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Subspace iteration for eigenproblems

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Program

- Galerkin approach
- Arnoldi type of methods
  Arnoldi
  Lanczos
  RKS (rational Krylov Sequence)
  ⋮
- ∘ IRA (Implicitly Restarted Arnoldi)
- Davidson type of methods
- Jacobi-Davidson
- Deflation
- Generalized eigenproblems

$$\boxed{\mathbf{A}\,\mathbf{x}_\lambda = \lambda\,\mathbf{x}_\lambda}$$

Galerkin approach

- Generate a subspace with basis $\mathbf{v}_1, \ldots, \mathbf{v}_k$.
- With $\mathbf{V} := [\mathbf{v}_1|\ldots|\mathbf{v}_k]$ find y and θ such that

$$\mathbf{r} := \mathbf{A}\mathbf{V}y - \theta\mathbf{V}y \perp \{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$$

$(\theta, \mathbf{V}y)$ **Ritz pair** w.r.t. **search space** span$(\mathbf{V})$.
$(\theta, \mathbf{V}y)$ with **residual** $\mathbf{r}$ approximates $(\lambda, \mathbf{x}_\lambda)$.

In practice. $k \ll n$

∘ Generate an orthonormal system $\mathbf{v}_1, \ldots, \mathbf{v}_k$:
$\mathbf{z}$ expansion vector $\mathbf{V}$ $\Rightarrow$ $\mathbf{v}_{k+1} :=$ modGS$_{\mathbf{V}}(\mathbf{z})$.
∘ solve the small problem

$$\mathbf{V}^*\mathbf{A}\mathbf{V}y = \theta\,y$$

Subspace iteration

1. **Start:**

   Choose an initial subspace $\mathbf{V}$.

2. **Repeat:**
   - Compute $\mathbf{W} \leftarrow \mathbf{A}\mathbf{V}$, $H \leftarrow \mathbf{V}^*\mathbf{W}$.
   - Compute a desired eigenpair (θ, y) of H (with $\|y\| = 1$).
   - Compute $\mathbf{u} \leftarrow \mathbf{V}y$,

     $\mathbf{r} \leftarrow \mathbf{A}\,\mathbf{u} - \theta\,\mathbf{u}$.
   - **Stop if** satisfied.
   - Compute an expansion vector $\mathbf{z}$
   - $\mathbf{V} \leftarrow$ ModGS$([\,\mathbf{V}\,|\,\mathbf{z}\,])$

Choices for the expansion vector

with initial search subspace span$(\mathbf{v}_1)$.

Arnoldi's method ['51]

$$\mathbf{z} = \mathbf{A}\mathbf{v}_k.$$

Then $H := \mathbf{V}^*\mathbf{A}\mathbf{V}$ is upper Hessenberg.

Lanczos' method if $\mathbf{A}^* = \mathbf{A}$ ['50]

$$\mathbf{z} = \mathbf{A}\mathbf{v}_k.$$

Then $H := \mathbf{V}^*\mathbf{A}\mathbf{V}$ is tridiagonal.

Search space span$(\mathbf{V})$ $=$ Krylov subspace

$$\text{span}\big(\mathbf{v}_1, \mathbf{A}\mathbf{v}_1, \ldots, \mathbf{A}^{k-1}\mathbf{v}_1\big).$$

Arnoldi (Lanczos) favors extremal eigenvalues

Exponential Arnoldi [Meerbergen & Sadkane '96]

$$\mathbf{z} = \exp(\mathbf{A})\mathbf{v}_k.$$

Approach favors eigenvalues λ with Re(λ) large
(amplifies $\mathbf{x}_\lambda$-comp. with $\exp(\lambda)$)

In practice.
With $\mathbf{U}$ orthornormal matrix of basisvectors of Krylov subspace span$(\mathbf{v}_k, \mathbf{A}\mathbf{v}_k, \ldots, \mathbf{A}^m\mathbf{v}_k)$
and $H' := \mathbf{U}^*\mathbf{A}\mathbf{U}$ take $\mathbf{z} = \mathbf{U}[\exp(H')e_1]$

Arnoldi (Lanczos) favors extremal eigenvalues

Shift-and-Invert-Arnoldi

Select target $\tau \in \mathbb{C}$.

$$\mathbf{z} = (\mathbf{A} - \tau\,\mathbf{I})^{-1}\mathbf{v}_k.$$

Then $H = \mathbf{V}^*\mathbf{A}\mathbf{V}$ is upper Hessenberg.

Approach favors eigenvalues close to τ
(amplifies $\mathbf{x}_\lambda$-comp. with $\frac{1}{\lambda-\tau}$)

Rational Krylov Sequence [Ruhe '84, '93]

$$\mathbf{z} = (\mathbf{A} - \tau_k\,\mathbf{I})^{-1}(\mathbf{A} - \sigma_k\mathbf{I})\mathbf{v}_k.$$

(amplifies $\mathbf{x}_\lambda$-comp. with $\frac{\lambda-\sigma_k}{\lambda-\tau_k}$)

However, for large problems,
"solve $(\mathbf{A} - \tau\,\mathbf{I})\mathbf{z} = \mathbf{v}_k$"
is expensive and has to be done accurately.

$\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ orthogonal basis search space.

Put $\mathbf{V}_k = [\mathbf{v}_1|\ldots|\mathbf{v}_k]$.

Arnoldi ['51]

Expansion vector $\mathbf{v}_{k+1}$ computed as

$$\mathbf{v}_{k+1} = \text{modGS}_{\mathbf{V}_k}(\mathbf{A}\mathbf{v}_k).$$

Then $\boxed{\mathbf{A}\,\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{H}_k}$

with $\underline{H}_k$ $(k+1) \times k$ upper Hessenberg.

Solve $H_k\,y - \theta\,y = 0$. Take $\mathbf{u} = \mathbf{V}_k\,y$.

$$\boxed{\mathbf{A}\,\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{H}_k}$$

$(H_k - \theta\, I)\, y = 0, \qquad \mathbf{u} := \mathbf{V}_k\, y$

The Arnoldi residual

$$\begin{aligned}\mathbf{r} &:= (\mathbf{A} - \theta\,\mathbf{I})\mathbf{u}\\ &= (\mathbf{A} - \theta\,\mathbf{I})\mathbf{V}_k\, y\\ &= \mathbf{V}_{k+1}\,(\underline{H}_k - \theta\, I)\, y\end{aligned}$$

$$\mathbf{r} \ = h_{k+1\,k}\; e_k^* y\; \mathbf{v}_{k+1}$$

$$\|\mathbf{r}\| = |h_{k+1\,k}|\,|e_k^* y|$$

$\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ orthogonal basis search space.

Put $\qquad \mathbf{V}_k = [\mathbf{v}_1|\ldots|\mathbf{v}_k]$.

Arnoldi ['51]

Expansion vector $\mathbf{v}_{k+1}$ computed as

$$\mathbf{v}_{k+1} = \text{modGS}_{\mathbf{V}_k}(\mathbf{A}\mathbf{v}_k).$$

Then $\qquad \boxed{\mathbf{A}\,\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{H}_k}$

with $\quad \underline{H}_k \quad (k+1)\times k$ upper Hessenberg.

Implicitly Restarted Arnoldi [Sorensen 92]

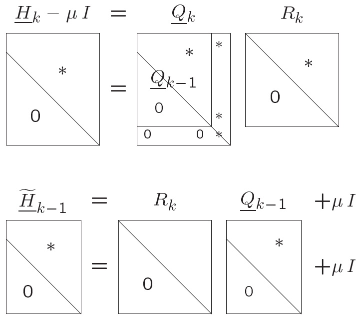
Select polynomial $\Psi(\lambda) = (\lambda - \mu_\ell)\cdots(\lambda - \mu_1)$.

