Multiresolution homogenization of operators in separated form

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The Numerical Homogenization Problem

Let S_h be a discretization of a differential operator w/scale parameter (step size) h.

(Examples of interest are $\mu(\mathbf{x})\Delta$ or $\nabla \cdot (\mu(\mathbf{x})\nabla)$.

Numerical homogenization problem:

- Find S_{2h} so that the action of S_{2h} approximates that of S_h on some (possibly even coarser) subspace.

- If possible, identify S_{2h} as a discretization of an operator of the same or related form.

- Otherwise, find algorithms for efficient computation of S_{2h}.

- Go to even coarser scales ($4h$, $8h$, ...)

Outline

1. Overview of multiresolution (wavelet-based) homogenization

2. Explicit formulas for coefficients of homogenized operators

3. Homogenization of operators in separated form

The Numerical Homogenization Problem

Multiscale Representation of Operators

Let H and G be orthogonal projection matrices where $HH^T + GG^T = I$.

If H and G are derived from a wavelet basis, they represent projections onto a *coarse scale* and the complementary wavelet space.

Alternatively, H may be viewed as a local-averaging operator; G is a local difference operator.

Vectors are decomposed as $s_v = Hv$ and $d_v = Gv$.

For a matrix S, we use the *standard form*:

$$\mathbf{A}_S = GSG^T, \ \ \mathbf{B}_S = GSH^T$$

$$\mathbf{C}_S = HSG^T, \ \ \mathbf{T}_S = HSH^T$$

In 2D, we use tensor products: $H_2 = H \otimes H$, $G_2 = (H \otimes G, G \otimes H, G \otimes G)$; similarly in 3D and higher.

Schur complement homogenization

Given equation

$$S_h u = f$$

we write it in standard form

$$\begin{pmatrix} \mathbf{A}_{S_h} & \mathbf{B}_{s_h} \\ \mathbf{C}_{S_h} & \mathbf{T}_{S_h} \end{pmatrix} \begin{pmatrix} d_u \\ s_u \end{pmatrix} = \begin{pmatrix} d_f \\ s_f \end{pmatrix}$$

and (formally) eliminate d_u:

$$(\mathbf{T}_{S_h} - \mathbf{C}_{S_h}\mathbf{A}_{S_h}^{-1}\mathbf{B}_{S_h})s_u = s_f - \mathbf{C}_{S_h}\mathbf{A}_{S_h}^{-1}d_f$$

So, we have $S_{2h} = \mathbf{R}_{S_h} = \mathbf{T}_{S_h} - \mathbf{C}_{S_h}\mathbf{A}_{S_h}^{-1}\mathbf{B}_{S_h}$.

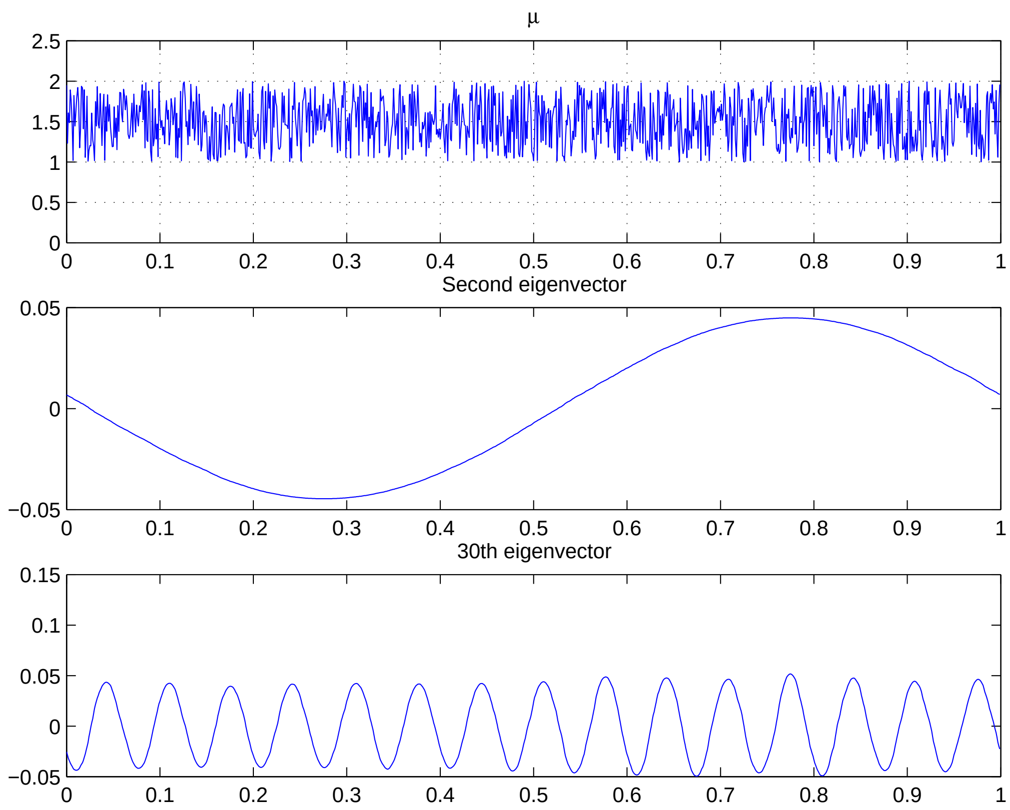
(Later, we use a convenient property of the Schur complement:)

$$\mathbf{T}_{S_h} - \mathbf{C}_{S_h}\mathbf{A}_{S_h}^{-1}\mathbf{B}_{S_h} = (\mathbf{T}_{(S_h)^{-1}})^{-1}$$

Eigenvalues and eigenvectors

Our homogenization procedure finds S_{2h} so that its *smaller* eigenvalues and corresponding eigenvectors are good approximations of those of S_h.

