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Scientific Computing

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Computational Science

- Design and analysis of numerical methods that are

  robust, accurate, efficient and versatile

- Focus on a large class of problems (as linear equations, least square problems, eigenvalue problems, . . .)
- Focus on one (class of) numerical method(s)

Scientific Computing

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- specifically for one family of practical problems only (as Navier Stokes, electronics, . . .)
- Combines several methods, methods that are most suitable for specific subproblems. Find optimal parameters.

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As we will learn today, problems from SC may lead to interesting new classes of problems in CS.

Program

- Multigrid (PDEs)
- Compressed Sensing (MRI)
- Model order reduction (Electronics)
- Relax to the max (QCD)

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Sparse reconstruction

With $\mathbf{A}$ an $n \times n$ matrix and $\mathbf{b}$ an n-vector: $\mathbf{A}\mathbf{x}^\star = \mathbf{b}$.

Suppose for $\mathcal{J} \subset \{1, 2, \ldots, n\}$ only $\mathbf{b}(\mathcal{J})$ is available.

Can we solve $(*)$ $\mathbf{A}(\mathcal{J}, :)\mathbf{x} = \mathbf{b}(\mathcal{J})$ to obtain $\mathbf{x}^\star$?

Here we use Matlab notation.

Sparse reconstruction

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Can we solve $(*)$ $\mathbf{A}(\mathcal{J}, :)\mathbf{x} = \mathbf{b}(\mathcal{J})$ to obtain $\mathbf{x}^\star$?

Generally, no:
$\mathbf{x}^\star + \mathbf{y}$ solves $(*)$ for any $\mathbf{y} \in \mathcal{N}(\mathbf{A}(\mathcal{J}, :))$
and for the least norm solution $\mathbf{x}_{\mathsf{LN}}$ we may have that

$$\|\mathbf{x}_{\mathsf{LN}}\|_2 \ll \|\mathbf{x}^\star\|_2.$$

Sparse reconstruction

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Can we solve $(*)$ $\mathbf{A}(\mathcal{J}, :)\mathbf{x} = \mathbf{b}(\mathcal{J})$ to obtain $\mathbf{x}^\star$?

However, in some applications it is known that

$$\|\mathbf{x}^\star\|_0 \equiv \#\{i \mid x_i^\star \neq 0\} \ll n,$$

the solution vector $\mathbf{x}^\star$ is **sparse**, d-**sparse**, where $d \equiv \|\mathbf{x}^\star\|_0$.

Sparse reconstruction

With $\mathbf{A}$ an $n \times n$ matrix and $\mathbf{b}$ an n-vector: $\mathbf{A}\mathbf{x}^\star = \mathbf{b}$.

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However, in some applications it is known that

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the solution vector $\mathbf{x}^\star$ is **sparse**.

Idea. Solve $\min \|\mathbf{x}\|_0$ such that $\mathbf{A}(\mathcal{J}, :)\mathbf{x} = \mathbf{b}(\mathcal{J})$.

Is $\mathbf{x}_{\min} = \mathbf{x}^\star$?

Compressed sensing: an example

Let $n = 2^m$ and let $\mathbf{x}^\star$ be such that $\|\mathbf{x}^\star\|_0 = 3$.
Can we "sense" $\mathbf{x}^\star$ by only inspecting a few coordinates?

Select $\mathcal{J} \subset \{1, \ldots, n\}$ randomly such that $|\mathcal{J}| = 8$.

a) Take $\mathbf{x}(\mathcal{J}) \equiv \mathbf{x}^\star(\mathcal{J})$ and $\mathbf{x}$ is zero elsewhere.

b) View $\mathbf{x}^\star$ as a function on $\{1, 2, \ldots, 2^m\}$.
Let $\mathbf{A} = \mathcal{F}$ be the Fourier transform, $\mathbf{b} = \mathbf{A}\mathbf{x}^\star = \widehat{\mathbf{x}}^\star$.
Find $\mathbf{x}$ such that $\|\mathbf{x}\|_0 = 3$ and $\widehat{\mathbf{x}}(\mathcal{J}) = \widehat{\mathbf{x}}^\star(\mathcal{J})$.

What is the probability that $\mathbf{x} = \mathbf{x}^\star$?

If $|\mathcal{J}| = 1$ we would already know that $\mathbf{x}^\star \neq \mathbf{0}$

$\mathcal{J}$ random to avoid aliasing.

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Note that in a) $\mathbf{A} = \mathbf{I}$.

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Conclusion. Depending on $\mathbf{A}$ the idea might work.

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What is the probability that $\mathbf{x} = \mathbf{x}^\star$?

In, for instance MRI, $\mathbf{A}$ is a 2 (or 3) dimensional Fourier transform. The MRI scanner measures $\mathbf{b}$, the Fourier transform of the (discretized) density function $\mathbf{x}$ of water in the scanned tissue. Measuring $\mathbf{b}$ only partially would reduce the scanning time (by a factor $|\mathcal{J}|/n$). With respect to, for instance, an appropriate wavelet basis, $\mathbf{x}$ is sparse, i.e., $\|\mathbf{x}\|_0 \ll n$. However the value of $\|\mathbf{x}\|_0$ is unknown.

Sparse reconstruction

Idea. Solve $\min \|\mathbf{x}\|_0$ such that $\mathbf{A}(\mathcal{J},:)\mathbf{x} = \mathbf{b}(\mathcal{J})$.

$\|\mathbf{x}\|_0$ is not a norm and leads to mathematical problems.

Alternative:

Solve $\min \|\mathbf{x}\|_1$ such that $\mathbf{A}(\mathcal{J},:)\mathbf{x} = \mathbf{b}(\mathcal{J})$.

Sparse reconstruction

$$\mathbf{x}_{\min} \equiv \text{argmin}\{\|\mathbf{x}\|_1 \mid \mathbf{x} \in \mathbb{R}^n \text{ st } \mathbf{A}(\mathcal{J},:)\mathbf{x} = \mathbf{A}(\mathcal{J},:)\mathbf{x}^\star\}$$

For $\mathbf{A} = \mathcal{F}$ (1,2, or 3-d), $d < k < n$ and random $\mathcal{J} \subset \{1,\ldots,n\}$, $|\mathcal{J}| = k$, consider the following statement.

Statement.

For all $\mathbf{x}^\star$ with $\|\mathbf{x}^\star\|_0 = d$, we have that $\mathbf{x}^\star = \mathbf{x}_{\min}$.

Theorem. The statement holds with high probability, where the probability depends on the ratios $d : k : n$.

No such result if $\|\cdot\|_1 \rightsquigarrow \|\cdot\|_2$!

Sparse reconstruction

$$\mathbf{x}_{\min} \equiv \text{argmin}\{\|\mathbf{x}\|_1 \mid \mathbf{x} \in \mathbb{R}^n \text{ st } \mathbf{A}(\mathcal{J},:)\mathbf{x} = \mathbf{A}(\mathcal{J},:)\mathbf{x}^\star\}$$

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Typical conditions: if $\frac{k}{d} \geq \frac{1}{\mu} \ln \frac{n}{d}$, then the probability that the statement is not correct is less than $2\exp(-k\mu)$. μ is some fix constant (as $\mu = 0.003$) independent of d, k, n.

Sparse reconstruction

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Expanation. Let $\mathcal{V} \subset \mathbb{R}^n$ be a random k-dim. subspace. Let $\mathbf{x} \in \mathbb{R}^n$ with the orthogonal component $\mathbf{x}_V$ in $\mathcal{V}$. Then

$$\text{Prob}\left(\left|1 - \frac{n}{k}\frac{\|\mathbf{x}_V\|_2^2}{\|\mathbf{x}\|_2^2}\right| > 2\epsilon\right) \leq 2\exp(-k/\epsilon^2).$$

There are only a 'few' d-sparse vectors: all d-sparse vectors are likely to be "sensed" in a random k dimensional subspace.

Sparse reconstruction

$$\mathbf{x}_{\min} \equiv \text{argmin}\{\|\mathbf{x}\|_1 \mid \mathbf{x} \in \mathbb{R}^n \text{ st } \mathbf{A}(\mathcal{J},:)\mathbf{x} = \mathbf{A}(\mathcal{J},:)\mathbf{x}^\star\}$$

For $\mathbf{A} = \mathcal{F}$ (1,2, or 3-d), $d < k < n$ and random $\mathcal{J} \subset \{1,\ldots,n\}$, $|\mathcal{J}| = k$, consider the following statement.

Statement.

For all $\mathbf{x}^\star$ with $\|\mathbf{x}^\star\|_0 = d$, we have that $\mathbf{x}^\star = \mathbf{x}_{\min}$.

Theorem. The statement holds with high probability, where the probability depends on the ratios $d : k : n$.

In practice $\widetilde{\mathbf{b}} \equiv \mathbf{A}(\mathcal{J},:)\mathbf{x}^\star + \delta_b$ is measured with $\|\delta_b\|_2 \leq \delta$.

Solve $\min \|\mathbf{x}\|_1$ such that $\|\mathbf{A}(\mathcal{J},:)\mathbf{x} - \widetilde{\mathbf{b}}\|_2 \leq \delta$.

The following statement holds with high probability.

Statement. For some modest constant κ, we have

$\|\mathbf{x}^\star - \mathbf{x}_{\min}\|_2 \leq \kappa\delta$ for all $\mathbf{x}^\star$ with $\|\mathbf{x}^\star\|_0 = d$.

Sparse reconstruction

Some general observations.

- Similar results for some other classes of matrices.
- Whether minimisation resolves $\mathbf{x}^\star$ depends on $\mathbf{A}(\mathcal{J},:)$
  ($\mathbf{A} = \mathbf{I}$ not solvable, $\mathbf{A} = \mathcal{F}$ solvable)
  and the number of non-zeros of $\mathbf{x}^\star$, not on the values or the location (index) of the non-zeros.
- Some randomness (in selecting $\mathcal{J}$) is required.
- $\mathbf{A}$ (that is, $\mathbf{A}(\mathcal{J},:)$) will not be sparse
  (otherwise $\mathbf{b}$ is sparse if $\mathbf{x}$ is sparse).

  Nevertheless $\mathbf{c} = \mathbf{A}(\mathcal{J},:)\mathbf{u}$ might be efficiently computable
  (if $\mathbf{A} = \mathcal{F}$ then FFT can be used
  to compute $\mathbf{c}' \equiv \mathbf{A}\mathbf{u}$ and $\mathbf{c} = \mathbf{c}'(\mathcal{J})$).

Constrained 1-norm minimisation

Let $\mathbf{A}$ be an $k \times n$ matrix, $k < n$ and $\mathbf{b}$ a k-vector.
With $f(\mathbf{x}) \equiv \frac{1}{2}\|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2$ and $g(\mathbf{x}) \equiv \|\mathbf{x}\|_1$, solve

$$\mathbf{x}_{\text{min}} = \text{argmin}\{g(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n \text{ st } f(\mathbf{x}) = \delta^2\}$$

Standard approach. Find $\lambda \in \mathbb{R}$ (**Lagrange multiplier**) and $\mathbf{x}$ (solution) that solve the **Lagrange equation**

$$\nabla f(\mathbf{x}) + \lambda \nabla g(\mathbf{x}) = \mathbf{0} \quad \& \quad f(\mathbf{x}) = \delta^2.$$

Note that, with the solution $\tau = \lambda$, the minimizer $\mathbf{x}$ of $f + \tau g$,

$$\mathbf{x}_{\text{min}} = \text{argmin}\{f(\mathbf{x}) + \tau g(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n\}$$

also solves the Lagrange equation.

However, g is **not** differentiable.

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$$\mathbf{x}_{\text{min}} = \text{argmin}\{g(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n \text{ st } f(\mathbf{x}) = \delta^2\}$$

Find appropriate $\tau > 0$. Solve

$$\mathbf{x}_{\text{min}} = \text{argmin}\{\rho(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n\} \quad \text{with} \quad \rho \equiv f + \tau g.$$

Note that with $g(\mathbf{x}) = \|\mathbf{x}\|_2^2$ gives Tykhonov regularisation.

1-norm regularisation

Let $\mathbf{A}$ be an $k \times n$ matrix, $k < n$ and $\mathbf{b}$ a k-vector.
With $f(\mathbf{x}) \equiv \frac{1}{2}\|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2$ and $g(\mathbf{x}) \equiv \|\mathbf{x}\|_1$, solve

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$$\mathbf{x}_{\min} = \operatorname{argmin}\{\rho(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n\} \quad \text{with} \quad \rho \equiv f + \tau g.$$

Example. Soft threshholding

$$s_\tau(\mathbf{b})_j \equiv \operatorname{sign}(b_j)\, \max(|b_j| - \tau, 0)$$

solves the minimisation for $\mathbf{A} = \mathbf{I}$:

$$s_\tau(\mathbf{b}) = \operatorname{argmin}\{\tfrac{1}{2}\|\mathbf{b} - \mathbf{x}\|_2^2 + \tau\|\mathbf{x}\|_1 \mid \mathbf{x} \in \mathbb{R}^n\}$$

Proof. Find $t_{\min} = \operatorname{argmin}\{\frac{1}{2}|\beta - t|^2 + \tau\,|t| \mid t \in \mathbb{R}\}$.

1-norm regularisation

Let $\mathbf{A}$ be an $k \times n$ matrix, $k < n$ and $\mathbf{b}$ a k-vector.
With $f(\mathbf{x}) \equiv \frac{1}{2}\|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2$ and $g(\mathbf{x}) \equiv \|\mathbf{x}\|_1$, solve

$$\mathbf{x}_{\min} = \operatorname{argmin}\{\rho(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n\} \quad \text{with} \quad \rho \equiv f + \tau g.$$

Towards an iterative solution method.
Let $\mathbf{x}_0$ be an approximate solution.
For updating $\mathbf{x}_0$, use Taylor expansion to bound f.
$\nabla f(\mathbf{x}) = -\mathbf{A}^*(\mathbf{b} - \mathbf{A}\mathbf{x})$. Select an $L \geq \lambda_{\max}(\mathbf{A}^*\mathbf{A})$. Then

$$\begin{aligned} f(\mathbf{x}) &\leq f(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0, \nabla f(\mathbf{x}_0)) + \tfrac{1}{2}L\|\mathbf{x} - \mathbf{x}_0\|_2^2 \\ &= d_0 + \tfrac{1}{2}L\|\mathbf{x} - \mathbf{x}_0'\|_2^2, \end{aligned}$$

where

$$d_0 \equiv f(\mathbf{x}_0) - \tfrac{1}{2L}\|\nabla f(\mathbf{x}_0)\|_2^2, \quad \mathbf{x}_0' \equiv \mathbf{x}_0 - \tfrac{1}{L}\nabla f(\mathbf{x}_0).$$

In particular,

$$\min \rho(\mathbf{x}) \leq d_0 + \min\{\tfrac{1}{2}L\|\mathbf{x} - \mathbf{x}_0'\|_2^2 + g(\mathbf{x})\} \leq \rho(\mathbf{x}_0).$$

The second term is minimised by $\mathbf{x}_1 \equiv s_{\tau/L}(\mathbf{x}_0')$.

Iterative Shrinkage-Thresholdong Algorithm

Find an $L > \lambda_{\max}(\mathbf{A}^*\mathbf{A})$.

ISTA

Select an $\mathbf{x}_0$. $\mathbf{x} = \mathbf{x}_0$

Repeat

$\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}, \quad \mathbf{s} = \mathbf{A}^*\mathbf{r}$

$\mathbf{x} \leftarrow \mathbf{x} + \frac{1}{L}\mathbf{s}$

$\mathbf{x} \leftarrow s_{\tau/L}(\mathbf{x})$

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$\mathbf{x} \leftarrow \mathbf{x} + \frac{1}{L}\mathbf{s}$

$\mathbf{x} \leftarrow s_{\tau/L}(\mathbf{x})$

Observations.

- If $\tau = 0$, then $s_0(\mathbf{x}) = \mathbf{x}$ and ISTA = Richardson with damping parameter $\frac{1}{L}$ for solving $\mathbf{A}^*\mathbf{A}\mathbf{x} = \mathbf{A}^*\mathbf{b}$.

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Repeat

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$\mathbf{x} \leftarrow \mathbf{x} + \frac{1}{L}\mathbf{s}$

$\mathbf{x} \leftarrow s_{\tau/L}(\mathbf{x})$

Observations.

- It can be proved that, for some modest κ,

$$\rho(\mathbf{x}_k) - \rho(\mathbf{x}^\star) \leq \kappa/k.$$

  Often, ISTA appears to converge slowly (conform upperbound).

