Preconditioning for Data Assimilation Problems

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Four-dimensional Variational Assimilation (4D-Var)

4D-Var aims to find the solution of a numerical forecast model that best fits sequences of observations distributed in space over a finite time interval.

Minimise cost function

$$J(\mathbf{v}_0) = (\mathbf{v}_0 - \mathbf{v}_0^B)^T \mathcal{B}^{-1} (\mathbf{v}_0 - \mathbf{v}_0^B) + \sum_{i=0}^{n} (\mathcal{H}(\mathbf{v}_i) - \mathbf{y}_i)^T \mathcal{R}^{-1} (\mathcal{H}(\mathbf{v}_i) - \mathbf{y}_i)$$

with constraint $\mathbf{v}_i = \mathcal{M}^{i,0}(\mathbf{v}_0)$.

analysis	$\mathbf{v}_0$
background (short-term forecast)	$\mathbf{v}_0^B$
observations	$\mathbf{y}$
observation operator	$\mathcal{H}$
model dynamics	$\mathbf{v}_{i+1} = \mathcal{M}(\mathbf{v}_i)$
background error covariance matrix	$\mathcal{B}$
observation error covariance matrix	$\mathcal{R}$

Incremental 4D-Var

- Linearise $\mathcal{H}$, $\mathcal{M}$ and solve resulting unconstrained optimisation problem iteratively:

$$\bar{H}^i_{k-1} \equiv \left.\frac{\partial \mathcal{H}^i}{\partial \mathbf{v}}\right|_{\mathbf{v}=\mathbf{v}_{k-1}}, \qquad \bar{M}^{i,0}_{k-1} \equiv \left.\frac{\partial \mathcal{M}^{i,0}}{\partial \mathbf{v}}\right|_{\mathbf{v}=\mathbf{v}_{k-1}}$$

- Hessian of the cost function is

$$\mathbb{H} = \mathcal{B}^{-1} + \widehat{H}^T \widehat{\mathcal{R}}^{-1} \widehat{H}$$

where
$$\begin{aligned} \widehat{H} &= [(\bar{H}^0)^T, (\bar{H}^1 \bar{M}^{1,0})^T, \ldots, (\bar{H}^N \bar{M}^{N,0})^T]^T \\ \widehat{\mathcal{R}} &= \texttt{bldiag}(\mathcal{R}_i), \quad i = 1, \ldots, N. \end{aligned}$$

- Cannot store $\mathbb{H}$ as a matrix: action of applying $\mathbb{H}$ to a vector is available, but expensive (involves both forward and backward model solves).

Approximating the inverse Hessian

- Motivation:
  - $\mathbb{H}^{-1}$ approximates the Posterior Covariance Matrix which can be used to find confidence intervals and carry out *a posteriori* error analysis.
  - $\mathbb{H}^{-1/2}$ can be used in ensemble forecasting.
  - $\mathbb{H}^{-1}$, $\mathbb{H}^{-1/2}$ can be used for preconditioning in a Gauss-Newton method.
- Potential issues:
  - Evaluating $\mathbb{H}\mathbf{v}$ is expensive in terms of computing time and memory (involves both forward and backward model solves with a sequence of tangent linear and adjoint problems).
  - No obvious equivalent option exists for evaluating $\mathbb{H}^{-1}\mathbf{v}$.

First-level preconditioning

- Precondition $\mathbb{H}$ based on the background covariance matrix (control variable transform):

$$H = (\mathcal{B}^{1/2})^T \mathbb{H} \mathcal{B}^{1/2} = I + (\mathcal{B}^{1/2})^T \widehat{H}^T \widehat{\mathcal{R}}^{-1} \widehat{H} \mathcal{B}^{1/2}$$

- Eigenvalues of H are bounded below by one: more details on the full eigenspectrum can be found in Haben et al. (2011), Tabeart et al. (2018).