Then, after **implicit restart**,

$$\mathbf{A}\widetilde{\mathbf{V}}_{k-\ell} = \widetilde{\mathbf{V}}_{k+1-\ell}\,\widetilde{\underline{H}}_{k-\ell}$$
$$\Psi(\mathbf{A})\mathbf{v}_1 = \gamma\,\tilde{\mathbf{v}}_1.$$

Can be computed without MVs and DOTs!

$$\mathbf{A}\,\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{H}_k$$



With $\quad \widetilde{\mathbf{V}}_i := \mathbf{V}_{i+1}\,\underline{Q}_i, \quad \widetilde{\underline{H}}_{k-1} = \underline{Q}_k^*\,\underline{H}_k\,\underline{Q}_{k-1}$

we have $\qquad \underline{Q}_k\,\widetilde{\underline{H}}_{k-1} = \underline{H}_k\,\underline{Q}_{k-1}$

$$\mathbf{A}\widetilde{\mathbf{V}}_{k-1} = \widetilde{\mathbf{V}}_k\,\widetilde{\underline{H}}_{k-1}$$

and $\quad (\mathbf{A} - \mu\,\mathbf{I})\mathbf{V}_k = \mathbf{V}_{k+1}(\underline{H}_k - \mu\, I) = \widetilde{\mathbf{V}}_k\, R_k$

$$\mathbf{A}\,\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{H}_k$$

Lemma. $\quad \underline{H}_k - \mu\, I = \underline{Q}_k\, R_k$.

With $\quad \widetilde{\mathbf{V}}_i := \mathbf{V}_{i+1}\,\underline{Q}_i, \quad \widetilde{\underline{H}}_{k-1} = \underline{Q}_k^*\,\underline{H}_k\,\underline{Q}_{k-1}$

we have $\qquad \mathbf{A}\widetilde{\mathbf{V}}_{k-1} = \widetilde{\mathbf{V}}_k\;\widetilde{\underline{H}}_{k-1}$

and, $\qquad (\mathbf{A} - \mu\,\mathbf{I})\mathbf{v}_1 = \gamma\,\tilde{\mathbf{v}}_1, \qquad$ *for some* γ.

Theorem. $\Psi(\lambda) := (\lambda - \mu_\ell)\cdots(\lambda - \mu_1)$.

Then $\qquad \mathbf{A}\widetilde{\widetilde{\mathbf{V}}}_{k-\ell} = \widetilde{\widetilde{\mathbf{V}}}_{k+1-\ell}\;\widetilde{\widetilde{\underline{H}}}_{k-\ell}$

and $\qquad \Psi(\mathbf{A})\mathbf{v}_1 = \gamma\,\tilde{\tilde{\mathbf{v}}}_1, \qquad$ *for some* γ.

where $\quad \widetilde{\widetilde{\mathbf{V}}}_{k-\ell} := \mathbf{V}_k\, Q', \quad \widetilde{\widetilde{\underline{H}}}_{k-\ell} = Q^*\,\underline{H}_k\, Q'$.

[Sorensen 92]

An implicit restart step

$$\mathbf{A}\,\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{H}_k$$

$\underline{Q}'$ is $\underline{Q}$ without last row and last column

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Select  μ_1, ..., μ_ℓ ∈ ℂ
Set  H = H_k,  Q̃ = I_k
For j = 1, ..., ℓ do
   Factorise  H − μ_j I_{k+1−j} = Q R
   Compute
     H ← R Q' + μ_j I_{k−j}
     Q̃ ← Q̃ Q
end for
Set   H̃̃_{k−ℓ} = H
Compute   Ṽ̃_{k+1−ℓ} = V_{k+1} Q̃,
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$$\mathbf{A}\,\widetilde{\widetilde{\mathbf{V}}}_{k-\ell} = \widetilde{\widetilde{\mathbf{V}}}_{k+1-\ell}\,\widetilde{\widetilde{\underline{H}}}_{k-\ell}$$

$$\underline{H}_k - \mu\, I = \underline{Q}_k\, R_k, \qquad \widetilde{\underline{H}}_{k-1} = R_k\underline{Q}_{k-1} + \mu\, I$$

Proposition. $\underline{H}_k$ irreducible

$$\mu \in \sigma(H_k) \ \Rightarrow \sigma(\widetilde{H}_{k-1}) = \sigma(H_k)\backslash\{\mu\}$$

Proof. $\mu \in \sigma(H_k)$ then $H_k - \mu$ singular and $\underline{Q}_k e_k = e_{k+1}$.

Lemma. $\underline{Q}_k e_k = e_{k+1}$.

Then, with $\tilde{Q}_k := [\underline{Q}_{k-1}\,|\,q]$ orthonormal,

$$\tilde{Q}_k^*\, H_k\, \tilde{Q}_k = \begin{bmatrix}\widetilde{H}_{k-1} & * \\ 0 & \mu\end{bmatrix}$$

Proof. With $\tilde{R}_k := R_k - \rho\, e_k e_k^*$ such that $e_k^* \tilde{R}_k = 0$,

we have $H_k = \tilde{Q}_k\,\tilde{R}_k + \mu$.

$$e_k^*\tilde{R}_k\tilde{Q}_k = 0, \ \ \tilde{R}_k\tilde{Q}_k[e_1, \ldots, e_{k-1}] = R_k\underline{Q}_{k-1} - \rho\, e_k e_k^*\,\underline{Q}_{k-1}$$
$$= R_k\underline{Q}_{k-1} - \eta\, e_k e_{k-1}^*.$$

Hence $\qquad \tilde{Q}_k^*\, H_k\, \tilde{Q}_k = \tilde{R}_k\,\tilde{Q}_k + \mu = \begin{bmatrix}\widetilde{H}_{k-1} & * \\ 0 & \mu\end{bmatrix}$

[Ruhe 84,93]

$\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ orthogonal basis search space.

Put $\qquad \mathbf{V}_k = [\mathbf{v}_1|\ldots|\mathbf{v}_k]$.

RKS (Rational Krylov Sequence)

Select $\ \mu_k \in \mathbb{C}, \ \ \vec{t} \in \mathbb{C}^k$.

Compute expansion vector $\mathbf{v}_{k+1}$ as

$$\mathbf{v}_{k+1} = \text{modGS}_{\mathbf{V}_k}\left((\mathbf{A} - \mu_k\,\mathbf{B})^{-1}\mathbf{B}\mathbf{V}_k\,\vec{t}\right).$$

Then $\quad \mathbf{A}\,\mathbf{V}_{k+1}\,\vec{h} = \mathbf{B}\,\mathbf{V}_{k+1}\,\left(\mu_k\,\vec{h} + \vec{t}\right)$.

Hence $\qquad \boxed{\mathbf{A}\,\mathbf{V}_{k+1}\,\underline{H}_k = \mathbf{B}\,\mathbf{V}_{k+1}\,\underline{K}_k}$

with $(\underline{H}_k, \underline{K}_k)$ strongly irreducible Hessenberg

Solve $\ (K_k - \theta\, H_k)\,\vec{y} = 0$. Take $\ \mathbf{u} := \mathbf{V}_{k+1}\,\underline{H}_k\,\vec{y}$.

Suppose $\underline{H}_k$ and $\underline{K}_k$ are Hessenberg.

Definition.

- $\underline{H}_k$ is **irreducible** if $h_{j+1,j} \neq 0 \ \ \forall j$
- $(\underline{H}_k, \underline{K}_k)$ **strongly irreducible** if

  $\underline{H}_k$ irreducible and
  $\underline{K}_k - \mu\,\underline{H}_k$ full rank $\ \forall\mu$.

Property. If $\underline{H}_k$ is irreducible then

$$\underline{K}_k = \underline{H}_k\, D + T$$

for some diagonal $D = D(\underline{H}_k, \underline{K}_k)$
and upper triangular $T = T(\underline{H}_k, \underline{K}_k)$.

Proof. $\quad D = \text{diag}(k_{j+1,j}/h_{j+1,j})$.

In RKS: $\quad D = \text{diag}(\mu_1, \ldots, \mu_k)$
$\qquad\qquad T = [\vec{t}_1, \ldots, \vec{t}_k]$.