- Convergence estimate does not depend on $\lambda_{\min}(\mathbf{A}^*\mathbf{A})$.

Iterative Shrinkage-Thresholdong Algorithm

Find an $L > \lambda_{\max}(\mathbf{A}^*\mathbf{A})$.

ISTA

Select an $\mathbf{x}_0$. $\mathbf{x} = \mathbf{x}_0$

Repeat

$\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}, \quad \mathbf{s} = \mathbf{A}^*\mathbf{r}$

$\mathbf{x} \leftarrow \mathbf{x} + \frac{1}{L}\mathbf{s}$

$\mathbf{x} \leftarrow s_{\tau/L}(\mathbf{x})$

Observations.

- **FastISTA** combines the last two iterates for $\mathcal{O}(1/k^2)$ convergence.
  Combination based on upperbounds for $\rho(\mathbf{x}_k) - \rho(\mathbf{x}^\star)$.

Iterative Shrinkage-Thresholdong Algorithm

Find an $L > \lambda_{\max}(\mathbf{A}^*\mathbf{A})$.

ISTA

Select an $\mathbf{x}_0$. $\mathbf{x} = \mathbf{x}_0$

Repeat

$\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}, \quad \mathbf{s} = \mathbf{A}^*\mathbf{r}$

$\mathbf{x} \leftarrow \mathbf{x} + \frac{1}{L}\mathbf{s}$

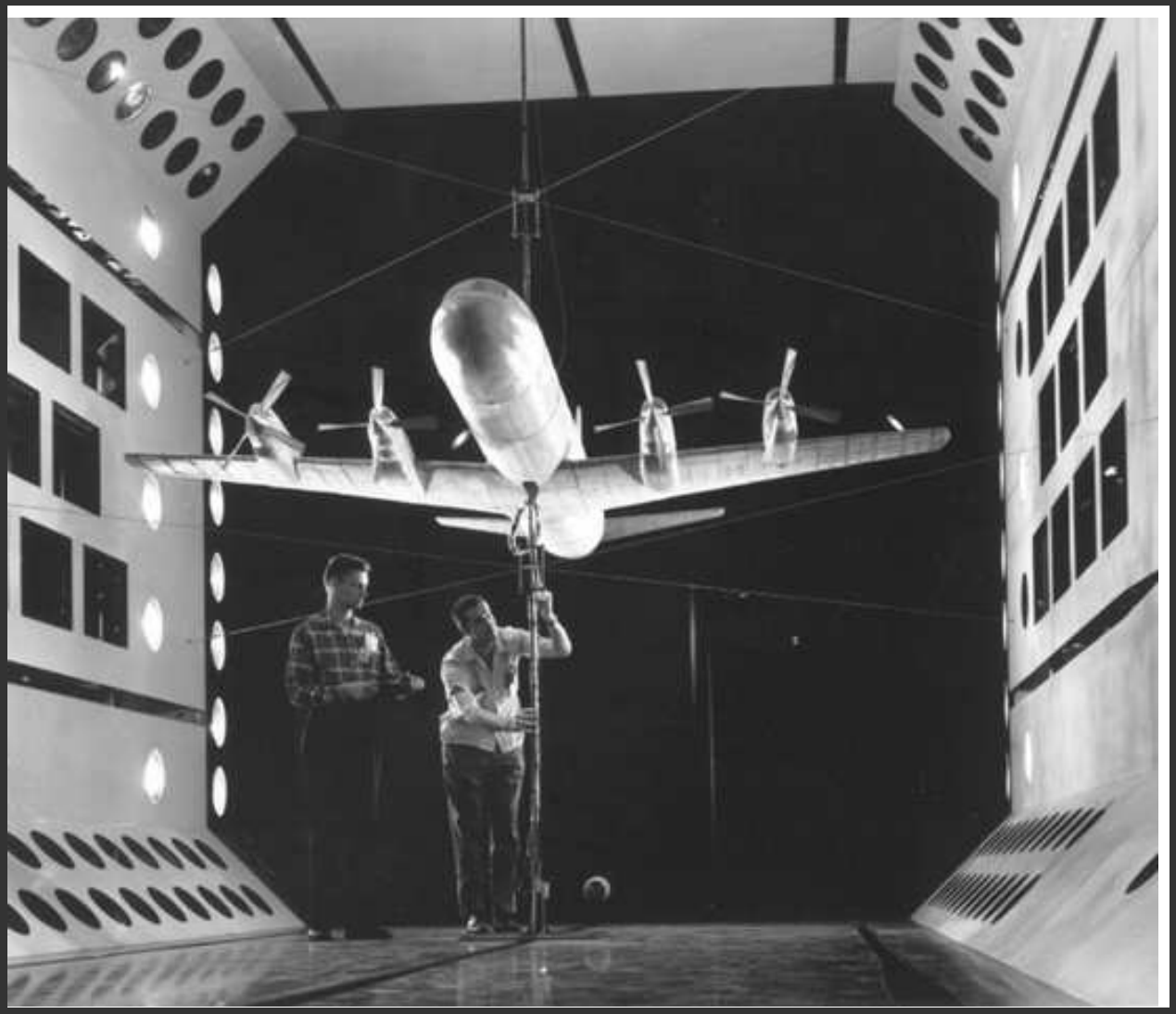
$\mathbf{x} \leftarrow s_{\tau/L}(\mathbf{x})$

Observations.

• Subspace acceleration may not work well: a basis transform of the $\mathbf{x}$ may spoil the sparsity of the vectors.

Program

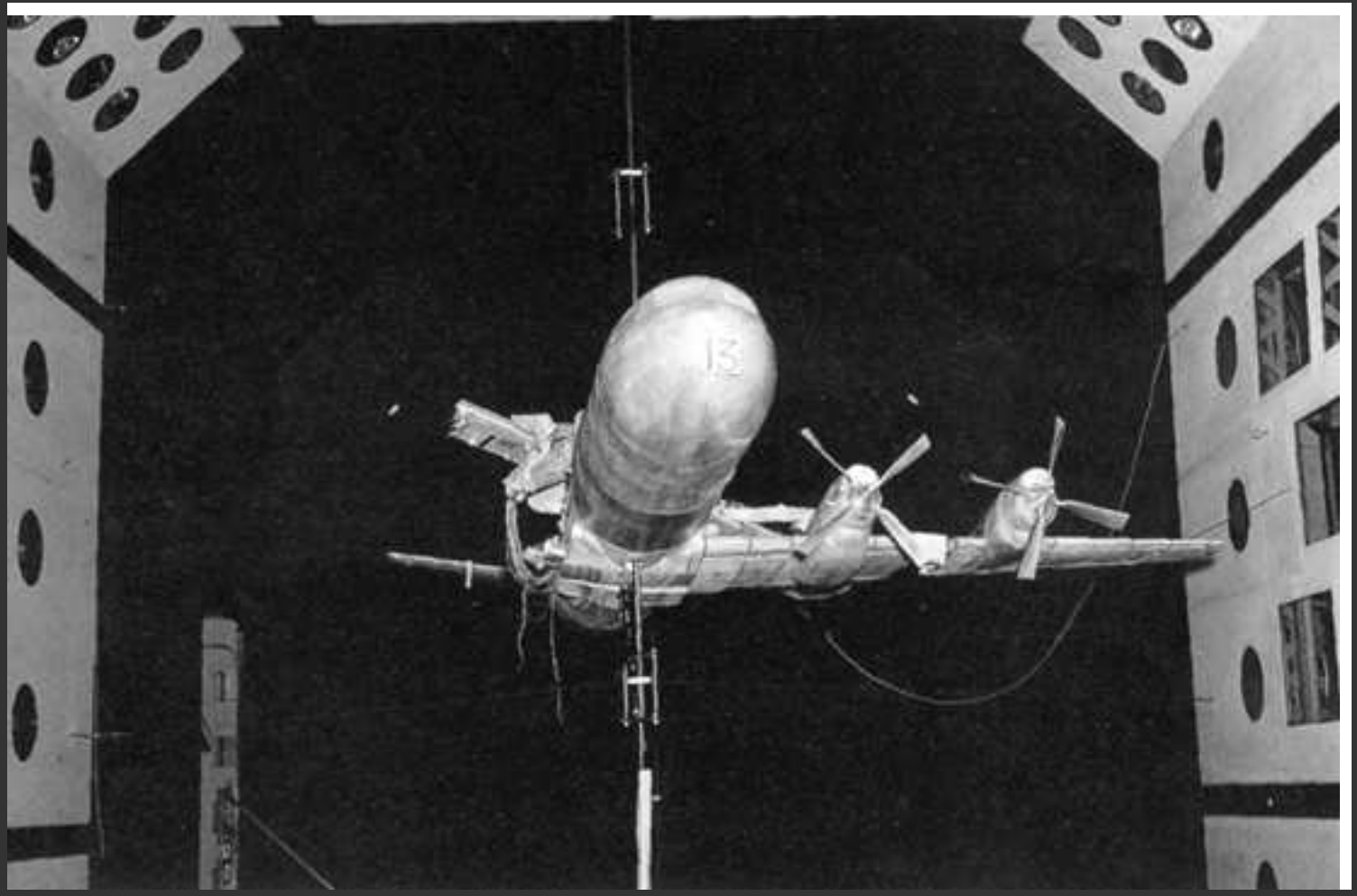
- Multigrid (PDEs)
- Compressed Sensing (MRI)
- Model order reduction (Electronics)
- Relax to the max (QCD)



Airplanes can vibrate

Vibrations are fuelled by turbulence in the airflow

Flutter



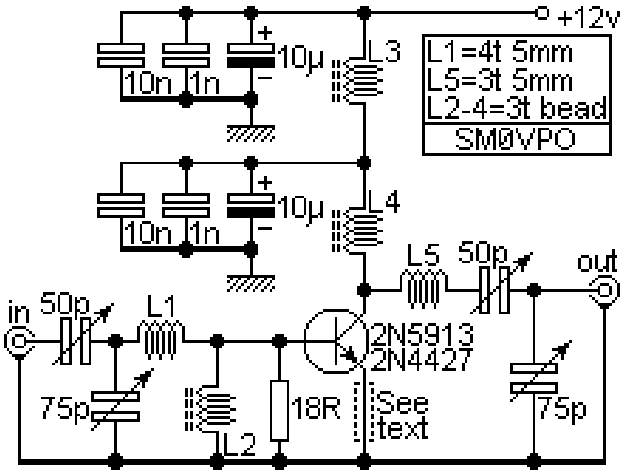
Possibly with a dramatic effect (within a fraction of a second)

Erasmus bridge, Rotterdam, Netherlands

Dynamical properties affected by rain

Effects of a large earthquake in Taiwan

Electrical Circuits.



This system contains also non-linear elements

linearization $\rightsquigarrow$ linear system

Dynamical systems. The (given) quantities $(\mathbf{A}, \mathbf{E}, \mathbf{b}, \mathbf{c}, d)$ define a linear, time invariant, dynamical system:

$$\begin{cases} \mathbf{E}\,\dot{\mathbf{x}}\,(t) &= \mathbf{A}\,\mathbf{x}(t) + \mathbf{b}\,u(t) \\ y(t) &= \mathbf{c}^*\mathbf{x}(t) + d\,u(t) \end{cases}$$

$\mathbf{A}$ (**state space**) and $\mathbf{E}$ are $n \times n$ matrices

n is the number of **states** or **order** of the system.

$\mathbf{E}$ may be non-singular, but $(\mathbf{A}, \mathbf{E})$ is a regular pencil

$s \rightsquigarrow \det(s\mathbf{E} - \mathbf{A})$ not trivial on $\mathbb{C}$.

$\mathbf{b}$ (**input**), $\mathbf{c}$ (**output**) n-vectors,

$d \in \mathbb{R}$, $t \rightsquigarrow u(t)$ given real-valued (**control**) function on $\mathbb{R}$.

The function $t \rightsquigarrow y(t)$ is the function of interest:

the **output** of the system.

$$\begin{cases} \mathbf{E}\,\dot{\mathbf{x}}(t) &= \mathbf{A}\,\mathbf{x}(t) + \mathbf{b}\,u(t) \\ y(t) &= \mathbf{c}^*\mathbf{x}(t) + d\,u(t) \end{cases}$$

Examples

Electrical Circuits.

Characteristics.

- In electronic chips: n is huge, $10^4 \sim 10^8$.
- **A**, **E** are sparse, G is not structured.
- Entries of **A** and **E** do *not* vary smoothly, neighboring entries may differ order of magnitudes.

$$\begin{cases} \mathbf{E}\,\dot{\mathbf{x}}(t) &= \mathbf{A}\,\mathbf{x}(t) + \mathbf{b}\,u(t) \\ y(t) &= \mathbf{c}^*\mathbf{x}(t) + d\,u(t) \end{cases}$$

Examples

Power systems.

$$\begin{cases} \mathbf{E}\,\dot{\mathbf{x}}(t) &= \mathbf{A}\,\mathbf{x}(t) + \mathbf{b}\,u(t) \\ y(t) &= \mathbf{c}^*\mathbf{x}(t) + d\,u(t) \end{cases}$$

Examples

Technical constructions.

Structural mechanics $\rightsquigarrow$

set of partial differential equation.

Discretization of the spatial part $\rightsquigarrow$

dynamical system.

Input from forcing acting on certain points,

Interested in the response at certain points (output).

$$\begin{cases} \mathbf{E}\,\dot{\mathbf{x}}(t) &= \mathbf{A}\,\mathbf{x}(t) + \mathbf{b}\,u(t) \\ y(t) &= \mathbf{c}^*\mathbf{x}(t) + d\,u(t) \end{cases}$$

---

b is $n \times 1$, u is real-valued **single input**

c is $n \times 1$, y is real-valued **single outut**:

Single **I**nput **S**ingle **O**utput (SISO) system.

In practice.

b is $n \times m$, u is $\mathbb{R}^m$-valued **multiple input**

c is $n \times p$, y is $\mathbb{R}^p$-valued **multiple outut**:

Multiple **I**nput **M**ultiple **O**utput (MIMO) system.

Non-linear (apply linearization), n in the range $10^4 - 10^8$.

A, **E** are sparse, and (often) unstructured.

$$\begin{cases} \mathbf{E}\,\dot{\mathbf{x}}(t) &= \mathbf{A}\,\mathbf{x}(t) + \mathbf{b}\,u(t) \\ y(t) &= \mathbf{c}^*\mathbf{x}(t) + d\,u(t) \end{cases}$$

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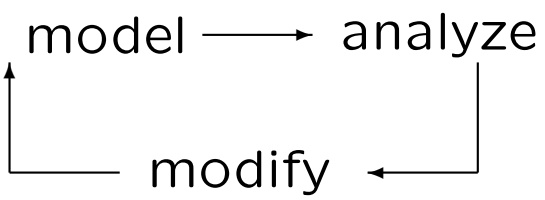
Design.



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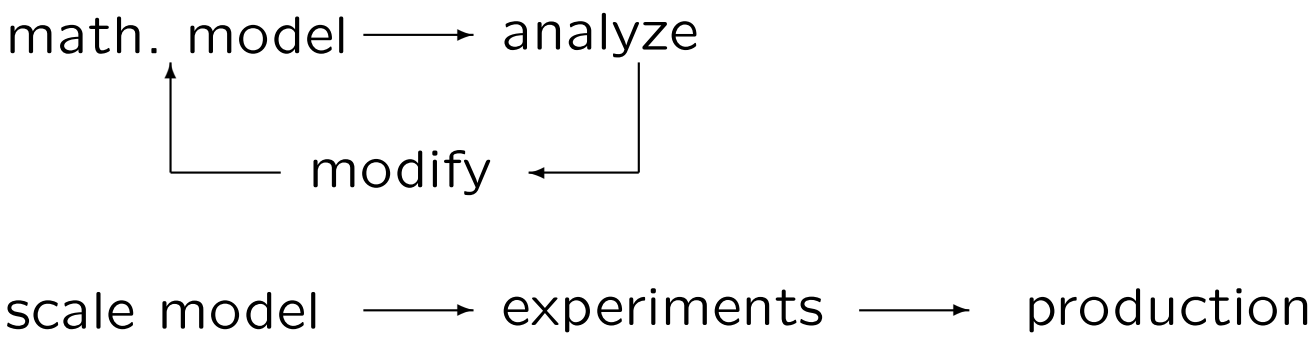

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Transfer function

Analysis strategy. Apply Laplace transform:

for $s \in \mathbb{C}$, consider $u(t) \equiv e^{st}$ $(t \in \mathbb{R})$

then $\mathbf{x}(t) = (s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b}\,e^{st}$

and $y(t) = \left[\mathbf{c}^*(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b} + d\right] e^{st}$

$$\boxed{H(s) \equiv \mathbf{c}^*(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b} + d}$$

is the **transfer function** of the system.

