A multilevel preconditioner for data assimilation with 4D-Var

Alison Ramage and Kirsty Brown,
Mathematics and Statistics,
University of Strathclyde,
Glasgow, Scotland

Igor Gejadze,
National Research Institute of
Science and Technology for
Environment and Agriculture,
Montpelier, France

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

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Physical model

- Evolution equation:

$$\begin{aligned}\frac{\partial\varphi(t)}{\partial t} &= F(\varphi(t)) + f(t),\\ \varphi(0) &= u,\end{aligned}$$

$$u \in X, \quad t \in (0,T), \quad f,\varphi \in Y = L_2(0,T;X)$$

true initial state	$\bar{u}$
true state evolution	$\bar{\varphi}$
observation operator	$C_{obs} : Y \to Y_{obs}$
observation error	ξ_o
observations	$\varphi_{obs} = C_{obs}\bar{\varphi} + \xi_o$
background error	ξ_b
background function	$u_b = \bar{u} + \xi_b$

Data assimilation problem

- represent model in operator form via control-to-state mapping

$$\varphi = R^{cts}(u)$$

- assume errors ξ_o, ξ_b are normal, unbiased and mutually uncorrelated with positive definite covariance operators

$$V_b(\cdot) = E[\langle \cdot, \xi_b \rangle_X \; \xi_b], \qquad V_o(\cdot) = E[\langle \cdot, \xi_o \rangle_{Y_{obs}} \; \xi_o]$$

- DA problem: find $v \in X$ which minimises

$$J(v) = \frac{1}{2}\langle V_b^{-1} v, v \rangle_X + \frac{1}{2}\langle V_o^{-1} C_{obs} R^{cts}(u) v, C_{obs} R^{cts}(u) v \rangle_{Y_{obs}}$$

Hessian operator

- define associated tangent linear operator

$$R'(u)v = \lim_{\tau \to 0} \frac{R^{cts}(u + \tau v) - R^{cts}(u)}{\tau}, \quad \forall v \in X$$

and adjoint

$$\langle v, R'^*(u)v^* \rangle_X = \langle R'(u)v, v^* \rangle_Y, \quad \forall v \in X \,, \forall v^* \in Y$$

- Hessian of DA problem:

$$\mathcal{H}(u) = V_b^{-1} + R'^*(u) C^*_{obs} V_o^{-1} C_{obs} R'(u)$$

Incremental 4D-Var

- Represent functions using a finite-dimensional basis.
- Rewrite as an unconstrained minimisation problem using Lagrange's method.
- Incremental approach: linearise evolution operator and solve linearised problem iteratively.
- Require a discrete version of the 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:

$$\mathcal{H} = V_b^{-1} + R^T C_{obs}^T V_o^{-1} C_{obs} R$$

- 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

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

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

First level preconditioning

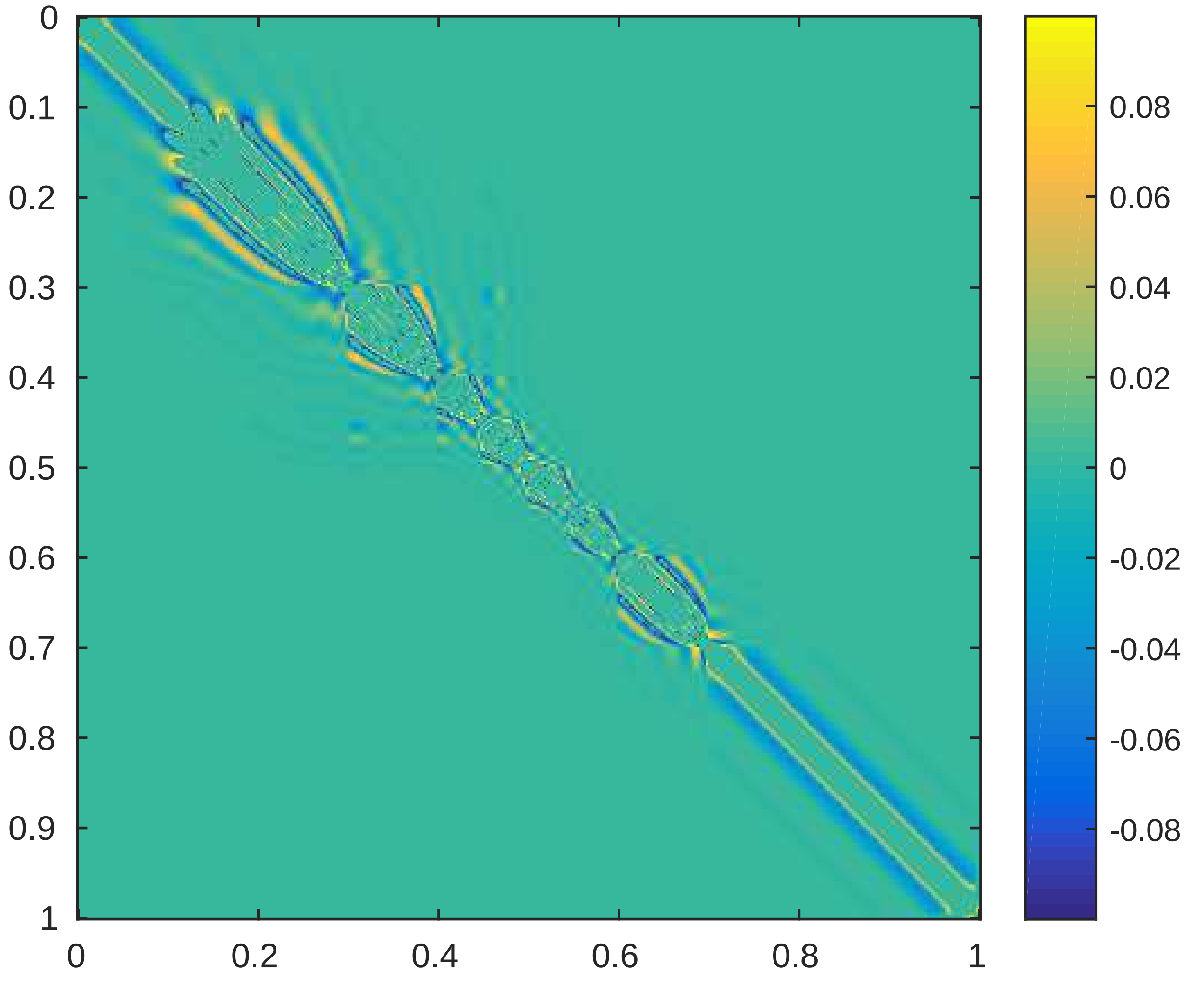
- Use the background covariance matrix V_b.
- Projected Hessian:

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

- 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.
  [HABEN ET AL., COMPUTERS & FLUIDS 46 (2011)]
- This makes H amenable to limited-memory approximation.

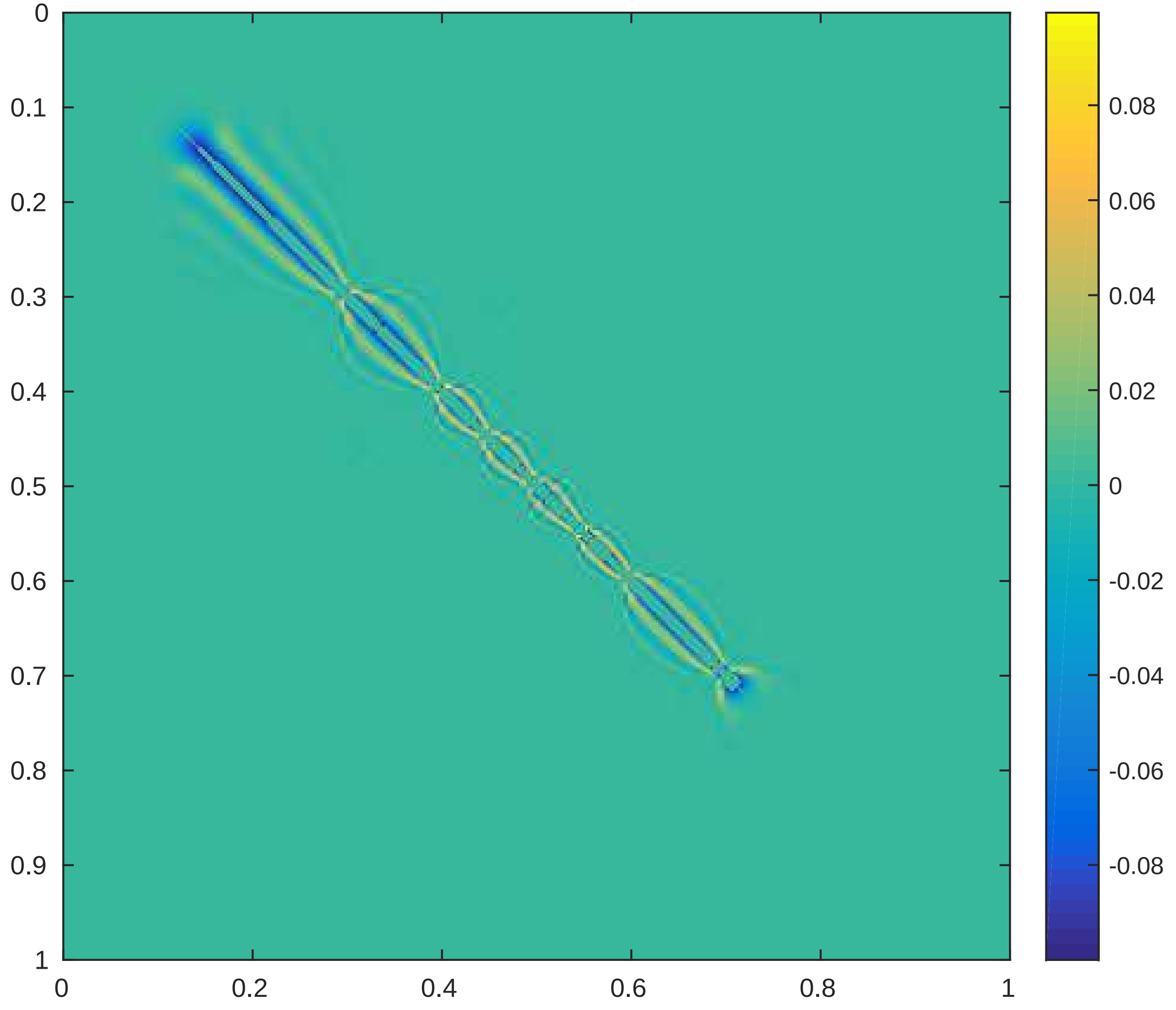
Correlation matrix

- $\mathcal{H}^{-1}$ (scaled to have unit diagonal)



Preconditioned correlation matrix

- H^{-1} (after first level preconditioning)



Limited-memory approximation

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

- Construct approximation

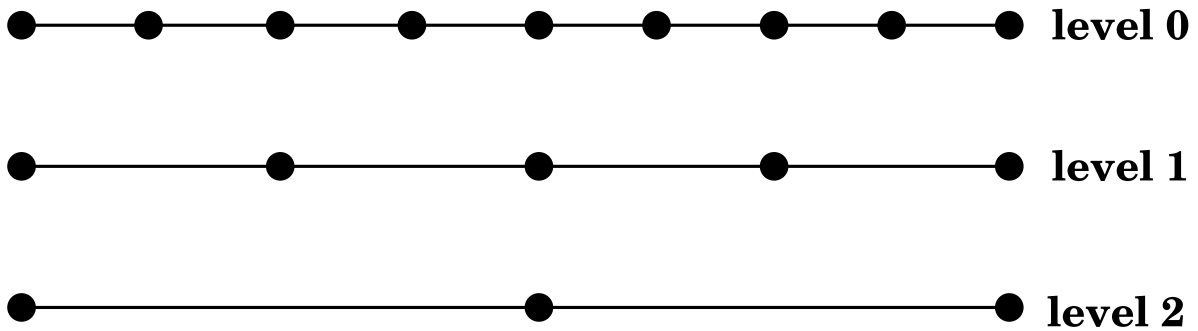
$$H \approx I + \sum_{i=1}^{n_e} (\lambda_i - 1)\mathbf{u}_i\mathbf{u}_i^T$$

- 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

- IDEA: Construct a multilevel approximation to H^{-1} based on a sequence of nested grids.
- 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 concept

- Given a symmetric positive definite operator A_0 available on the finest grid level in matrix-vector product form:

1. represent A_0 on the coarsest grid level;
