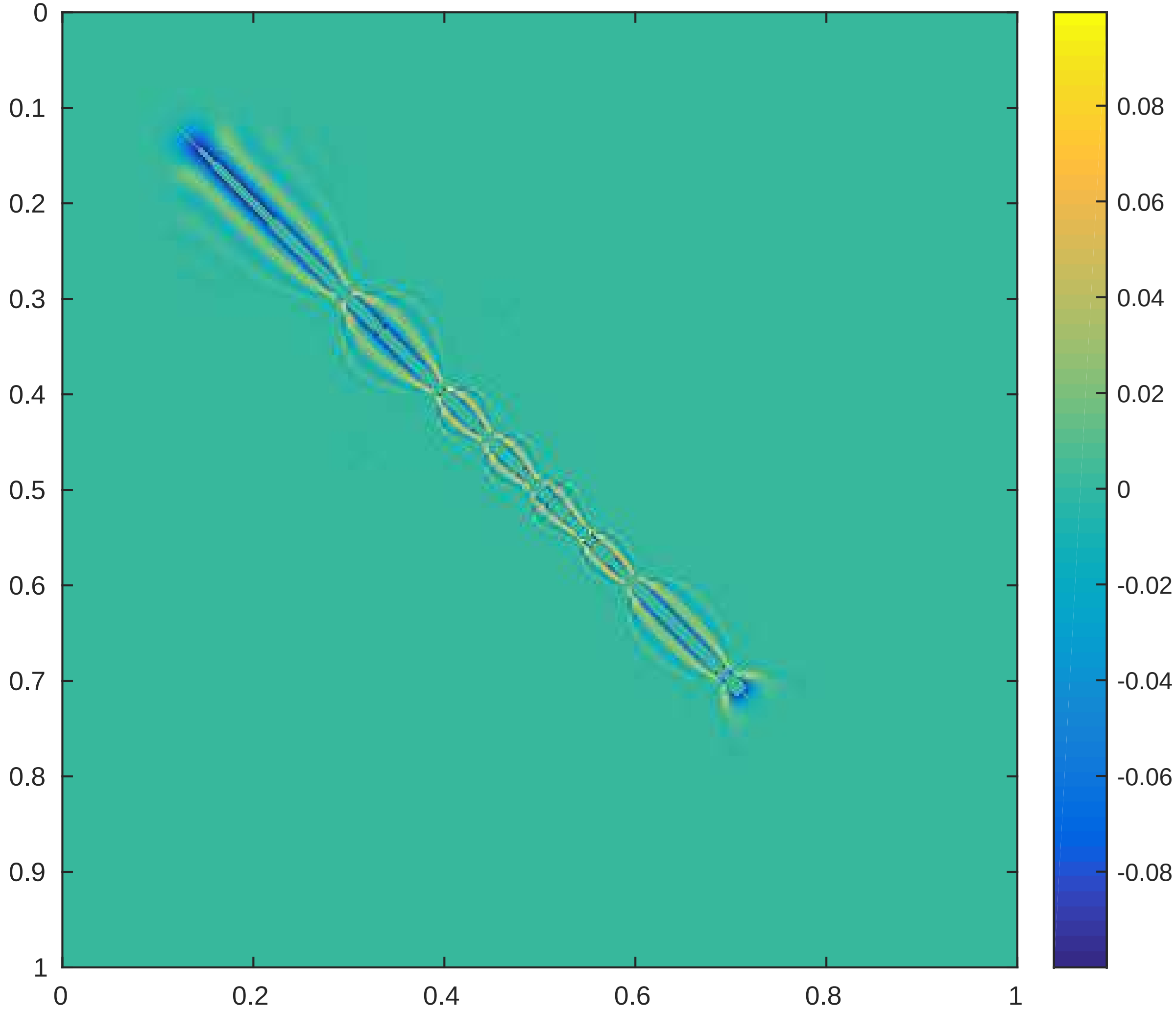
Correlation matrix

- inverse Hessian scaled to have unit diagonal



Preconditioned correlation matrix

- after first level preconditioning has been applied



Limited-memory approximation

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

- Construct approximation

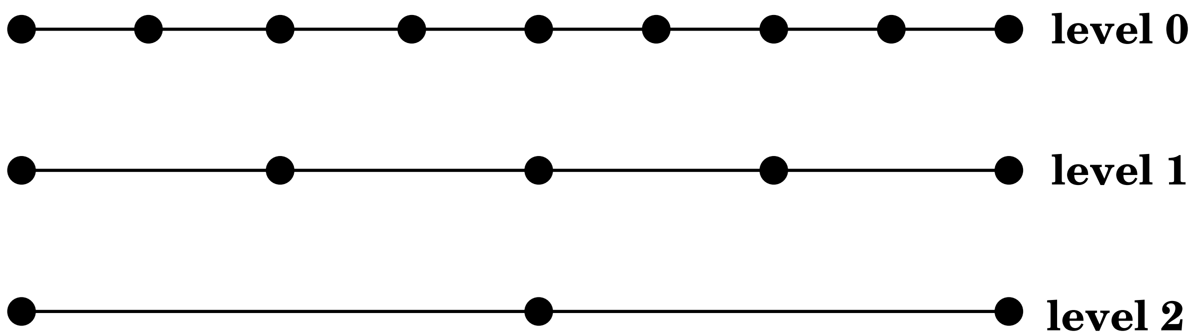
$$H \approx I + \sum_{i=1}^{n_e} (\lambda_i - 1)\mathbf{u}_i\mathbf{u}_i^T$$

- 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) to represent Hessian H_0
- Grid level k contains $m_k = m/2^k + 1$ nodes.



- Identity matrix I_k on grid level k.

Grid transfers with "correction"

- Grid transfer based on piecewise cubic splines:
  - Restriction matrix R_c^f from $k = f$ to $k = c$.
  - Prolongation matrix P_f^c from $k = c$ to $k = f$.
- Construct new 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 $\tilde{H}_{0\to k}^{-1/2}$:

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

Preconditioners

- Construct $B_k^{k+1} = I_k$ on level $k+1$, apply on level k.

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

- For other levels, construct preconditioners recursively:

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

- 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

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

Algorithm

- use $N_e = (n_0, n_1, \ldots, n_c)$ eigenvalues at each level

```
[Λ,𝒰]=mlpre(H_0,n_0, n_1, ..., n_c)
for  k = k_c, k_c − 1, ..., 0
   compute by the Lanczos method
   and store in memory
      {λ_k^i, U_k^i}, i = 1, ..., n_k of H̃_{0→k}
   using preconditioners B_{k,k+1} and B^T_{k,k+1}
end
```

- storage:

$$\Lambda = \left[\lambda^1_{k_c}, \ldots, \lambda^{n_{k_c}}_{k_c}, \lambda^1_{k_c-1}, \ldots, \lambda^{n_{k_c-1}}_{k_c-1}, \ldots, \lambda^1_0, \ldots, \lambda^{n_0}_0\right],$$

$$\mathcal{U} = \left[U^1_{k_c}, \ldots, U^{n_{k_c}}_{k_c}, U^1_{k_c-1}, \ldots, U^{n_{k_c-1}}_{k_c-1}, \ldots, U^1_0, \ldots, U^{n_0}_0\right].$$