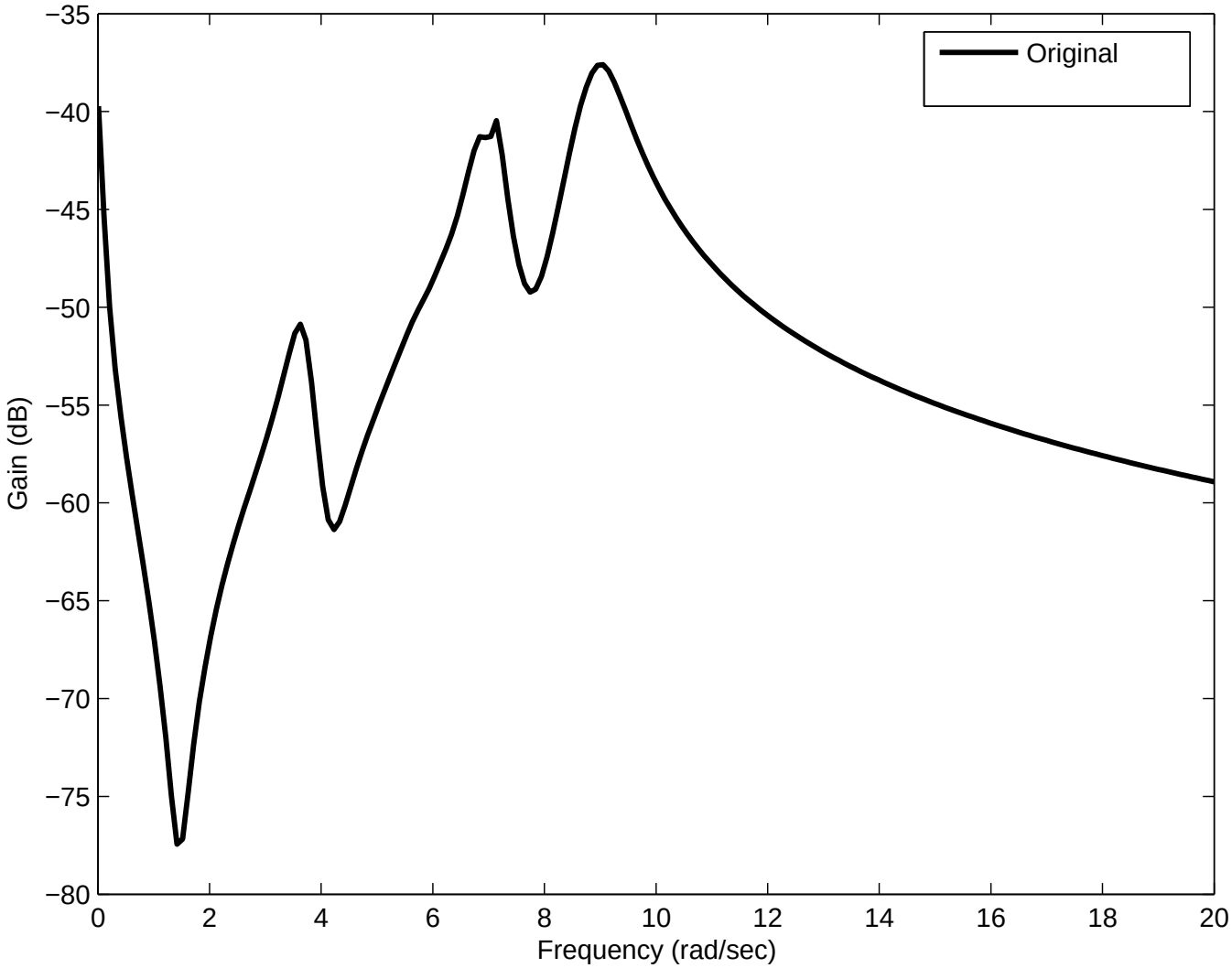
$$H(s) \equiv \mathbf{c}^*(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b} + d$$

The transfer function describes

how the system responses at the output

to an harmonic oscillation with frequency ω if $s = 2\pi i\omega$.

New England test system [... 96]



Bode plot: $\omega \rightsquigarrow |H(2\pi i\omega)|$ on decibel scale.

$n = 66$ (Solid line —).

$$H(s) \equiv \mathbf{c}^*(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b} + d$$

The transfer function describes

how the system responses at the output

to an harmonic oscillation with frequency ω if $s = 2\pi i\omega$.

In a design stage,
depending on the application, oscillations with frequencies

in a certain range have to "damped"
(to avoid flutter, for earthquake resistancy,. . .)

in other ranges have to be "amplified"
(radio receivers, amplifiers, equalizers,. . .)

$$H(s) \equiv \mathbf{c}^*(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b} + d$$

The transfer function describes

how the system responses at the output

to an harmonic oscillation with frequency ω if $s = 2\pi i\omega$.

Computational obstacles.

- n large
- H needed for a wide range of ω (i.e., $s = 2\pi i\omega \in i\mathbb{R}$),
- preconditioners are hard to include
(preconditioner for $\mathbf{A}$ is not a preconditioner for $\mathbf{A} - s\mathbf{E}$),
- solutions required for a number of systems
(in a design stage).

$$H(s) \equiv \mathbf{c}^*(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b} + d$$

The transfer function describes

how the system responses at the output

to an harmonic oscillation with frequency ω if $s = 2\pi i\omega$.

Computational obstacles.

- n large
- H needed for a wide range of ω (i.e., $s = 2\pi i\omega \in i\mathbb{R}$),
- preconditioners are hard to include

(preconditioner for $\mathbf{A}$ is not a preconditioner for $\mathbf{A} - s\mathbf{E}$),

- solutions required for a number of systems

(when a non-linear system is to be analyzed).

Model Order Reduction

Find a kth order system $(\widetilde{A}, \widetilde{E}, \widetilde{b}, \widetilde{c}, d)$ with $k \ll n$ such that

- $\|y(t) - \widetilde{y}(t)\|$ 'small' all u
  (2-norm, Hankel-norm,. . .)
- preservation of (physical and numerical) properties
  (as, stability, passivity,. . .)
- computationally efficient and stable
- cheap measurement for the error
  (when constructing reduced system)

- preserve structure (from 2nd order system)
- realizable
- fit in existing simulation software

Approaches

MOR

- Balanced truncation,
  Hankel norm appr.
- Padé approximation,
  moment matching
- Modal approximation

Eigenvalue computation

- QZ (dense systems)
  (n not large)
- Bi-Lanczos & Arnoldi
- (Jacobi–)Davidson

Approaches

MOR

- Balanced truncation,
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  moment matching
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For ease of explanation, in the remainder $\mathbf{E} = \mathbf{I}$

Approaches

MOR

- Balanced truncation, Hankel norm appr.
- Padé approximation, moment matching
- Modal approximation

Eigenvalue computation

- QZ (dense systems) (n not large)
- Bi-Lanczos & Arnoldi
- (Jacobi–)Davidson

Find $n \times k$ matrices $\mathbf{V}_k$, $\mathbf{W}_k$ such that $\mathbf{W}_k^* \mathbf{V}_k = I_k$.

Project the system

$$\widetilde{A} \equiv \mathbf{W}_k^* \mathbf{A} \mathbf{V}_k, \quad \widetilde{b} \equiv \mathbf{W}_k^* \mathbf{b}, \quad \widetilde{c} \equiv \mathbf{V}_k^* \mathbf{c}$$

Approaches

MOR

- Balanced truncation, Hankel norm appr.
- Padé approximation, moment matching
- Modal approximation

Eigenvalue computation

- QZ (dense systems) (n not large)
- Bi-Lanczos & Arnoldi
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Project the system

$$\widetilde{A} \equiv \mathbf{W}_k^* \mathbf{A} \mathbf{V}_k, \quad \widetilde{b} \equiv \mathbf{W}_k^* \mathbf{b}, \quad \widetilde{c} \equiv \mathbf{V}_k^* \mathbf{c}$$

Note that $\mathbf{W}_k^* (\mathbf{A} - \sigma \mathbf{I}) \mathbf{V}_k = \widetilde{A} - \sigma I_k$.

If $(\widetilde{A} - \sigma I_k) y = \widetilde{b}$ and $\mathbf{x}_k \equiv \mathbf{V}_k y \quad \Rightarrow \quad (\mathbf{A} - \sigma \mathbf{I}) \mathbf{x}_k \approx \mathbf{b}$ and
$\mathbf{c}^* (\mathbf{A} - \sigma \mathbf{I})^{-1} \mathbf{b} \approx \mathbf{c}^* \mathbf{x}_k = \mathbf{c}^* \mathbf{V}_k y = \widetilde{c}^* y = \widetilde{c}^* (\widetilde{A} - \sigma I_k)^{-1} \widetilde{b}$

Approaches

MOR

- Balanced truncation, Hankel norm appr.
- Padé approximation, **moment matching**
- Modal approximation

Eigenvalue computation

- QZ (dense systems) (n not large)
- **Bi-Lanczos & Arnoldi**
- (Jacobi–)Davidson

$$H(s) = \mathbf{c}^*(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b} + d$$

$|s|$ large

$(s\mathbf{I}-\mathbf{A})^{-1} = s^{-1}(\mathbf{I}-s^{-1}\mathbf{A})^{-1} = s^{-1}(\mathbf{I}+s^{-1}\mathbf{A}+s^{-2}\mathbf{A}^2+\ldots)$:

Take

$$\text{span}(\mathbf{V}_k) \equiv \mathcal{K}_k(\mathbf{A},\mathbf{b}) = \text{span}(\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^{k-1}\mathbf{b})$$

$\mathbf{W}_k = \mathbf{V}_k$ (Arnoldi) or, $\text{span}(\mathbf{W}_k) \equiv \mathcal{K}_k(\mathbf{A}^*, \mathbf{c})$ (bi-Lanczos)

Approaches

MOR

- Balanced truncation, Hankel norm appr.
- Padé approximation, **moment matching**
- Modal approximation

Eigenvalue computation

- QZ (dense systems) (n not large)
- **Bi-Lanczos & Arnoldi**
- (Jacobi–)Davidson

$$H(s) = \mathbf{c}^*(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b} + d$$

$|s|$ small

$(s\mathbf{I} - \mathbf{A})^{-1} = (s\mathbf{A}^{-1} - \mathbf{I})^{-1}\mathbf{A}^{-1} = -(\mathbf{I} + s\mathbf{A}^{-1} + \ldots)\mathbf{A}^{-1}$:

Take $\quad \text{span}(\mathbf{V}_k) \equiv \mathcal{K}_k(\mathbf{A}^{-1}, \mathbf{A}^{-1}\mathbf{b})$

$\mathbf{W}_k = \mathbf{V}_k$ or, $\quad \text{span}(\mathbf{W}_k) \equiv \mathcal{K}_k(\mathbf{A}^{-*}, \mathbf{c})$

Approaches

MOR

- Balanced truncation,
  Hankel norm appr.
- Padé approximation,
  moment matching
- Modal approximation

Eigenvalue computation

- QZ (dense systems)
  (n not large)
- **Bi-Lanczos & Arnoldi**
- (Jacobi–)Davidson

$$H(s) = \mathbf{c}^*(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b} + d$$

$|s - s_0|$ small

$$(s\mathbf{I} - \mathbf{A})^{-1} = ((s - s_0)\mathbf{I} + (s_0\mathbf{I} - \mathbf{A}))^{-1} =$$
$$((s - s_0)(s_0\mathbf{I} - \mathbf{A})^{-1} + \mathbf{I})^{-1}(s_0\mathbf{I} - \mathbf{A})^{-1}$$

Approaches

MOR

- Balanced truncation,
  Hankel norm appr.
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- Modal approximation

Eigenvalue computation

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  (n not large)
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- (Jacobi–)Davidson

Arnoldi

- $\mathbf{V}_k$ orthonormal, spans $\mathcal{K}_k((s_0\mathbf{I}-\mathbf{A})^{-1},(s_0\mathbf{I}-\mathbf{A})^{-1}\mathbf{b})$.
- Take $\mathbf{W}_k = \mathbf{V}_k$. Project onto $\mathbf{V}_k$.

Variants: block versions,

Rational **K**rylov **S**equence,

two-sided versions **bi-Lanczos**

...

Approaches

MOR

- Balanced truncation, Hankel norm appr.
- Padé approximation, moment matching
- **Modal approximation**

Eigenvalue computation

- QZ (dense systems) (n not large)
- Bi-Lanczos & Arnoldi
- **(Jacobi–)Davidson**

Modal approximations.

Compute $\mathbf{V}_k$, $\mathbf{W}_k$ $k \times n$ matrices with columns appropriate right, left, respectively eigenvectors $\mathbf{A}$,.

$$H(s) = \mathbf{c}^*(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b} + d$$

Dominant poles

λ is **pole** of H if $\lim_{s\to\lambda} |H(s)| = \infty$.

Poles are eigenvalues of $\mathbf{A}$: for non-zero $\mathbf{v}_i$, $\mathbf{w}_i$

$$\mathbf{A}\mathbf{v}_i = \lambda_i \mathbf{v}_i \qquad \text{right eigenvectors}$$
$$\mathbf{w}_i^*\mathbf{A} = \lambda_i \mathbf{w}_i^* \qquad \text{left eigenvectors}$$

Select $(\mathbf{v}_i, \mathbf{w}_i, \lambda_i)$ such that

- $\lambda_i \neq \lambda_j \quad (i \neq j)$
- $\mathbf{b} = \sum \beta_i \mathbf{v}_i, \qquad \mathbf{c} = \sum \gamma_i \mathbf{w}_i$
- scaled such that $\mathbf{w}_i^*\mathbf{v}_i = 1$ if $\mathbf{w}_i^*\mathbf{v}_i \neq 0$.

$$H(s) = \mathbf{c}^*(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b} + d$$

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$$H(s) = \sum_{i=1}^{n'} \frac{R_i}{s - \lambda_i} + d, \qquad R_i = (\mathbf{c}^*\mathbf{v}_i)(\mathbf{w}_i^*\mathbf{b})$$

R_i are the **residuals**. **Note.** $R_i = 0$ if $\mathbf{w}_i^*\mathbf{v}_i = 0$.

Dominant poles

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A pole λ_i is '**dominant**' if $\dfrac{|R_i|}{|\mathrm{Re}(\lambda_i)|}$ is large.

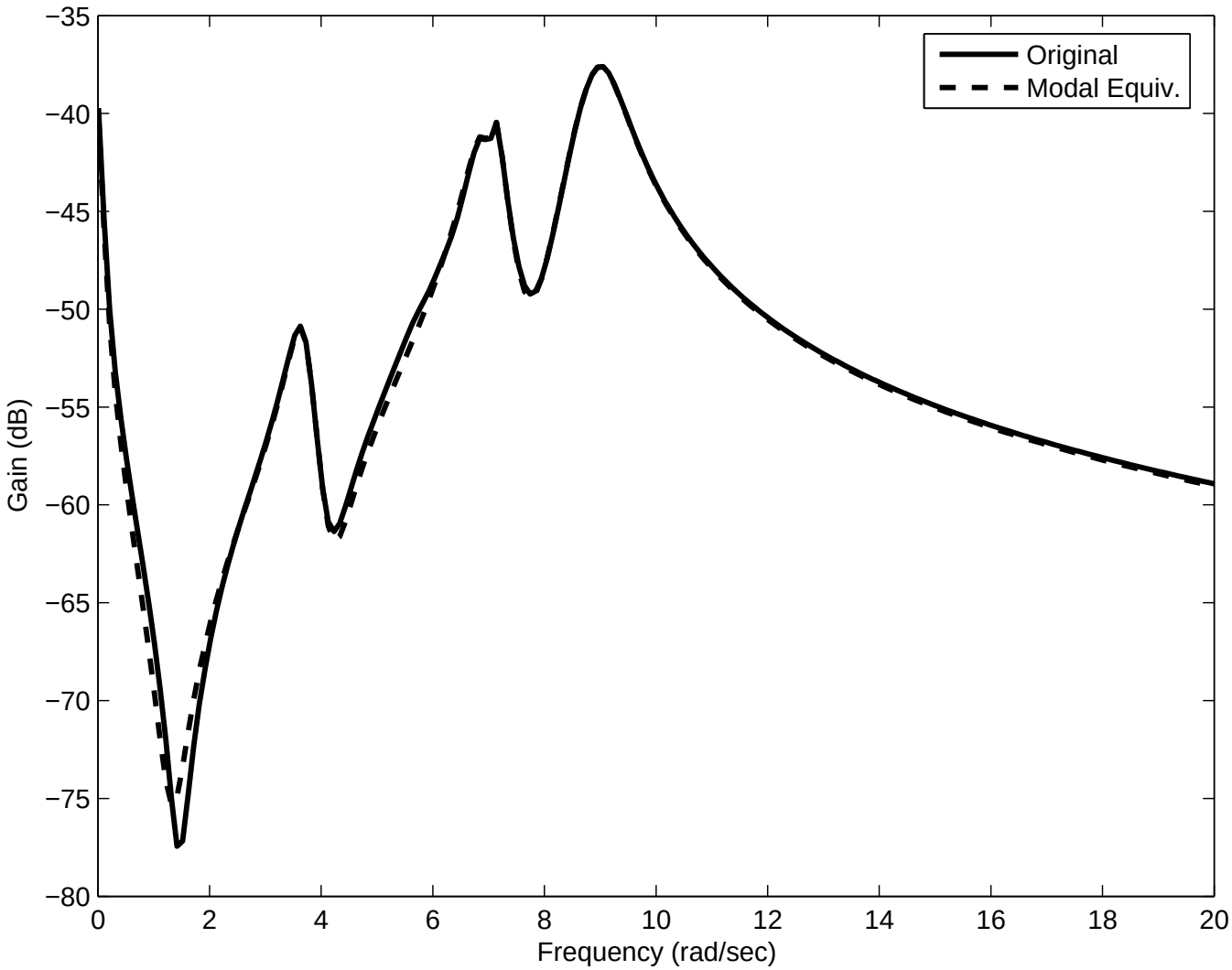
(determine the high peaks in the Bode plot.)