A RKS expansion step

$$\mathbf{A}\,\mathbf{V}_k\,\underline{H}_{k-1} = \mathbf{B}\,\mathbf{V}_k\,\underline{K}_{k-1}$$

Select a $\mu \in \mathbb{C}$ and a $\vec{t} \in \mathbb{C}^k$

Solve $\tilde{\mathbf{v}}$ from $(\mathbf{A} - \mu\,\mathbf{B})\tilde{\mathbf{v}} = \mathbf{V}_k\,\vec{t}$

$\vec{h} = \mathbf{V}_k^*\,\tilde{\mathbf{v}}$, $\tilde{\mathbf{v}} \leftarrow \tilde{\mathbf{v}} - \mathbf{V}_k\,\vec{h}$

$h = \|\tilde{\mathbf{v}}\|$, $\mathbf{v}_{k+1} = \tilde{\mathbf{v}}/h$

$\mathbf{V}_{k+1} = [\mathbf{V}_k \,|\, \mathbf{v}_{k+1}]$

$\underline{H}_k = \begin{bmatrix} \underline{H}_{k-1} & \vec{h} \\ 0\dots0 & h \end{bmatrix}$, $\underline{K}_k = \begin{bmatrix} \underline{K}_{k-1} & \mu\,\vec{h} + \vec{t} \\ 0\dots0 & \mu\,h \end{bmatrix}$

$$\mathbf{A}\,\mathbf{V}_{k+1}\,\underline{H}_k = \mathbf{B}\,\mathbf{V}_{k+1}\,\underline{K}_k$$

Selecting the anti-shift μ_k

Examples

- $\mu_k = \theta$, $\vec{t} = \vec{y}$ with $(K_k - \theta\,H_k)\,\vec{y} = 0$.

However:
LU-factorisation $\mathbf{A} - \mu_k\,\mathbf{B}$ may be expensive.

- $\mu_k = \mu_\ell$, $\vec{t} = e_k$

- $\mu_k = \mu_\ell$, $\vec{t} = \vec{y}$

$$\boxed{\mathbf{A}\,\mathbf{V}_{k+1}\,\underline{H}_k = \mathbf{B}\,\mathbf{V}_{k+1}\,\underline{K}_k}$$

$(K_k - \theta\,H_k)\,\vec{y} = 0$, $\qquad \mathbf{u} := \mathbf{V}_{k+1}\,\underline{H}_k\,\vec{y}$

The RKS residual

$$\begin{aligned} \mathbf{r} &:= (\mathbf{A} - \theta\,\mathbf{B})\mathbf{u} \\ &= (\mathbf{A} - \theta\,\mathbf{B})\mathbf{V}_{k+1}\,\underline{H}_k\,\vec{y} \\ &= \mathbf{B}\mathbf{V}_{k+1}\,(\underline{K}_k - \theta\,\underline{H}_k)\,\vec{y} \end{aligned}$$

$$\mathbf{r} = (k_{k+1\,k} - \theta\,h_{k+1\,k})\;e_k^*\vec{y}\;\mathbf{B}\mathbf{v}_{k+1}$$

$$\|\mathbf{r}\| = \|\mathbf{B}\mathbf{v}_{k+1}\|\,|k_{k+1\,k} - \theta\,h_{k+1\,k}|\,|e_k^*\vec{y}|$$

$\underline{H}_k$, $\underline{K}_k$ Hessenberg. $\quad \underline{H}_k$ with QR-decomp.

$$\underline{H}_k = \underline{Q}_k\,R_k.$$

Let $q \in \mathbb{C}^{k+1}$, $\|q\| = 1$ such that $q^*\underline{Q}_k = 0$.

$\underline{Z}_{k-1}$ orthogonal $k \times (k-1)$ Hessenberg s.t.

$$q^*\,\underline{K}_k\,\underline{Z}_{k-1} = 0$$

Put

$$\underline{\widetilde{H}}_{k-1} := \underline{Q}^*\,\underline{H}_k\,\underline{Z}_{k-1} \;\&\; \underline{\widetilde{K}}_{k-1} := \underline{Q}^*\,\underline{K}_k\,\underline{Z}_{k-1}$$

Lemma.
$(\underline{\widetilde{H}}_{k-1}, \underline{\widetilde{K}}_{k-1})$ is strongly irreducible
if $(\underline{H}_k, \underline{K}_k)$ is strongly irreducible.

$$\boxed{\begin{array}{l} \mathbf{C}\,\mathbf{V}_{k+1}\,\underline{K}_k = \mathbf{V}_{k+1}\,\underline{H}_k \quad \text{with} \\ (\underline{H}_k, \underline{K}_k) \text{ strongly irr. Hessenberg,} \end{array}}$$

Lemma. Factorize $\quad \underline{K}_k - \sigma\,\underline{H}_k = \underline{Q}_k\,R_k$.
With q and $\underline{Z}_{k-1}$ such that
$[\underline{Q}_k, q]$ unitary and
$[\underline{Z}_{k-1}, (\bar{\sigma}\underline{K}_k + \underline{H}_k)^*\,q]$ unitary Hessenberg

With
$$\begin{aligned} \widetilde{\mathbf{V}}_k &:= \mathbf{V}_{k+1}\,\underline{Q}_k \\ \underline{\widetilde{H}}_{k-1} &:= \underline{Q}_k^*\,\underline{H}_k\,\underline{Z}_{k-1} \\ \underline{\widetilde{K}}_{k-1} &:= \underline{Q}_k^*\,\underline{K}_k\,\underline{Z}_{k-1} \end{aligned}$$

we have $\quad \mathbf{C}\,\widetilde{\mathbf{V}}_k\,\underline{\widetilde{K}}_{k-1} = \widetilde{\mathbf{V}}_k\,\underline{\widetilde{H}}_{k-1}$,
$(\underline{\widetilde{H}}_{k-1}, \underline{\widetilde{K}}_{k-1})$ strongly irr. Hessenberg,
$D(\underline{\widetilde{H}}_{k-1}, \underline{\widetilde{K}}_{k-1}) := \text{diag}(\mu_2, \dots, \mu_k)$.

$\mu_k = 0 \;\Rightarrow\; \text{span}(\mathbf{I} - \sigma\,\mathbf{C})\mathbf{V}_k = \text{span}\big(\widetilde{\mathbf{V}}_k\big)$.

$$\boxed{\begin{array}{l} \mathbf{A}\,\mathbf{V}_{k+1}\,\underline{H}_k = \mathbf{B}\,\mathbf{V}_{k+1}\,\underline{K}_k \quad \text{with} \\ (\underline{H}_k, \underline{K}_k) \text{ strongly irr. Hessenberg,} \end{array}}$$

Theorem. For $\tau_1, \dots, \tau_\ell$, consider

$$\Phi := \prod_{j=1}^{\ell} (\mathbf{A} - \mu_{k+1-j}\mathbf{B})^{-1}(\mathbf{A} - \tau_j\,\mathbf{B})$$

Then $\;\mathbf{A}\,\widetilde{\mathbf{V}}_{k+1-\ell}\,\underline{\widetilde{H}}_{k-\ell} = \mathbf{B}\,\widetilde{\mathbf{V}}_{k+1-\ell}\,\underline{\widetilde{K}}_{k-\ell}$
$(\underline{\widetilde{H}}_{k-\ell}, \underline{\widetilde{K}}_{k-\ell})$ strongly irr. Hessenberg,
$D(\underline{\widetilde{H}}_{k-\ell}, \underline{\widetilde{K}}_{k-\ell}) := \text{diag}(\mu_{\ell+1}, \dots, \mu_k)$.
$\text{span}\Big(\Phi\left(\mathbf{V}_{k+1-\ell}\right)\Big) = \text{span}\Big(\widetilde{\mathbf{V}}_{k+1-\ell}\Big)$

Proof. With $\mathbf{C}_j := (\mathbf{A} - \mu_{k+1-j}\mathbf{B})^{-1}\mathbf{B}$, $\sigma_j := \tau_j - \mu_{k+1-j}$

$$(\mathbf{A} - \mu_{k+1-j}\mathbf{B})^{-1}(\mathbf{A} - \tau_j\,\mathbf{B}) = \mathbf{I} - \sigma_j\,\mathbf{C}_j$$

An implicitly restarted RKS step

$\sigma_j = \tau_j - \mu_{k+1-j}$,

Set $\underline{H} = \underline{H}_k$, $\underline{K} = \underline{K}_k$, $\tilde{Q} = \underline{I}_k$

For $j = 1, \dots, \ell$ do
  Factorise $\underline{K} - \sigma_j\,\underline{H} = \underline{Q}\,R$
  Compute q such that $[\underline{Q}, q]$ unitary
  Compute $\underline{Z}$ such that
    $[\underline{Z}, (\bar{\sigma}_j\,\underline{K} + \underline{H})^*q]$ unitary Hess.
  Compute $\quad \underline{H} \leftarrow \underline{Q}^*\,\underline{H}\,\underline{Z}$
    $\underline{K} \leftarrow \underline{Q}^*\,\underline{K}\,\underline{Z}$
    $\underline{\tilde{Q}} \leftarrow \underline{\tilde{Q}}\,\underline{Q}$
end for

Set $\quad \underline{\widetilde{H}}_{k-\ell} = \underline{H}$, $\underline{\widetilde{K}}_{k-\ell} = \underline{K}$

Compute $\quad \widetilde{\mathbf{V}}_{k+1-\ell} = \mathbf{V}_{k+1}\,\underline{\tilde{Q}}$,

Alternatives

Davidson's method [Davidson '75]

$$\mathbf{z} = (\text{diag}(\mathbf{A}) - \theta\,\mathbf{I})^{-1}\mathbf{r}$$

with $\quad \mathbf{r} := \mathbf{A}\mathbf{u} - \theta\,\mathbf{u}$ $\;(\mathbf{u} := \mathbf{V}y,\; \mathbf{V}^*\mathbf{A}\mathbf{V}y = \theta y)$.