For discretizations of $\mu(\mathbf{x})\Delta$ or $\nabla \cdot (\mu(\mathbf{x})\nabla)$, these eigenspaces correspond to longer-wavelength, less oscillatory subspaces.



Wavelet-based Homogenization of Eigenvalue Problems

Given eigenvalue problem

$$S_h u = \lambda u \Rightarrow \begin{pmatrix} \mathbf{A}_{S_h} & \mathbf{B}_{s_h} \\ \mathbf{C}_{S_h} & \mathbf{T}_{S_h} \end{pmatrix} \begin{pmatrix} d_u \\ s_u \end{pmatrix} = \lambda \begin{pmatrix} d_u \\ s_u \end{pmatrix} \tag{1}$$

eliminate fine-scale variable to achieve

$$(\mathbf{T}_{S_h} - \mathbf{C}_{S_h}(\mathbf{A}_{S_h} - \lambda I)^{-1}\mathbf{B}_{S_h})s_u = \lambda s_u.$$

Linear approximation in λ:

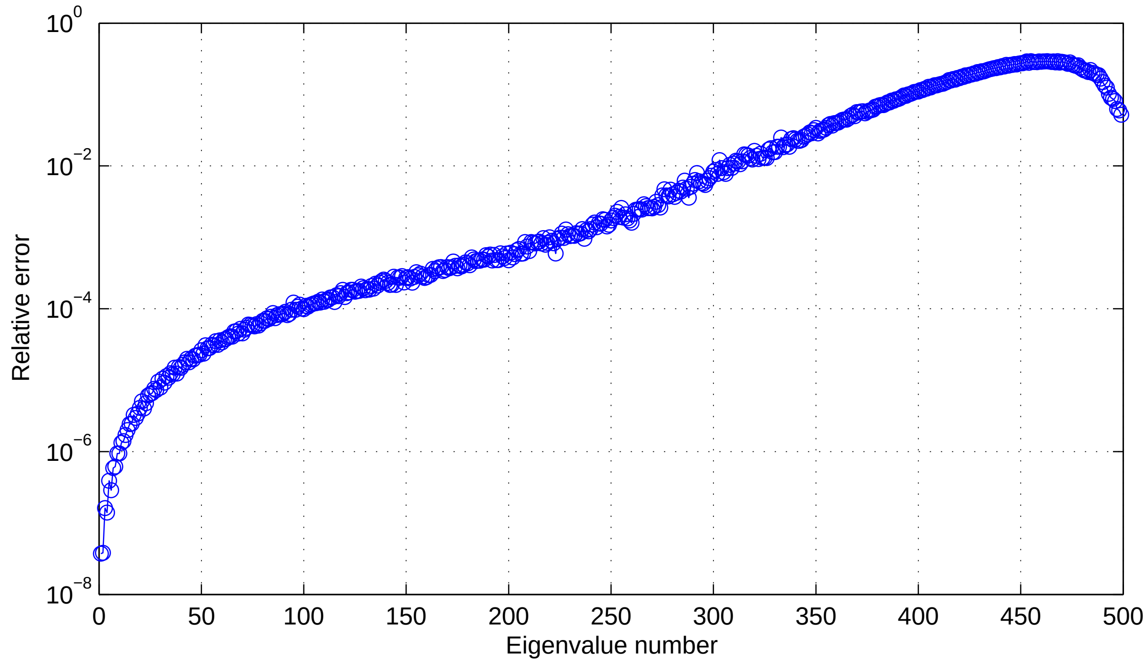
$$(\mathbf{T}_{S_h} - \mathbf{C}_{S_h}\mathbf{A}_{S_h}^{-1}\mathbf{B}_{S_h})s_u = \lambda s_u \tag{2}$$

or

$$\mathbf{R}_{S_h} s_u = \lambda s_u$$

Eigenvalue approximation

Smaller eigenvalues of $\mathbf{R}_{S_h}$ are known to be good approximations of those of S_h. (Coult 1997, Beylkin + Coult 1998)



Here we use $S_h = \Delta_- V \Delta_+$, V diagonal w/pseudorandom entries, $h = \frac{1}{1000}$, wavelets with 8 vanishing moments. Eigenvalues of $\mathbf{R}_{S_h}$ and S_h are compared. (Using more vanishing moments results in better accuracy for larger eigenvalues.)

Wavelet-based (multiresolution) homogenization

- Use Schur complement to eliminate fine-scale variables and compute a coarse-scale operator $\mathbf{R}_{S_h}$

- $\mathbf{R}_{S_h}$ has smaller eigenvalues that approximate those of S_h well

- $\mathbf{R}_{S_h}$ has a sparse (banded) approximation

How can we characterize $\mathbf{R}_{S_h}$ as an *operator*?

Can we extract a coarse-scale *medium* from $\mathbf{R}_{S_h}$?

What separability properties does $\mathbf{R}_{S_h}$ have?

Explicit formulas for homogenized coefficients

Homogenization of μ

Given S_h as a discretization of $\mu(\mathbf{x})\Delta$ or $\nabla \cdot (\mu(\mathbf{x})\nabla)$, what can be said about the *form* of $\mathbf{R}_{S_h}$? Can it be identified as a discretization of some (possibly different) differential operator?

A.C. Gilbert. A Comparison of multiresolution and classical one-dimensional homogenization schemes. *Appl. Comput. Harmon. Anal.* 5, 1–35 (1998)

M. Dorobantu, B. Engquist. Wavelet-based numerical homogenization. *SIAM. J. Numer. Anal.* Vol. 35, No. 2, pp. 540-559, April 1998

U. Andersson, B. Engquist, G. Ledfelt, O. Runborg. A contribution to wavelet-based subgrid modeling. *Appl. Comput. Harmon. Anal.* 7, 151–164 (1999)

Y. Capdeboscq, M.S. Vogelius. Wavelet based homogenization of a 2 dimensional elliptic problem. *Preprint*, 2002.

Engquist et. al. showed that if $S_h = \Delta_- V \Delta_+$, then $\mathbf{R}_{S_h} = \Delta_- \tilde{V} \Delta_+$ where $\tilde{V}$ is strongly diagonally-dominant (and similarly in 2D) when using the Haar basis and first-order finite-differences for $\Delta_\pm$.

