Matrix balancing for field of values type inclusion regions

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The challenge

Given large sparse A or routine `mv(A,x)`.

Want:

- high quality inclusion region;
- fast.

Applications:

- eigenvalue localization;
- stability;
- convergence behavior linear solvers;
- etc.

Motivation

Inclusion regions

Largest eigenvalue of `A = grcar(10000) + 5I`:

- `eigs`: fail
- `krylov_schur` (Stewart 2001): $\mathcal{O}(5000)$ MVs, accuracy?
- Good FoV based eigenvalue inclusion region: $10 - 20$ MVs.

Motivation

Field of values

Field of values:

- cheap to approximate numerically;
- convex;
- guaranteed to contain all eigenvalues;
- often relatively tight around eigenvalues, but not always!

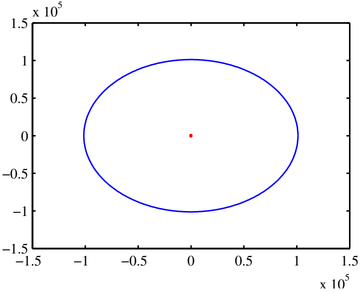


Figure: Tolosa before balancing

Motivation
Balancing

Balancing badly scaled A may:

- dramatically improve quality of FoV as inclusion region;
- improve accuracy of eigenvalue computations;
- improve convergence behaviour.

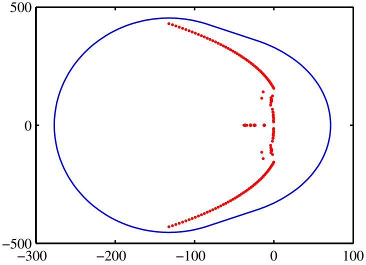


Figure: Tolasa after balancing

Definitions

Field of values:

$$W(A) \equiv \{\mathbf{x}^* A \mathbf{x} : \|\mathbf{x}\|_2 = 1\}$$

Spectral radius:

$$\rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|$$

Numerical radius:

$$r(A) \equiv \max_{z \in W(A)} |z|$$

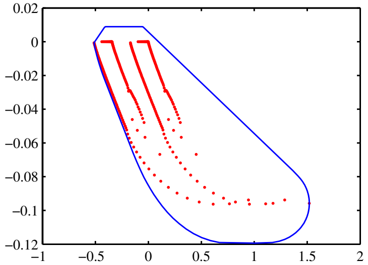


Figure: Quantum Chemistry

Math

Ideally:

$$\frac{r(A)}{\rho(A)} \approx 1$$

Unbalanced:

$$\frac{r(A)}{\rho(A)} \gg 1$$

Balancing:

Replace A by $D^{-1}AD$, usually: $\|D^{-1}AD\| \ll \|A\|$.

Effect:

$\frac{1}{2}\|A\| \leq r(A) \leq \|A\|$ (Theorem)

$$\frac{r(D^{-1}AD)}{\rho(D^{-1}AD)} = \frac{r(D^{-1}AD)}{\rho(A)} \ll \frac{r(A)}{\rho(A)}$$

$W(A) \equiv \{\mathbf{x}^* A \mathbf{x} : \|\mathbf{x}\|_2 = 1\}, \qquad \rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|, \qquad r(A) \equiv \max_{z \in W(A)} |z|$

Results

Quebec Hydroelectric Power System

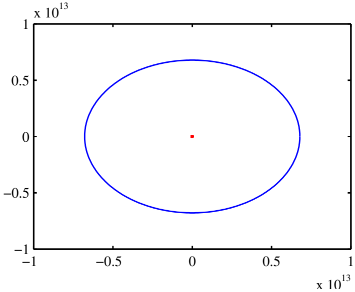


Figure: Unbalanced

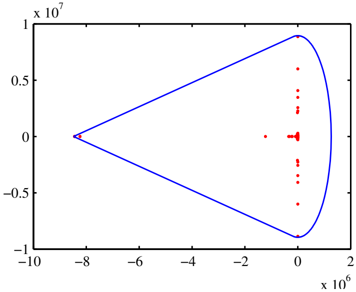


Figure: Balanced

Results

Table: $r(A)/\rho(A)$ for different matrices and methods.