Practice.

dominant poles $\ll$ # poles $<$ # eigenvalues $\leq n$

Approach. Project onto (and work in) the spaces spanned by the eigenvectors associated with dominant poles: **b** onto the space spanned by appropriate right eigenvectors, **c** onto the space of appropriate left eigenvectors.

New England test system



Bode plot: $\omega \rightsquigarrow |H(2\pi i\omega)|$ on decibel scale.

$n = 66$ (Solid line —).

Modal approximation of order $k = 11$ (dashed $- -$).

Practice.

dominant poles $\ll$ # poles $<$ # eigenvalues $\leq n$

Approach. Project onto (and work in) the spaces spanned by the eigenvectors associated with dominant poles: **b** onto the space spanned by appropriate right eigenvectors, **c** onto the space of appropriate left eigenvectors.

How to compute the dominant poles and associated eigenvectors?

$$H(s) = \sum_{i=1}^{n'} \frac{R_i}{s - \lambda_i} + d, \qquad R_i = (\mathbf{c}^* \mathbf{v}_i)(\mathbf{w}_i^* \mathbf{b})$$

[Aguirre 93, Varga 95, Green Limebeer 95]

A pole λ_i is '**dominant**' if $\dfrac{|R_i|}{|\mathrm{Re}(\lambda_i)|}$ is large.

[Hamdan Nayfeh 89]

In our convergence **analysis**:

A pole λ_i is **dominant** if $|R_i| > |R_j|$ for all j.

Definition. (two-sided) **Rayleigh quotient**

$$\rho(\mathbf{x}, \mathbf{y}) = \rho(\mathbf{A}, \mathbf{x}, \mathbf{y}) \equiv \frac{\mathbf{y}^* \mathbf{A} \mathbf{x}}{\mathbf{y}^* \mathbf{x}} \quad \text{provided} \quad \mathbf{y}^* \mathbf{x} \neq 0$$

Note that $\mathbf{y}^* \mathbf{x}$ can be 0

$$H(s) = \sum_{i=1}^{n'} \frac{R_i}{s - \lambda_i} + d, \qquad R_i = (\mathbf{c}^* \mathbf{v}_i)(\mathbf{w}_i^* \mathbf{b})$$

[Aguirre 93, Varga 95, Green Limebeer 95]

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$$\rho(\mathbf{x}) \equiv \rho(\mathbf{x}, \mathbf{x})$$

Dominant Pole Algorithm

Select $s_0 \in \mathbb{C}$ and $tol > 0$.

Set $\nu = 1$, $s = s_0$

While $\nu > tol$ repeat

$\quad$ Solve $(s\mathbf{I} - \mathbf{A})\mathbf{x} = \mathbf{b}$ for $\mathbf{x}$

$\quad$ Solve $(s\mathbf{I} - \mathbf{A})^*\mathbf{y} = \mathbf{c}$ for $\mathbf{y}$

$\quad$ $s = \dfrac{\mathbf{y}^*\mathbf{A}\mathbf{x}}{\mathbf{y}^*\mathbf{x}}$

$\quad$ $\nu = \max(\|\mathbf{A}\mathbf{x} - s\mathbf{x}\|_2, \|\mathbf{y}^*\mathbf{A} - s\mathbf{y}^*\|_2)$

end while

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$\quad$ $s = \dfrac{\mathbf{y}^*\mathbf{A}\mathbf{x}}{\mathbf{y}^*\mathbf{x}}$

$\quad$ $\nu = \max(\|\mathbf{A}\mathbf{x} - s\mathbf{x}\|_2, \|\mathbf{y}^*\mathbf{A} - s\mathbf{y}^*\|_2)$

end while

Note. For the moment, assume exact LU-decomposition $s\mathbf{I} - \mathbf{A}$ is feasible.

DPA is Newton $\Rightarrow$

if $s_k \to \lambda_i$, then convergence is quadratic

Theorem. $\mathbf{A}\mathbf{v} = \mathbf{v}\lambda$ and $\mathbf{w}^*\mathbf{A} = \lambda\mathbf{w}^*$, $\mathbf{w}^*\mathbf{v} = 1$.

Apply DPA. Then

$$\mathbf{x}_k \to \mathbf{v} \quad \Leftrightarrow \quad \mathbf{y}_k \to \mathbf{w} \quad \Leftrightarrow \quad s_{k+1} = \rho(\mathbf{x}_k, \mathbf{y}_k) \to \lambda.$$

If convergence, then quadratic convergence:

$$\|\mathbf{v} - \mathbf{x}_{k+1}\| \leq \kappa \, \|\mathbf{v} - \mathbf{x}_k\|_2 \, \|\mathbf{w} - \mathbf{y}_k\|_2$$

$$\|\mathbf{w} - \mathbf{y}_{k+1}\| \leq \kappa \, \|\mathbf{v} - \mathbf{x}_k\|_2 \, \|\mathbf{w} - \mathbf{y}_k\|_2$$

[Ostrowski 59, Parlett 74]

Two-sided Rayleigh quotient iteration:

$\mathbf{x}$ and $\mathbf{y}$ right, left, respectively, eigenvector approximations

use, not only

the best available eigenvalue approximation $s \equiv \rho(\mathbf{x}, \mathbf{y})$

but also the best available eigenvector approximation

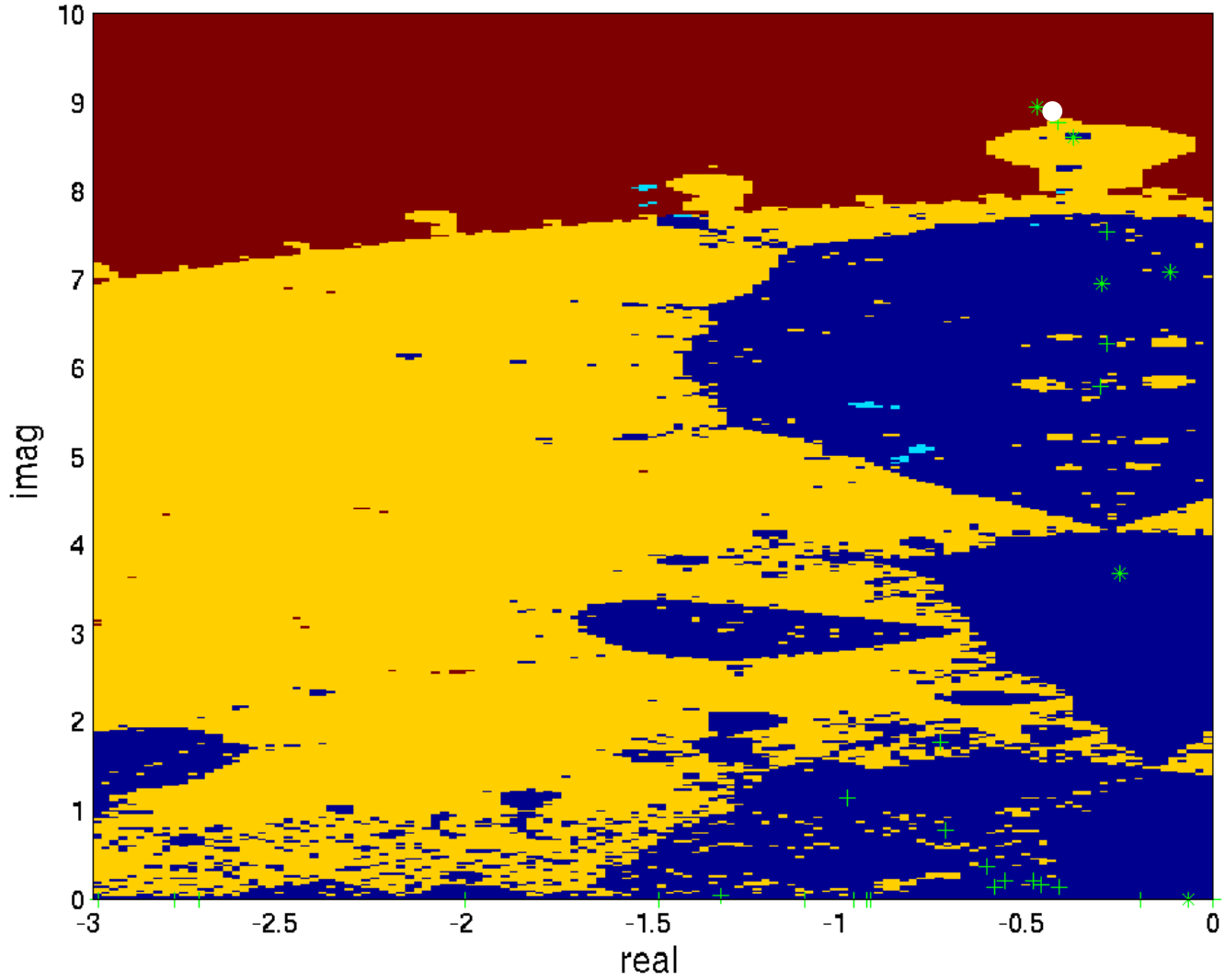
$$\mathbf{x} \leftarrow (s\mathbf{I} - \mathbf{A})^{-1}\mathbf{x} \quad \text{and} \quad \mathbf{y}^* \leftarrow \mathbf{y}^*(s\mathbf{I} - \mathbf{A})^{-1},$$

$$s = \frac{\mathbf{y}^*\mathbf{A}\mathbf{x}}{\mathbf{y}^*\mathbf{x}}$$

[Ostrowski 59, Parlett 74]

Theorem. Cubic convergence.

Part of the complex plane



Dominant pole $-0.456 \pm 8.96i$ (white •).
DPA converges for s_0 in red and yellow
RQI converges for s_0 in red and light blue
Dark blue convergence to less dominant poles.

Why is the convergence region of DPA so much bigger than the convergence region of RQI?

Heuristics. Recal $R_i = (\mathbf{c}^*\mathbf{v}_i)(\mathbf{w}_i^*\mathbf{b})$.

DPA keeps using info from $\mathbf{b}$ and $\mathbf{c}$:

$$\mathbf{x} = (s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b}, \quad \mathbf{y}^* = \mathbf{c}^*(s\mathbf{I} - \mathbf{A})^{-1}$$

RQI convergences faster (cubically)

but tends to converge to eigenvalue closest to s_0.

Selecting initial shift s_0

DPA: $s_0 = \dfrac{\mathbf{c}^*\mathbf{A}\mathbf{b}}{\mathbf{c}^*\mathbf{b}}$. Reasonable? What if $\mathbf{c}^*\mathbf{b} = 0$?

RQI: $\mathbf{x}_0 = \mathbf{b}$, $\mathbf{y}_0 = \mathbf{c}$. Reasonable? What if $\mathbf{c}^*\mathbf{b} = 0$?

Recall that **b** represents input, **c** represents output.

Therefore,

Select s_0.

In RQI: $\mathbf{x}_0 = (s_0\mathbf{I} - \mathbf{A})^{-1}\mathbf{b}$, $\mathbf{y}_0^* = \mathbf{c}^*(s_0\mathbf{I} - \mathbf{A})^{-1}$.

We stop if $\nu \leq 10^{-8}$.

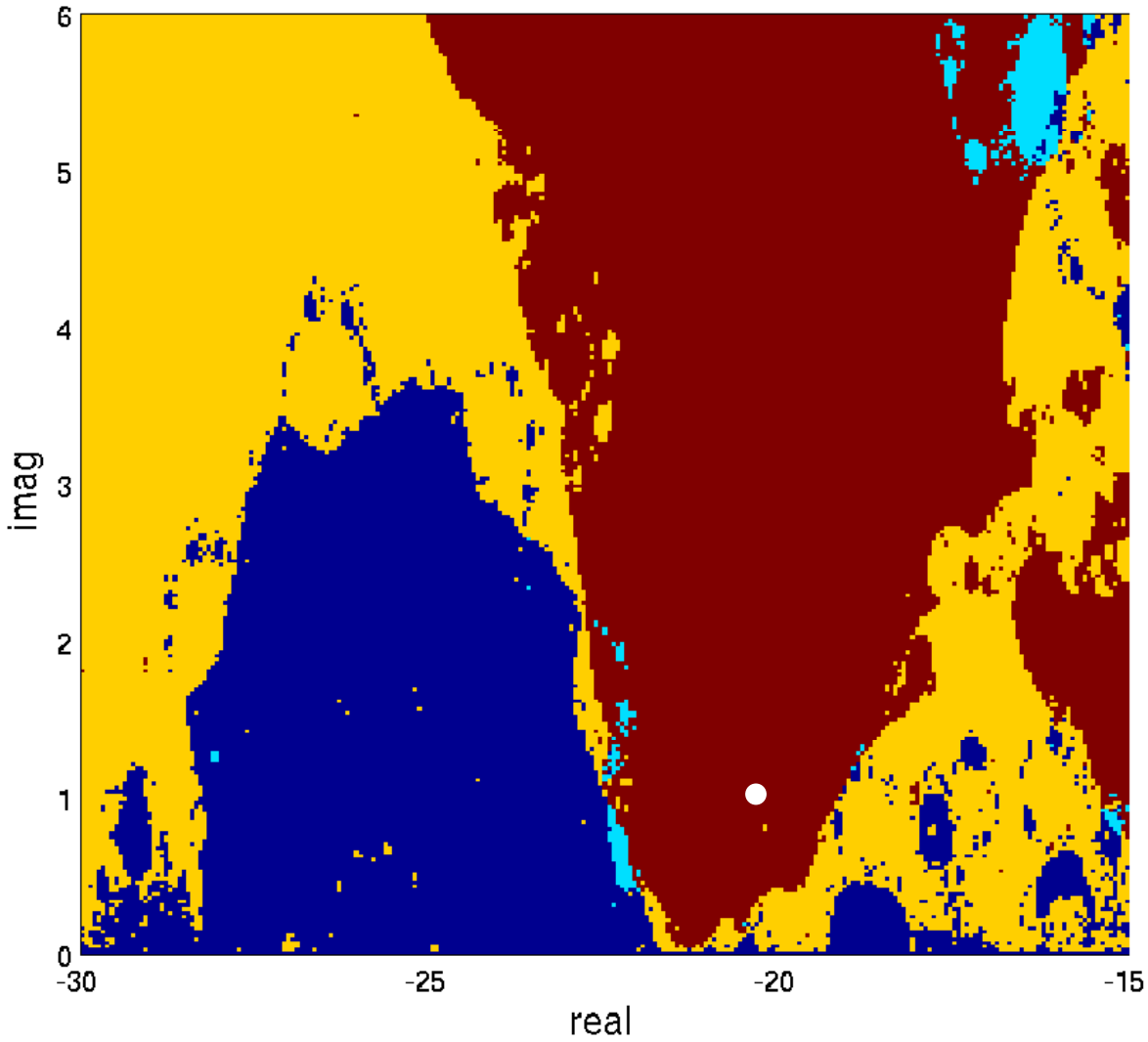
[Rommes Martins 06]

Example. Brazilian Interconnect Power System.