Example

- Test using 1D Burgers' equation with initial condition

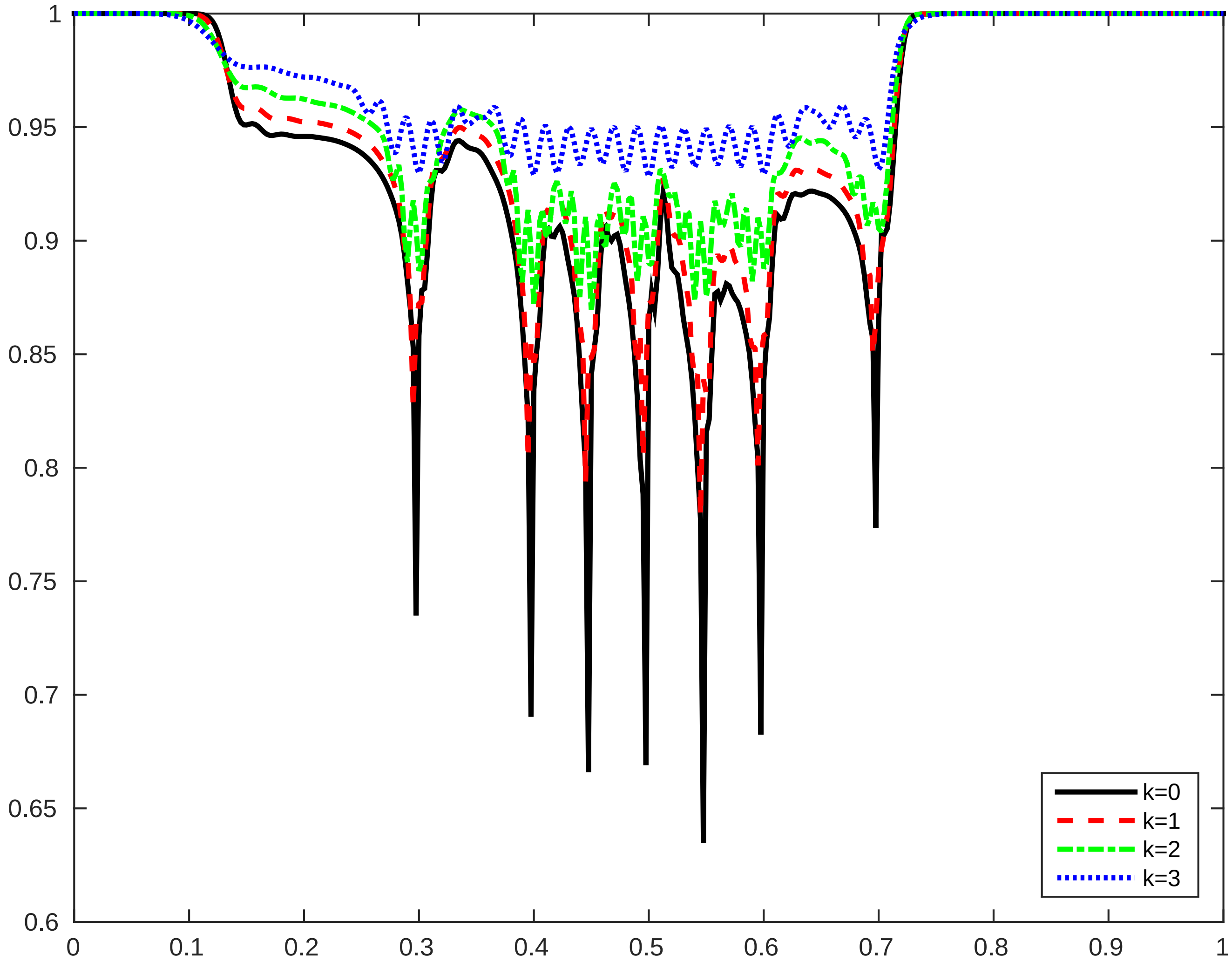
$$f(x) = 0.1 + 0.35\left[1 + \sin\left(4\pi x + \frac{3\pi}{2}\right)\right], \qquad 0 < x < 1$$

- 1D uniform grid with 7 sensors located at 0.3, 0.4, 0.45, 0.5, 0.55, 0.6, and 0.7 in $[0, 1]$.

- Multilevel preconditioning with four grid levels:

k	0	1	2	3
grid points	401	201	101	51

Diagonal of H^{-1}



Assessing approximation accuracy

- Riemannian distance:

$$\delta(A,B) = \left\| ln(B^{-1}A) \right\|_F = \left(\sum_{i=1}^{n} ln^2 \lambda_i \right)^{1/2}$$

- Compare eigenvalues of H^{-1} and $\tilde{H}^{-1}$ on the finest grid level $k = 0$ using