Others have explored various approximations of $\mathbf{A}^{-1}$, or found explicit formulae for $\tilde{V}$ in the case of periodic coefficients.

Explicit formula for homogenized coefficients

We consider two cases:

1. $S_h = \Delta_- V \Delta_+$ (discretization of $\frac{d}{dx}\mu(x)\frac{d}{dx}$)

2. $S_h = VL$ (discretization of $\mu(x)\Delta$ in any dimension)

In both cases we derive an approximation of $\mathbf{R}_{S_h}$ which includes an *explicit formula* for the homogenized coefficients.

Homogenized coefficients of $S_h = \Delta_- V \Delta_+$

Assume $(S_h)^{-1}$ exists (or restrict it to a subspace where it does); define $K = \Delta_+^{-1}$. Using properties of Schur complements, we find

$$\mathbf{R}_{S_h} = \mathbf{R}_{\Delta_-} \mathbf{N}^{-1} \mathbf{R}_{\Delta_+}$$

where

$$\mathbf{N} = \mathbf{R}_{\Delta_+} \mathbf{C}_K \mathbf{A}_W \mathbf{C}_K^T \mathbf{R}_{\Delta_-} + \mathbf{R}_{\Delta_+} \mathbf{C}_K \mathbf{B}_W + \mathbf{C}_W \mathbf{C}_K^T \mathbf{R}_{\Delta_-} + \mathbf{T}_W$$

and

$$W = V^{-1}.$$

$\mathbf{R}_{\Delta_\pm}$ is a differentiation matrix of the same approximation order as $\Delta_\pm$.

$\mathbf{N}$ is diagonally dominant. We seek to identify $\mathbf{N}$ with pointwise multiplication by some vector; $\mathbf{N}$ is not diagonal so we must make another approximation to do this.

Homogenized coefficients of $S_h = \Delta_- V \Delta_+$

We approximate $\mathbf{N}$ via *mass-lumping*; in place of $\mathbf{N}$ we use a diagonal matrix $\tilde{\mathbf{N}}$ whose action on constant vectors is the same as $\mathbf{N}$.

If o is a vector of ones, then $\mathbf{R}_{\Delta_+} o = 0$, $\mathbf{T}_W o = \frac{1}{\sqrt{2}} H w$, $\mathbf{B}_W o = \frac{1}{\sqrt{2}} G w$, where $w = \text{diag}(W)$.

We find

$$\text{diag}(\tilde{\mathbf{N}}) = \frac{1}{\sqrt{2}} (H v^{-1} + \mathbf{R}_{\Delta_+} \mathbf{C}_K G v^{-1})$$

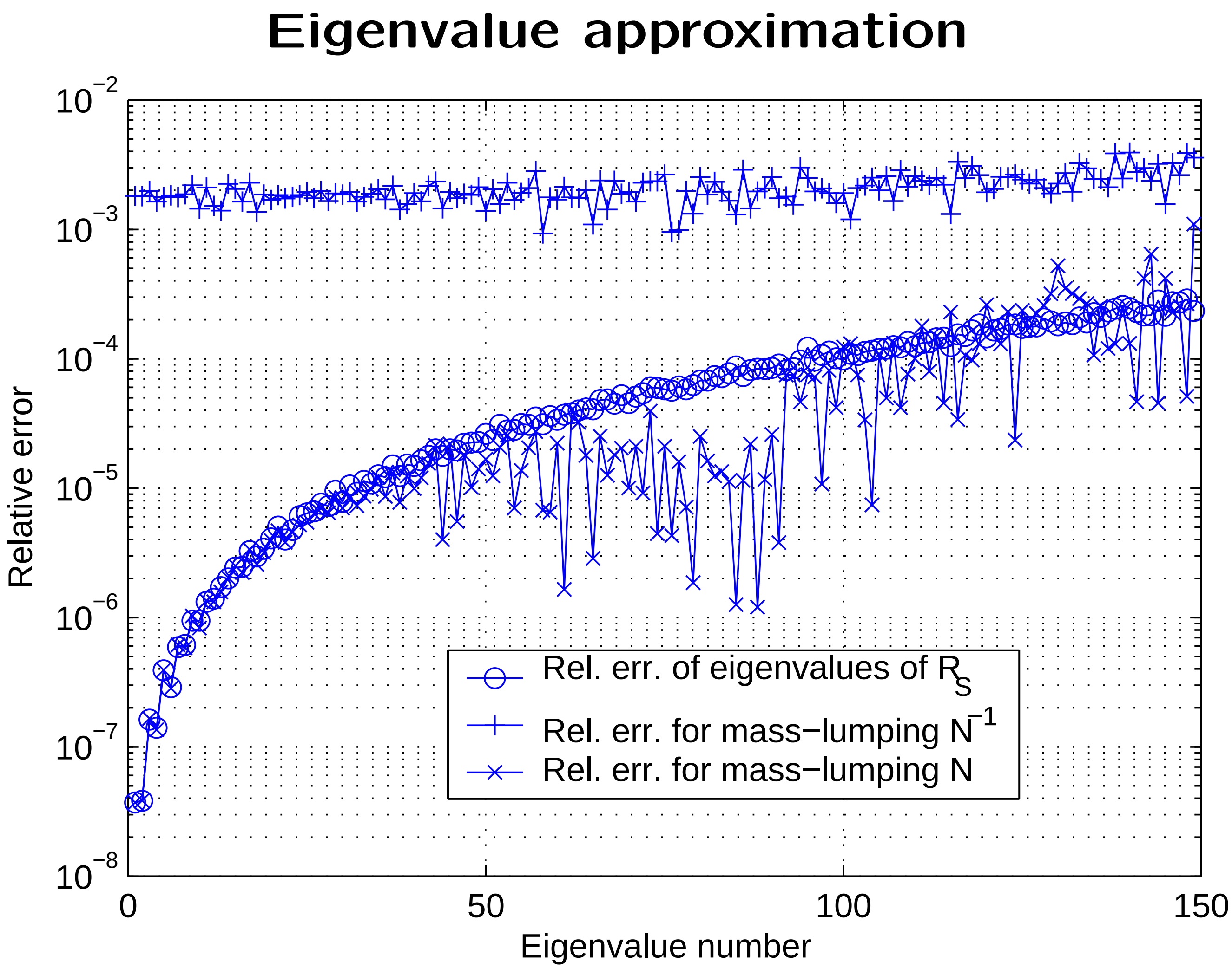
where v is the diagonal of V.