$\mathbf{A}$ and $\mathbf{E}$ are of dimension $n = 13,251$, $\mathbf{E}$ is singular.

Both $\mathbf{b}$ and $\mathbf{c}$ have only one non-zero entry, $\mathbf{c}^*\mathbf{E}\mathbf{b} = 0$.

Part of the complex plane



Average number of steps
DPA: 7.2
RQI: 6.0

In red region
DPA: 6.1
RQI: 5.9

Dominant pole $-20.5 \pm 1.1i$ (white •).
DPA converges for s_0 in red and yellow
RQI converges for s_0 in red and light blue
Dark blue convergence to less dominant poles.

Conclusions

- DPA has better global convergence than RQI to dominant poles for a large class of dynamical systems:

DPA has (much) larger convergence areas for dominant poles than RQI, becoming larger with increasing dominance.

- The local cubic convergence of RQI versus the local quadratic convergence of DPA leads to a small advantage for RQI in iteration steps (typically, 10%–20%)

- The computational costs per step are $\approx$ the same (DPA slightly more efficient).

Program

- Multigrid (PDEs)
- Compressed Sensing (MRI)
- Model order reduction (Electronics)
- Relax to the max (QCD)

Problem

$$\boxed{\mathbf{Ax}=\mathbf{b}}$$

Compute efficiently a $\widetilde{\mathbf{x}}$ with residual accuracy ϵ (i.e., $\|\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}\| \leq \epsilon$)

Properties of the square matrix $\mathbf{A}$:

- The matrix $\mathbf{A}$ is expensive to store (dimension, density)

but

- we have a device that approximates $\mathbf{Au}$ by $\mathcal{A}_\eta(\mathbf{u})$ s.t.

$$\mathcal{A}_\eta(\mathbf{u}) = \mathbf{Au} + \mathbf{f} \quad \text{with} \quad \|\mathbf{f}\| \leq \eta \, \|\mathbf{A}\| \, \|\mathbf{u}\|,$$

η is the relative accuracy of the matrix-vector mult.,

- is more costly for higher 'rel. accuracy' (i.e., smaller η).

$$\mathcal{A}_\eta(\mathbf{u}) = \mathbf{A}\mathbf{u} + \mathbf{f} \quad \text{with} \quad \|\mathbf{f}\| \leq \eta \, \|\mathbf{A}\| \, \|\mathbf{u}\|$$

Computation $\mathcal{A}_\eta(\mathbf{u})$ more costly for smaller η

Examples.

- In floating point arithmetic: $\eta = \mathcal{O}$(rel. machine prec.)
- Schurcomplement systems
- Matrix sign functions

⋮

Schurcomplement system

Fields of applications.

- Domain decomposition [Bouras Fraysse 00, Bouras Fraysse Giraud 00]
- Oceanography [van den Eshof S. van Gijzen 03]
- Optimisation
- CFD
- Electronic circuit simulation

⋮

Schurcomplement system

$$\begin{bmatrix} \mathbf{H} & \mathbf{B}_1^* \\ \mathbf{B}_2 & -\mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{z} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{0} \end{bmatrix}$$

is equivalent to the **Schurcomplement** system (i.e., eliminate $\mathbf{y}$, solve for $\mathbf{z}$, as in Lecture 11):

Schurcomplement

$$\underbrace{\left(\mathbf{C} + \mathbf{B}_2 \mathbf{H}^{-1} \mathbf{B}_1^* \right)}_{\mathbf{A}} \underbrace{\mathbf{z}}_{\mathbf{x}} = \underbrace{\mathbf{B}_2 \mathbf{H}^{-1} \mathbf{g}}_{\mathbf{b}} .$$

To compute $\mathbf{c} = \mathbf{A}\mathbf{u}$ with relative accuracy η, use sufficiently many steps of an iterative meth. to solve $\mathbf{H}\tilde{\mathbf{u}} = \mathbf{B}_1^* \mathbf{u}$

higher accuracy (=smaller η) requires more iterative steps.

Matrix sign functions

Fields of applications.

- Quantum Chromodynamics (QCD)

[Cundy van den Eshof Frommer Krieg Lippert Schäfer 04]

Computational challenge.

- Monte Carlo simulations:

  very high dimensional linear systems are repeatedly solved

  b random, **A** some randomness.

[Neuberger 98]

Lattice QCD and the overlap operator

$$\mathbf{A} = \rho\,\Gamma_5 + \mathrm{sign}(\mathbf{H}), \text{ where } \rho \geq 1,\ \Gamma_5 \equiv \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{bmatrix}$$

Properties H

- $\mathbf{H}$ is explicitly available (coeff. from stochastic process)
- $\mathbf{H}$ is sparse and Hermitian $(\mathbf{H}^* \equiv \bar{\mathbf{H}}^\top = \mathbf{H})$
- $\mathbf{H}$ is high-dimensional $(16^4 \cdot 12 \approx 0.79\,10^6,\ 32^4 \cdot 12 = 12.5\,10^6)$
- $\mathrm{sign}(\mathbf{H}) \equiv \mathbf{V}\,\mathrm{sign}(\Lambda)\,\mathbf{V}^*$, where $\mathbf{H} = \mathbf{V}\Lambda\mathbf{V}^*$, Λ diagonal and $\mathrm{sign}(\lambda) \equiv \lambda/|\lambda|$

Properties A.

- $\Gamma_5\,\mathbf{H} \neq \mathbf{H}\,\Gamma_5$,
- $\mathbf{A}^* = \mathbf{A} \not> \mathbf{0}$,
- No preconditioner for $\mathbf{A}$.

No problem computing $\mathbf{Hu}$. **What about $\mathbf{Au}$?**

Via $\mathrm{sign}(\mathbf{H})\mathbf{u}$? Computing eigensystem $\mathbf{H}$ is not feasable.

[van den Eshof Frommer Lippert Schilling van den Vorst 02]

Computing the sign of a matrix

$\text{sign}(\lambda) = \frac{\lambda}{\sqrt{\lambda^2}}$

$$\text{sign}(\mathbf{H}) = \mathbf{H}(\mathbf{H}^2)^{-\frac{1}{2}} = \mathbf{H} f(\mathbf{H}^2), \quad \text{where} \quad f(\lambda) \equiv 1/\sqrt{\lambda}$$

Determine scalars ω_i, τ_i (explicit solutions are available)

such that $$f(\lambda) \approx \sum_{i=1}^{m} \omega_i \frac{1}{\lambda + \tau_i} \quad \Rightarrow$$

$$\text{sign}(\mathbf{H})\mathbf{u} \approx \sum_{i=0}^{m} \omega_i \mathbf{H} \underbrace{(\mathbf{H}^2 + \tau_i \mathbf{I})^{-1}\mathbf{u}}$$

Solve with CG
(multishift CG)

Computation **Au** to high accuracy is very costly.
Costs are higher if higher accuracy is required.

Approach

- **Use a Krylov subspace method**

only MVs and basic linear algebra operations (AXPYs, DOTs)

- **Relax the MV**: replace $\mathbf{Au}_k$ by $\mathcal{A}_{\eta_k}(\mathbf{u}_k)$
- **Relax to the max,**

i.e., apply a relaxation strategy that selects η_k 'as large as possible' (η_k step dependent) without

  - **disturbing the speed of convergence**
  - **spoiling the residual accuracy (i.e. $\|\mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}\| \lesssim \epsilon$)**

Note. If the MV changes per step

$\Rightarrow$ **not** a Krylov subspace method

Conclusions

- 'Relax to the max' strategy exists.

For optimal profits

- Choose your basis for expansion wisely
- Use internal updates (low quality)
  and external updates (high quality)

Subspace method

Repeat until convergence, i.e., $\|\mathbf{r}_k\| \leq \texttt{tol}$

1) **Expand** the subspace $\mathcal{U}_k = \text{span}(\mathbf{U}_k)$
   with the vector $\mathbf{A}\mathbf{u}_k$. Here, $\mathbf{U}_k \equiv [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_k]$.
   Note. The vector $\mathbf{A}\mathbf{u}_k$ may be modified (orthogonalised against ...) to form $\mathbf{u}_{k+1}$
2) **Extract** some suitable approximate solution $\mathbf{x}_k \in \mathcal{U}_k$

The basis vectors $\mathbf{u}_j$ of $\mathcal{U}_k$ that are being multiplied by $\mathbf{A}$ to expand the search subspace form the **basis for expansion**. The basis vectors $\mathbf{w}_j$ of $\mathcal{U}_k$ that are actually used to update $\mathbf{x}_k$, $\mathbf{x}_k = \sum_{j \leq k} \mathbf{w}_j \alpha_j$, form the **basis for extraction**.

Methods as GMRES use the same basis for expansion and extraction, methods as GCR, CG use different basis.

Extraction strategies (optimal methods)

- **Galerkin**

  $\mathbf{x}_k \in \mathcal{U}_k$ such that $\mathbf{b} - \mathbf{A}\mathbf{x}_k \perp \mathcal{U}_k$

Particular implementations

General **A**:	**FOM**
Symmetric **A**:	**ORTHORES, CG**

Properties: may have many high peaks in convergence curve

- **Minimal residuals**

  $\mathbf{x}_k \in \mathcal{U}_k$ such that $\|\mathbf{b} - \mathbf{A}\mathbf{x}_k\|$ is minimal

Particular implementations

General **A**:	**GMRES, GCR**
Symmetric **A**:	MINRES, CR

Properties: monotonic convergence curve

$$\mathcal{A}_\eta(\mathbf{u}) = \mathbf{A}\mathbf{u} + \mathbf{f} \quad \text{with} \quad \|\mathbf{f}\| \leq \eta \, \|\mathbf{A}\| \, \|\mathbf{u}\|$$

Computation $\mathcal{A}_\eta(\mathbf{u})$ more costly for smaller η

Are highly accurate MVs required?

Question: How to **"relax to the max"**

that is, how to select η 'as large as possible' without

- disturbing the speed of convergence
- spoiling the residual accuracy (i.e. $\|\mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}\| \lesssim \epsilon$)

Analysis strategy

Our analysis is based on estimating the **residual gap**:

$$\text{res.-gap}_k \equiv \Big| \| \underbrace{\mathbf{b} - \mathbf{A}\mathbf{x}_k}_{\text{true residual}} \| - \rho_k \Big|, \quad \text{where} \quad \rho_k = \|\mathbf{r}_k\|_2$$

with $\mathbf{x}_k$ and ρ_k as **computed** by the method.
On convergence (i.e., $\rho_k \leq \epsilon$), the residual gap determines the **residual accuracy**, i.e, the size of $\|\mathbf{b} - \mathbf{A}\mathbf{x}_k\|_2$.

- Computed residual norms ρ_k are available and in many methods the computed residual $\mathbf{r}_k$ as well.
- Computation of true residuals would require additional MVs. Expensive!

We focus on the **accuracy** (residual gap). Strategies that allow high accuracy (i.e., small res. gap) also appear not to hamper convergence (experimental evidence only).

Analysis strategy

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- Computed residual norms ρ_k are available and in many methods the computed residual $\mathbf{r}_k$ as well.
- Computation of true residuals would require additional MVs. Expensive!

Note that

$$| \, \|\mathbf{b} - \mathbf{A}\mathbf{x}_k\|_2 - \rho_k \, | \leq \|(\mathbf{b} - \mathbf{A}\mathbf{x}_k) - \mathbf{r}_k\|_2.$$

Examples. For methods as CG, Bi-CGSTAB,. . . :

```
...
while ...
    ...
    c = Au, compute α
    x ← x + αu
    r ← r − αc
```

In computation: $\mathbf{c} = \mathbf{A}\mathbf{u} + \mathbf{f}$ with $\|\mathbf{f}\| \leq \eta \|\mathbf{A}\| \, \|\mathbf{u}\| \;\; \Rightarrow$

$$\begin{aligned} \text{res.-gap}_k &\leq \sum \|\alpha_j \mathbf{f}_j\| \leq \|\mathbf{A}\| \sum \eta_j \|\alpha_j \mathbf{u}_j\| \\ &\leq \mathcal{C}(\mathbf{A}) \sum \eta_j \|\alpha_j \mathbf{c}_j\| \leq \mathcal{C}(\mathbf{A}) \sum \eta_j (\|\mathbf{r}_j\| + \|\mathbf{r}_{j+1}\|), \end{aligned}$$

where we sum over all $j = 1, \ldots, k$.

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where we sum over all $j = 1, \ldots, k$.

Relaxation strategy. Take $\eta_j = \epsilon / (\|\mathbf{r}_j\| + \|\mathbf{r}_{j+1}\|)$.

Then $\quad \text{res.-gap}_k \leq k\epsilon$.

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where we sum over all $j = 1, \ldots, k$.

Relaxation strategy. Take $\eta_j = \epsilon/(\|\mathbf{r}_j\| + \|\mathbf{r}_{j+1}\|)$.

Then $\text{res.-gap}_k \leq k\epsilon$.

However, when computing $\mathbf{c}_j$, $\mathbf{r}_{j+1}$ is unknown.

Examples. For methods as CG, Bi-CGSTAB,. . . :

```
...
while ...
    ...
    c = Au, compute α
    x ← x + αu
    r ← r − αc
```

In computation: $\mathbf{c} = \mathbf{A}\mathbf{u} + \mathbf{f}$ with $\|\mathbf{f}\| \leq \eta \|\mathbf{A}\| \, \|\mathbf{u}\| \;\; \Rightarrow$

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where we sum over all $j = 1, \ldots, k$.

Relaxation strategy. Take $\eta_j = \epsilon / \|\mathbf{r}_j\|$.

Then $\text{res.-gap}_k \leq \epsilon \sum \text{peak}_j$, where $\text{peak}_j \equiv 1 + \dfrac{\|\mathbf{r}_{j+1}\|}{\|\mathbf{r}_j\|}$.

If the convergence does not exhibit peaks, is the choice

$$\boxed{\eta_j = \frac{\epsilon}{\rho_j} \quad \text{with} \quad \rho_j = \|\mathbf{r}_j\|}$$

a good relaxation strategy (also for methods that are not of the type as on the previous transparancy)? Here, ρ_j is the norm of the residual as computed by the method.

A simple example. In example

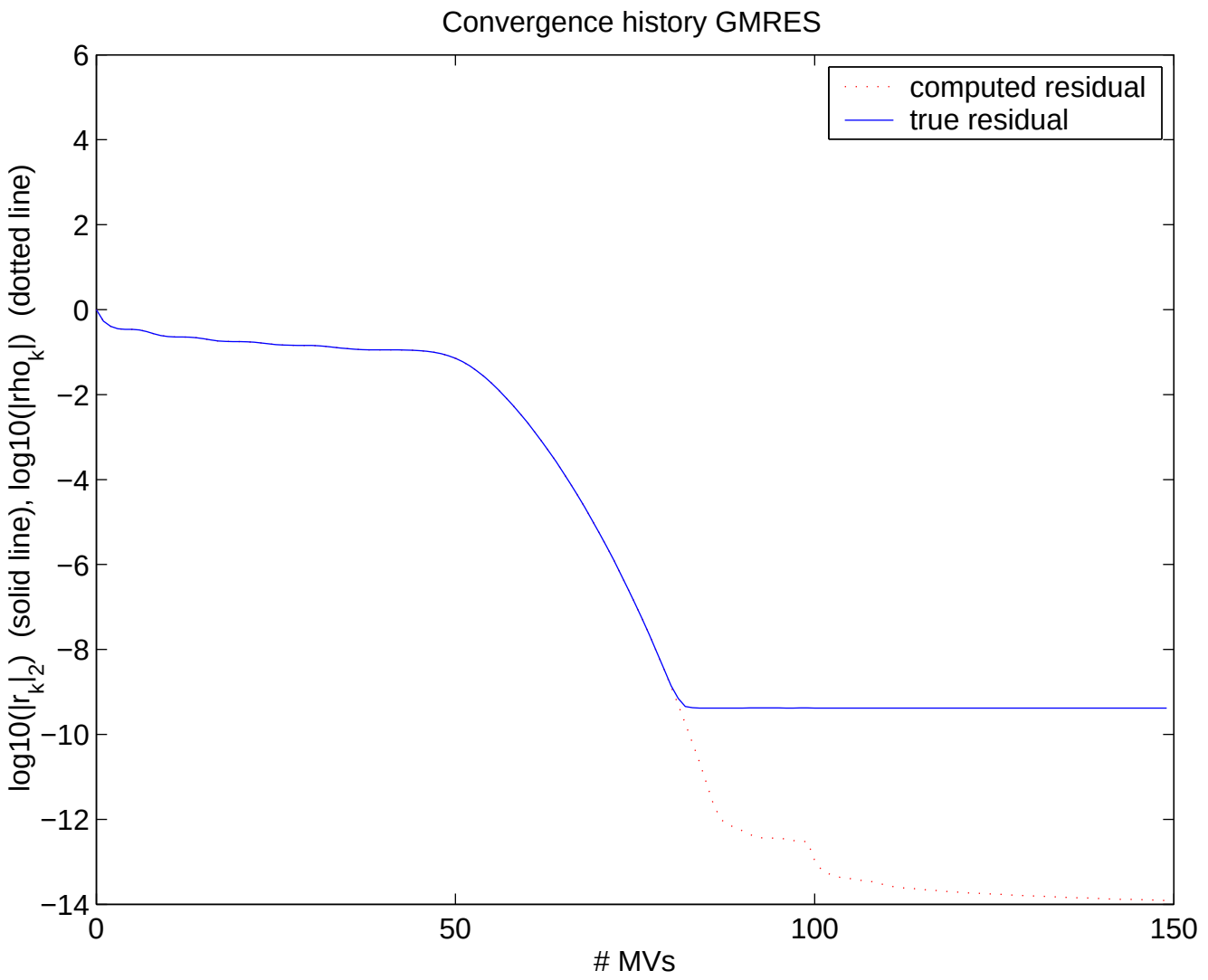
$$\mathbf{A} = \text{diag}(1:3:300) - 13.6156\,\mathbf{I}, \qquad \mathcal{C}(\mathbf{A}) \approx 4.6\,10^2.$$

$\mathcal{A}_\eta(\mathbf{u}) \equiv \mathbf{A}\mathbf{u} + \mathbf{f}$ with $\mathbf{f}$ random such that $\|\mathbf{f}\| = \eta\,\|\mathbf{A}\|\,\|\mathbf{u}\|$

Expansion at step j by $\mathcal{A}_{\eta_j}(\mathbf{v}_j)$ with η_j as above

($\mathbf{v}_j$ is the expansion vector as selected by the method).