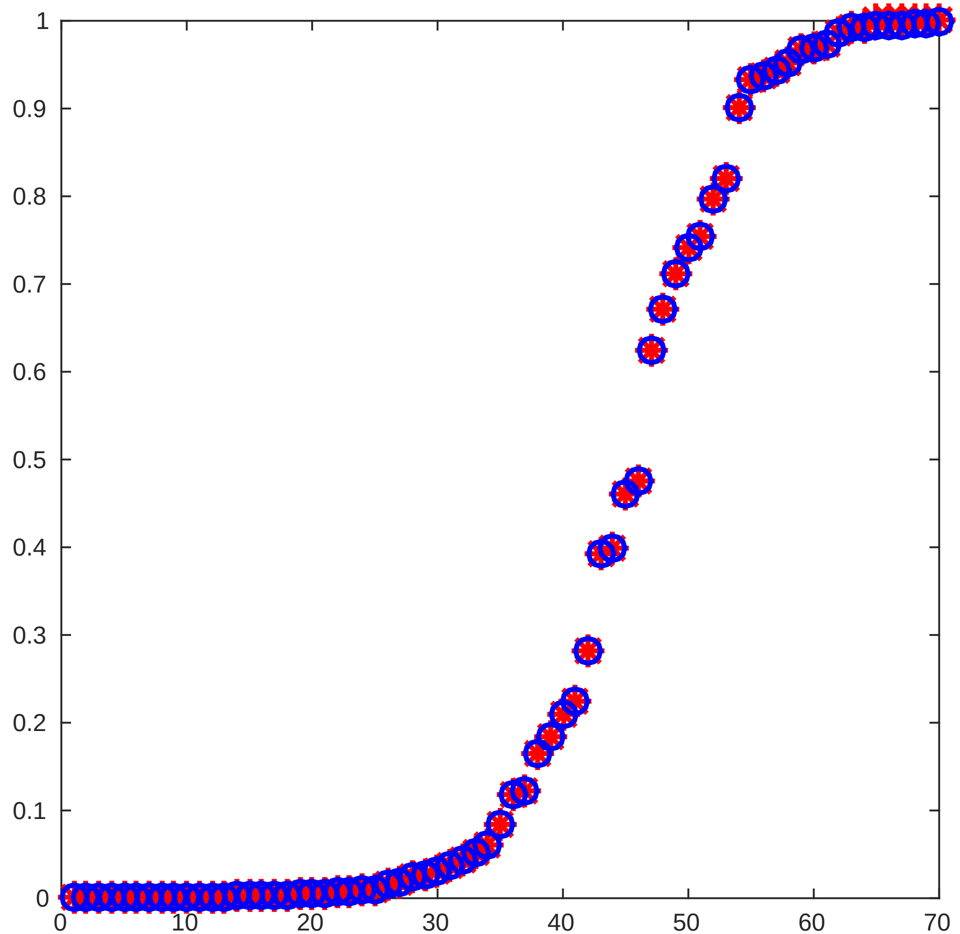
$$D = \frac{\delta(H^{-1}, \tilde{H}^{-1})}{\delta(H^{-1}, I)}$$

- Vary number of eigenvalues chosen on each grid level

$$N_e = (n_0, n_1, n_2, n_3)$$

Eigenvalues of the inverse Hessian

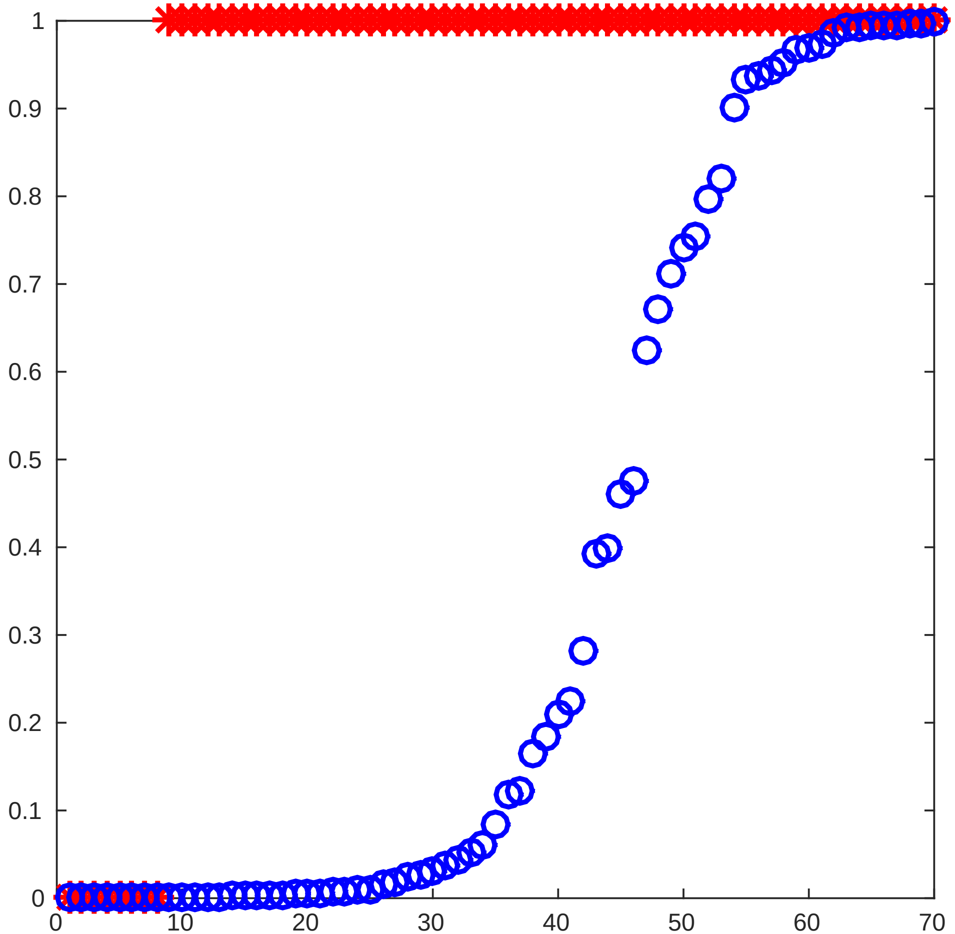
- Exact (blue circles), approximated (red stars)



