# Padé via Lanczos for multiple right-hand sides 

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## Outline

(joint work with Zhaojun Bai)
(1) Motivation
(2) Fast alternatives

- Modal truncation
- AMLS
- Lanczos method
(3) Further analysis

4 Numerical examples

## Vibration problems

A car window is subjected to vibrations from outside, including wind. Glass manufacturers want to compute the transmission of noise through windscreens.


## Fourier analysis

- Solve

$$
\left(K-\omega^{2} M\right) x=f
$$

with $K, M: n \times n$ sparse matrices, symmetric.

- $\omega \in \Omega=\left[\omega_{\min }, \omega_{\max }\right]$.

We also define $\Omega^{2}=\left[\omega_{\text {min }}^{2}, \omega_{\text {max }}^{2}\right]$

- $x$ is called the frequency response function.



## Alternatives: modal truncation

- Consider the eigendecomposition

$$
K u_{j}=\lambda_{j} M u_{j}
$$

- The solution of $\left(K-\omega^{2} M\right) x=f$ is

$$
x=\sum_{j=1}^{n} u_{j} \frac{u_{j}^{*} f}{\lambda_{j}-\omega^{2}}
$$

- Rational function with poles $\lambda_{j}$.


## Alternative: modal truncation

$$
x=\sum_{j=1}^{n} u_{j} \frac{u_{j}^{*} f}{\lambda_{j}-\omega^{2}} \approx \sum_{j=1}^{k} u_{j} \frac{u_{j}^{*} f}{\lambda_{j}-\omega^{2}}
$$



## Alternative: AMLS

The solution of

$$
\left(K-\omega^{2} M\right) x=f
$$

for $\omega \in \Omega$ is split into two parts.

- Let $U_{p}=\left[u_{1}, \ldots, u_{p}\right]$ be the eigenvectors corresponding to the eigenvalues in $\Omega^{2}$.
- Solve the $p \times p$ problem

$$
U_{p}^{*}\left(K-\omega^{2} M\right) U_{p} z=U_{p}^{*} f
$$

- Solve the remainder

$$
\left(K-\omega^{2} M\right) y=\left(I-M U_{p} U_{p}^{*}\right) f
$$

- $x=U_{p} z+y$


## Alternative: AMLS

- Preconditioner for the 'remainder' system :

$$
(K-\sigma M)^{-1}
$$

- Preconditioned system is

$$
A y=b
$$

with

$$
\begin{aligned}
b & =\left(I-M U_{p} U_{p}^{*}\right)(K-\sigma M)^{-1} f \\
A & =(K-\sigma M)^{-1}\left(K-\omega^{2} M\right)
\end{aligned}
$$

- In AMLS [Bennighof \& Kaplan, 1998], [Ko \& Bai, 2007] $K-\sigma M$ is diagonal


## Alternative: Lanczos process

- Use a Krylov method for solving $A y=b$
- Since $x^{*} M A y=y^{*} M A x$, we use the Lanczos method with $M$ inner product
- Lanczos method:

1. Let $v_{1}=b /\|b\|_{M}$
2. For $j=1, \ldots, k$
2.1. Compute Krylov vector $v_{j+1}=A v_{j}$.
2.2. Orthogonalize $v_{j+1}$ against $v_{1}, \ldots, v_{j}$
so that $v_{j+1}^{*} M V_{j}=0$.

- Lanczos vectors $V_{k}=\left[v_{1}, \ldots, v_{k}\right]$.
- Recurrence relation: $A V_{k}-V_{k} T_{k}=\beta_{k} v_{k+1} e_{k}^{*}$ with $T_{k}$ tridiagonal
- $y=V_{k} T_{k}^{-1} e_{1}\|b\|_{M}$


## Shifted Lanczos method

- Recall that

$$
\begin{gathered}
A=(K-\sigma M)^{-1}\left(K-\omega^{2} M\right) \\
(K-\sigma M)^{-1}\left(K-\omega^{2} M\right) V_{k}-V_{k} T_{k}=\beta_{k} v_{k+1} e_{k}^{*}
\end{gathered}
$$

- $V_{k}$ and $T_{k}$ can be computed from the shifted Lanczos method.

$$
(K-\sigma M)^{-1} M \tilde{V}_{k}-\tilde{V}_{k} \tilde{T}_{k}=\tilde{\beta}_{k} \tilde{v}_{k+1} e_{k}^{*}
$$

- $V_{k}=\tilde{V}_{k}$ and $T_{k}=I+\left(\sigma-\omega^{2}\right) \tilde{T}_{k}$


## Shifted linear systems

- Analyzed in the context of model reduction methods
- Feldman, Freund, Bai, Grimme, Sorensen, Van Dooren, Ruhe, Skoogh, Olsson, Simoncini, M., ...
- Connection with eigendecomposition
- Connection with iterative linear solvers
- Connection with rational approximation (Padé)
- Recycling Ritz vectors for parameterized systems: Kilmer \& de Sturler 2006


## Spectral analysis of deflated iterative method



- Let $B=\left.A\right|_{\left\{U_{p}\right\}^{\perp}{ }_{M}}$
- Black eigenvalues only: $B$ is positive definite
- Eigenvalues of $B$ clustered around 1
- spectral radius of $I-B$ is smaller than one


## Inexact deflation

- Be careful for deflation with Ritz vectors
[Darnell, Morgan, Wilcox 2007]
- Reason is that the system's residual need not be small

$$
r(\omega)=R_{p} z_{p}+v_{k+1} \zeta_{k}
$$

with $R_{p}$ coming from deflation of Ritz vectors and $v_{k+1}$ the residual term of the iterative method.