GMRES



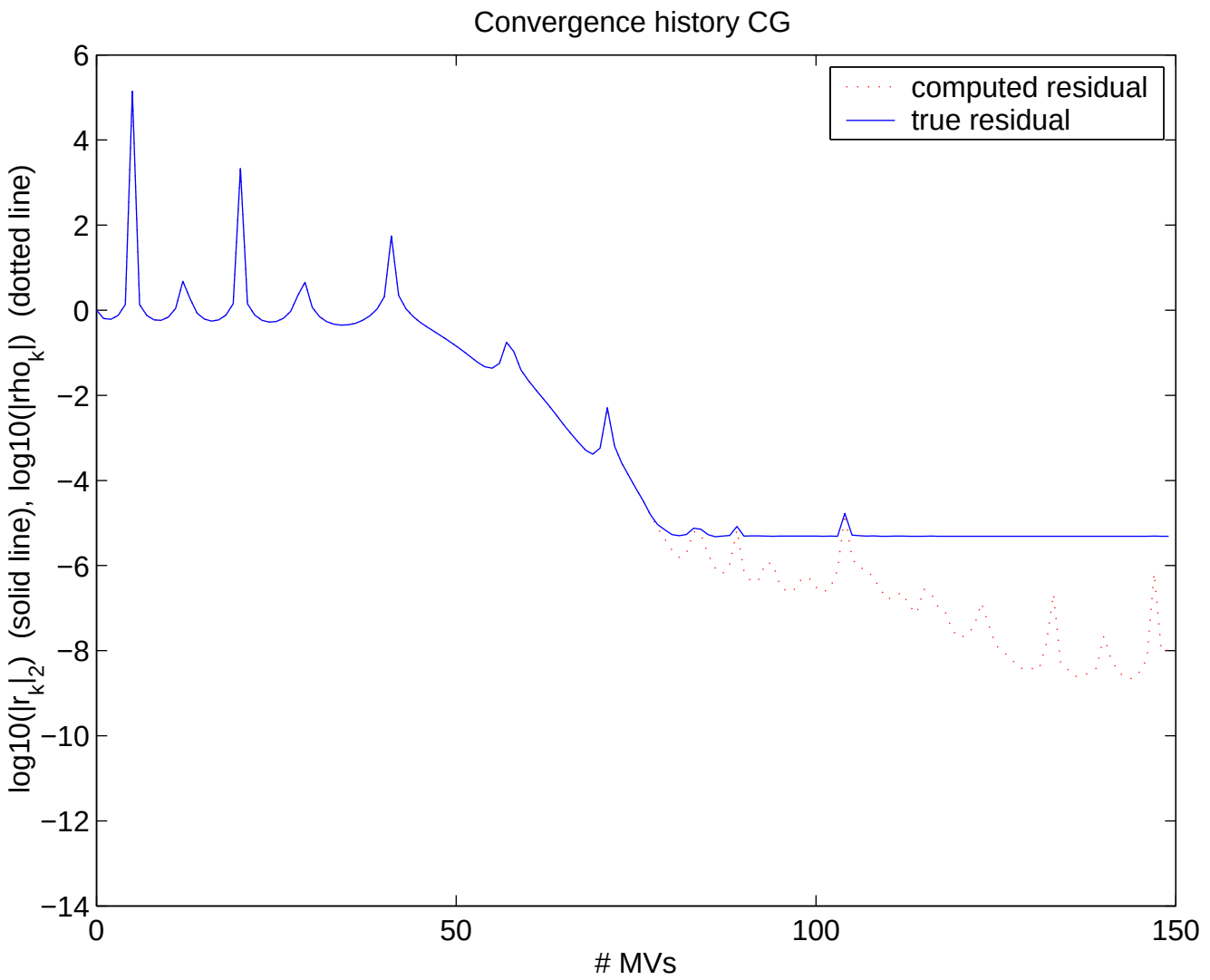
k versus $\|\text{true residual}\|$ —
k versus computed residual norm $\cdots$

$\epsilon = 10^{-12}, \quad \eta_k = \epsilon/\rho_k$

$\mathbf{A} = \text{diag}(1:3:300) - 13.6156\,\mathbf{I}$

$\mathcal{C}(\mathbf{A}) \approx 4.6\,10^2$

CG



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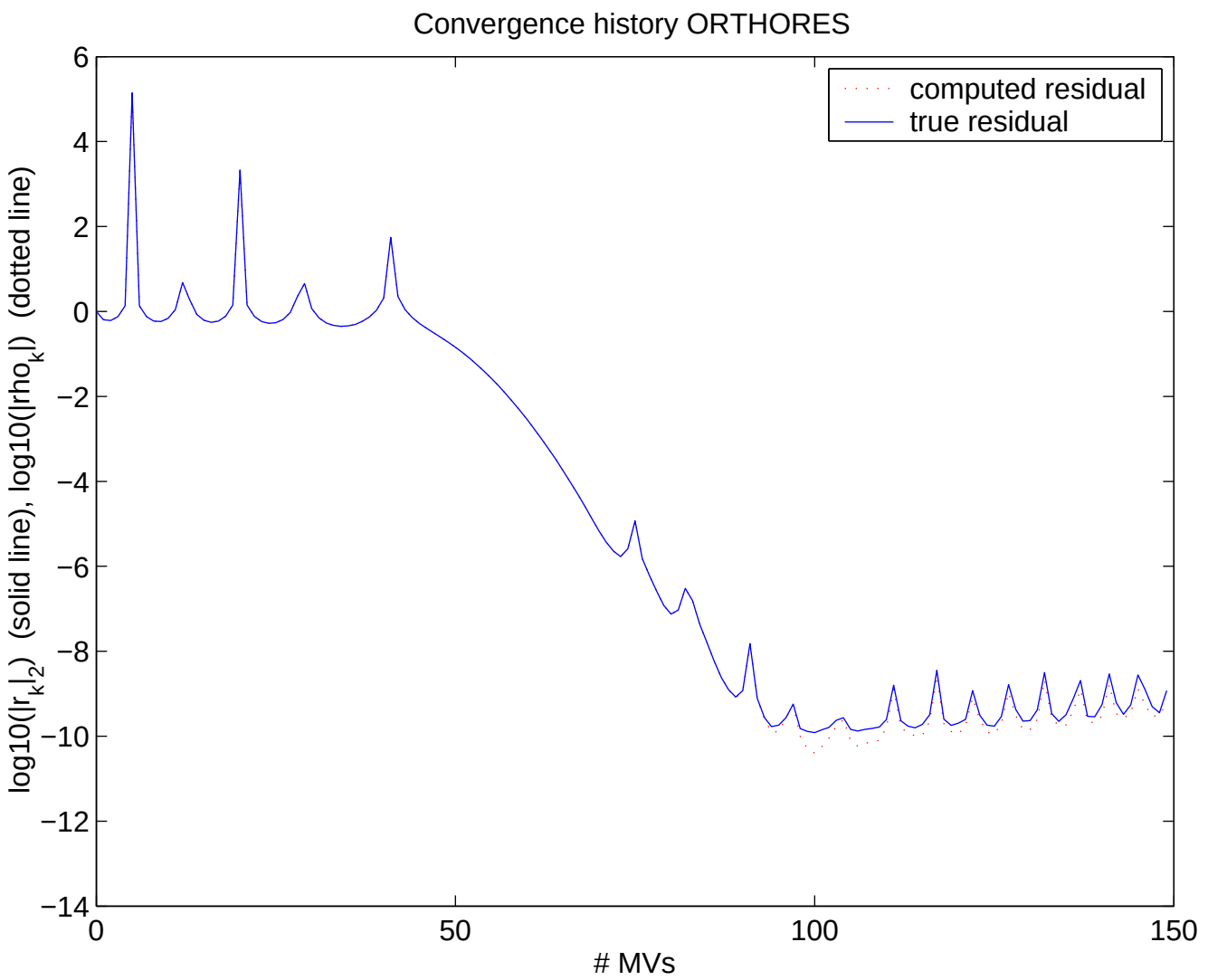
ORTHORES



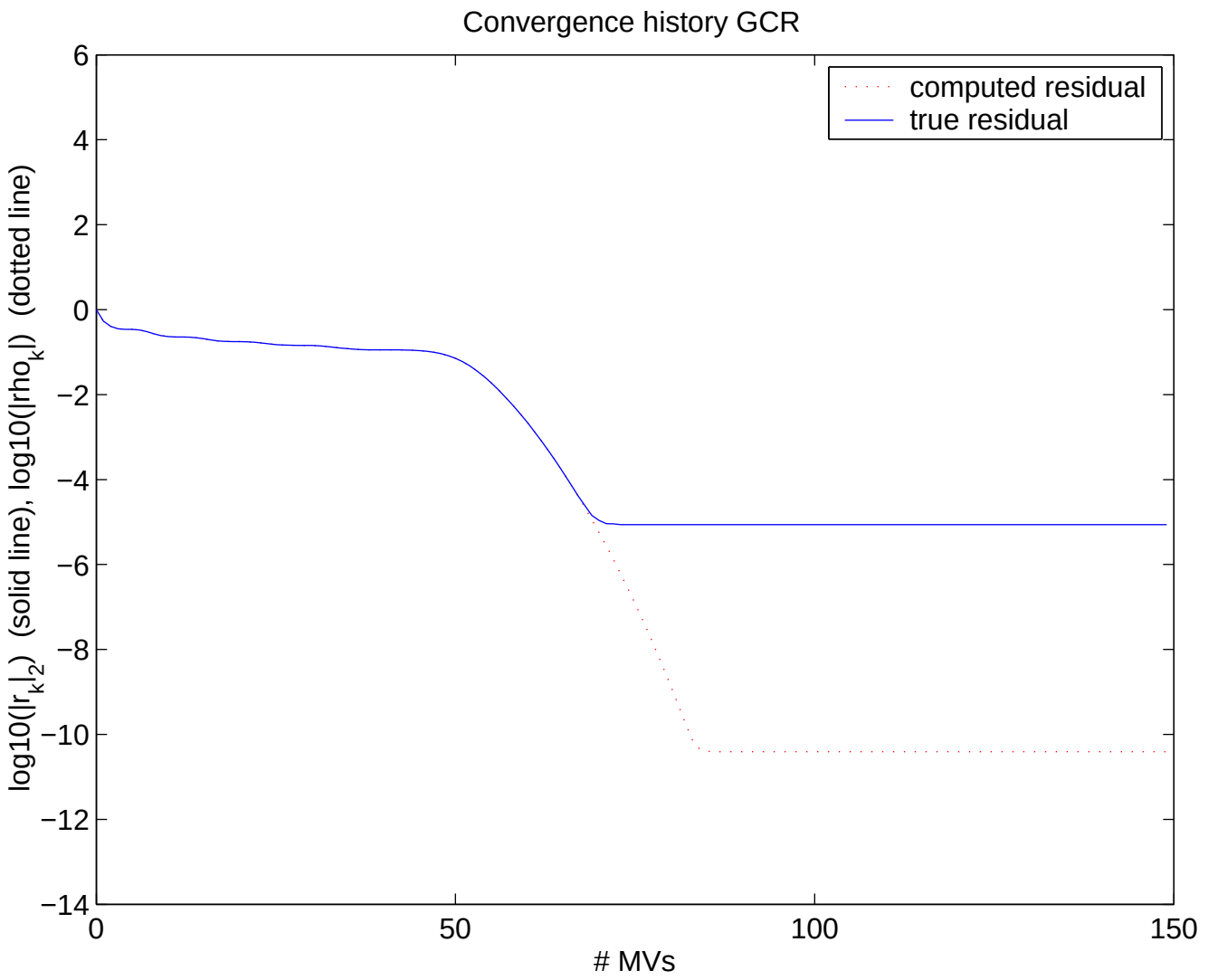
k versus ||true residual|| —
k versus computed residual norm $\cdots$

$\epsilon = 10^{-12}, \quad \eta_k = \epsilon/\rho_k$

$\mathbf{A} = \mathrm{diag}(1:3:300) - 13.6156\,\mathbf{I}$

$\mathcal{C}(\mathbf{A}) \approx 4.6\,10^2$

GCR



k versus $\|\text{true residual}\|$ —
k versus computed residual norm $\cdots$

$\epsilon = 10^{-12}, \quad \eta_k = \epsilon/\rho_k$

$\mathbf{A} = \text{diag}(1:3:300) - 13.6156\,\mathbf{I}$

$\mathcal{C}(\mathbf{A}) \approx 4.6\,10^2$

$$\mathbf{A}\mathbf{U}_k + \mathbf{F}_k \quad \text{with} \quad \|\mathbf{f}_j\| \le \eta_j \|\mathbf{A}\| \|\mathbf{u}_j\|, \quad \mathbf{x}_k = \mathbf{U}_k y_k,$$

$$\|(\mathbf{b} - \mathbf{A}\mathbf{x}_k) - \mathbf{r}_k\| = \|\mathbf{F}_k y_k\|_2 \le \sum_{j \le k} \eta_j \, \|\mathbf{A}\| \, \|\mathbf{u}_j\| \, |e_j^* y_k|$$

$$\mathbf{AU}_k + \mathbf{F}_k \quad \text{with} \quad \|\mathbf{f}_j\| \leq \eta_j \|\mathbf{A}\| \|\mathbf{u}_j\|, \quad \mathbf{x}_k = \mathbf{U}_k y_k,$$

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Observations.

- $\mathbf{x}_k = \mathbf{U}\, y_k = \sum_{j \leq k} \mathbf{u}_j (e_j^* y_k)$:

  $\mathbf{u}_j (e_j^* y_k)$ is the component of $\mathbf{x}_k$ in the direction $\mathbf{u}_j$.

- In all methods:

  $\mathbf{AU}_k + \mathbf{F}_k$ copied from algorithm

  y_k requires some manipulation (without $\mathbf{A}$)

  Analysis assumes that the MV is the only source of errors

$$\mathbf{AU}_k + \mathbf{F}_k \quad \text{with} \quad \|\mathbf{f}_j\| \le \eta_j \|\mathbf{A}\| \|\mathbf{u}_j\|, \quad \mathbf{x}_k = \mathbf{U}_k y_k,$$

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- In all methods:

  $\mathbf{AU}_k + \mathbf{F}_k$ copied from algorithm

  y_k requires some manipulation (without $\mathbf{A}$)

  Analysis assumes that the MV is the only source of errors

- Estimate is 'sharp' (no specific directions in perturbs).
- Growth in η_j ($j \uparrow$) to be compensated by small $\|\mathbf{u}_j (e_j^* y_k)\|$.

$$\mathbf{A}\mathbf{U}_k + \mathbf{F}_k \quad \text{with} \quad \|\mathbf{f}_j\| \leq \eta_j \|\mathbf{A}\| \|\mathbf{u}_j\|, \quad \mathbf{x}_k = \mathbf{U}_k y_k,$$

$$\|(\mathbf{b} - \mathbf{A}\mathbf{x}_k) - \mathbf{r}_k\| = \|\mathbf{F}_k y_k\|_2 \leq \sum_{j \leq k} \eta_j \, \|\mathbf{A}\| \, \|\mathbf{u}_j\| \, |e_j^* y_k|$$

Observations (cont.).