Thus we have

$$\mathbf{R}_{S_h} \approx \mathbf{R}_{\Delta_-} \tilde{V} \mathbf{R}_{\Delta_+}$$

where the diagonal of $\tilde{V}$ is given by

$$\sqrt{2} (H v^{-1} + \mathbf{R}_{\Delta_+} \mathbf{C}_K G v^{-1})^{-1}$$



Our approximation appears to provide similar (or even slightly better) accuracy of eigenvalues as the exact $\mathbf{R}_{S_h}$, though we have no proof yet. Note that mass-lumping $\mathbf{N}^{-1}$ results in very poor accuracy.

Homogenized coefficients of $S_h = \Delta_- V \Delta_+$

Homogenized coefficients via mass-lumping:

$$\sqrt{2}(Hv^{-1} + \mathbf{R}_{\Delta_+}\mathbf{C}_K G v^{-1})^{-1}$$

Some remarks:

- If Gv^{-1} is constant, the formula reduces to $\sqrt{2}(Hv^{-1})^{-1}$, a *local harmonic mean.*

- If v^{-1} is cell-periodic w/period 2, the formula reduces exactly to the harmonic mean.

- $\mathbf{R}_{\Delta_+}$ and $\mathbf{C}_K$ have sparse (banded) approximations.

Homogenized coefficients of $S_h = VL$

We define $Q = L^{-1}$ (Q is a discretization of Δ^{-1}; this will be important later). We derive

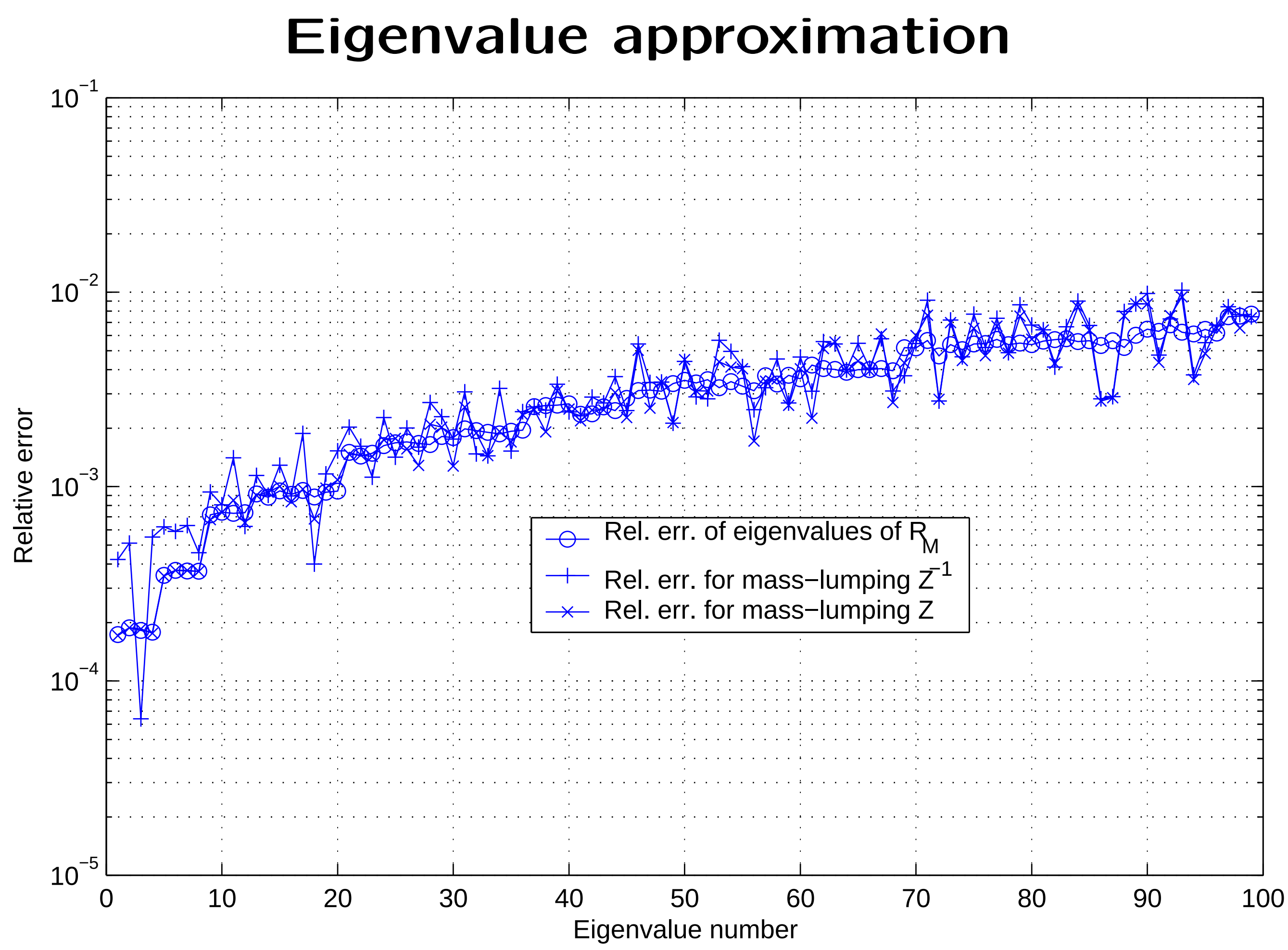
$$\mathbf{R}_{S_h} = \mathbf{Z}^{-1}\mathbf{R}_L$$