Matrix	spbal	K&B	Az	ATz	Cutoff
af23560	1.01	1.02	—	1.08	1.29
bcsstk29	1.00	1.00	2.32	—	1.00
cry10000	1.00	1.00	3.87	1.53	1.00
dw8192	1.00	1.00	4.64	1.03	1.12
e40r0000	1.00	1.00	—	1.00	1.00
grcar10000	1.08	1.08	3.88	—	2.52
memplus	1.00	1.00	3.36	—	1.00
olm5000	1.00	1.01	—	1.64	1.54
rw5151	0.98	0.98	—	9.79	2.22
sherman3	1.00	1.00	1.06	1.00	1.00
tols4000	1.01	3.27	—	2.55	5.08
utm5940	0.95	0.94	7.20	—	1.36

`spbal`, Az, ATz, Cutoff by (Chen, Demmel 2000)

$W(A) \equiv \{\mathbf{x}^* A \mathbf{x} : \|\mathbf{x}\|_2 = 1\}, \qquad \rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|, \qquad r(A) \equiv \max_{z \in W(A)} |z|$

Conclusions

Field of values:

- simple;
- cheap;
- often tight.

Balancing:

- simple (e.g., `B = spbalance(A)`);
- fast (e.g., 0.25ms for `A = tols4000`);
- it's super effective!

"Krylov & Balancing" (K&B) shows high quality inclusion regions can be created for large sparse A with only a few (e.g., 20) MVs.

Computing the Field of Values

Small Dense Matrices

(Johnson 1978)

Step 1

For a few $\alpha \in [0, 2\pi)$ compute

$$\lambda_\alpha = \frac{1}{2}\lambda_{\max}(e^{i\alpha}A + (e^{i\alpha}A)^*)$$

and the corresponding eigenvector $\mathbf{x}_\alpha$.

Step 2

Compute the convex hull of

$$\{\mathbf{x}_\alpha^* A \mathbf{x}_\alpha : \alpha\}.$$

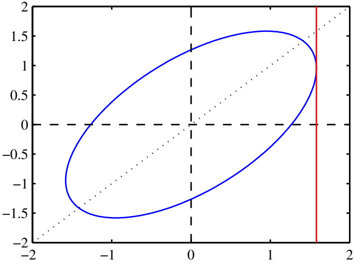


Figure: Example where $\alpha = \pi/4$.

$$W(A) \equiv \{\mathbf{x}^* A\mathbf{x} : \|\mathbf{x}\|_2 = 1\}, \qquad \rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|, \qquad r(A) \equiv \max_{z \in W(A)} |z|$$

Computing the Field of Values

Large Sparse Matrices

Step 1

Create basis V_k for Krylov subspace

$$\mathrm{span}\{\mathbf{v}_1, A\mathbf{v}_1, \ldots, A^{k-1}\mathbf{v}_1\}$$

and compute $H_k = V_k^* A V_k$.

Step 2

Compute $W(H_k)$. Why?
Ritz values approximate exterior eigenvalues well and

$$W(H_k) \subseteq W(H_{k+1}) \subseteq W(A).$$

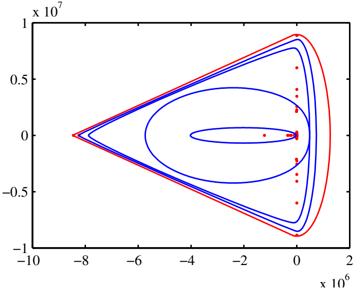


Figure: $W(H_2), \ldots, W(H_5)$.

$W(A) \equiv \{\mathbf{x}^* A\mathbf{x} : \|\mathbf{x}\|_2 = 1\}$, $\rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|$, $r(A) \equiv \max_{z \in W(A)} |z|$

The Krylov and Balancing Method

Easy as π!