$$N_e = (64, 0, 0, 0)$$
$$D = 2.98e - 4$$

Eigenvalues of the inverse Hessian

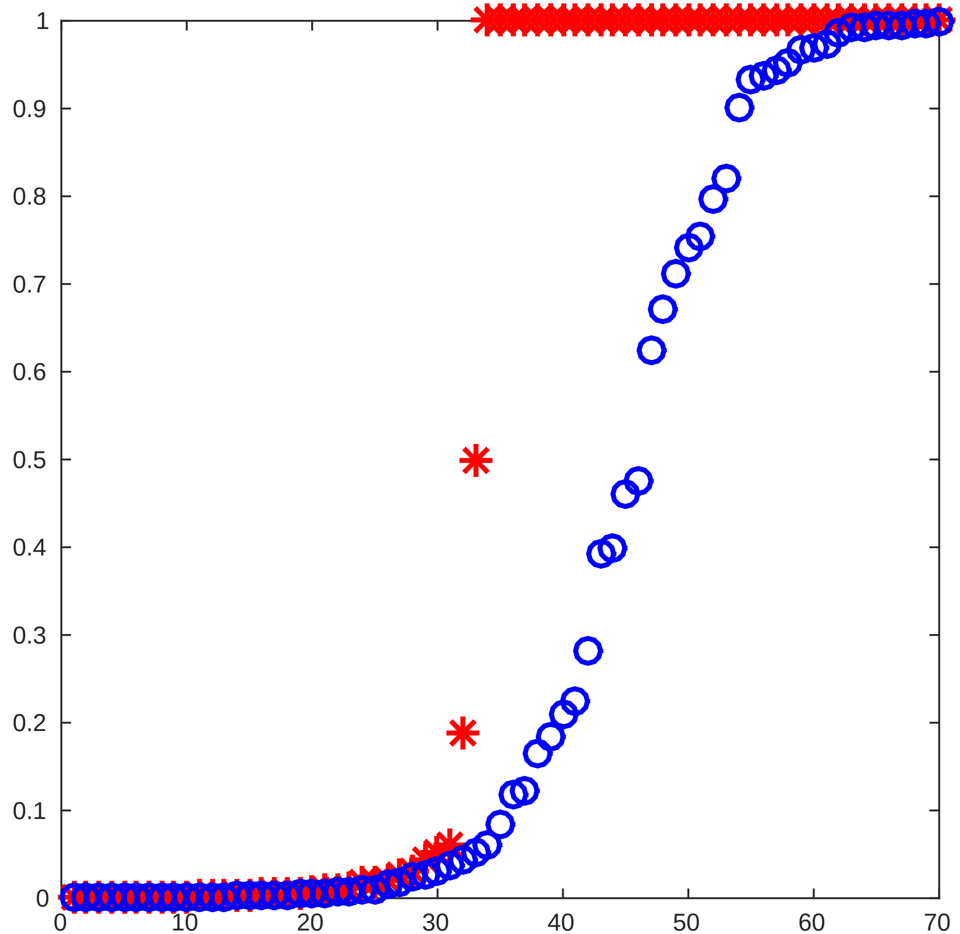
- Exact (blue circles), approximated (red stars)