where $\mathbf{Z} = \mathbf{R}_L\mathbf{C}_Q\mathbf{B}_W + \mathbf{T}_W$. We approximate $\mathbf{Z}$ via mass-lumping to achieve

$$\mathbf{R}_{S_h} \approx \tilde{V}\mathbf{R}_L$$

where $\tilde{V}$ is diagonal w/ entries

$$\sqrt{2}(Hv^{-1} + \mathbf{R}_L\mathbf{C}_Q G v^{-1})^{-1}$$



$S_h = VL$, V diagonal w/random entries, 40×40 spatial discretization. Again, our approximation appears to provide similar accuracy of eigenvalues as the exact $\mathbf{R}_{S_h}$, though we have no proof yet.

Homogenized coefficients of $S_h = VL$

$$\sqrt{2}(Hv^{-1} + \mathbf{R}_L \mathbf{C}_Q G v^{-1})^{-1}$$

Remarks:

- This result holds in any number of dimensions.
- $\mathbf{R}_L$ is a discretization of Δ of same approximation order as L.
- Reduces to local harmonic mean/harmonic mean in certain cases.
- $\mathbf{R}_L$ and $\mathbf{C}_Q$ have sparse approximations.
- Homogenized medium is *isotropic*.

Homogenization of operators in separated form

Separated representations: $S = VL$

We have $S = VL = V(D^x_- D^x_+ + D^y_- D^y_+)$, and $V = \sum_{k=1}^{r} \sigma_k x_k \otimes y_k$, so

$$S = (\sum_{k=1}^{r} \sigma_k (x_k D^x_- D^x_+ \otimes y_k + x_k \otimes D^y_- D^y_+ y_k)$$

with separation rank $\rho(S) \leq 2r$. (We use *rank* as shorthand for *separation rank*.)

What can be determined about $\rho(\mathbf{R}_S)$?

We use

$$\mathbf{R}_S \approx \tilde{V}\mathbf{R}_L$$

where

$$\mathrm{diag}(\tilde{\mathrm{V}}) = \sqrt{2}(\mathrm{Hv}^{-1} + \mathbf{R}_\mathrm{L}\mathbf{C}_\mathrm{Q}\mathrm{Gv}^{-1})^{-1}$$

Note that $\rho(\tilde{V}\mathbf{R}_L) \leq \rho(\tilde{V})\rho(\mathbf{R}_L)$.

Separated representations: $S = VL$

We have

$$\rho(\tilde{V}\mathbf{R}_L) \leq \rho(\tilde{V})\rho(\mathbf{R}_L).$$

and

$$\rho(\tilde{V}^{-1}) \leq \rho(Hv^{-1}) + \rho(\mathbf{R}_L\mathbf{C}_Q Gv^{-1})$$

H and G are totally separated, so $\rho(Hv^{-1}) \leq \rho(v^{-1}), \rho(Gv^{-1}) \leq \rho(v^{-1})$.

The main influence on $\rho(\tilde{V}^{-1})$ thus appears to be $\rho(\mathbf{R}_L\mathbf{C}_Q)$

Estimates of $\rho(\mathbf{C}_Q), \rho(\mathbf{R}_L)$, and $\rho(\tilde{V})$

Recall that since Q is a discretization of Δ^{-1}, we may find a separated representation valid on the annulus $(\sum_{i=1}^{d} \xi_i^2)^{1/2} \in [\delta D, D]$ where the rank depends logarithmically on δ.

In 1D, the Fourier symbol of $\mathbf{C}_Q = \mathcal{O}(\xi^{m-2})$, where m is the number of vanishing moments of the wavelet basis.

In 2D and higher we achieve similar results - thus $\mathbf{C}_Q$, w/ accuracy $\mathcal{O}(\delta D)^{m-2}$, is the restriction of Δ^{-1} to a subset of the annulus $[\delta D, D]$.

We expect $\rho(\mathbf{R}_L) = d$ since $\mathbf{R}_L$ is a discretization of Δ. So, we hope to achieve the bound

$$\rho(\tilde{V}^{-1}) \leq (1 + d\rho(\mathbf{C}_Q))\rho(v^{-1})$$

For a *vector* f, what is the relationship between $\rho(f)$ and $\rho(f^{-1})$?

$$S_h = \Delta_-^x V \Delta_+^x + \Delta_-^y V \Delta_+^y$$

Except for special cases, (e.g. periodic v) a mass-lumped approximation for homogenized coefficients has not been found. We do know:

- $\mathbf{R}_{S_h}$ has a sparse representation in wavelet basis
- $\mathcal{O}(N = n^d)$ algorithms exist for computing $\mathbf{R}_{S_h}$
- $\mathbf{R}_{S_h}$ has eigenvalue-approximating property
- The homogenized operator may be *anisotropic*

Homogenization in separated form

Even banded approximations arising from sparse wavelet representations are *expensive* in multiple dimensions.

So we represent S_h in separated form, and compute

$$\mathbf{R}_{S_h} = \mathbf{T}_{S_h} - \mathbf{C}_{S_h}\mathbf{A}_{S_h}^{-1}\mathbf{B}_{S_h}$$

using separated linear algebra.

Inverse via Newton-Schulz iteration

$$M_{i+1} = 2M_i - M_i\mathbf{A}M_i$$

If $\|\mathbf{A}M_0 - I\| < 1$ then M_i converges quadratically to $\mathbf{A}^{-1}$.