Step 1

Compute $H_k = V_k^* A V_k$ for, say, $k = 20$.
(Remember: need H_k anyway for $W(A)$.)

Step 2

Balance H_k (e.g. using Matlab's `balance`).

Step 3

???

Step 2

Profit!!!

$$W(A) \equiv \{\mathbf{x}^* A \mathbf{x} : \|\mathbf{x}\|_2 = 1\}, \qquad \rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|, \qquad r(A) \equiv \max_{z \in W(A)} |z|$$

Dealing with outliers

Recall

$$\lambda_\alpha = \frac{1}{2}\lambda_{\max}(e^{i\alpha}A + (e^{i\alpha}A)^*)$$

Assume:

$$\lambda_{\max} = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = \lambda_{\min}$$

With outliers

$$\lambda_\alpha = \frac{1}{2}\lambda_2(e^{i\alpha}A + (e^{i\alpha}A)^*)$$

Or λ_3, λ_4, etc.

$$W(A) \equiv \{\mathbf{x}^* A\mathbf{x} : \|\mathbf{x}\|_2 = 1\}, \qquad \rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|, \qquad r(A) \equiv \max_{z \in W(A)} |z|$$

Example

```
A = rand(1000);
```

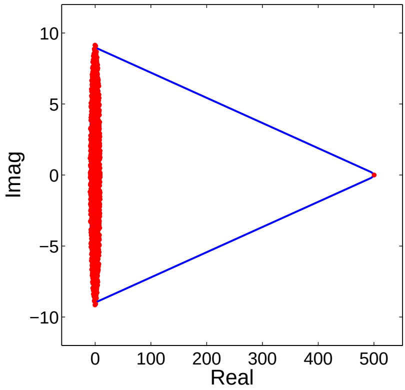


Figure: Original

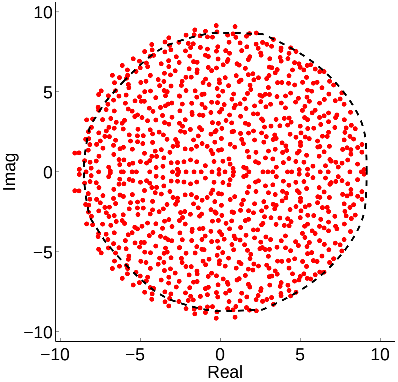


Figure: Higher-order FoV

Exclusion regions

Idea

Shift-and-invert: eigenvalues of $(A - \tau I)^{-1}$ are $(\lambda - \tau)^{-1}$ and

$$\Lambda(A) = \bigcap_{\tau \in \mathbb{C} \setminus \Lambda(A)} \frac{1}{W((A - \tau I)^{-1})} + \tau$$

(Hochstenbach, Singer, Zachlin 2008, 2013)

Example

- Incl. region $W(H_k)$
- Excl. region $1/W((H_k - \tau_j I)^{-1}) + \tau_j$
- Random starting on S^{n-1}
- Krylov dimension $k = 20$

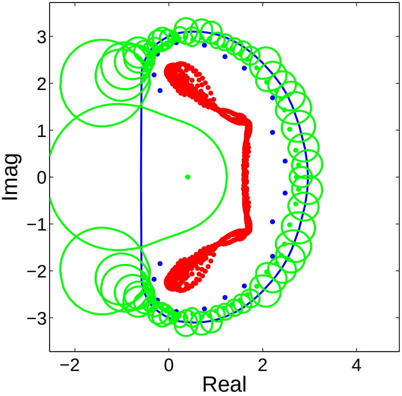


Figure: grcar

$$W(A) \equiv \{\mathbf{x}^* A \mathbf{x} : \|\mathbf{x}\|_2 = 1\}, \qquad \rho(A) \equiv \max_{\lambda \in \Lambda(A)} |\lambda|, \qquad r(A) \equiv \max_{z \in W(A)} |z|$$

spbalance

Parlett–Reinsch (1969):

- gebal (LAPACK);
- balanc (EISPACK);
- balance (MATLAB).

Chen–Demmel (2000):

- spbalance.