$$N_e = (8, 0, 0, 0)$$
$$D = 7.71e - 1$$

Eigenvalues of the inverse Hessian

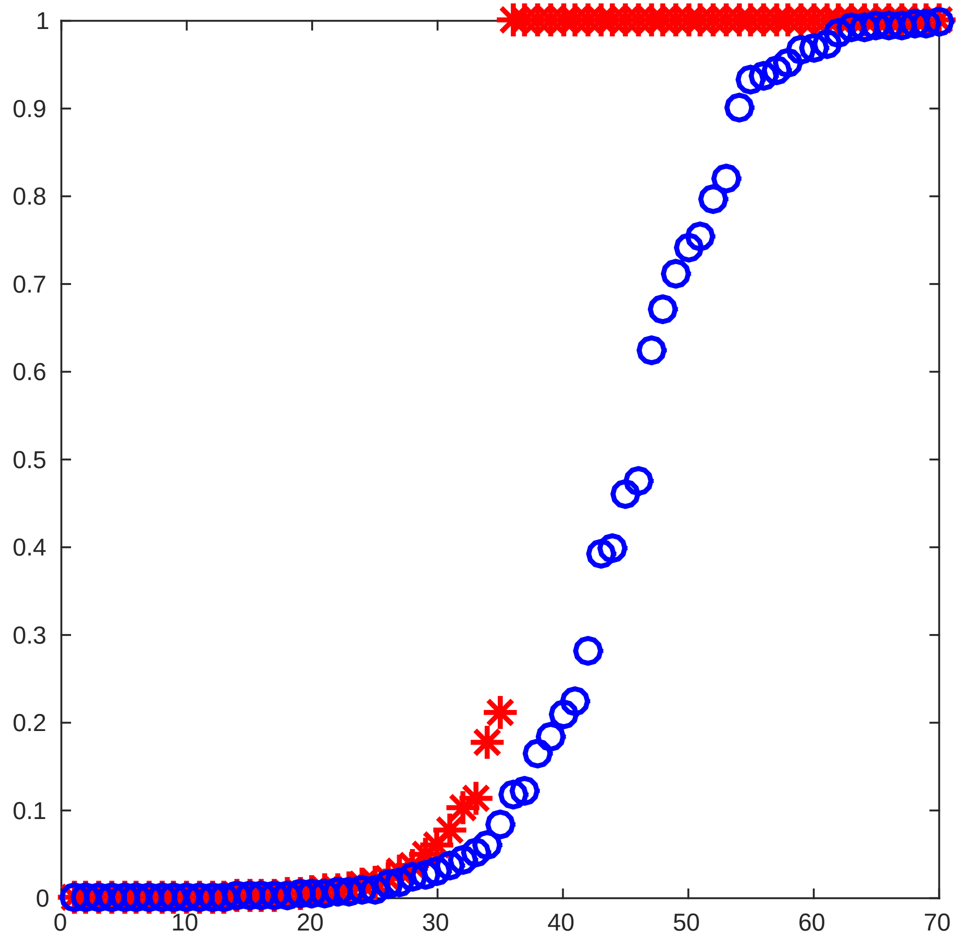
- Exact (blue circles), approximated (red stars)