## Eigenvalue solver

- Use Ritz pairs of the Lanczos method
- Ritz values: $T_{k} z=\theta z$
- Ritz vectors: $\hat{u}=V_{k} z$
- No exact eigenpairs
- But interesting properties as we now see:


## Convergence of Ritz vectors

- Eigenvalues in $\Omega^{2}$ are computed fairly accurately

- If $\|A \hat{y}-b\|_{M} \leq \gamma\|y\|_{M}$ for all $\omega \in \Omega$
- then $\rho_{j}=\left\|A \hat{u}_{j}-\hat{u}_{j} \hat{\theta}_{j}\right\|_{M}$ with

$$
\rho_{j} \leq \frac{\gamma}{\left|\lambda_{j}-\sigma\right|}
$$

## Methods

- DRHSL or init-CG
- Solve $U_{p}^{T}(K-\sigma M)^{-1}\left(K-\omega^{2} M\right) U_{p} z=U_{p}^{T} f$
- Compute Krylov space for $A=(K-\sigma M)^{-1} M$ and $\left(I-U_{p} U_{p}^{T} M\right)(K-\sigma M)^{-1} f$
- Solve tridiagonal system
- Add the two components of the solution
- DML
- Solve $U_{p}^{T}(K-\sigma M)^{-1}\left(K-\omega^{2} M\right) U_{p} z=U_{p}^{T} f$
- Compute Krylov space for $B=\left(I-U_{p} U_{p}^{T} M\right)(K-\sigma M)^{-1} M\left(I-U_{p} U_{p}^{T} M\right)$ and $\left(I-U_{p} U_{p}^{T} M\right)(K-\sigma M)^{-1} f$
- Project $A$ on $\left[U_{p} V_{k}\right]$
- In exact arithmetic both methods do the same thing
- DML is more expensive in operations and memory
- but may be more reliable since deflation is imposed explicitly


## Padé via Lanczos

- Lanczos method:

$$
\hat{x}=\sum_{j=1}^{k} \hat{u}_{j} \frac{\hat{u}_{j}^{*} f}{\hat{\lambda}_{j}-\omega^{2}}
$$

- First $k$ moments of $\hat{x}$ and $x$ match.
- With exact deflation:

$$
\hat{x}=\sum_{j=1}^{p} u_{j} \frac{u_{j}^{*} f}{\lambda_{j}-\omega^{2}}+\sum_{j=p+1}^{k} \hat{u}_{j} \frac{\hat{u}_{j}^{*} f}{\hat{\lambda}_{j}-\omega^{2}}
$$

- First $k-p$ moments of $\hat{x}$ and $x$ match.
- Interpolation in the $p$ deflated eigenvalues.


## Applications

- AMLS frequency sweeping
- Multiple right-hand sides:
- Parameterized Lanczos for right-hand side 1
- Keep Ritz vectors
- Recycle Ritz vectors for coming right-hand sides
- Changing $\sigma$ : recycle Ritz vectors for new pole.


## Windscreen

- Glaverbel-BMW windscreen
- grid : 3 layers of $60 \times 30$ HEX08 elements $(n=22,692)$
- $\Omega=[0,100]$
- First run:
- unit point force at one of the corners
- Use Lanczos method with $k=20$ vectors.
- We keep the Ritz values in $\left[0,2 \times 100^{2}\right]: p=14$


## Windscreen

- Second run with other right-hand side
- Perform 6 additional Lanczos steps

- The largest $\kappa(\hat{B})$ is 1.9813 .
- Six iterations reduce the error in the $M \hat{B}$ norm by $2 \cdot 10^{-5}$.


## Acoustic cavity



- $n=48,158$
- Frequency range : [0, 10000]
- 202 right-hand sides
- matrix factorization: 8 seconds
- Lanczos method with 40 vectors: 6 seconds


## Acoustic cavity (cont.)

- 2nd right-hand side: keep the 31 Ritz values in $\left[0,2 \times 10.000^{2}\right]$.
- 9 additional Lanczos iterations recycling 31 Ritz vectors: 2 seconds


With recycling



## Multiple eigenvalues

- 3D Laplacian on a cube.
- 30 Lanczos iterations with first right-hand side
- Recycle 22 Ritz pairs
- Run 8 iterations with the second right-hand side