2. use a local preconditioner to improve the eigenvalue distribution;
3. build a limited memory approximation to its inverse using the Lanczos method (which forms the basis of the local preconditioner at the next coarsest level);
4. move up one grid level and repeat.

Multilevel algorithm for H^{-1}

- 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} 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

```
[$\Lambda$,$\mathcal{U}$]=$mlevd$($H_0$,$N_e$)
for   $k = k_c, k_c - 1, \ldots, 0$
   compute by the Lanczos method
   and store in memory
       $\{\lambda_k^i, U_k^i\}$, $i = 1, \ldots, n_k$ of $\tilde{H}_{0\to k}$
   using preconditioner $B_k^{k+1}$
end
```

- storage:

$$\begin{aligned} \Lambda &= \left[\lambda_{k_c}^1, \ldots, \lambda_{k_c}^{n_{k_c}}, \lambda_{k_c-1}^1, \ldots, \lambda_{k_c-1}^{n_{k_c-1}}, \ldots, \lambda_0^1, \ldots, \lambda_0^{n_0}\right], \\ \mathcal{U} &= \left[U_{k_c}^1, \ldots, U_{k_c}^{n_{k_c}}, U_{k_c-1}^1, \ldots, U_{k_c-1}^{n_{k_c-1}}, \ldots, U_0^1, \ldots, U_0^{n_0}\right]. \end{aligned}$$