- $\mathbf{x}_k$ depends on the extraction method, not on basis $\mathbf{U}_k$

$$\mathbf{A}\mathbf{U}_k + \mathbf{F}_k \quad \text{with} \quad \|\mathbf{f}_j\| \le \eta_j \|\mathbf{A}\| \|\mathbf{u}_j\|, \quad \mathbf{x}_k = \mathbf{U}_k y_k,$$

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Observations (cont.).

- $\mathbf{x}_k$ depends on the extraction method, not on basis $\mathbf{U}_k$

However, on termination $\mathbf{x}_k \approx \mathbf{x} \;\Rightarrow$ no essential difference between Galerkin $\mathbf{x}_k^{\text{Gal}}$ and minimal residual $\mathbf{x}_k^{\text{mr}}$.

Hence,

$\mathbf{U}_k$ ill-conditioned $\Rightarrow$ some $\|\mathbf{u}_j\| \, |e_j^* y_k|$ large

Basis used for expansion exact MV

- Orthogonal basis $\mathbf{u}_k \perp \mathbf{u}_j$

Particular implementations:

FOM	**ORTHORES**	Galerkin
GMRES	MINRES	Min. res.
general **A**	symmetric **A**	

- '**A**-Orthogonal' basis $\mathbf{A}\mathbf{u}_k \perp \mathbf{u}_j$

Particular implementations:

	CG	Galerkin
GCR	CR	Min. res.
general **A**	symmetric **A**	

Note. '**A**-Orthogonal' basis guaranteed to be
a (well-conditioned) basis only if **A** positive definite.

$$\text{res-gap}_k \le \sum_{j \le k} \mu_j, \qquad \mu_j \equiv \eta_j \, \|\mathbf{A}\| \, \|\mathbf{u}_j\| \, |e_j^* y_k|$$

Estimates for exact MVs & orthogonal $\mathbf{U}_k$

Galerkin: $\boxed{\mu_j \le \eta_j \, \mathcal{C}(\mathbf{A}) \left(\|\mathbf{r}_j^{\text{mr}}\| + \|\mathbf{r}_k^{\text{Gal}}\| \right)}$ FOM ORTHORES

Min. res.: $\boxed{\mu_j \le \eta_j \, \mathcal{C}(\mathbf{A}) \, \|\mathbf{r}_j^{\text{mr}}\|}$ GMRES

$$\text{res-gap}_k \leq \sum_{j \leq k} \mu_j, \qquad \mu_j \equiv \eta_j \, \|\mathbf{A}\| \, \|\mathbf{u}_j\| \, |e_j^* y_k|$$

Estimates for exact MVs & orthogonal $\mathbf{U}_k$

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Min. res.: $\boxed{\mu_j \leq \eta_j \, \mathcal{C}(\mathbf{A}) \, \|\mathbf{r}_j^{\text{mr}}\|}$ GMRES

If $\mathbf{A}$ is positive definite

Galerkin:
min. res.: $\boxed{\mu_j \leq \eta_j \, \mathcal{C}(\mathbf{A}) \, \|\mathbf{r}_j^{\text{mr}}\|}$

Theoretical results are sharp (experimental evidence)

Alternative analysis: [Simoncini Szyld, 2003]

$$\text{res-gap}_k \le \sum_{j \le k} \mu_j, \qquad \mu_j \equiv \eta_j \, \|\mathbf{A}\| \, \|\mathbf{u}_j\| \, |e_j^* y_k|$$

Estimates for exact MVs & A-orth. $\mathbf{U}_k$

Galerkin:

$$\boxed{\mu_j \le \eta_j \, \mathcal{C}(\mathbf{A}) \left(\|\mathbf{r}_j^{\text{Gal}}\| + \|\mathbf{r}_{j+1}^{\text{Gal}}\| \right)}$$

CG

Min. res.:

$$\boxed{\mu_j \le \eta_j \, \mathcal{C}(\mathbf{A}) \left(\|\mathbf{r}_j^{\text{Gal}}\| + \|\mathbf{r}_{j+1}^{\text{Gal}}\| \frac{\|\mathbf{r}_{j+1}^{\text{mr}}\|}{\|\mathbf{r}_j^{\text{mr}}\|} \right)}$$

GCR

$$\text{res-gap}_k \le \sum_{j \le k} \mu_j, \qquad \mu_j \equiv \eta_j \, \|\mathbf{A}\| \, \|\mathbf{u}_j\| \, |e_j^* y_k|$$

Estimates for exact MVs & A-orth. $\mathbf{U}_k$

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CG

Min. res.:

$$\boxed{\mu_j \le \eta_j \, \mathcal{C}(\mathbf{A}) \left(\|\mathbf{r}_j^{\text{Gal}}\| + \|\mathbf{r}_{j+1}^{\text{Gal}}\| \frac{\|\mathbf{r}_{j+1}^{\text{mr}}\|}{\|\mathbf{r}_j^{\text{mr}}\|} \right)}$$

GCR

If $\mathbf{A}$ is positive

Galerkin:
min. res.:

$$\boxed{\mu_j \le \eta_j \, \mathcal{C}(\mathbf{A}) \, \|\mathbf{r}_j^{\text{mr}}\|_2}$$

Theoretical results are sharp (experimental evidence)

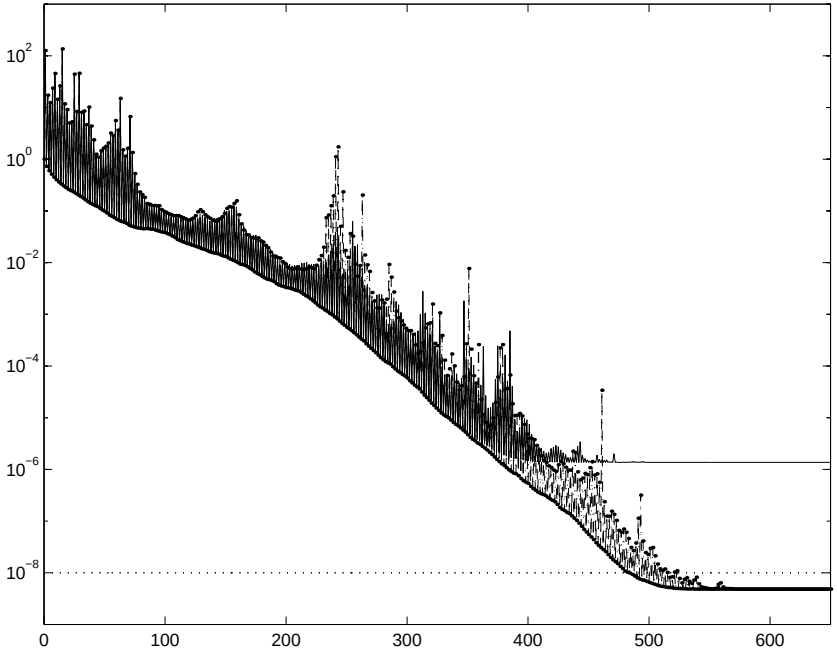
But

MV is not exact . . .

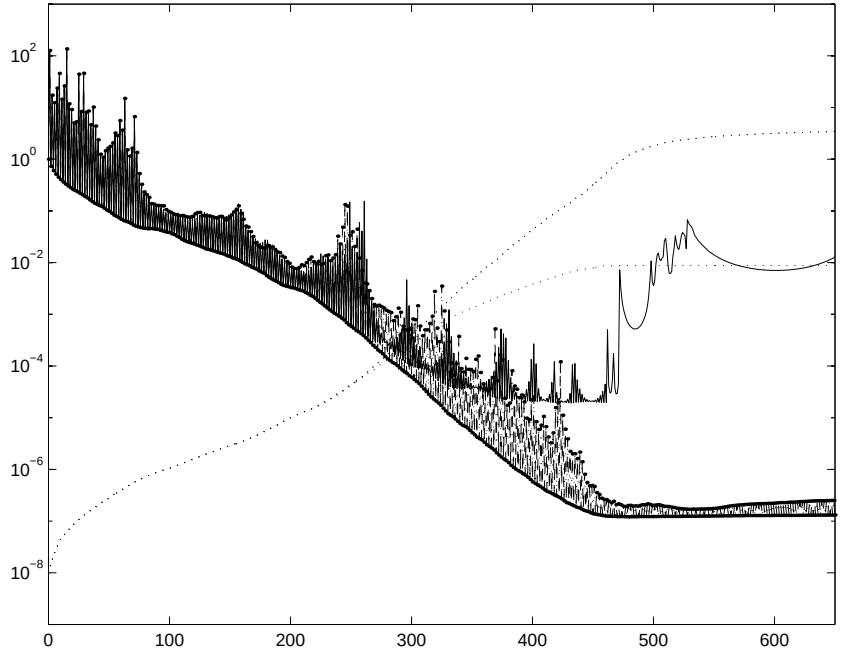
and rounding errors play a role

Example from QCD

$\mathbf{D}_W =$ `CONF6.0-0.0014x4.2000` (Matrix market, $n = 3072$)



$\epsilon = 10^{-8}, \quad \eta_k = \epsilon$

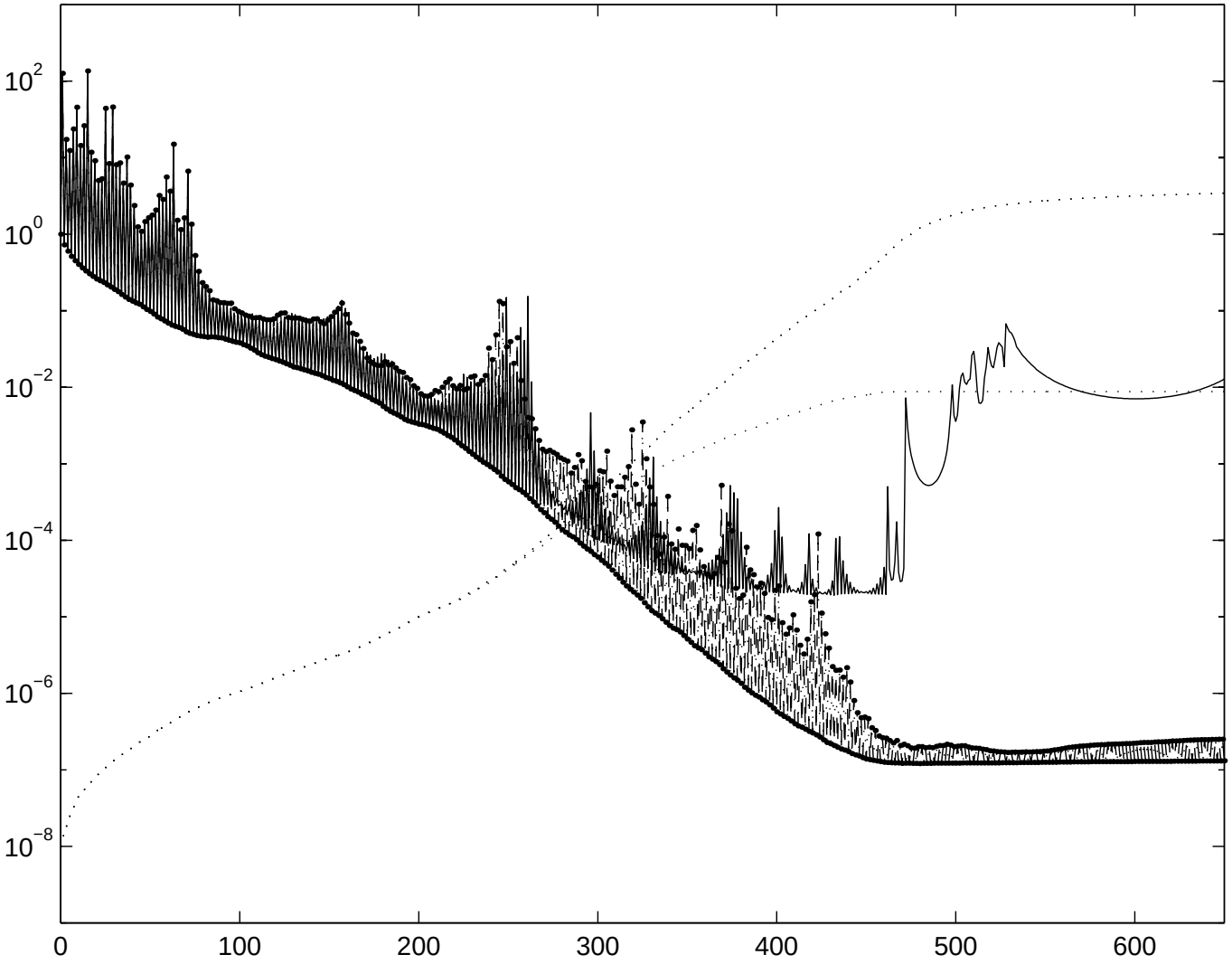


$\epsilon = 10^{-8}, \quad \eta_k = \epsilon/\rho_k$

k versus $\|$true residual$\|$
CG —
ORTHORES $- \cdot -$
η_k $\cdots$

$\mathbf{A} \equiv \Gamma_5 \mathbf{D}_W, \quad \mathbf{b}$ normalized random

(Amplification right picture)



k versus ‖true residual‖
CG —
ORTHORES $- \cdot -\cdot$
(coincides with Rutishauser)
η_k $\cdots$

Total costs of MVs

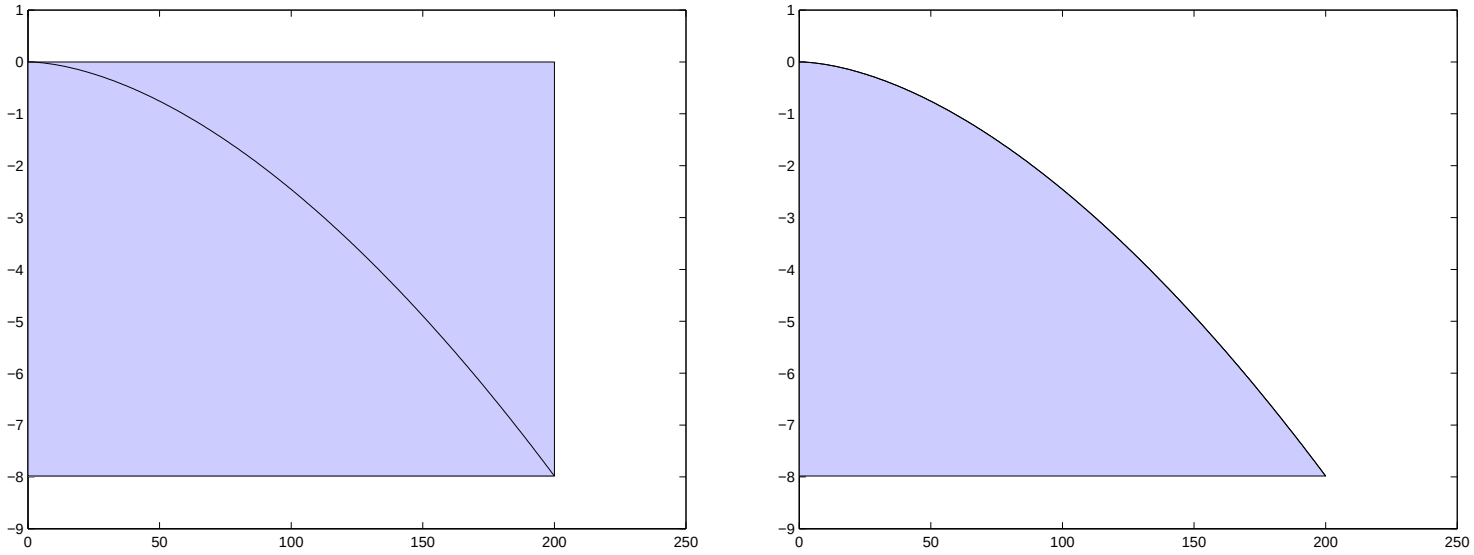
Assume: costs $\mathcal{A}_\eta(\mathbf{u})$ are $\sim -\log \eta$.