Generalized Davidson [Morgan '90]

$$\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{I} \quad \text{and} \quad \mathbf{z} = \mathbf{M}^{-1}\mathbf{r}$$

If $\quad \mathbf{z} = (\mathbf{A} - \theta\,\mathbf{I})^{-1}\mathbf{r}$ $\quad$ then **stagnation**.

If $\quad \mathbf{z} = \mathbf{r} = (\mathbf{A} - \theta\,\mathbf{I})\mathbf{u}$ $\quad$ then **Arnoldi**:
$\text{span}(\mathbf{v}_1, \dots, \mathbf{v}_k, \mathbf{A}\mathbf{v}_k) =$
$\qquad \text{span}(\mathbf{v}_1, \dots, \mathbf{v}_k, (\mathbf{A} - \theta\,\mathbf{I})\mathbf{u})$.

Expansion with Ritz vectors

$$\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{I}$$

Inexact Shift-and-Invert,

$$\mathbf{z} = \mathbf{M}^{-1}\mathbf{v}_k,$$

aims for eigensolution $\mathbf{M}$.

Generalized Davidson,

$$\mathbf{z} = \mathbf{M}^{-1}(\mathbf{A} - \theta\,\mathbf{I})\mathbf{u},$$

aims for eigensolution $\mathbf{M}^{-1}(\mathbf{A} - \lambda\,\mathbf{I})\mathbf{x}_\lambda = 0$.

A Gen. Davidson $\approx$ Cayley Transform Arnoldi:

$$\mathbf{z} = (\mathbf{A} - \tau\,\mathbf{I})^{-1}(\mathbf{A} - \sigma\,\mathbf{I})\mathbf{u}.$$

Exponential Arnoldi (for efficient expansion):

$$\mathbf{z} = \exp(\mathbf{A} - \theta\,\mathbf{I})\mathbf{u} \quad (\approx \mathbf{U}[\exp(H')e_1]\,).$$

$$\boxed{\mathbf{A}\,\mathbf{x}_\lambda = \lambda\,\mathbf{x}_\lambda}$$

Towards optimal expansion

Consider the Ritz approximation $(\theta, \mathbf{u} := \mathbf{V}y)$.

$$\theta := \frac{\mathbf{u}^*\mathbf{A}\,\mathbf{u}}{\mathbf{u}^*\mathbf{u}}, \qquad \mathbf{r} := \mathbf{A}\,\mathbf{u} - \theta\,\mathbf{u} \perp \mathbf{V}$$

Find $\mathbf{z} \perp \mathbf{u}$ such that $\mathbf{x}_\lambda = \mathbf{u} + \mathbf{z}$.

$$(\mathbf{A} - \lambda\,\mathbf{I})\,\mathbf{z} = -\mathbf{r} + (\lambda - \theta)\,\mathbf{u}$$

or, equivalently,

$$\begin{cases} \mathbf{u}^*\mathbf{A}\mathbf{x}_\lambda = \lambda\,\mathbf{u}^*\mathbf{x}_\lambda \\ \left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)(\mathbf{A} - \lambda\,\mathbf{I})\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r} \end{cases}$$

[S. & van der Vorst '96]

Jacobi-Davidson

Since λ is unknown:

solve $\mathbf{z} \perp \mathbf{u}$ (approximately) from

the correction equation

$$\boxed{\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)(\mathbf{A} - \theta\,\mathbf{I})\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}}$$

[S., van der Vorst '96]

Jacobi-Davidson

1. **Start:**
   Choose initial orth. matrix $\mathbf{V}$.
2. **Repeat:**
   - Compute $\mathbf{W} \leftarrow \mathbf{A}\mathbf{V}$, $H \leftarrow \mathbf{V}^*\mathbf{W}$.
   - Compute a desired eigenpair (θ, y) of H (with $\|\,y\,\| = 1$).
   - Compute $\mathbf{u} \leftarrow \mathbf{V}y$, $\mathbf{r} \leftarrow \mathbf{A}\,\mathbf{u} - \theta\,\mathbf{u}$.
   - **Stop if** satisfied.
   - Solve (approximately) $$(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,(\mathbf{A} - \theta\,\mathbf{I})\,(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,\mathbf{z} = -\mathbf{r}.$$
   - $\mathbf{V} \leftarrow$ ModGS($[\,\mathbf{V}\,|\,\mathbf{z}\,]$)

Solve approximately

$$\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)(\mathbf{A} - \theta\,\mathbf{I})\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}.$$

Any preconditioned it. method can be used.

Preconditioning: $\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{I}$

Preconditioning equation:

$$\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{M}\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}$$

Solution:

$$\mathbf{M}\,\mathbf{z} = -\mathbf{r} + \alpha\,\mathbf{u} \quad \text{such that} \quad \mathbf{z} \perp \mathbf{u},$$

or

$$\mathbf{z} = -\mathbf{M}^{-1}\mathbf{r} + \alpha\,\mathbf{M}^{-1}\mathbf{u} \quad \& \quad \alpha = \frac{\mathbf{u}^*\mathbf{M}^{-1}\mathbf{z}}{\mathbf{u}^*\mathbf{M}^{-1}\mathbf{u}}.$$

Solve approximately

$$\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)(\mathbf{A} - \theta\,\mathbf{I})\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}$$

$$\neq$$

Solve approximately

$$\left.\begin{array}{l}(\mathbf{A} - \theta\,\mathbf{I})\,\mathbf{z}_r = \mathbf{r} \\ (\mathbf{A} - \theta\,\mathbf{I})\,\mathbf{z}_u = \mathbf{u}\end{array}\right\} \;\&\; \begin{array}{l}\mathbf{z} = -\mathbf{z}_r + \alpha\,\mathbf{z}_u \\ \text{s.t. } \mathbf{z} \perp \mathbf{u}\end{array}$$

except if

"solve appr." = 1 step with fixed precond. $\mathbf{M}$.

Example. With static polynomial method p:

$$p\left(\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)(\mathbf{A} - \theta\,\mathbf{I})\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\right) \neq$$

$$\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)p\,(\mathbf{A} - \theta\,\mathbf{I})\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)$$

Related methods

with $\mathbf{M}$ a fixed preconditioner

Expand the search space by the sol. $\mathbf{z}$ of

- $\mathbf{M}\,\mathbf{z} = -\mathbf{r} + \alpha\,\mathbf{u}$ & $\alpha = \mathbf{u}^*\mathbf{M}^{-1}\mathbf{z}/\mathbf{u}^*\mathbf{M}^{-1}\mathbf{u}$
  Olsen's method ['90 for symm. $\mathbf{A}$]
- $\mathbf{M}\,\mathbf{z} = -\mathbf{r}$
  Generalized Davidson [Morgan '90]
- $\mathbf{M}\,\mathbf{z} = \mathbf{u}$
  Inexact Shift-and-Invert.

$$\mathbf{z} = -\mathbf{M}^{-1}\mathbf{r} + \alpha\,\mathbf{M}^{-1}\mathbf{u}$$

Extreme choices

- $\mathbf{M} = \mathbf{I}$:
  $\mathbf{z} = -\mathbf{r} + \alpha\,\mathbf{u} = -\mathbf{A}\,\mathbf{u} + (\theta + \alpha)\mathbf{u} \sim \mathbf{A}\,\mathbf{u}$.

  J-D $\equiv$ Gen. Dav. $\equiv$ Arnoldi.
  Inexact Shift-and-Invert stagnates.
- $\mathbf{M} = \mathbf{A} - \theta\,\mathbf{I}$:
  $\mathbf{z} = -\mathbf{u} + \alpha\,(\mathbf{A} - \theta\,\mathbf{I})^{-1}\mathbf{u} \sim (\mathbf{A} - \theta\,\mathbf{I})^{-1}\mathbf{u}$.