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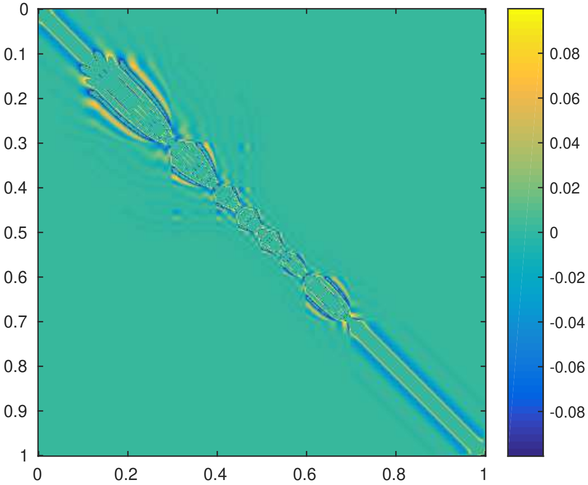
- Hessian linear system (within a Gauss-Newton method):

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

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

Correlation matrix

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



Preconditioned correlation matrix

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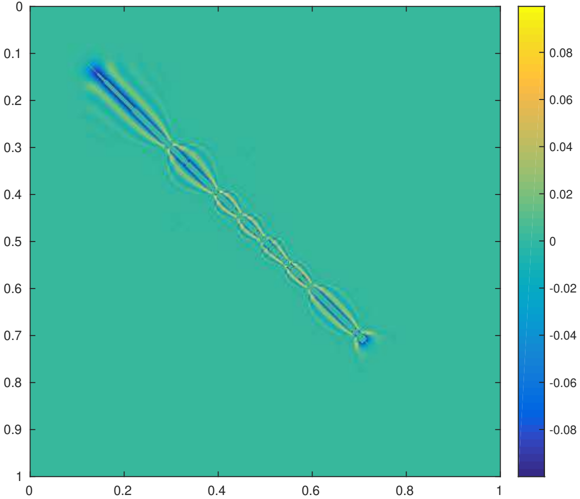


Limited-memory approximation for H^{-1}

- H amenable to limited-memory approximation.
- Find n_e leading eigenvalues and orthonormal eigenvectors using the Lanczos method (needs only $H\mathbf{v}$).
- Construct approximation

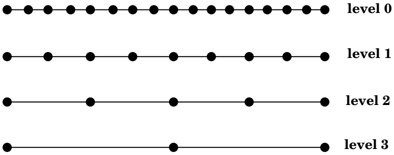
$$H \approx I + \sum_{i=1}^{n_e} (\lambda_i - 1)\mathbf{u}_i \mathbf{u}_i^T$$

- Can also use this to easily approximate matrix powers (including H^{-1} and $H^{-1/2}$):

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

Multilevel limited-memory approximation

- Sequence of grid levels $k = 0, 1, 2, \ldots$.



- Matrix H_0 is available on finest grid $k = 0$.
- Construct a multilevel approximation to H_0^{-1} based on limited-memory approximations on a sequence of nested grids.
- Need grid transfer operators (more shortly).
- Identity matrix I_k on grid level k.
- $[H]_{\to k}$ means "matrix H transferred to grid level k".

Grid transfers for vectors

- Coarse grid level $k = c$; fine grid level $k = f$.
- Restriction matrix R; prolongation matrix P: assume "perfect interpolation", i.e., $RP = I_c$.
- Split fine grid vector into two parts:

$$\mathbf{v}_f \quad = \quad \mathbf{v}_f^{(1)} + \mathbf{v}_f^{(2)} \quad = \quad (I_f - PR)\mathbf{v}_f + PR\mathbf{v}_f.$$

- Restrict $\mathbf{v}_f$ to coarse grid:

$$\mathbf{v}_c^{(1)} = R\mathbf{v}_f^{(1)} = R(I_f - PR)\mathbf{v}_f = (R - (RP)R)\mathbf{v}_f = \mathbf{0}$$

$$\mathbf{v}_c^{(2)} = R\mathbf{v}_f^{(2)} = (RP)R\mathbf{v}_f = R\mathbf{v}_f.$$

- Modes in $\mathbf{v}_f^{(1)}$ are not supported on coarse grid.