Example

- Test using 1D Burgers' equation with initial condition

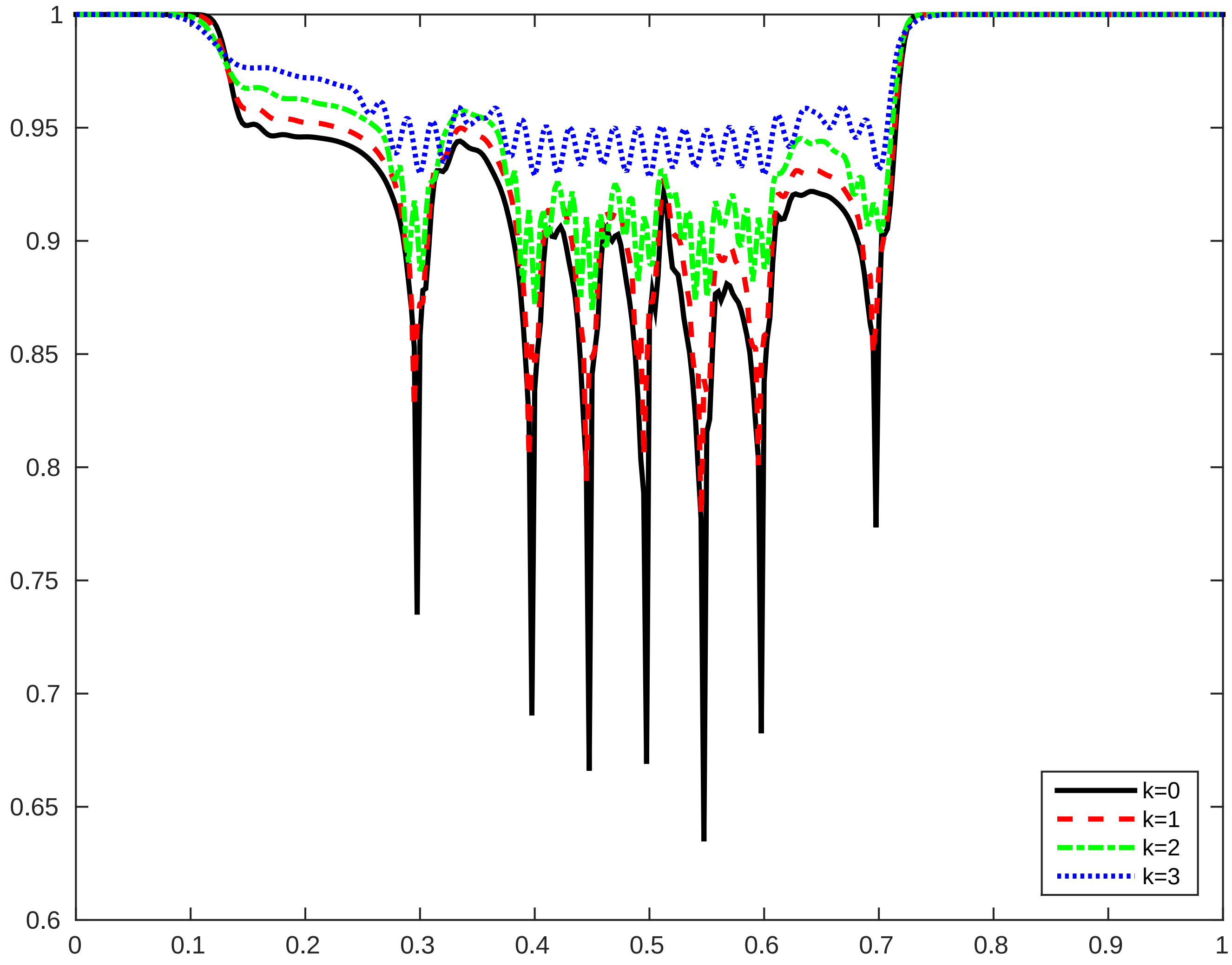
$$f(x) = 0.1 + 0.35\left[1 + \sin\left(4\pi x + \frac{3\pi}{2}\right)\right], \qquad 0 < x < 1$$

- 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

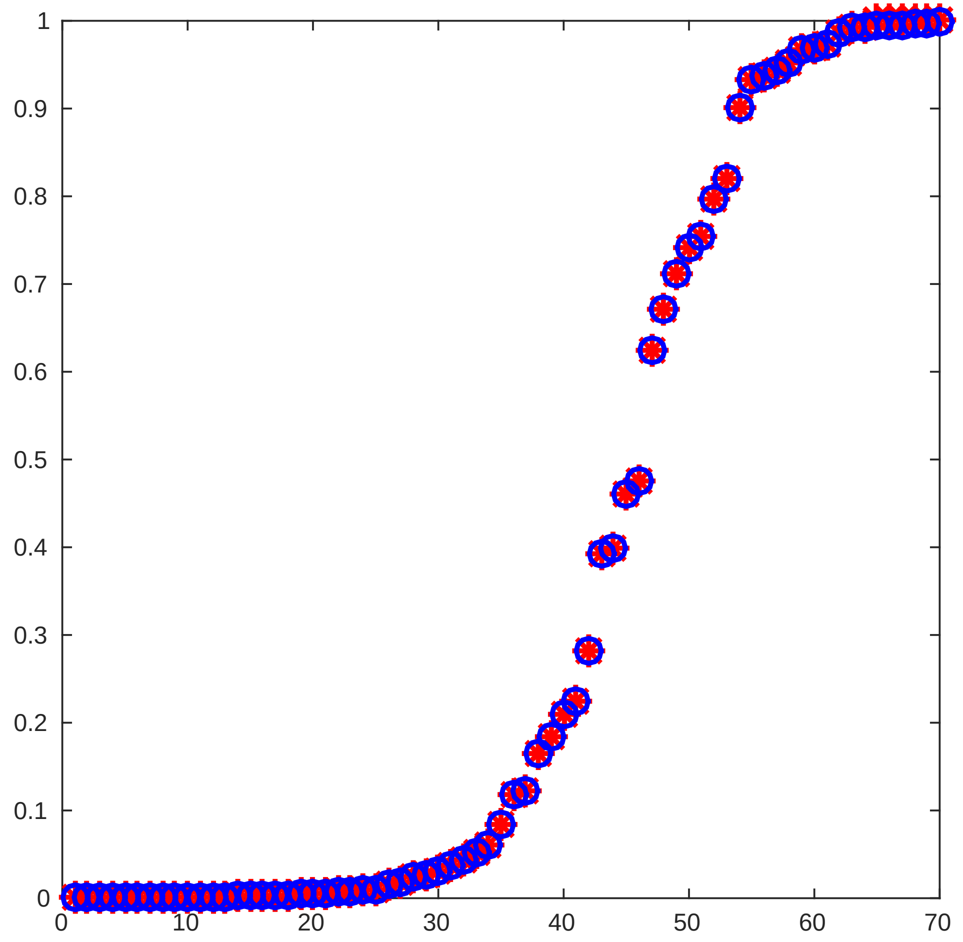
$$D = \frac{\delta(H^{-1}, \tilde{H}^{-1})}{\delta(H^{-1}, I)}$$