Sparse Parlett–Reinsch with improved permutation phase.

spbalance

Permutation phase

What?

Find P such that

$$P^T A P = \begin{bmatrix} X_{11} & \dots & X_{1b} \\ 0 & \ddots & \vdots \\ 0 & 0 & X_{bb} \end{bmatrix}$$

is block upper triangular.

Why?

$$\Lambda(A) = \bigcup_i \Lambda(X_{ii})$$

spbalance

Scale phase

What?

Compute (diagonal) D_i such that

$$D_i^{-1} X_{ii} D_i$$

is balanced.

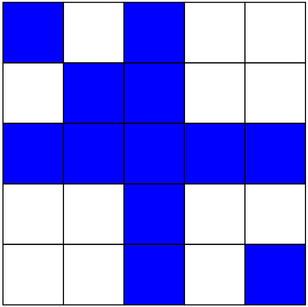
Why?

$$B = D^{-1} P^T A P D = \begin{bmatrix} D_1^{-1} X_{11} D_1 & \dots & D_1^{-1} X_{1b} D_b \\ 0 & \ddots & \vdots \\ 0 & 0 & D_b^{-1} X_{bb} D_b \end{bmatrix}$$

spbalance

Scale phase cont'd

1. Compute $C_j \equiv \|X_{ii}(:,j)\|_1$, $R_j \equiv \|X_{ii}(j,:)\|_1$, exclude $X_{ii}(j,j)$.
2. While $C_j < R_j$ ($C_j > R_j$) increase (decrease) $D_i(j,j)$.
3. Iterate over j until convergence.



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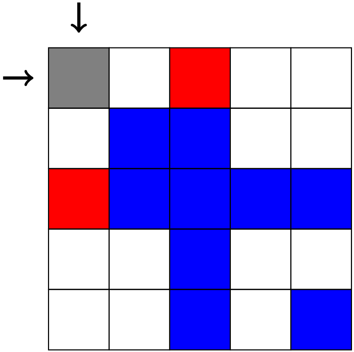

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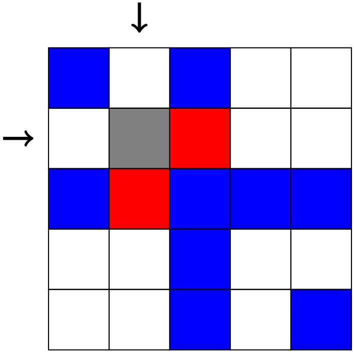

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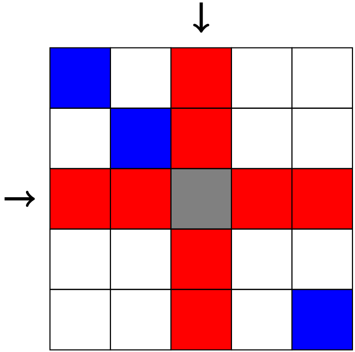

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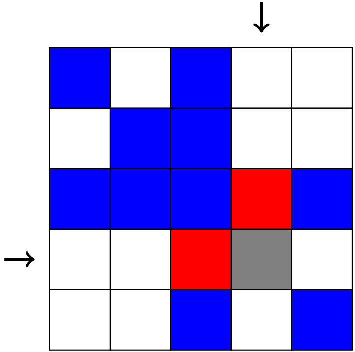

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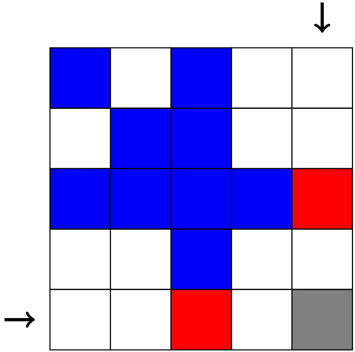

Summary

1
FoV and balancing $\rightsquigarrow$ high quality inclusion region.

2
Computing FoV for large sparse $A \rightsquigarrow$ K&B.

2
Many extensions.

3
Balancing with Parlett–Reinsch.