New Approaches to Generalized Problem

$$\boxed{\mathbf{Ax} = \mathbf{Bx}\lambda}$$

- Subspace Projection Framework
- Truncated Reduction to Condensed Form
- The QZ-method and Implicit Restarting
- Another Point of View –

  Projection onto Generated and Derived Spaces
- Shift-Invert, Projection, Newton Sequences

Partial Reduction to Condensed Form

Motivation:

$$\begin{aligned} \mathbf{AV} &= \mathbf{WH}, \\ \mathbf{BV} &= \mathbf{WR}. \end{aligned}$$

Truncate:

$$\begin{aligned} \mathbf{AV}_k &= \mathbf{W}_k\mathbf{H}_k + \mathbf{F}_k \ , \quad \text{with} \quad \mathbf{W}_k^T\mathbf{F}_k = 0, \\ \mathbf{BV}_k &= \mathbf{W}_k\mathbf{R}_k, \end{aligned}$$

$\mathbf{V}_k$ and $\mathbf{W}_k$ orthonormal

$\mathbf{H}_k$ Hessenberg
$\mathbf{R}_k$ Triangular

Two Points of View

- Truncate Reduction to Condensed Form
  - Generalize Arnoldi/Lanczos

- Generate a **V** - sequence ... Derive a **W** - sequence
  - Generate **V** sequence to contain Newton Steps
  - Generate **V** sequence to contain Pre-conditioned or quasi-Newton Steps

Generalize Arnoldi ($\mathbf{B} = \mathbf{I}$)

k-step Arnoldi reduction

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_k\mathbf{H}_k + \mathbf{F}_k,$$

with $\mathbf{V}_k^T\mathbf{V}_k = \mathbf{I}_k$ and $\mathbf{V}_k^T\mathbf{F}_k = 0$.

Krylov property implies $\mathbf{F}_k = \mathbf{f}_k e_k^T$

$$\mathbf{F}_k = (\mathbf{I} - \mathbf{V}_k\mathbf{V}_k^T)\mathbf{A}\mathbf{V}_k.$$

Generalize Projection for $\mathbf{Ax} = \mathbf{Bx}\lambda$

k-step generalized Arnoldi reduction

$$\begin{aligned} \mathbf{F}_k &= (\mathbf{I} - \mathbf{W}_k \mathbf{W}_k^T)\mathbf{A}\mathbf{V}_k, \\ \mathbf{B}\mathbf{V}_k &= \mathbf{W}_k \mathbf{R}_k. \end{aligned}$$

where $\mathbf{W}_k^T \mathbf{W}_k = \mathbf{V}_k^T \mathbf{V}_k = \mathbf{I}_k$.

Note: $\mathbf{F}_k$ is orthogonal to $Range(\mathbf{B}\mathbf{V}_k)$,

Relation to Standard Arnoldi

Substitution $\mathbf{V}_k = \mathbf{B}^{-1}\mathbf{W}_k\mathbf{R}_k$
gives both

$$(\mathbf{A}\mathbf{B}^{-1})\mathbf{W}_k = \mathbf{W}_k\hat{\mathbf{H}}_k + \hat{\mathbf{f}}_k\mathbf{e}_k^T$$

and

$$(\mathbf{B}^{-1}\mathbf{A})\mathbf{V}_k = \mathbf{V}_k\tilde{\mathbf{H}}_k + \tilde{\mathbf{f}}_k\mathbf{e}_k^T$$

where $\hat{\mathbf{H}}_k = \mathbf{H}_k\mathbf{R}_k^{-1}$, $\tilde{\mathbf{H}}_k = \mathbf{R}_k^{-1}\mathbf{H}_k$

and $\hat{\mathbf{f}}_k = \mathbf{f}_k/\rho_{kk}$, $\tilde{\mathbf{f}}_k = \mathbf{B}^{-1}\mathbf{f}_k$,

Remark:

Replace$\mathbf{A}$ with $\mathbf{B}$

Replace $\mathbf{B}$ with $\mathbf{A} - \sigma\mathbf{B}$

Equivalent to shift-invert Arnoldi with $(\mathbf{A} - \sigma\mathbf{B})^{-1}\mathbf{B}$.

Generated and Derived Spaces

Generated sequence $\{\mathbf{v}_j\}$

What is required for rapid convergence?