- Vary number of eigenvalues chosen on each grid level

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

Eigenvalues of the inverse Hessian

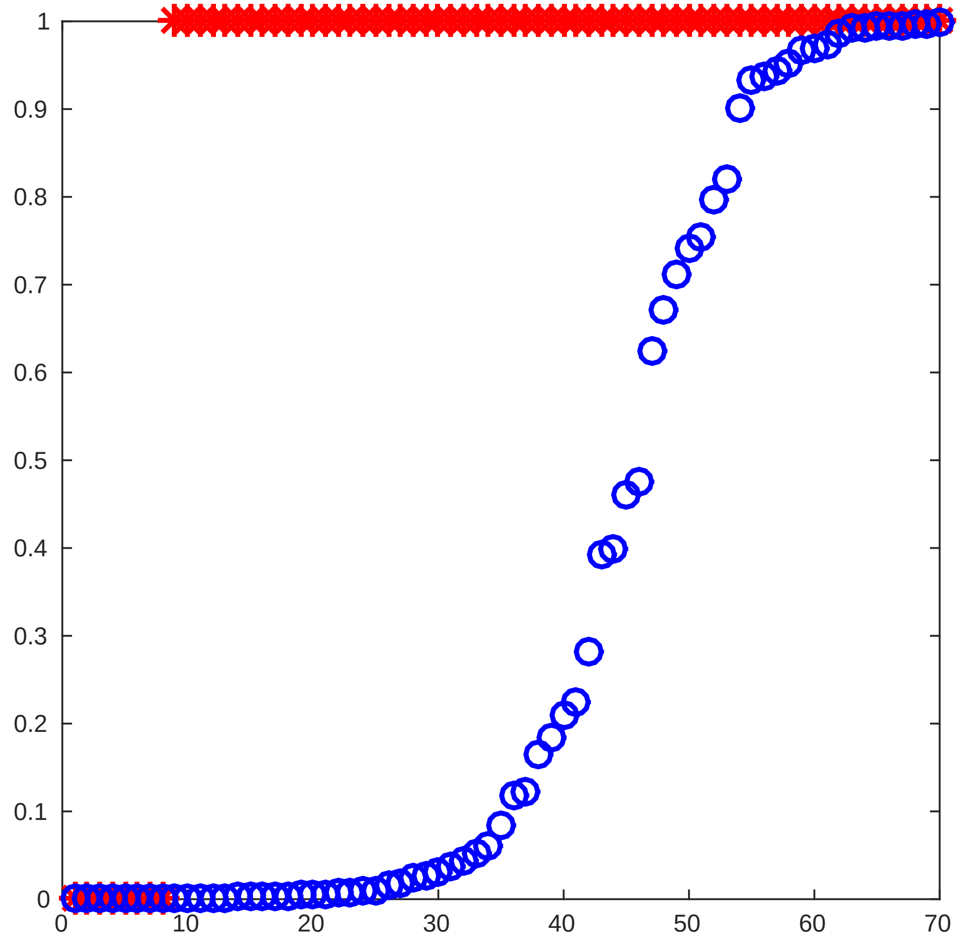
- Exact (blue circles), approximated (red stars)