Grid transfers for matrices

- Consider action of coarse grid matrix H_c on a fine grid vector:

$$\begin{aligned}[H_c]_{\to f}\mathbf{v}_f &= \mathbf{v}_f^{(1)} + PH_cR\mathbf{v}_f^{(2)} \\ &= (I_f - PR)\mathbf{v}_f + PH_c(RP)R\mathbf{v}_f \\ &= (P(H_c - I_c)R + I_f)\mathbf{v}_f\end{aligned}$$

- This motivates matrix transfer operators
  - From coarse grid to fine grid

$$[H_c]_{\to f} = P(H_c - I_c)R + I_f$$

  - From fine grid to coarse grid

$$[H_f]_{\to c} = R(H_f - I_f)P + I_c$$

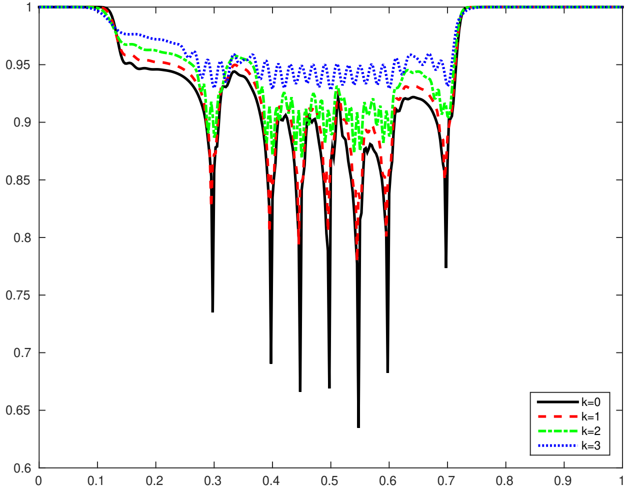
Test problem 1

- Model is 1D Burgers' equation.
- Discretise evolution equation on a grid with $m+1$ nodes (level 0) to represent full Hessian H_0.
- Grid level k contains $m_k = m/2^k + 1$ nodes.
- 1D uniform grid with 7 sensors located at 0.3, 0.4, 0.45, 0.5, 0.55, 0.6, and 0.7 in $[0, 1]$.
- Construct a multilevel approximation to H^{-1} with four grid levels:

k	0	1	2	3
grid points	401	201	101	51

Hessian in a multilevel framework

- Diagonal of H^{-1} on various grid levels:



Eigenvalues of Hessian at each level

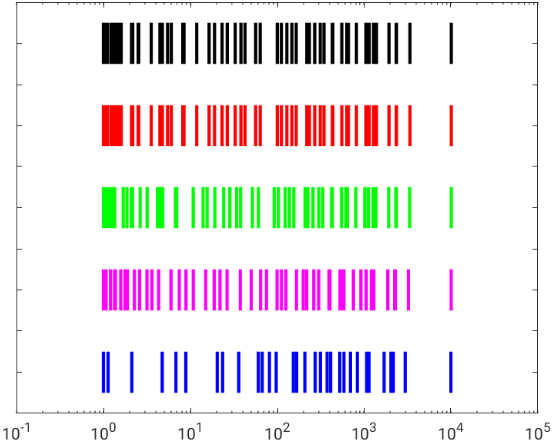
H_0

$H_0 = [H_0]_{\to 0}$

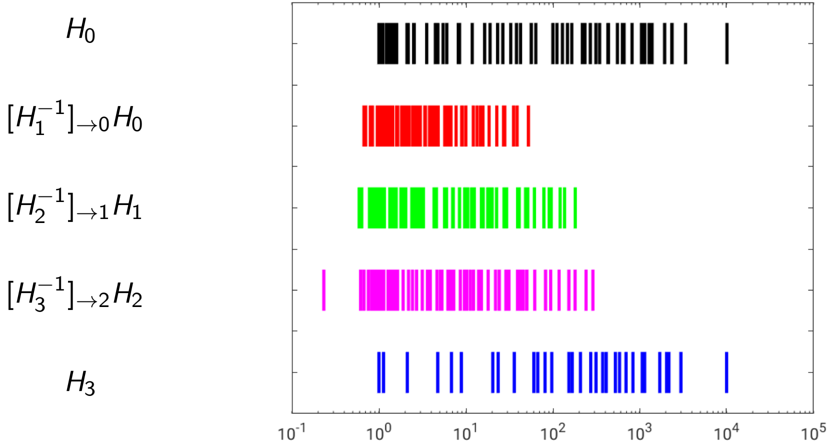
$H_1 = [H_0]_{\to 1}$

$H_2 = [H_0]_{\to 2}$

$H_3 = [H_0]_{\to 3}$



Eigenvalues of preconditioned Hessian at each level



Motivating idea

- Eigenvalues of $[H_c^{-1/2}]_{\to f}\ H_f\ [H_c^{-1/2}]_{\to f}$ should be clustered around 1.