Generate Derived $\mathbf{W}$ Sequence

Partial Reduction of the pair $(\mathbf{A}, \mathbf{B})$

$$\begin{aligned} \mathbf{V}_j &\leftarrow (\mathbf{V}_{j-1}, \mathbf{v}_j); \\ \mathbf{B}\mathbf{V}_j &= \mathbf{W}_j \mathbf{R}_j; \\ \mathbf{A}\mathbf{V}_j &= \mathbf{W}_j \mathbf{H}_j + \mathbf{F}_j; \end{aligned}$$

with $\mathbf{W}_j^T \mathbf{W}_j = \mathbf{V}_j^T \mathbf{V}_j = \mathbf{I}_j, \quad \mathbf{W}_j^T \mathbf{F}_j = 0$
Use classical Gram Schmidt othogonalization (with DGKS).

Newton-Like Methods

Suppose $\mathbf{H}\mathbf{y} = \mathbf{R}\mathbf{y}\theta$ and $\mathbf{x} = \mathbf{V}\mathbf{y}$

with $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$ and let $\lambda \in \sigma(\mathbf{A}, \mathbf{B})$ closest to θ

Let $\mathbf{q}$ corresponding eigenvector normalized $\mathbf{x}^H\mathbf{q} = 1$

Represent

$$\mathbf{q} = \mathbf{x} + \delta\mathbf{x}, \quad \lambda = \theta + \delta\theta,$$

with $\mathbf{x}^H\delta\mathbf{x} = 0$

Use $\mathbf{A}\mathbf{q} = \mathbf{B}\mathbf{q}\lambda$.

Second Order Approximation

$$(\mathbf{A} - \theta\mathbf{B})\delta\mathbf{x} = -(\mathbf{A} - \theta\mathbf{B})\mathbf{x} + \delta\theta\mathbf{B}\mathbf{x} + \delta\theta\mathbf{B}\delta\mathbf{x}$$

Newton-Like Methods contd. – JDQR

Since $\mathbf{x} = \mathbf{V}\mathbf{y}$,

$$-(\mathbf{A} - \theta\mathbf{B})\mathbf{x} + \delta\theta\mathbf{B}\mathbf{x} = -\mathbf{F}\mathbf{y} + \delta\theta\mathbf{W}\mathbf{R}\mathbf{y}$$

Plug in and Project both sides with $\mathbf{I} - \mathbf{W}\mathbf{W}^H$

$$(\mathbf{I} - \mathbf{W}\mathbf{W}^H)(\mathbf{A} - \theta\mathbf{B})(\mathbf{I} - \mathbf{V}\mathbf{V}^H)\delta\mathbf{x} = -\mathbf{F}\mathbf{y}$$

Take $\mathbf{v} = (\mathbf{I} - \mathbf{V}\mathbf{V}^H)\delta\mathbf{x}$ normalized.

Assures second order correction is a member of the updated spaces $\mathcal{S}_{\mathbf{V}}$ and $\mathcal{S}_{\mathbf{W}}$ when $\mathbf{v}$ is adjoined

Reduced Basis - Molecular Dynamics

Typical Molecular Dynamics Simulation

$$m\ddot{\mathbf{x}}(t) = -\nabla\mathcal{V}(\mathbf{x}),$$

with $\mathbf{x}(0) = \mathbf{x}_o$ and $\dot{\mathbf{x}}(t)$ from a Gaussian distribution for the corresponding temperature

Form

$$\mathbf{C} = (\mathbf{x}_1, \mathbf{x}_2, ...\mathbf{x}_m)$$

$$\mathbf{C} = \mathbf{U}\mathbf{S}\mathbf{V}^T \approx \mathbf{U}_k(\mathbf{S}_k)\mathbf{V}^T \;\text{ and }\; \mathbf{x}_j \approx (\mathbf{U}_k)\mathbf{y}_j$$

where $\mathbf{y}_j = (\mathbf{S}_k)\mathbf{V}\mathbf{e}_j$

Reduced Basis:

Substitute $\mathbf{x} = \mathbf{U}_k\mathbf{y}$, and then

$$m(\mathbf{U}_k)\ddot{\mathbf{y}} \; - \nabla\mathcal{V}(\mathbf{U}_k\mathbf{y})$$

Obtain $\mathbf{y}$ by solving the reduced equation

$$m\ddot{\mathbf{y}} \; - \mathbf{U}_k^T(\nabla\mathcal{V}(\mathbf{U}_k\mathbf{y}) \;\text{ with }\; \mathbf{x}(t) \approx \mathbf{U}_k\mathbf{y}(t)$$

Update SVD and Visualize

Update and Trucate SVD as time history evolves

Use Spatial Co-ordinates to locate active sites

Zoom and Replay active site trajectory

Potential for Data Compression is Enormous and Essential

Conclusions

1. Most important research topic:

   - Spectral Enhancement (Pre-Conditioning) without a factorization or accurate solve

2. To get the ARPACK software and other info

   visit `http://www.caam.rice.edu/software/ARPACK`

   Also see Netlib –Scalapack Directory