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

Eigenvalues of the inverse Hessian

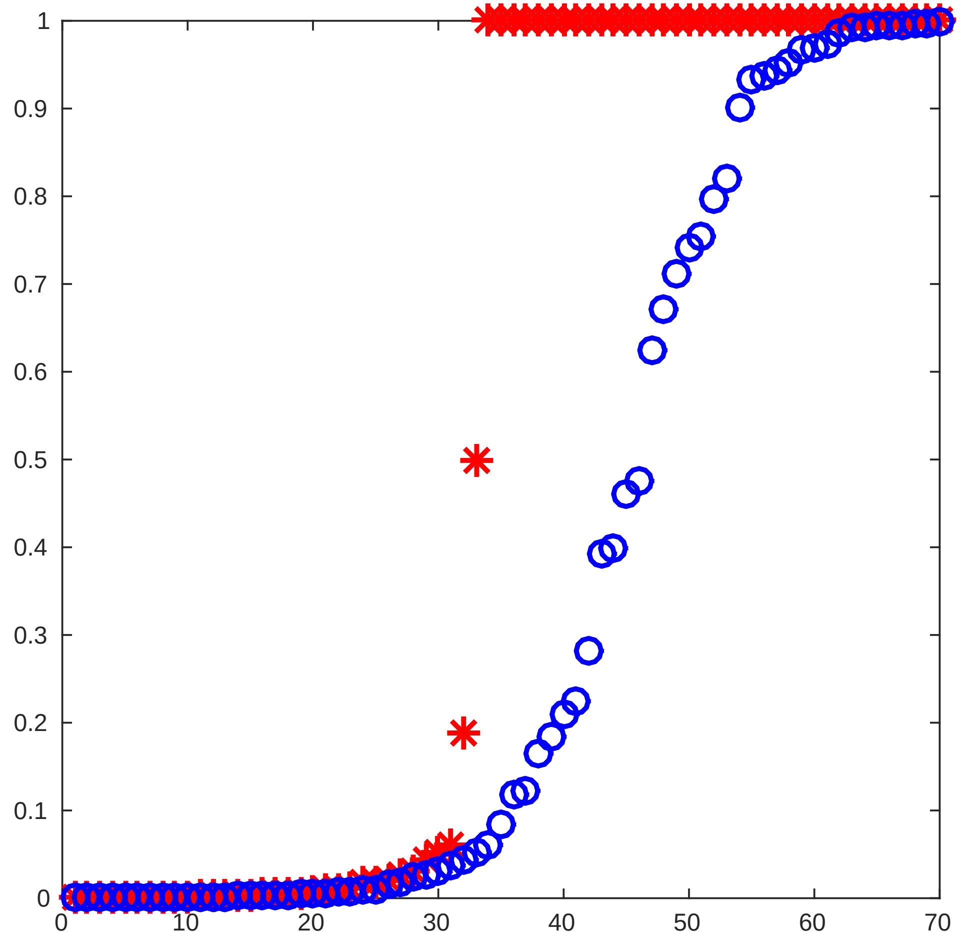
- Exact (blue circles), approximated (red stars)



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

Eigenvalues of the inverse Hessian

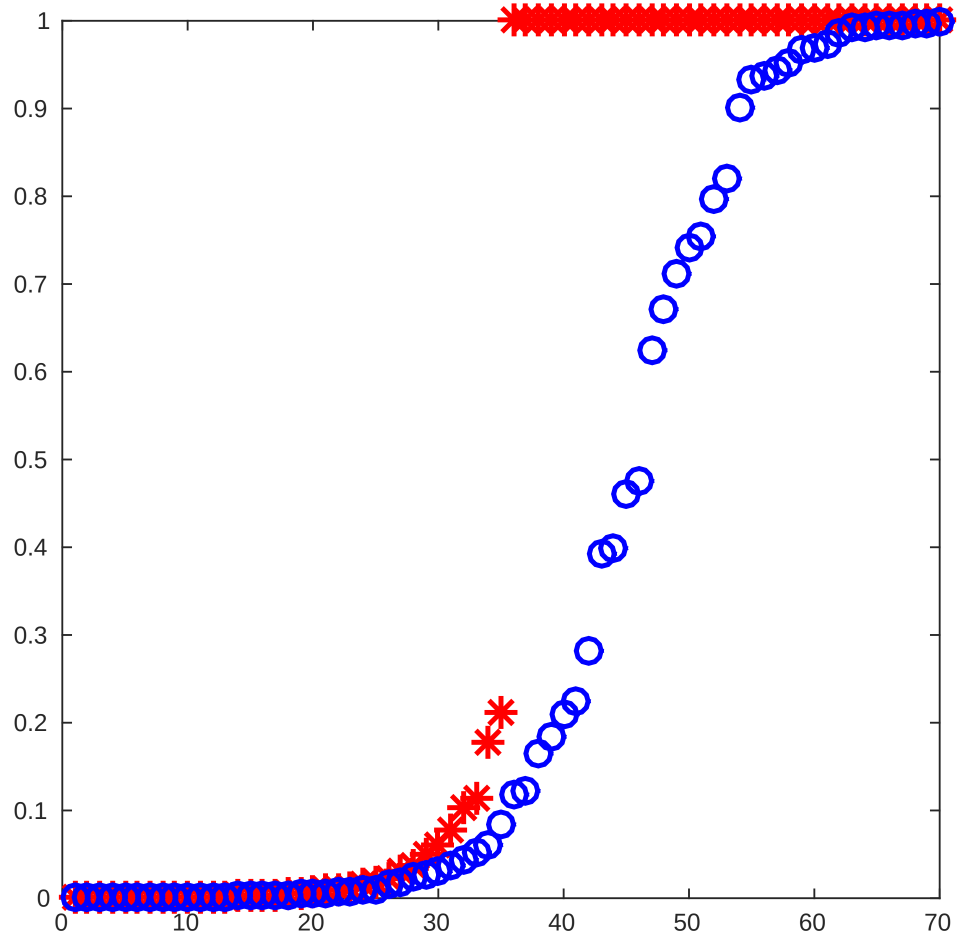
- Exact (blue circles), approximated (red stars)