- Construct an approximation to $H_c^{-1/2}$:
    - Precondition H_c to obtain $\tilde{H}_c = M^T H_c M$ with eigenvalues closer to 1.
    - Build $\hat{H}_c$, a limited memory approximation for $\tilde{H}_c$ using n_c eigenvalues with the Lanczos method.
    - Note that
    $$H_c^{-1} = M\tilde{H}_c^{-1}M^T \simeq M\hat{H}_c^{-1}M^T$$
    so
    $$H_c^{-1/2} = M\tilde{H}_c^{-1/2} \simeq M\hat{H}_c^{-1/2}.$$

- Use $\hat{M} = [M\hat{H}_c^{-1/2}]_{\to f}$ as a preconditioner on the level above.

Outline of multilevel concept

Step 1. Start on coarsest grid level.

Step 2. Represent H_0 on grid level k as $H_k = [H_0]_{\to k}$.

Step 3. Precondition this to obtain $\tilde{H}_k = M_k^T H_k M_k$.

Step 4. Build limited memory approximation $\hat{H}_k^{-1/2}$.

Step 5. Project $\hat{M}_k = M_k \hat{H}_k^{-1/2}$ to the level above to be used as preconditioner at the next coarsest level.

Step 6. Move up one grid level and repeat from step 2.

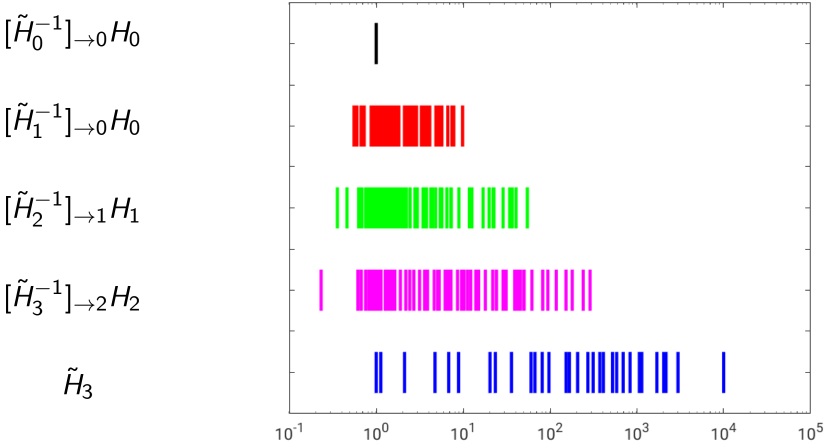
Preconditioners

- On coarsest grid, level $k+1$ does not exist so set $M_k = I_k$.
- For other levels, M_k is constructed on level $k+1$ and applied on level k.
- Preconditioners are constructed recursively:

$$M_k = [\hat{M}_{k+1}]_{\to k} = \left[M_{k+1} \hat{H}_{k+1}^{-1/2} \right]_{\to k}.$$

- At level 0, final inverse Hessian approximation H_{approx}^{-1} will contain eigenvalue information from all levels.

Eigenvalues of recursively preconditioned Hessians



Limited memory versions

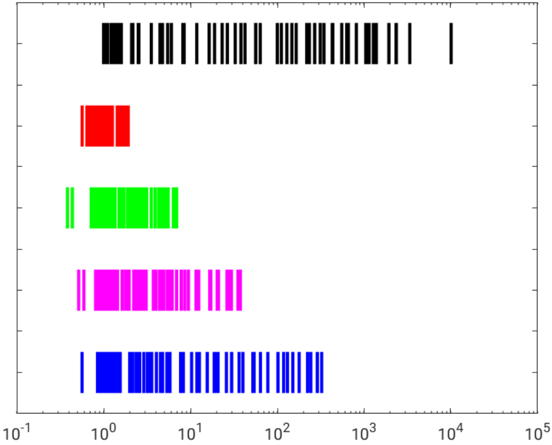
H_0

32 per level

16 per level

8 per level

4 per level



Algorithm in practice

- use $N_e = (n_0, n_1, \ldots, n_{k_c})$ eigenvalues at each level

```
[Λ,U]=MLalg(H_0,N_e)
for    k = k_c, k_c − 1, ..., 0
   compute by the Lanczos method
       {λ_k^i, U_k^i}, i = 1, ..., n_k of H̃_{0→k}
   using preconditioner M_k
end
```