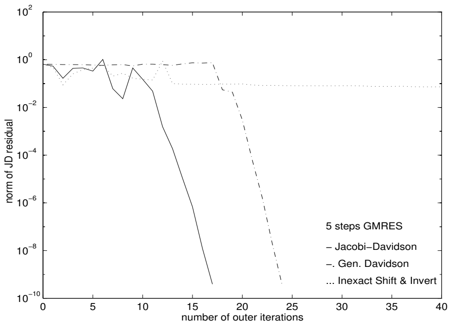
  J-D $\equiv$ Shift-and-Invert with optimal shift.
  Generalized Davidson stagnates.

$\lambda \approx 0$, $\mathbf{A} = \text{SHERMAN4} - .5\,\mathbf{I}$, $n = 1104$

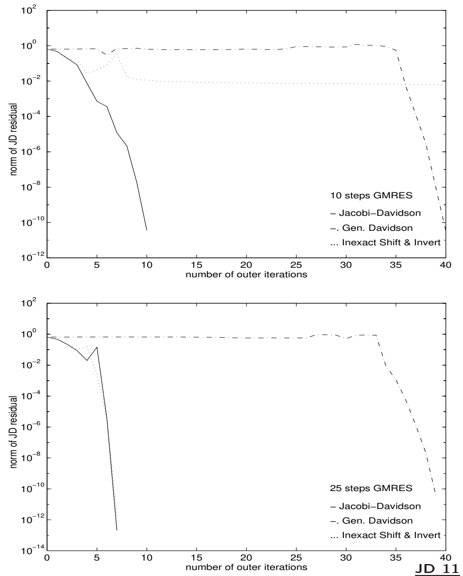
CorEq:

- $(\mathbf{I}-\mathbf{u}\,\mathbf{u}^*)(\mathbf{A}-\theta\,\mathbf{I})(\mathbf{I}-\mathbf{u}\,\mathbf{u}^*)\,\mathbf{z}=-\mathbf{r}$ [J-D]
- $(\mathbf{A}-\theta\,\mathbf{I})\,\mathbf{z}=-\mathbf{r}$ ["Davidson"]
- $(\mathbf{A}-\theta\,\mathbf{I})\,\mathbf{z}=\mathbf{u}$ ["Shift-and-Invert"]

m steps precond. GMRES with $\mathbf{M} = \text{ILU}(2)$.

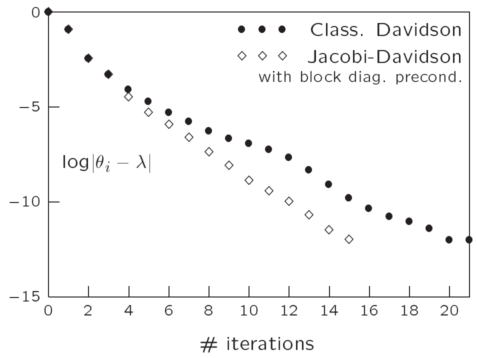


$m = 5$



[van Dam, van Lenthe '94]

Example [Quantum Chemistry]



$\mathbf{A}$ symmetric, $n \approx 50{,}000$

block diag. precond. with max. block size 66

J-D as a Newton scheme

Choose scaling vectors $\tilde{\mathbf{u}}$ and $\mathbf{w}$.

$$\mathbf{F}(\mathbf{u}) \equiv \mathbf{A}\,\mathbf{u} - \theta\,\mathbf{u}, \qquad \theta \equiv \theta(\mathbf{u}) \equiv \frac{\mathbf{w}^*\mathbf{A}\,\mathbf{u}}{\mathbf{w}^*\mathbf{u}}$$

$$\mathbf{F} : \{\mathbf{u}, \tilde{\mathbf{u}}^*\mathbf{u} = 1\} \to \{\mathbf{r} = \mathbf{F}(\mathbf{u}) \perp \mathbf{w}\}$$

$$\boxed{\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x} \quad \& \quad \tilde{\mathbf{u}}^*\mathbf{x} = 1} \quad \Leftrightarrow \quad \boxed{\mathbf{F}(\mathbf{x}) = 0}$$

Newton:

- solve $\mathbf{z} \perp \tilde{\mathbf{u}}$

$$\frac{\partial\,\mathbf{F}}{\partial\,\mathbf{u}}\mathbf{z} = -\mathbf{r} \equiv -\mathbf{F}(\mathbf{u})$$

- $\mathbf{u} \leftarrow \mathbf{u} + \mathbf{z}$

For $\mathbf{z} \perp \tilde{\mathbf{u}}$, $\displaystyle\frac{\partial\,\mathbf{F}}{\partial\,\mathbf{u}}\mathbf{z} = \left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{u}}\right)(\mathbf{A}-\theta\,\mathbf{I})\,\mathbf{z}$

Accelerated Newton:

- solve $\mathbf{z} \perp \tilde{\mathbf{u}}$

$$\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{u}}\right)(\mathbf{A}-\theta\,\mathbf{I})\left(\mathbf{I} - \frac{\mathbf{u}\,\tilde{\mathbf{u}}^*}{\tilde{\mathbf{u}}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}$$

- accelerated update

Inexact Newton: $\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{I}$.

Solve $\displaystyle\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{u}}\right)\mathbf{M}\left(\mathbf{I} - \frac{\mathbf{u}\,\tilde{\mathbf{u}}^*}{\tilde{\mathbf{u}}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}$:

$$\mathbf{z} = -\mathbf{M}^{-1}\mathbf{r} + \alpha\,\mathbf{M}^{-1}\mathbf{u} \quad \& \quad \alpha = \frac{\tilde{\mathbf{u}}^*\mathbf{M}^{-1}\mathbf{r}}{\tilde{\mathbf{u}}^*\mathbf{M}^{-1}\tilde{\mathbf{u}}}$$

$\alpha = 0$ if $\mathbf{M}$ maps $\tilde{\mathbf{u}}^\perp$ onto $\mathbf{w}^\perp$

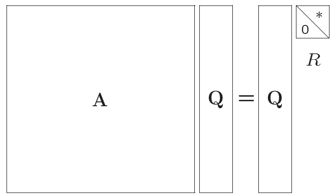
JDQR

[Fokkema, S, van der Vorst '96]

Compute m eigenvalues close to some $\tau \in \mathbb{C}$.

- Deflation
- Schur vectors
- Restart

Partial Schur form



$\mathbf{A}\,\mathbf{Q} = \mathbf{Q}\,R$ with $\mathbf{Q}^*\mathbf{Q} = \mathbf{I}$

R upper Δ

diag$(R) = (\lambda_1, \ldots, \lambda_m)$

$|\lambda_i - \tau|$ increases

If $R\,y_i = \lambda_i\,y_i$ then $\mathbf{A}\,\mathbf{Q}\,y_i = \lambda_i\,\mathbf{Q}\,y_i$.

Finding other eigenpairs

Expansion of the partial Schur form:

$$\mathbf{A}\,[\,\mathbf{Q}\,|\,\mathbf{q}\,] = [\,\mathbf{Q}\,|\,\mathbf{q}\,]\begin{bmatrix} R & s \\ & \lambda \end{bmatrix}$$

with $\mathbf{Q}^*\mathbf{q} = 0$.

Hence

$$(\mathbf{I}-\mathbf{Q}\,\mathbf{Q}^*)(\mathbf{A}-\lambda\,\mathbf{I})(\mathbf{I}-\mathbf{Q}\,\mathbf{Q}^*)\mathbf{q} = \mathbf{0}$$

which means that $(\lambda, \mathbf{q})$ is an eigenpair of $\widetilde{\mathbf{A}}$:

$$\widetilde{\mathbf{A}} := (\mathbf{I}-\mathbf{Q}\,\mathbf{Q}^*)(\mathbf{A}-\lambda\,\mathbf{I})(\mathbf{I}-\mathbf{Q}\,\mathbf{Q}^*)$$

JDQR: apply JD for $\widetilde{\mathbf{A}}$.