Graphical interpretation total costs MVs if convergence unaltered

$\eta_j = \epsilon$ $\eta_j = \epsilon / \|\mathbf{r}_j\|$

j versus $\log \|\mathbf{r}_j\|$

$\log \epsilon$



Total costs MVs (TC) $\sim$ size blue area

$$\mathrm{TC} \sim -\sum_{j \leq k} \log \epsilon \qquad \mathrm{TC} \sim -\sum_{j \leq k} (\log \epsilon - \log \|\mathbf{r}_j\|)$$

In case convergence accelerates:

+ reduces number of iteration steps :-)

− limitted profit from relaxing MVs :-(

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+ reduces number of iteration steps :-)

− limitted profit from relaxing MVs :-(

Alternatives: nest & relax MVs

Basic scheme:

for $k = 0, 1, \ldots$

Compute $\mathbf{u}_k$ (e.g., s.t. $\mathbf{A}\mathbf{u}_k \approx \mathbf{r}_k$)

$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{u}_k$

either $\mathbf{r}_{k+1} = \mathbf{r}_k - \mathbf{A}\mathbf{u}_k$

In "Compute $\mathbf{u}_k$", relax:

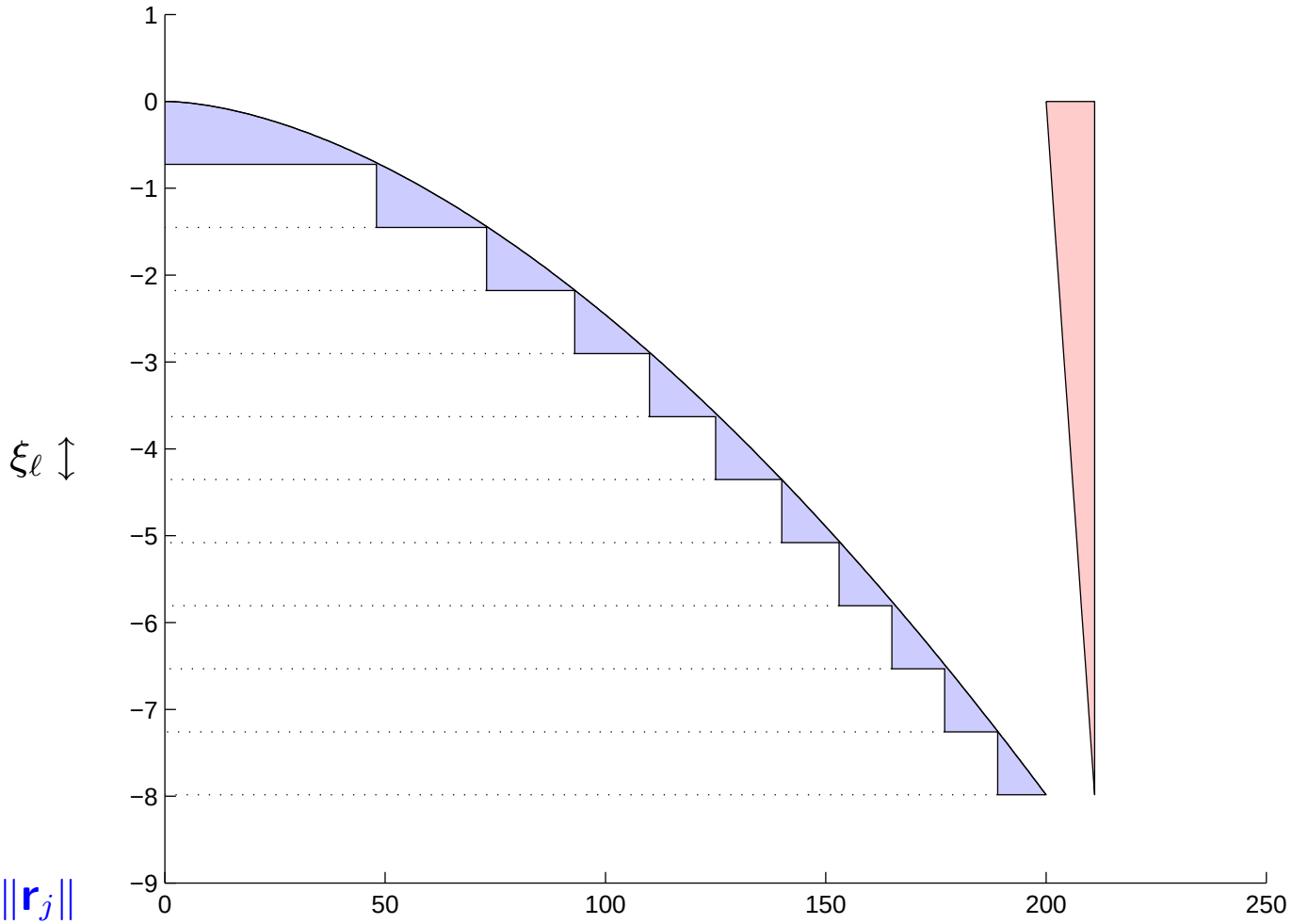
$\mathcal{A}_{\eta_k^{(i)}}(\ldots)$ with $\eta_k^{(i)} = \xi_k \frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_k^{(i)}\|}$.

In "update $\mathbf{r}_k$", relax:

$\mathcal{A}_{\eta_j}(\mathbf{u}_k)$ with $\eta_k = \epsilon \frac{\|\mathbf{r}_0\|}{\|\mathbf{r}_k\|}$

$$\mathcal{A}_\eta(\mathbf{u}) = \mathbf{A}\mathbf{u} + \mathbf{f} \qquad \|\mathbf{f}\| \leq \eta \, \|\mathbf{A}\| \, \|\mathbf{u}\|$$

Estimated costs with nesting & relaxed MV



TC $\sim$ size blue area (inner loop)
$+$ size red area (outer loop)

Alternative: nest & relax MVs

Inner iteration with (another) inexact solver.

Leads to a small number of outer iterations.

Advantages

- Only a few expensive MVs
- ◦ Modest accumulation of 'errors' MV

Drawback

- Loss of optimality Krylov solver $\Rightarrow$ more MVs in total

Solvers for the 'outer iteration' must be '**flexible**' (i.e. must cope with variable preconditioners), e.g.:

- **GMRES Repeated**
- **Flexible GMRES**

...

(See also Hernández et al 00, Golub et al 00, Carpentieri 02)

[van den Eshof S van Gijzen 03]

Schurcomplement system

Example from Oceanography (barotropic flow)

$$\begin{bmatrix} r\,\mathbf{L} - \mathbf{C} & \alpha\,\widetilde{\mathbf{L}} \\ -\widetilde{\mathbf{L}}^* & \mathbf{M} \end{bmatrix} \begin{bmatrix} \boldsymbol{\psi} \\ \boldsymbol{\zeta} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{0} \end{bmatrix}.$$

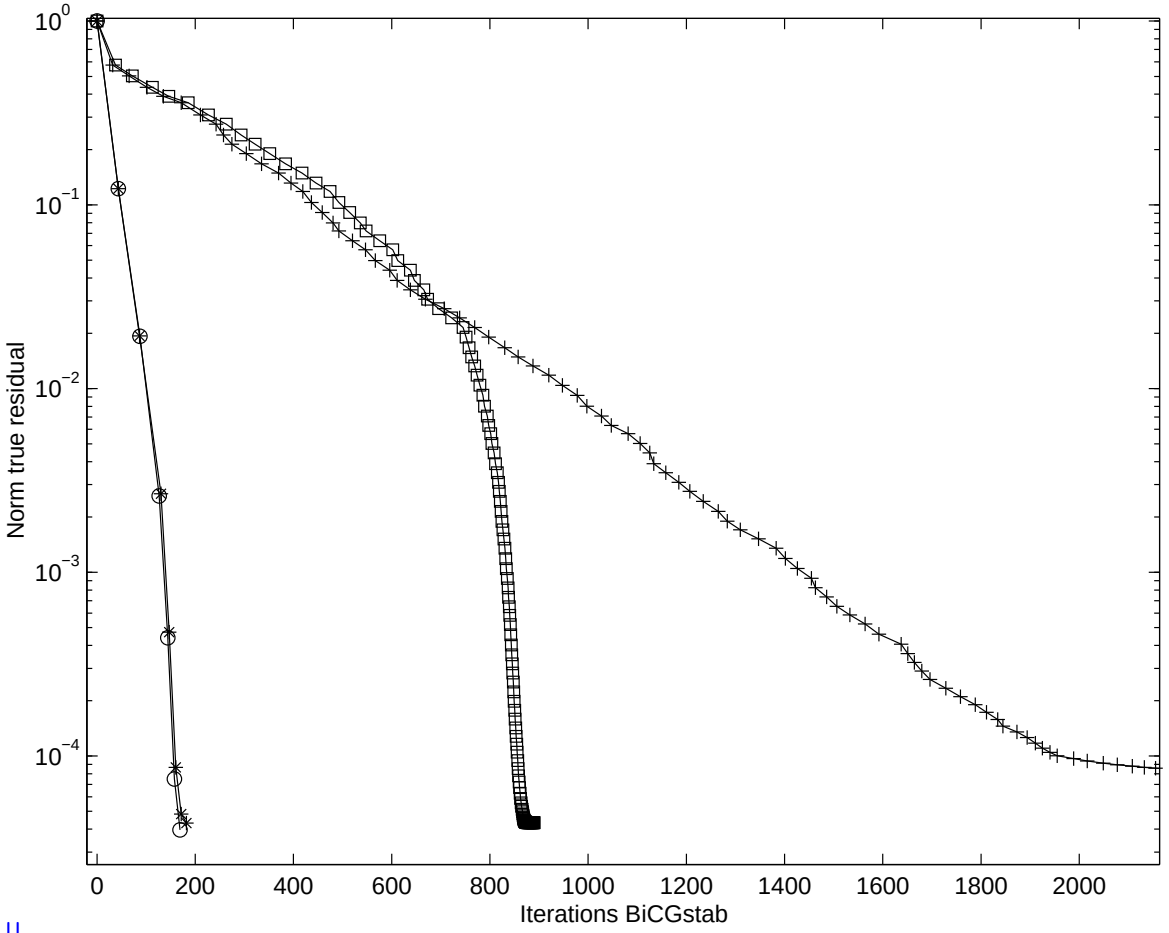
is equivalent to the Schur complement system

$$\underbrace{\left(\mathbf{M} + \alpha\,\widetilde{\mathbf{L}}^*(r\,\mathbf{L} - \mathbf{C})^{-1}\widetilde{\mathbf{L}} \right)}_{\mathbf{A}}\ \underbrace{\boldsymbol{\zeta}}_{\mathbf{x}} \;=\; \underbrace{\widetilde{\mathbf{L}}^*(r\,\mathbf{L} - \mathbf{C})^{-1}\mathbf{g}}_{\mathbf{b}}\,.$$

To get $\mathbf{Au}$ with relative accuracy η, use sufficiently many steps of Bi-CGSTAB to solve $(r\mathbf{L} - \mathbf{C})\tilde{\mathbf{u}} = \widetilde{\mathbf{L}}\mathbf{u}$

In example $n = 26\,455$. Costs $\sim$ # Bi-CGSTAB steps

[van den Eshof S van Gijzen 03]



$\epsilon_7 = \epsilon$, $\log\epsilon$

Costs versus $\log\|\mathbf{r}_j\|$

$+++$ GMRES, MV fixed prec. $\epsilon = 10^{-6}$

$\square\square$ GMRES, relaxed MV $\epsilon = 10^{-7}$

$**$ FGMRES(GMRES) & relaxed MV

$\circ\circ$ GMRESR(GMRES) & relaxed MV

[Cundy van den Eshof Frommer Krieg Lippert Schäfer 04]

Matrix sign function

$$(\rho \mathbf{I} + \Gamma_5 \operatorname{sign}(\mathbf{H}))\,\mathbf{x} = \mathbf{b}$$

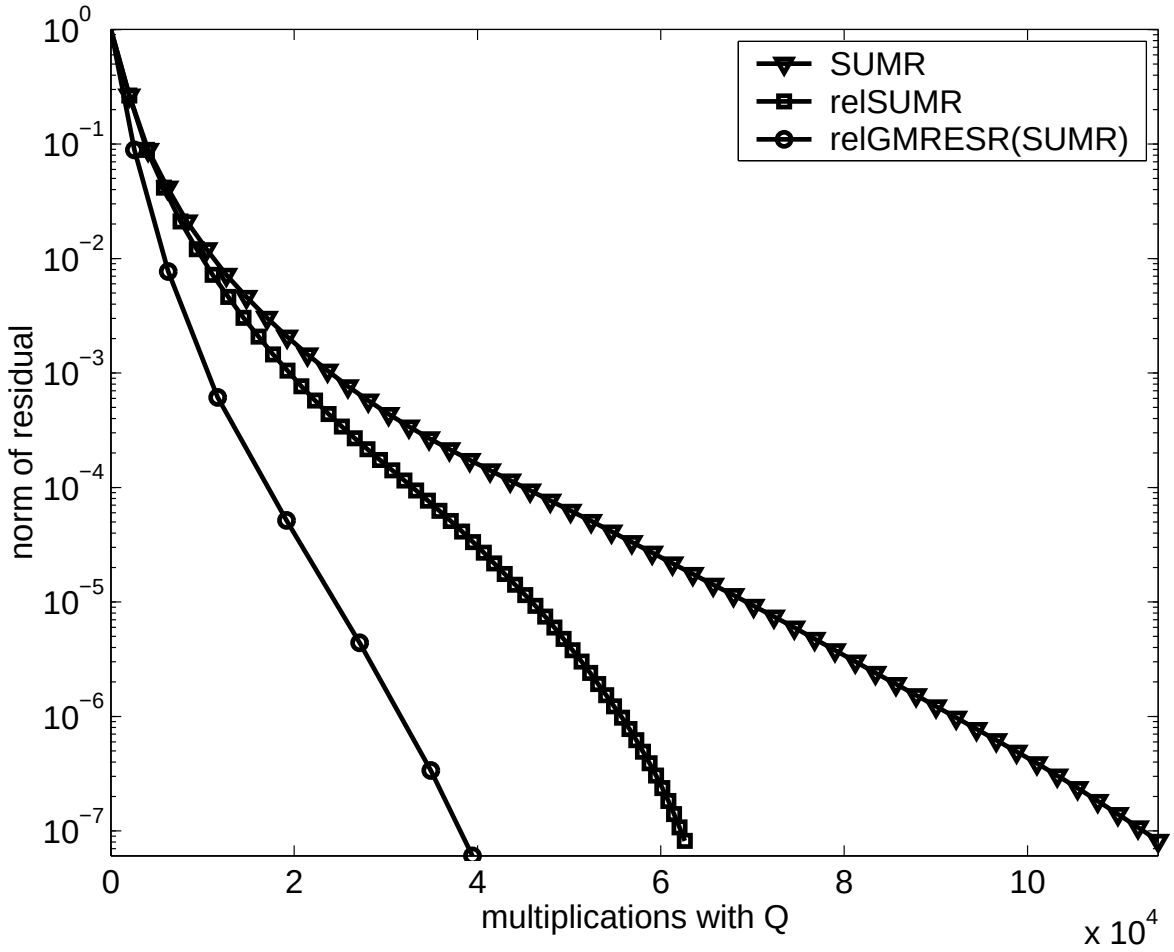
[Jagels Reichel 94]

Solve with **Shifted Unitary Minimal Residuals**
(efficient variant of GMRES for shifted unitary matrices)
and variants:

SUMR (`SUMR`),
relaxed SUMR (`relSUMR`),
relaxed GMRESR(relaxed SUMR) (`relGMRESR(SUMR)`)

In example, on a 8^4 lattice ($n = 49\,152$), $\rho = 1.22$.

[Cundy van den Eshof Frommer Krieg Lippert Schäfer 04]



On 16 processors of ALiCE (cluster computer Wuppertal)

Time in seconds, improvement factor in brackets

`SUMR` **2510** `relSUMR` **1500** **(1.67)** `relGMRESR(SUMR)` **576** **(4.36)**

[Cundy van den Eshof Frommer Krieg Lippert Schäfer 04]

Matrix sign function

$$(\rho \mathbf{I} + \Gamma_5 \operatorname{sign}(\mathbf{H}))\,\mathbf{x} = \mathbf{b}$$

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relaxed GMRESR(relaxed SUMR) (`relGMRESR(SUMR)`)

In example, on a 16^4 lattice ($n = 786\,432$), $\rho = 1.06$.

On 16 processors of ALiCE (cluster computer Wuppertal)

Time in seconds, improvement factor in brackets

`SUMR` **31550** `relSUMR` **18840** **(1.67)** `relGMRESR(SUMR)` **5974** **(5.28)**