Algorithm:

1. Compute $M_{i+1} = 2M_i - M_i\mathbf{A}M_i$ using separated matrix-matrix multiply.

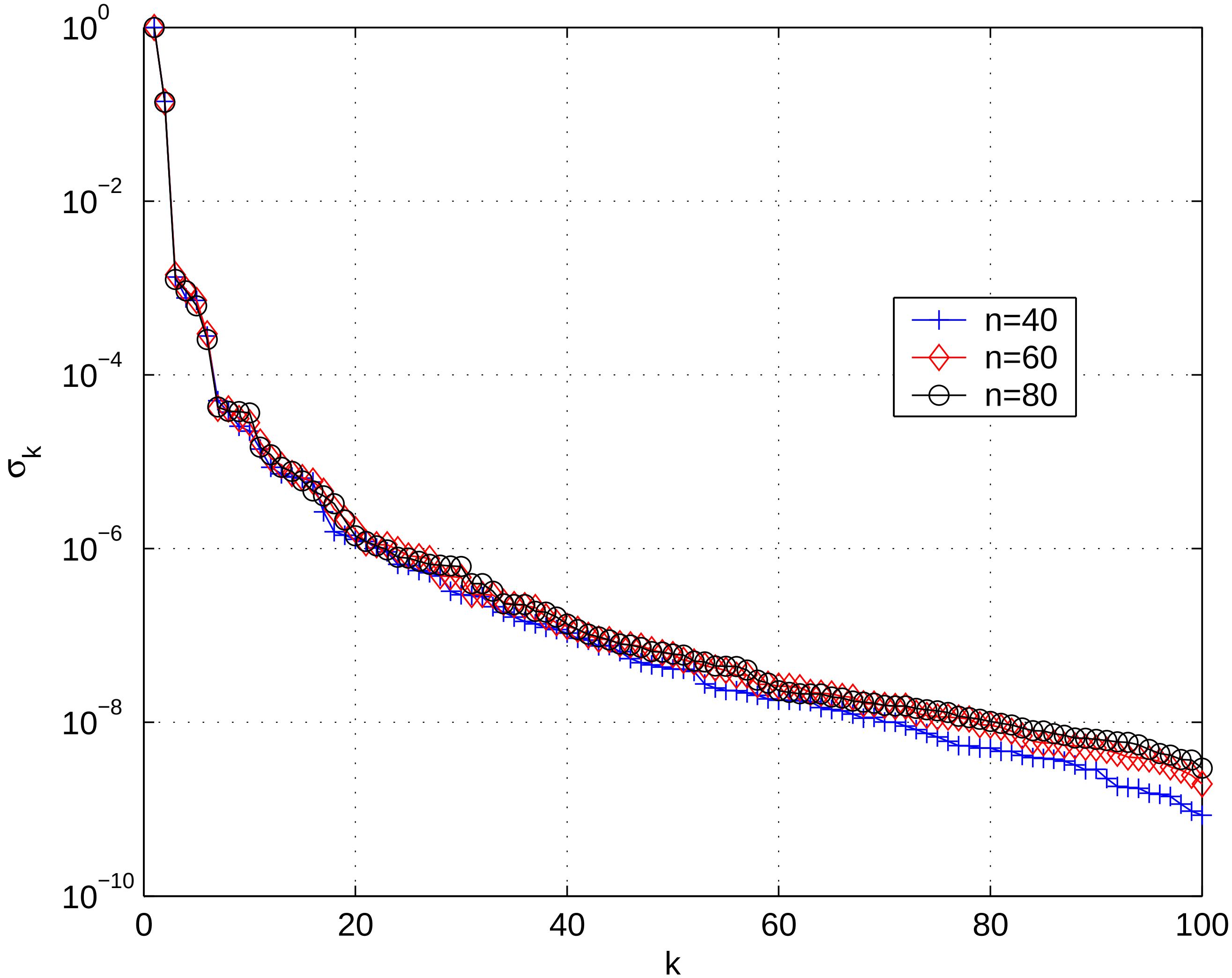
2. Apply rank reduction to M_{i+1}; repeat from 1 until $\|M_{i+1} - M_i\| \leq \epsilon$.

For fixed-rank banded matrices, cost per iteration is $\mathcal{O}(N^{\frac{1}{d}})$.

Number of iterations depends only weakly on N since $\mathbf{A}$ is well-conditioned.

Even if $\rho(\mathbf{A})$ and $\rho(\mathbf{A}^{-1})$ are small, how do we keep intermediate ranks small?