$$N_e = (0, 6, 13, 14)$$
$$D = 3.95e - 1$$

Eigenvalues of the inverse Hessian

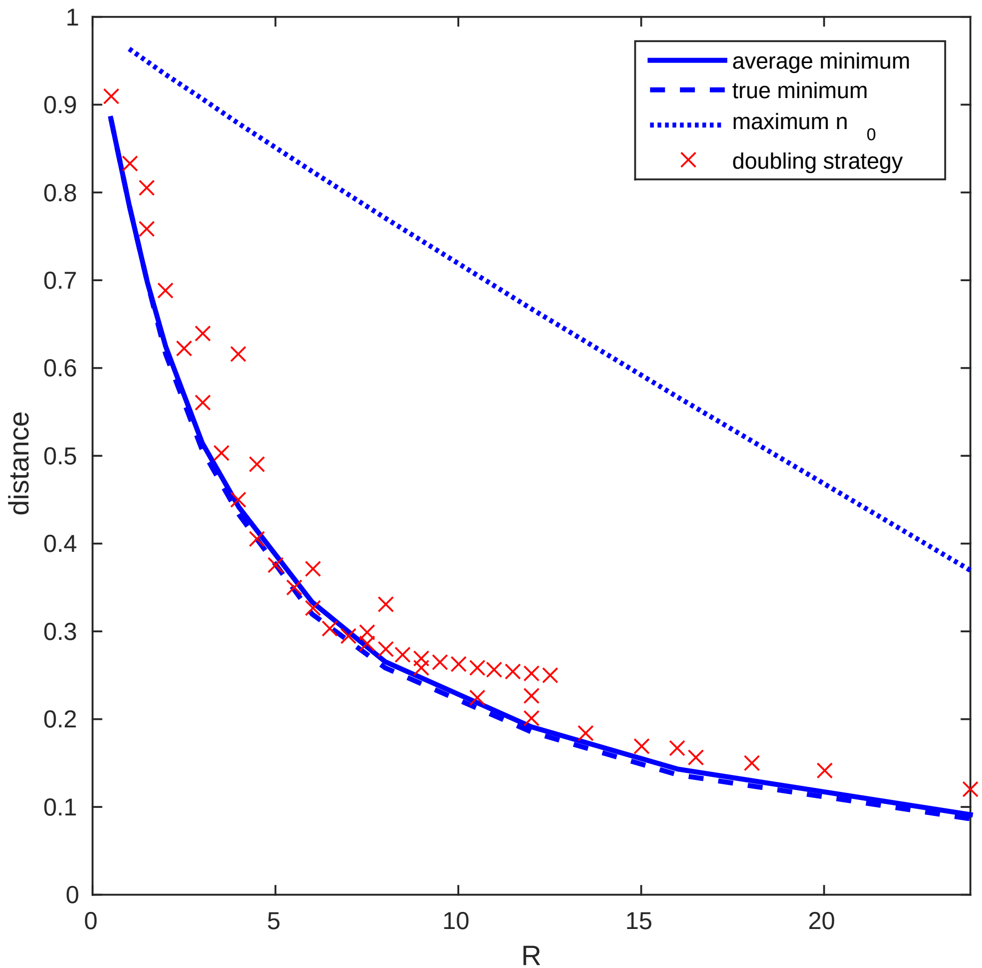
- Exact (blue circles), approximated (red stars)



$$N_e = (0, 0, 29, 6)$$
$$D = 3.39e - 1$$

Fixed memory ratio

- Fixed memory ratio $$R = \sum_{k=0}^{k_c} \frac{n_k}{2^k}$$



PCG iteration for one 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

Practical approach: version 1

- Assemble local Hessians for each sensor to form H_a, then apply mlpre to H_a.

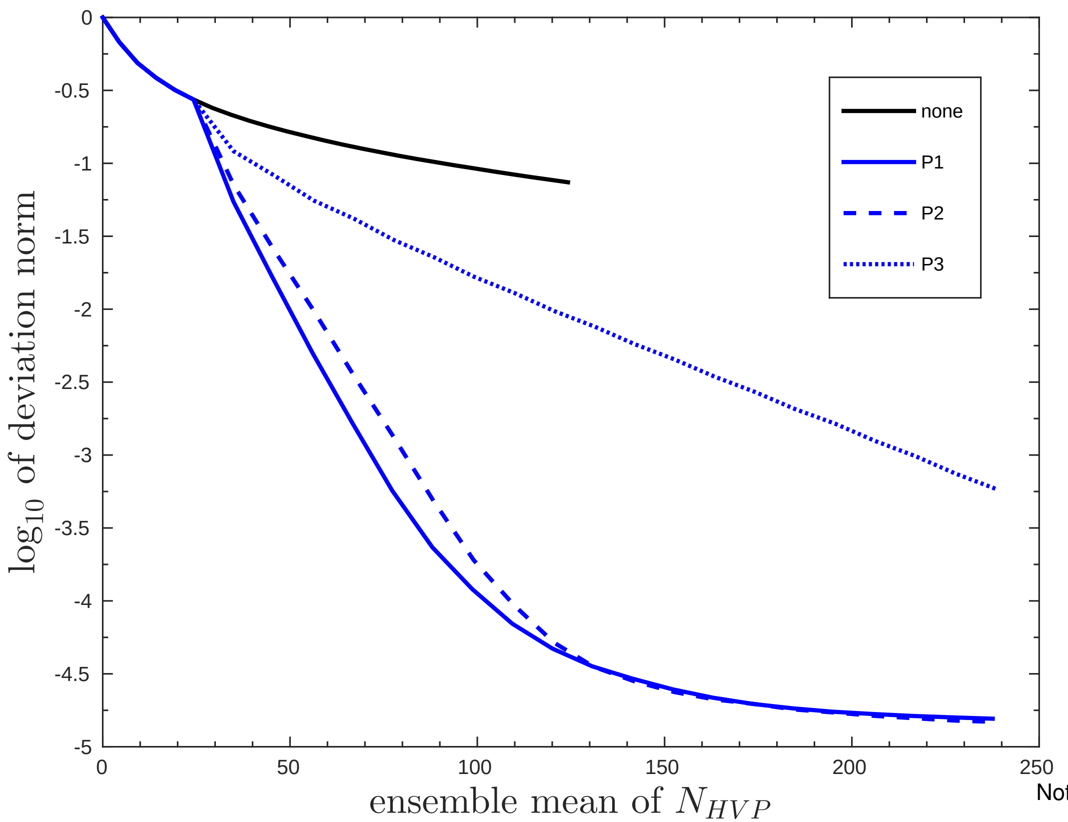
- Local Hessians cheaper to compute:
  - Potentially smaller area of influence.
  - Could run local rather than global model.
  - Compute local Hessians at level l.
  - Use limited-memory form with n_l eigenpairs.
  - Can be computed in parallel.