1. **Start:** Choose an initial space $\mathbf{V}$.
   - Set $\Lambda = [\,]$, $\mathbf{Q} = [\,]$
2. **Repeat:**
   a. Compute $\mathbf{W} \leftarrow \mathbf{A}\mathbf{V}$, $\quad H \leftarrow \mathbf{V}^*\mathbf{W}$

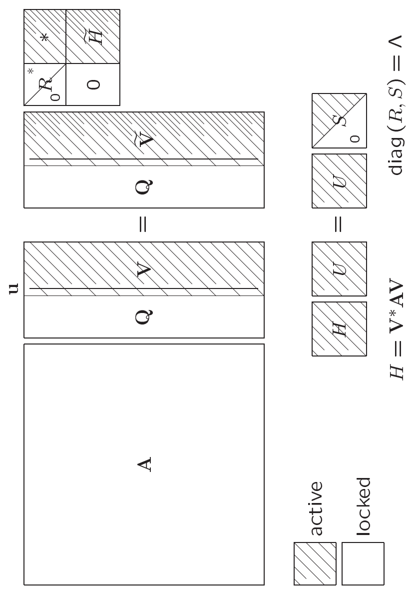
   b. Compute $H = USU^*$
   with $U^*U = I$, $\quad S$ upper Δ,
   $|S_{11} - \tau| \leq |S_{22} - \tau| \leq \ldots$.

   c. $\theta \leftarrow S_{11}$, $y \leftarrow Ue_1$, $\mathbf{u} \leftarrow \mathbf{V}y$,
   $\mathbf{r} \leftarrow \mathrm{ModGS}_{\mathbf{Q}}(\mathbf{A}\,\mathbf{u} - \theta\,\mathbf{u})$.

   d. **If** $\|\mathbf{r}\| \leq$ *tol*
   - $\Lambda \leftarrow [\Lambda\,|\,\theta]$, $\quad \mathbf{Q} \leftarrow [\mathbf{Q}\,|\,\mathbf{u}]$.
   - $J = [e_2\,|\,\ldots\,|\,e_{\mathrm{dim}(\mathbf{V})}]$,
     $\mathbf{V} \leftarrow \mathbf{V}(UJ)$, $U \leftarrow I$, $S \leftarrow J^*SJ$.
   - **Goto** 2.c.

   e. Solve (app.) $\mathbf{z} \perp \widetilde{\mathbf{Q}} \equiv [\mathbf{Q}\,|\,\mathbf{u}]$
   $(\mathbf{I} - \widetilde{\mathbf{Q}}\widetilde{\mathbf{Q}}^*)\,(\mathbf{A} - \theta\,\mathbf{I})\,(\mathbf{I} - \widetilde{\mathbf{Q}}\widetilde{\mathbf{Q}}^*)\,\mathbf{z} = -\mathbf{r}$.

   f. $\mathbf{V} \leftarrow \mathrm{ModGS}([\mathbf{V}\,|\,\mathbf{z}])$



Solving the preconditioning eq.

$$(\mathbf{I} - \mathbf{Q}\mathbf{Q}^*)\,\mathbf{M}\,(\mathbf{I} - \mathbf{Q}\mathbf{Q}^*)\,\mathbf{z} = -\mathbf{r}.$$

$\mathbf{M}\,\mathbf{z} = -\mathbf{r} + \mathbf{Q}\,y \quad$ such that $\quad \mathbf{z} \perp \mathbf{Q}$

$\Rightarrow$

$$\mathbf{z} = -\mathbf{M}^{-1}\mathbf{r} + \mathbf{M}^{-1}\mathbf{Q}\,y$$

& $\quad y = \underbrace{(\mathbf{Q}^*\,\mathbf{M}^{-1}\,\mathbf{Q})}_{\text{small matrix}}{}^{-1}\,\mathbf{Q}^*\,\mathbf{M}^{-1}\mathbf{r}.$

Restart

For λ close to a given **target** $\tau \in \mathbb{C}$

- For $\mathbf{V}$, compute $H := \mathbf{V}^*\mathbf{A}\mathbf{V}$

$$\left.\begin{array}{c} H = USU^* \text{ with } U^*U = I, \\ S \text{ upper triangular} \end{array}\right\} \text{QR}$$

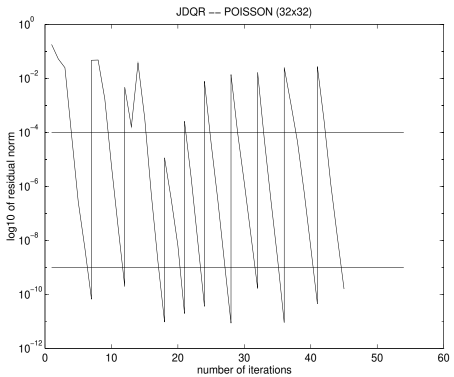
- Order S such that $\quad |s_{j,j} - \tau| \quad$ increases.
- Restart with $\mathbf{V} \leftarrow \mathbf{V}[u_1, \ldots, u_\ell]$ if necessary.

Properties JDQR

- Leads to partial Schur form.
- Employs orthonormal sets of vectors.
- Finds also multiple eigenvalues.
- Easy selection of wanted eigenvalues.
- No matrix inversion involved.
- Preconditioner can be included.
- Ingredients:
  vector updates, Dot-products, MVs,
  preconditioners
  QR for small problems.

Some practical notes

- After convergence of some eigenvectors, solution of correction equation easier.
- Number of pojections can be limited.
- Correction equation can be preconditioned.
  Preconditioner can be used more often:
  pays to make better preconditioning.
- For generalized eigenproblems:
  JD + QZ-reduction



2D Poisson Problem (32×32)
Target = 0d0
Max Dim = 15, Min Dim = 10
GMRES(10) plus ILU(0)
eps = 1d-9


```
lambda( 1): ( 9.0562E-03, 0.0000E+00 )
lambda( 2): ( 2.2599E-02, 0.0000E+00 )
lambda( 3): ( 2.2599E-02, 0.0000E+00 )
lambda( 4): ( 3.6143E-02, 0.0000E+00 )
lambda( 5): ( 4.5035E-02, 0.0000E+00 )
lambda( 6): ( 4.5035E-02, 0.0000E+00 )
lambda( 8): ( 5.8578E-02, 0.0000E+00 )
lambda( 7): ( 5.8578E-02, 0.0000E+00 )
lambda( 9): ( 7.6160E-02, 0.0000E+00 )
lambda(10): ( 7.6160E-02, 0.0000E+00 )
```

2D Poisson Problem (32×32)
Target = 0d0
Max Dim = 15, Min Dim = 10
GMRES(10) with ILU(0)
eps = 1d-9

Examples

Maximum dimension $\mathbf{V}$ is 15,

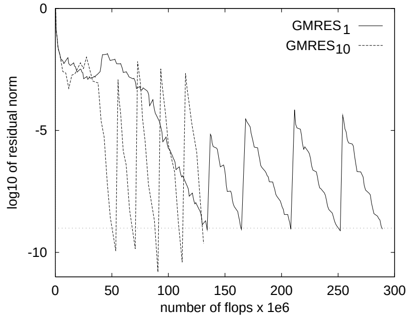
after restart dimension $\mathbf{V}$ is 10.

Accuracy correction equation: $\|\tilde{\mathbf{r}}_i\| \leq 2^{-j}\|\tilde{\mathbf{r}}_0\|$

DW4096: Square Dielectric Waveguide
standard eigenproblem

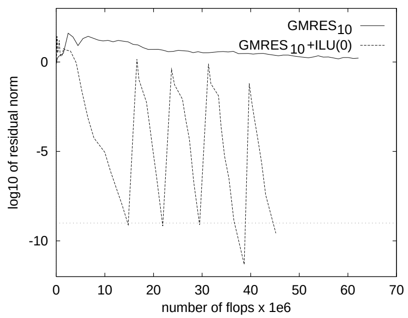
Searching for the five rightmost eigenvalues:

$$8.6479e-01, \quad 8.6528e-01, \quad 8.6564e-01, \quad 8.6594e-01, \quad 8.6657e-01$$



BWM2000: Brusselator wave model
standard eigenproblem

Searching for the five rightmost eigenvalues.