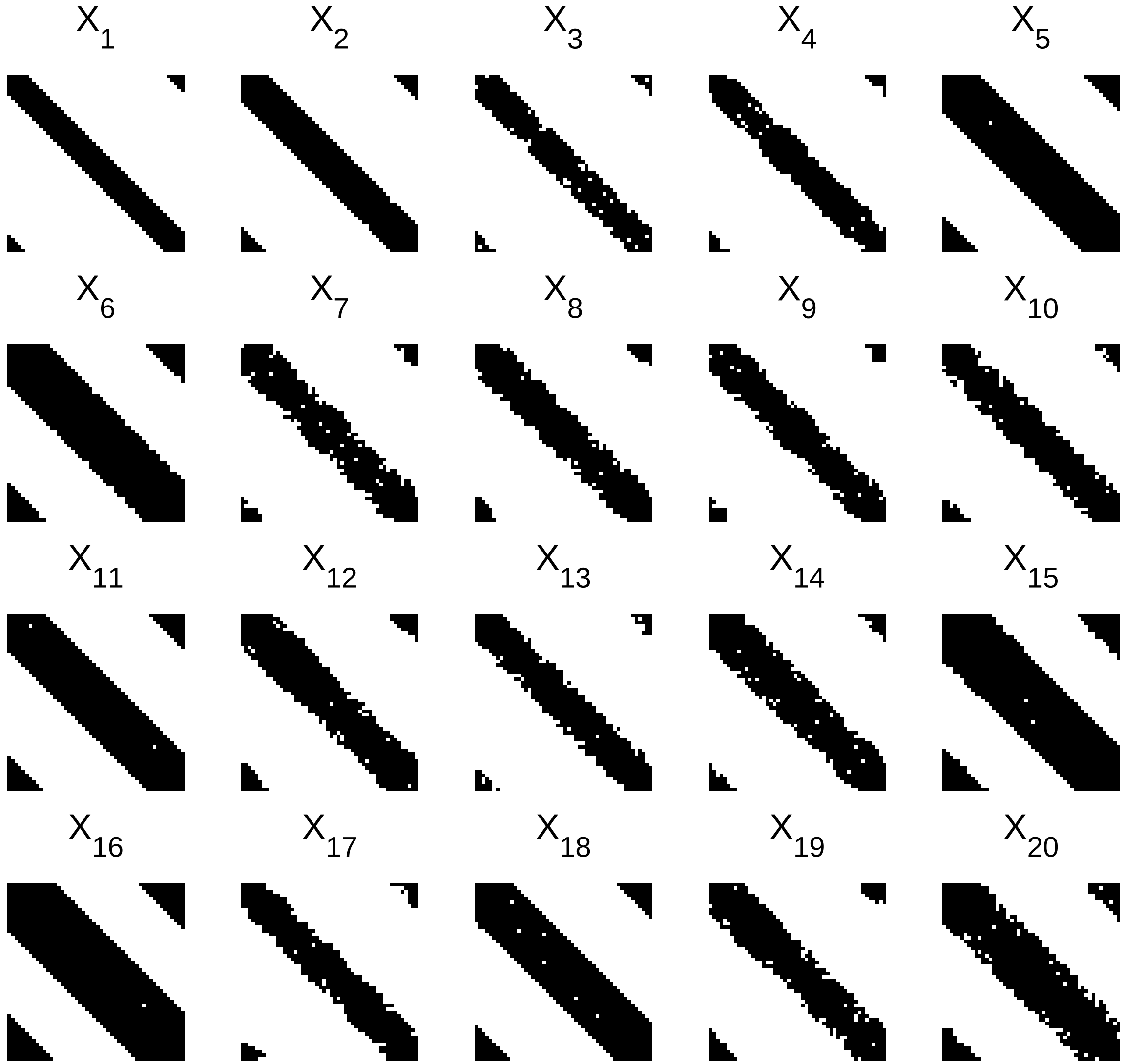
Numerical results: $\rho(\mathrm{R})$ vs. n



$$S = D_-^x V D_+^x + D_-^y V D_+^y, n = 40, 60, 80, \rho(S) = 4.$$

V chosen to be pseudorandom.

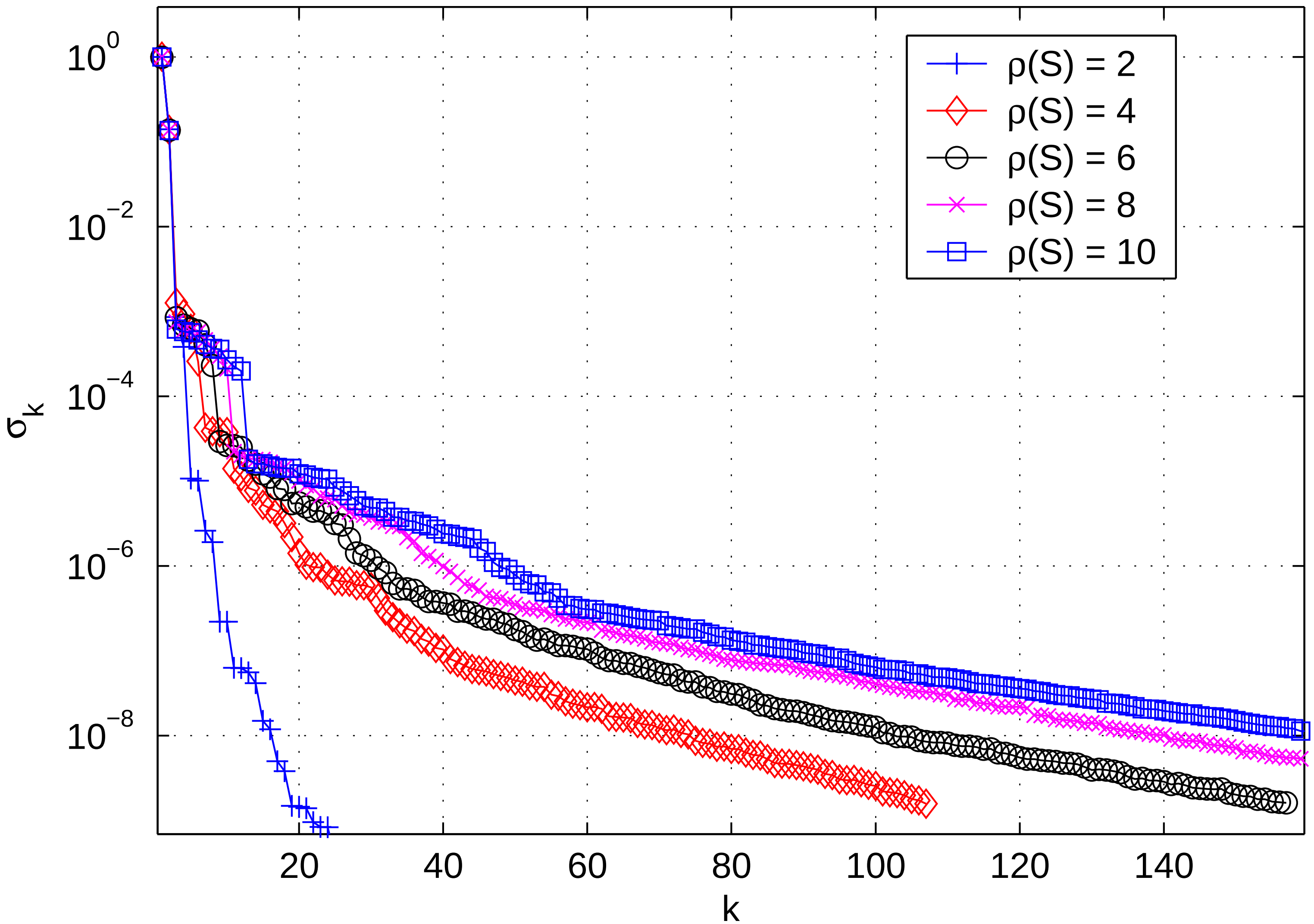
Banded matrices



$n = 50$, $\rho(S) = 4$, $\rho(R) = 20$
matrix entries truncated below threshold value.