- More memory required:
  - Need to store additional local Hessians.

Iteration counts

Preconditioner	N_e	l	n_l
P1	(200,0,0,0)	1	8
P2	(0,8,16,32)	1	8
P3	(0,4,8,16)	1	8

log(error) vs number of HVP



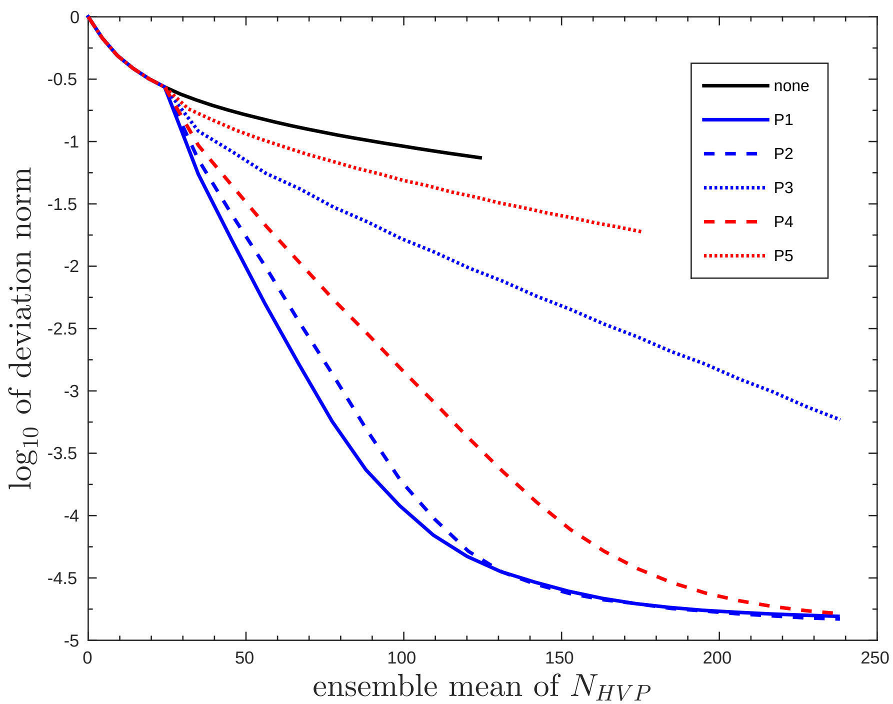
Practical approach: version 2

- Can reduce memory requirements further.
- Approximate local Hessians by applying mlpre to local inverse Hessians using N_e^l.
- Construct a reduced-memory assembled Hessian H_a^{rm}.
- Use mlpre again on H_a^{rm}.

Iteration counts

Preconditioner	N_e	l	n_l	N_e^l
P1	(200,0,0,0)	1	8	-
P2	(0,8,16,32)	1	8	-
P3	(0,4,8,16)	1	8	-
P4	(0,8,16,32)	1	8	(0,0,8,0)
P5	(0,8,16,32)	2	8	(0,0,0,8)

log(error) vs number of HVP



Conclusions and next steps

- Similar results with other configurations (e.g. moving sensors, different initial conditions).
- 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.

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- Now ready for two dimensions!

It is sometimes nice in Scotland. . .