Generalized eigenproblems

$$\mathbf{A}\,\mathbf{x}_\lambda = \lambda\,\mathbf{B}\,\mathbf{x}_\lambda$$

$\mathbf{V}$ <u>search space</u>, $\quad$ $\mathbf{W}$ <u>test space</u>

- Petrov-Galerkin approach:

$$\mathbf{W}^*\,\mathbf{A}\,\mathbf{V}\,y - \theta\,\mathbf{W}^*\,\mathbf{B}\,\mathbf{V}\,y = 0.$$

$$\mathbf{u} = \mathbf{V}\,y, \qquad \mathbf{r} := \mathbf{A}\,\mathbf{u} - \theta\,\mathbf{B}\,\mathbf{u}$$

- The correction equation:

$$\left(\mathbf{I} - \frac{\tilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\tilde{\mathbf{w}}}\right)(\mathbf{A} - \theta\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{u}\,\tilde{\mathbf{u}}^*}{\tilde{\mathbf{u}}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}$$

<u>**Th.**</u> $\quad \mathbf{w} \in \mathbf{W} \quad \& \quad \tilde{\mathbf{w}} = (\alpha\mathbf{A} + \beta\mathbf{B})\,\mathbf{u}$

& exact solve $\Rightarrow$ quadratic convergence.

$$\boxed{(\mathbf{A} - \lambda\,\mathbf{B})\,\mathbf{x} = 0}$$

Split $\quad \mathbf{x} = \mathbf{u} + \mathbf{z}_e \quad$ with $\quad \mathbf{z}_e \perp \tilde{\mathbf{u}}$.

$\mathbf{z}$ is the computed correction, $\quad \mathbf{z} \perp \tilde{\mathbf{u}}$.

Note $\quad \mathbf{x} - \mathbf{u} = \mathbf{z}_e, \quad \mathbf{x} - (\mathbf{u} + \mathbf{z}) = \mathbf{z}_e - \mathbf{z}$.

$(\mathbf{A} - \theta\,\mathbf{B})\,\mathbf{z}_e = -\mathbf{r} + (\lambda - \theta)\mathbf{B}\mathbf{x}, \qquad \mathbf{z}_e \perp \tilde{\mathbf{u}}$.

$\mathbf{P}(\mathbf{A} - \theta\,\mathbf{B})\,\mathbf{z} = -\mathbf{r}, \qquad \mathbf{z} \perp \tilde{\mathbf{u}}$

where $\quad \mathbf{P} \equiv \left(\mathbf{I} - \frac{\tilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\tilde{\mathbf{w}}}\right)$.

Hence $\quad \mathbf{P}(\mathbf{A} - \theta\,\mathbf{B})_{|\tilde{\mathbf{u}}^\perp}(\mathbf{z}_e - \mathbf{z}) = \mathbf{P}(\lambda - \theta)\,\mathbf{B}\mathbf{x}$.

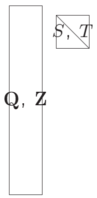
$$\lambda - \theta = \frac{\mathbf{w}^*(\mathbf{A} - \theta\,\mathbf{B})\mathbf{z}_e}{\mathbf{w}^*\mathbf{B}\mathbf{x}} = \mathcal{O}(\|\,\mathbf{z}_e\|).$$

$$\mathbf{P}\mathbf{B}\mathbf{x} = \mathcal{O}(\|\mathbf{x} - \mathbf{u}\|) = \mathcal{O}(\|\,\mathbf{z}_e\|) \quad \text{iff} \quad \mathbf{P}\mathbf{B}\mathbf{u} = 0.$$

Partial generalized Schur form

$\mathbf{A}\,\mathbf{Q} = \mathbf{Z}\,S \qquad \mathbf{Q}, \mathbf{Z}$ orth.,

$\mathbf{B}\,\mathbf{Q} = \mathbf{Z}\,T \qquad S, T$ upper $\triangle$.



$\mathbf{A}\,\mathbf{Q} = \mathbf{B}\,\mathbf{Q}\,\underbrace{T^{-1}S}_{\text{upper } \triangle} \qquad$ span$(\mathbf{Z})$ = span$(\mathbf{B}\,\mathbf{Q})$ = span$(\mathbf{C}\,\mathbf{Q})$

$\mathbf{C} := \alpha\,\mathbf{A} + \beta\,\mathbf{B}$

$\mathbf{Z}^*\mathbf{A}\,\mathbf{Q} = S \qquad \mathbf{V} \ni \mathbf{u} \rightarrow$ first column $\mathbf{Q}$

$\mathbf{Z}^*\mathbf{B}\,\mathbf{Q} = T \qquad \mathbf{W} \ni \mathbf{w} \rightarrow$ first column $\mathbf{Z}$

Natural choices in connection with QZ:

span$(\mathbf{W})$ = span$(\mathbf{C}\,\mathbf{V})$, $\quad \mathbf{w} = \mathbf{C}\,\mathbf{u}$.

Choosing spaces & projections

Select $\alpha, \beta \in \mathbb{C}$. $\quad$ Consider $\mathbf{C} := \alpha\,\mathbf{A} + \beta\,\mathbf{B}$.

$$\mathbf{u} = \mathbf{V}\,y, \quad \mathbf{r} = \mathbf{A}\,\mathbf{u} - \theta\,\mathbf{B}\,\mathbf{u}, \quad \mathbf{w} = \mathbf{C}\,\mathbf{u}$$

- The correction equation:

$$\left(\mathbf{I} - \frac{\mathbf{w}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{w}}\right)(\mathbf{A} - \theta\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}.$$

- The search space and test space:

$\mathbf{V}$ = modGS $([\,\mathbf{V}\,|\,\mathbf{z}\,])$, $\quad \mathbf{W}$ = modGS $([\,\mathbf{W}\,|\,\mathbf{C}\,\mathbf{z}\,])$

Preconditioning

$$\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{B}$$

$$\left(\mathbf{I} - \frac{\mathbf{w}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{w}}\right)\mathbf{M}\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}.$$

<u>Explicit left preconditioning</u>:

- The correction equation:

$$\left(\mathbf{I} - \frac{\mathbf{v}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{v}}\right)\mathbf{M}^{-1}(\mathbf{A} - \theta\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{v}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{v}}\right)\mathbf{z} = -\mathbf{r}'.$$

where

$$\mathbf{M}\,\mathbf{v} = \mathbf{w} = \mathbf{B}\,\mathbf{u} \quad \& \quad \mathbf{r}' = \left(\mathbf{I} - \frac{\mathbf{v}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{v}}\right)\mathbf{r}.$$

Choosing the mixture of $\mathbf{A}$ and $\mathbf{B}$

Aim for optimal appr. first "left Schur vector"

$$\mathbf{w} = \alpha\,\mathbf{A}\,\mathbf{u} + \beta\,\mathbf{B}\,\mathbf{u}$$

Inspiration:

$\mathbf{B} = \mathbf{I}$: choose $\quad \mathbf{w} = \mathbf{u} = 0\,\mathbf{A}\,\mathbf{u} + 1\,\mathbf{B}\,\mathbf{u}$.

$\mathbf{A} = \mathbf{I}$: choose $\quad \mathbf{w} = \mathbf{u} = 1\,\mathbf{A}\,\mathbf{u} + 0\,\mathbf{B}\,\mathbf{u}$.

$\mathbf{w} = 1\,\mathbf{A}\,\mathbf{u} + 0\,\mathbf{B}\,\mathbf{u}$ is "instable" choice

if $\mathbf{B} = \mathbf{I}$ and $\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \approx \mathbf{0}$

Select α, β such that

— $|\alpha|^2 + \beta^2 = 1$, $\beta \geq 0$, and

— $\|\alpha\,\mathbf{A}\,\mathbf{u} + \beta\,\mathbf{B}\,\mathbf{u}\|$ approximately maximal:

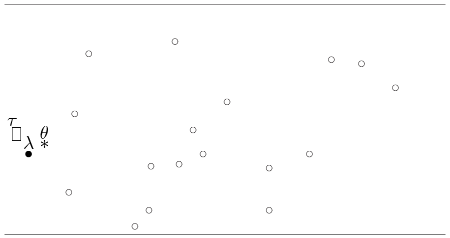
$$\mathbf{C} = \frac{\bar{\tau}}{\sqrt{1+|\tau|^2}}\mathbf{A} + \frac{1}{\sqrt{1+|\tau|^2}}\mathbf{B}$$

Selecting Ritz pairs

Suppose $\mathbf{A}$ normal, $\mathbf{B} = \mathbf{I}$.

$$\theta = \sum_i |\gamma_i|^2 \lambda_i \quad \text{with} \quad \mathbf{u} = \sum_i \gamma_i \mathbf{x}_i$$

Suppose τ outside hull spectrum:



If $\theta \approx \tau$ then wanted component large.