- storage:

$$\begin{aligned}\Lambda &= \left[\lambda_0^1, \ldots, \lambda_0^{n_0}, \lambda_1^1, \ldots, \lambda_1^{n_1}, \ldots, \lambda_{k_c}^1, \ldots, \lambda_{k_c}^{n_{k_c}}\right], \\ \mathcal{U} &= \left[U_0^1, \ldots, U_0^{n_0}, U_1^1, \ldots, U_1^{n_1}, \ldots, U_{k_c}^1, \ldots, U_{k_c}^{n_{k_c}}\right].\end{aligned}$$

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 H^{-1}_{approx} on the finest grid level $k = 0$ using distance function

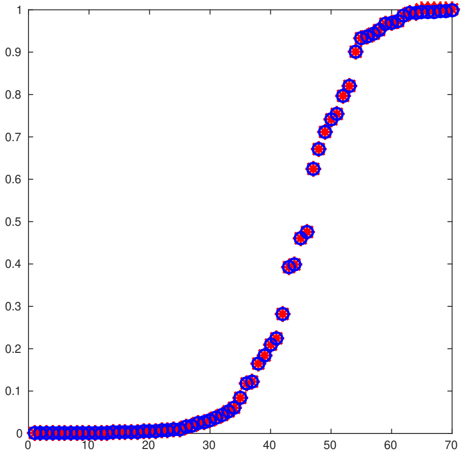
$$D = \frac{\delta(H^{-1}, H^{-1}_{approx})}{\delta(H^{-1}, I)}$$

- Vary number of eigenvalues chosen on each grid level

$$N_e = (n_0, n_1, \ldots, n_{k_c})$$

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

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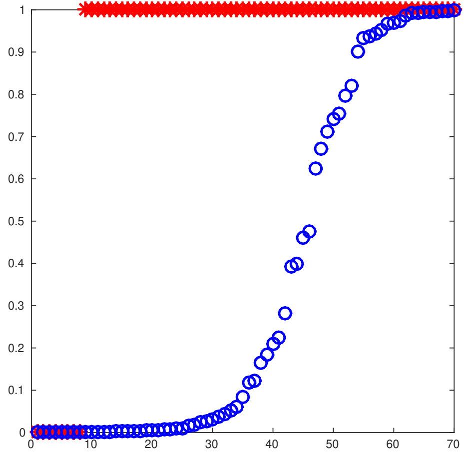

$$N_e = (8, 0, 0, 0)$$
$$D = 7.71e - 1$$

Eigenvalues of the inverse Hessian

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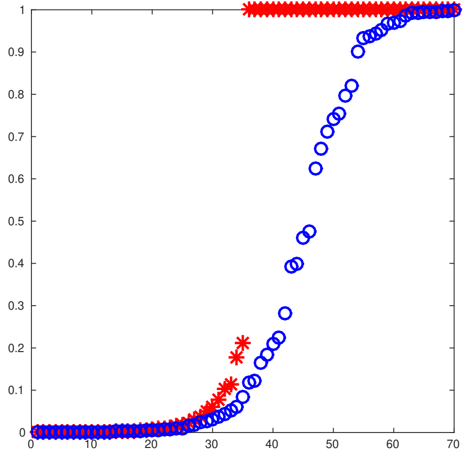
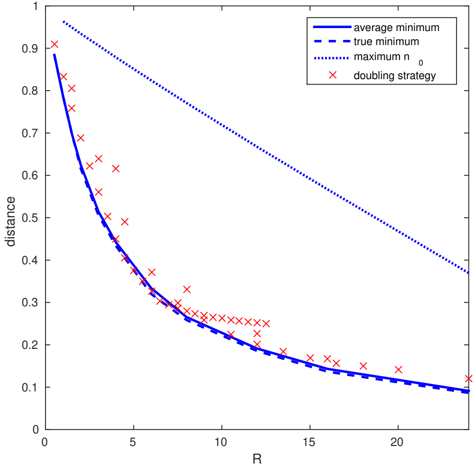