$\rho(\mathbf{R})$ vs. $\rho(S)$

$$S = D_-^x V D_+^x + D_-^y V D_+^y, n = 80.$$



$\rho(S)$ **vs.** $\rho(R)$

At a given truncation level, the relationship between $\rho(S)$ and $\rho(R)$ appears nearly linear:

At $\epsilon = 10^{-4}$, we have

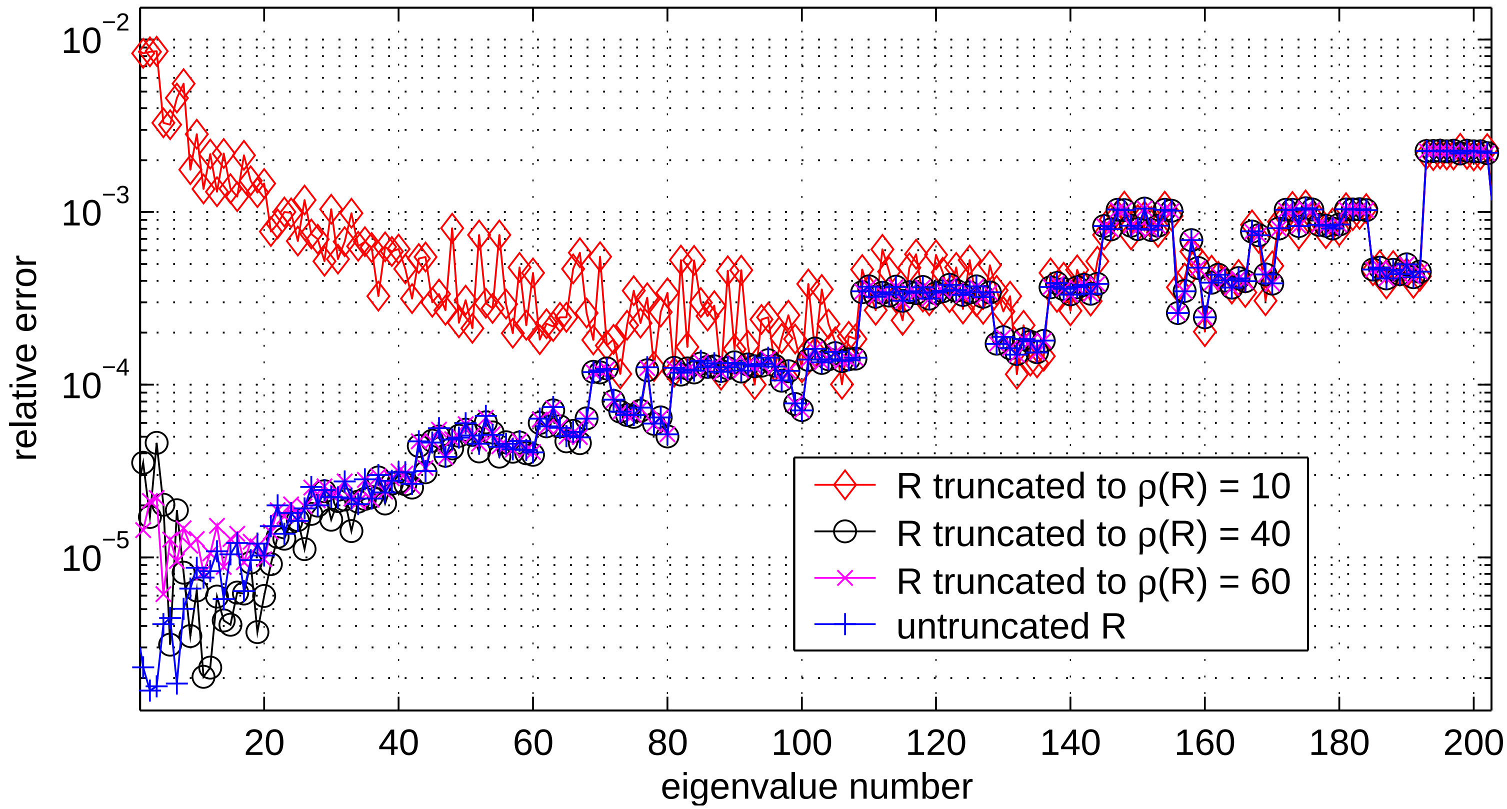
$\rho(S)$	4	6	8	10
$\rho(R)$	6	8	10	12

At $\epsilon = 10^{-6}$, we have

$\rho(S)$	4	6	8	10
$\rho(R)$	21	30	39	47

Eigenvalue approximation

The smaller eigenvalues of $\mathbf{R}$ approximate those of S well (see Beylkin + Coult 1998). Truncating separation values of $\mathbf{R}$ perturbs the eigenvalues.



$n = 80,\ \rho(S) = 4.$

Future Work

- More general estimates of $\rho(S)$ vs. $\rho(\mathbf{R}_S)$.
- Homogenized coefficients for $\nabla \cdot (\mu(\mathbf{x})\nabla)$
- Efficient 3D implementation.
- Wave propagation in highly heterogeneous media.

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