What if τ is in the interior of the hull spectrum?

Harmonic Ritz values

$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0} \quad \Leftrightarrow \quad (\mathbf{A} - \tau\,\mathbf{I})^{-1}\mathbf{x} = \frac{1}{\lambda - \tau}\mathbf{x}$:

if $\lambda \approx \tau$ then $1/(\lambda - \tau)$ extremal for $(\mathbf{A} - \tau\,\mathbf{I})^{-1}$.

<u>How to avoid inversion?</u>

Galerkin for $(\mathbf{A} - \tau\,\mathbf{I})^{-1}$, with

search space = test space = span($(\mathbf{A} - \tau\,\mathbf{I})\mathbf{V}$),

is equivalently to Petrov for $\mathbf{A}$, with

search space: $\mathbf{V}$; test space: $\mathbf{W} = (\mathbf{A} - \tau\,\mathbf{I})\mathbf{V}$.

Harmonic Ritz value := this Petrov value

For generalized eigenproblems, take

$$\text{span}(\mathbf{W}) = \text{span}((\mathbf{A} - \tau\,\mathbf{B})\mathbf{V}),$$

$$\mathbf{C} = \frac{1}{\sqrt{1+|\tau|^2}}\mathbf{A} - \frac{\tau}{\sqrt{1+|\tau|^2}}\mathbf{B}.$$

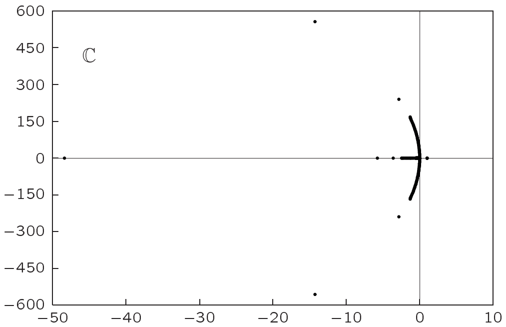
The problem

$$\boxed{\mathbf{A}\,\mathbf{x}_\lambda = \lambda\,\mathbf{B}\,\mathbf{x}_\lambda}$$

For MHD-problems:

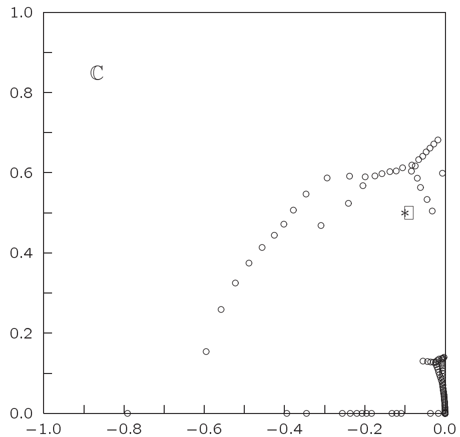
- $\mathbf{A}$ is non Hermitian
- $\mathbf{B}$ Hermitian, posidtive definite
- $\mathbf{A}$, $\mathbf{B}$ block tridiagonal
- interior eigenvalues
- very large order
- inversion unpractical

Spectrum MHD test problem

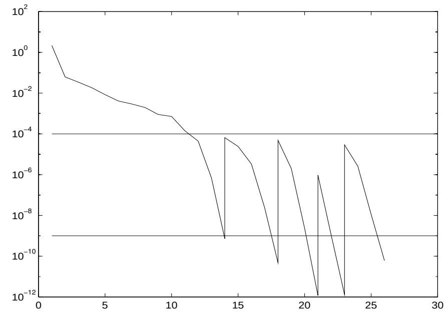


Entire spectrum MHD test problem ($n = 416$).
Correct eigenvalues (.) are shown.

Alfvén spectrum



MHD test problem ($n = 416$).
Correct eigenvalues ($\circ$), target ($*$).



MHD Problem (416)

Target = (-0.3, 0.5)

Max Dim = 15, Min Dim = 10

GMRES(10) with ILU(2)

eps = 1d-9


```
lambda( 1): ( -3.0929E-01, 4.6875E-01 )
lambda( 2): ( -3.4656E-01, 5.4689E-01 )
lambda( 3): ( -2.4103E-01, 5.2381E-01 )
lambda( 4): ( -3.7810E-01, 5.0716E-01 )
lambda( 5): ( -2.9401E-01, 5.8715E-01 )
```

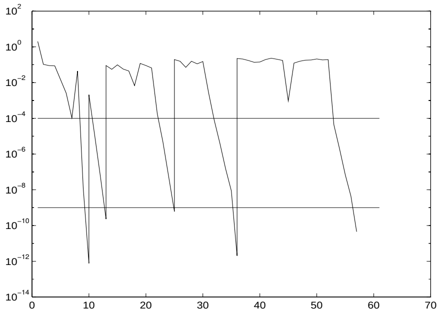
MHD Problem (416)

Target = (-0.3, 0.5)

Max Dim = 15, Min Dim = 10

GMRES(10) with ILU(2)

eps = 1d-9



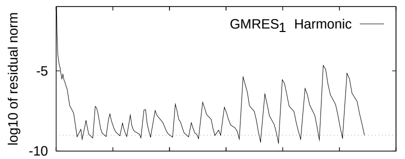
MHD Problem (1600)
Target = (-0.3, 0.5)
Max Dim = 15, Min Dim = 10
GMRES(10) with ILU(2)
eps = 1d-9

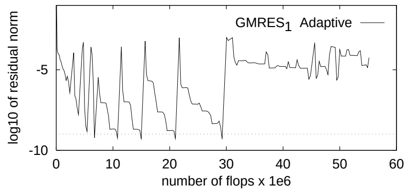
```
lambda( 1): ( -3.3746E-01, 4.8958E-01 )
lambda( 2): ( -3.5776E-01, 4.6050E-01 )
lambda( 3): ( -2.3839E-01, 4.4657E-01 )
lambda( 4): ( -3.8189E-01, 5.0369E-01 )
lambda( 5): ( -2.2157E-01, 5.3364E-01 )
```

MHD Problem (1600)
Target = (-0.3, 0.5)
Max Dim = 15, Min Dim = 10
GMRES(10) with ILU(2)
eps = 1d-9

MHD416

Searching for the Alfvén branch





ILU(2) for $\mathbf{A} - \tau\mathbf{B}$ is used as preconditioner.

Generalized eigenproblems

$$\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{B}\,\mathbf{x}$$

[Booten, Fokkema **MHD**]

$$\mathbf{P}(\lambda)\mathbf{x} := \mathbf{A}_0\,\mathbf{x} + \lambda\,\mathbf{A}_1\,\mathbf{x} + \ldots + \lambda^\ell\,\mathbf{A}_\ell\,\mathbf{x} = 0$$

[van Gijzen, Raeven **acoustics, con. mech.**]

- $$\mathbf{W}^*\mathbf{P}(\theta)\mathbf{V}y = 0$$
  $$\mathbf{u} = \mathbf{V}y, \quad \mathbf{w} = \mathbf{P}'(\theta)\mathbf{u}, \quad \mathbf{r} = \mathbf{P}(\theta)\mathbf{u}$$
- The correction equation:
  $$\left(\mathbf{I} - \frac{\mathbf{w}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{w}}\right)\mathbf{P}(\theta)\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}$$
- The spaces: $\mathbf{V} = \text{modGS}\,([\,\mathbf{V}\,|\,\mathbf{z}\,])$, ...

J-D

- is an accelerated inexact Newton scheme
  — quadratic convergence —
- relies on orthogonal projections
- allows any precond. it. method
  to solve the linear (Jacobian) system
- robust
- no inversion
- also for interior eigenvalues

J-D is not

- a Krylov subspace method,
- Davidson with Jacobi-preconditioning,
- a method that produces eigenvectors for
  a preconditioned eigenproblem

Current research

- Fine tuning inner-outer loop and problem.
- Assembly strategies.
- Stopping criterion.
- **Preconditioner.**
- Tracking strategies.

What to use?

- For small problems: QR-algorithm
- If matrices can be inverted
(systems can be solved exactly):
Shift-&-Invert Arnoldi with implicit restart
[Sorensen '92]
Rational Krylov Sequence with implicit restart
[Ruhe '84, '93]
- If matrix inversion is not feasible: JD