$$N_e = (0, 0, 29, 6)$$
$$D = 3.82e - 1$$

Fixed memory ratio

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



Eigenvalues of preconditioned Hessian

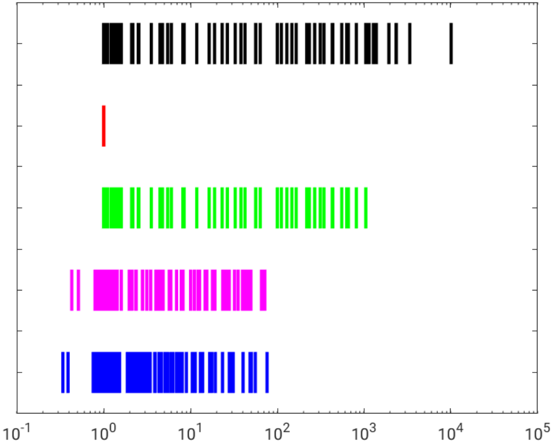
H_0

$(64, 0, 0, 0)$

$(8, 0, 0, 0)$

$(2, 4, 8, 16)$

$(0, 0, 29, 6)$



Example: PCG iteration for one Newton step

- Hessian linear system (within a Gauss-Newton method):

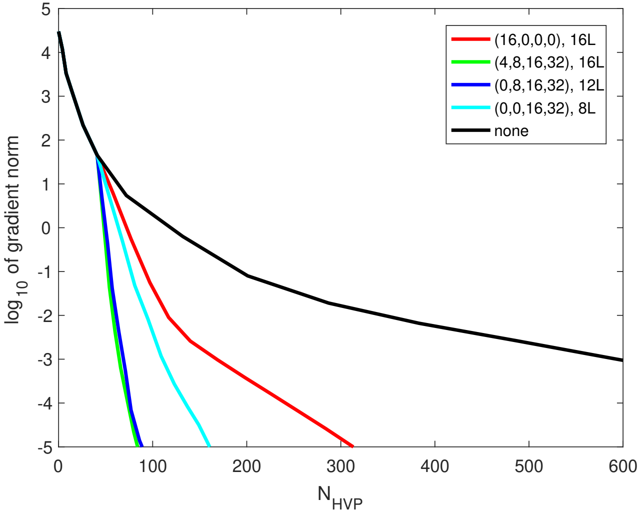
$$H(\mathbf{u}_k)\delta\mathbf{u}_k = G(\mathbf{u}_k)$$

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

- measurement units
  - storage: length of vector on finest grid L
  - solve cost: cost of HVP on finest grid HVP

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

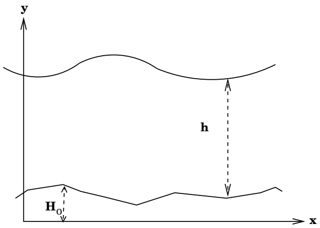
Solve cost measured in number of HVPs



Test problem 2

- Model is 1D shallow water equations for velocity u and geopotential $\phi = gh$.

$$\begin{aligned} \frac{Du}{Dt} + \frac{\partial \phi}{\partial x} &= -g\frac{\partial H_o}{\partial x} \\ \frac{D(\ln \phi)}{Dt} + \frac{\partial u}{\partial x} &= 0 \end{aligned}$$



- Uniformly spaced sensors.
- Four grid multilevel structure as before.

PCG iteration for one Newton step

- Background covariance matrix B constructed using a Laplacian correlation function.

	# PCG iterations			
Preconditioner	$n = 400$	$n = 800$	$n = 1600$	$n = 3200$
none	308	1302	5,879	25,085
ML(4,0,0,0)	38	34	34	47
ML(1,2,4,8)	31	29	28	37
ML(0,2,4,16)	27	26	24	32
ML(0,0,8,16)	26	25	24	30
ML(0,0,0,32)	23	19	19	24

PCG iteration for one Newton step

- Background covariance matrix B constructed using a Second-Order Auto-Regressive (SOAR) correlation function.

	# PCG iterations			
Preconditioner	$n = 400$	$n = 800$	$n = 1600$	$n = 3200$
none	509	2,277	10,453	43,915
ML(4,0,0,0)	39	35	35	44
ML(1,2,4,8)	28	26	26	34
ML(0,2,4,16)	23	22	21	27
ML(0,0,8,16)	22	21	20	26
ML(0,0,0,32)	19	16	15	20

Cost of building the preconditioner

- Costs shown so far have not included building the preconditioner.
- Repeated applications of Lanczos still expensive.
- Possibility of exploiting Lanczos/CG connection?
- May have coarser level information already available?
- Potential for using randomisation to compute eigenvalues?