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

Eigenvalues of the inverse Hessian

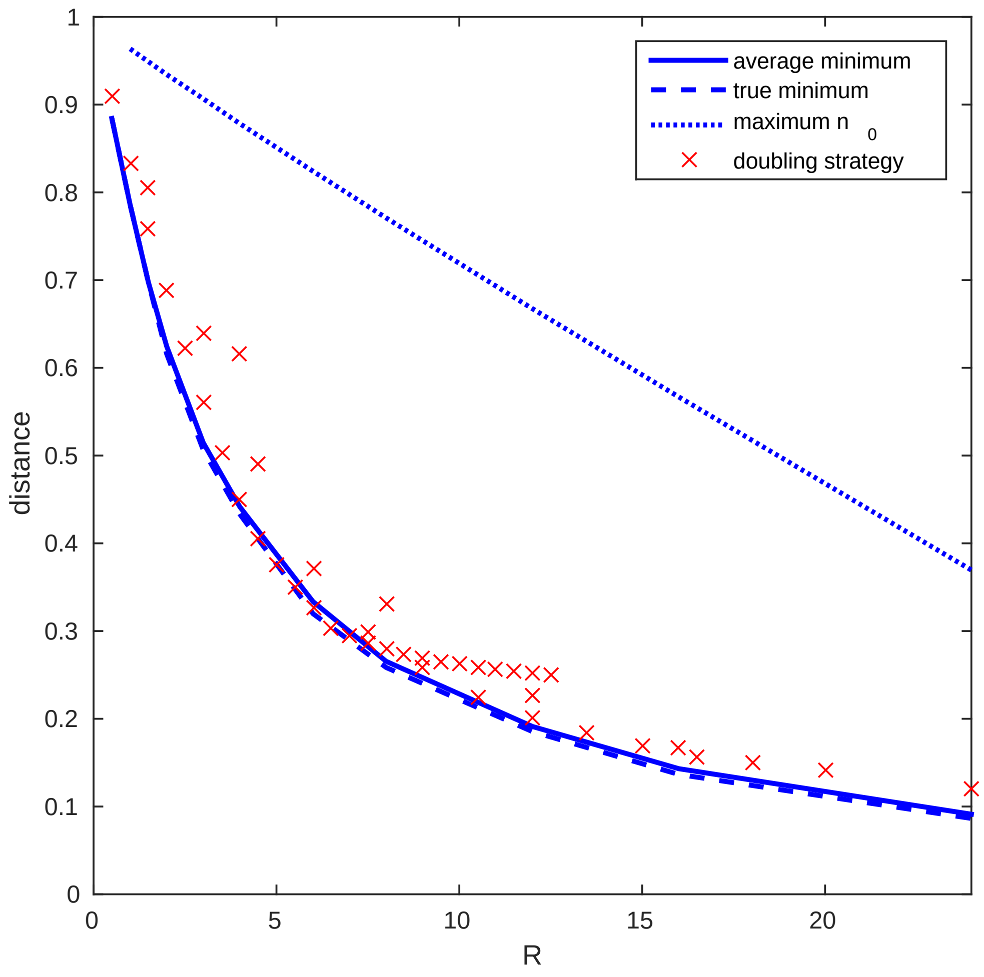
- Exact (blue circles), approximated (red stars)



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

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

Hessian decomposition

- partition domain into subregions and compute local Hessians H^l such that

$$H(u) = I + \sum_{l=1}^{L} (H^l(u) - I)$$

- fewer eigenvalues required for limited-memory representation of each H^l
- local Hessians can be computed in parallel
- H^l need not be computed at finest grid level:

$$H_k(u_k) = I_k + \sum_{l=1}^{L} (H_k^l(u_k) - I_k)$$

- could run local rather than global model

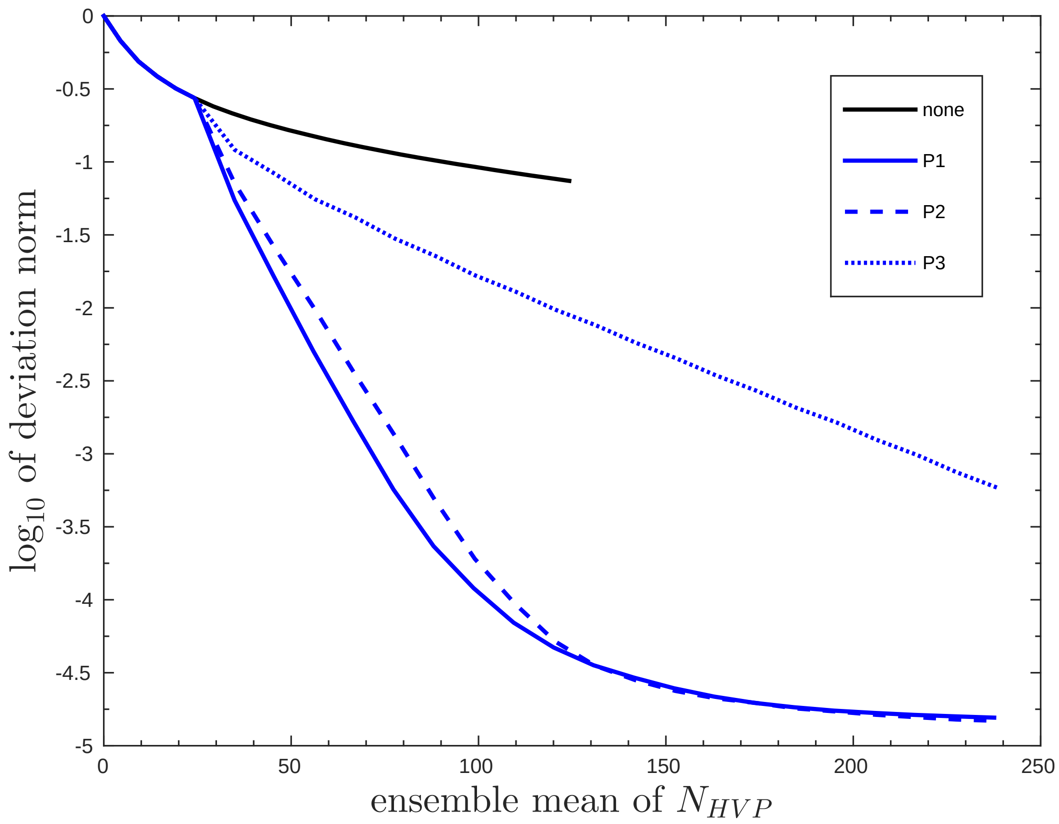
Practical approach: version 1

- Compute limited-memory approximations to local sensor-based Hessians on level l using n_l eigenpairs.
- Assemble these to form H_a, then apply mlevd to H_a based on a fixed N_e.
- Local Hessians cheaper to compute.
- Additional user-specified parameter(s) l, n_l needed.
- More memory required as local Hessians must also be stored.

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



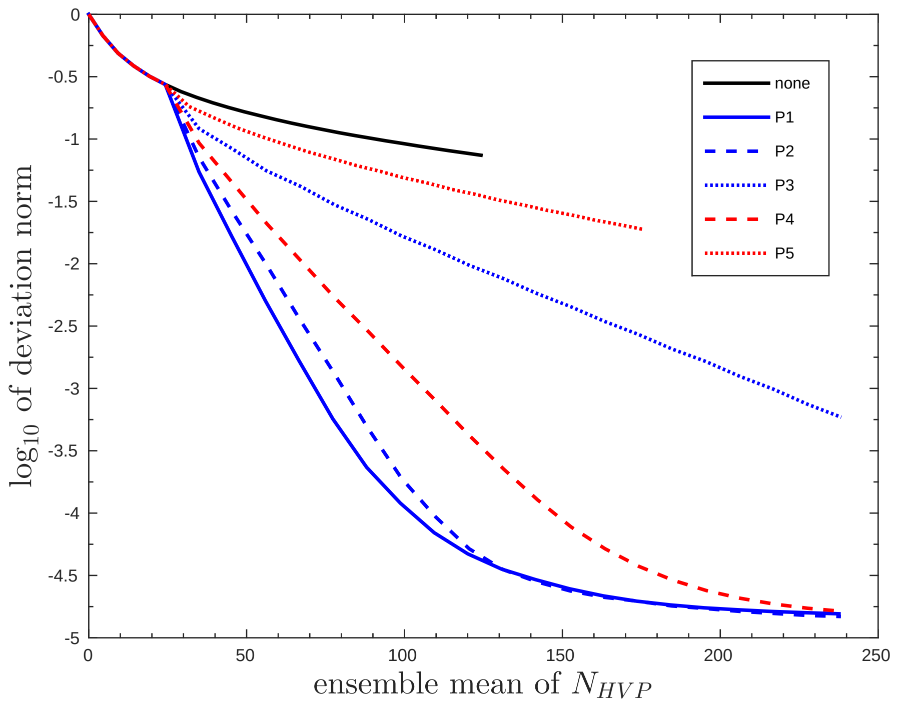
Practical approach: version 2

- Can reduce memory requirements further by using a multilevel approximation of each limited-memory local Hessian on level l using n_l eigenpairs.
- Approximate local Hessians by applying mlevd to local inverse Hessians based on N_e^l.
- Assemble these to form a reduced-memory assembled Hessian H_a^{rm}.
- Use mlevd again on H_a^{rm} based on N_e.

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) and other parameters is tricky.

- Now ready for two dimensions!

It is sometimes nice in Scotland. . .