Practical implementation: Hessian decomposition

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

$$H(\mathbf{v}) = I + \sum_{s=1}^{S} (H^s(\mathbf{v}) - I)$$

- computational advantages of local Hessians:
  - fewer eigenvalues required for limited-memory approximation;
  - can be calculated at a coarser grid level;
  - can use local rather than global models;
  - can be computed in parallel.

Practical approach: Version 1

1. Compute limited-memory approximations to local sensor-based Hessians on level k using n_k eigenpairs:

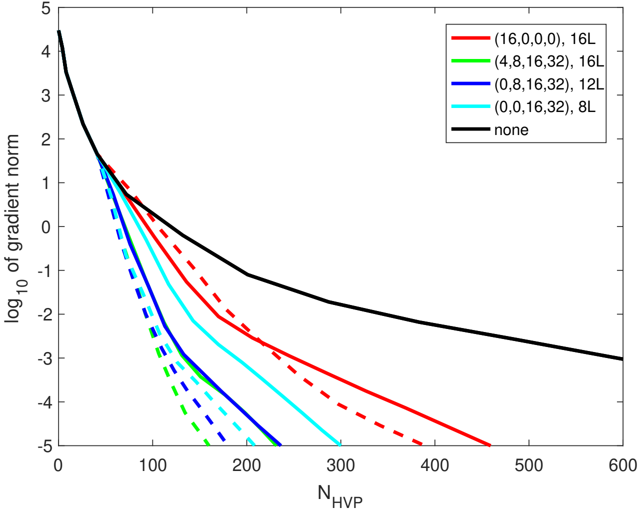
$$H_k^s \approx I + \sum_{i=1}^{n_k} (\lambda_i - 1)\mathbf{u}_i\mathbf{u}_i^T$$

2. Assemble these to form H_a.
3. Apply MLalg to H_a based on a fixed N_e.

- Advantage:
  - Local Hessians cheaper to compute.
- Disadvantages:
  - Additional user-specified parameter(s) n_k needed.
  - More memory required as local Hessians must also be stored.

Sample costs including building preconditioner

- Local Hessians with 8 eigenvalues at level 0 (solid lines) or level 1 (dashed lines).



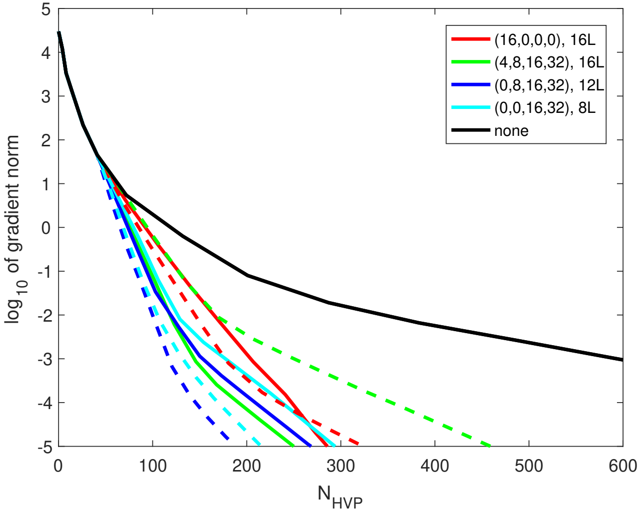
Practical approach: Version 2

1. Approximate each local Hessian H_k^s by applying MLalg to local inverse Hessians based on $N_{e,k}$.
2. Assemble these to form reduced-memory Hessian H_a^{rm}.
3. Use MLalg again on H_a^{rm} based on N_e.

- Advantage:
  - Requires less memory than Version 1.
- Disadvantage:
  - Additional user-specified parameter(s) $N_{e,k}$ needed.

Version 2: cost including building preconditioner

- Local Hessians with 8 eigenvalues at level 0 (solid lines) or level 1 (dashed lines) with $N_{e,k} = (8, 4, 0, 0)$ ML approx.



Concluding remarks

- Algorithm based solely on repeated use of Lanczos at each level (for building limited-memory approximations).
- Tricky to identify the optimal number of eigenvalues to use at each level: good rule of thumb available but analysis would be better!
- Full algorithm may not always be practical, but we have developed practical implementations based on Hessian decompositions.
- Also works well for other configurations (e.g. moving sensors, different initial conditions).
- Potential for extension to higher dimensions and other applications.

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