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Dynamical systems and Iterative Eigensolvers

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Non Hermitian Eigenvalue problem

$$\mathbf{A}\mathbf{p} = \mathbf{B}\mathbf{p}\lambda \quad \mathbf{A}, \mathbf{B} \in \mathbb{C}^{n \times n} \quad \mathbf{p} \in \mathbb{C}^{n}$$

- Suppose the matrices are large and only available via matrix vector products
- Only want a small number of eigenvalues and eigenvectors, say the leftmost

$$\mathrm{Re}(\lambda_1) < \mathrm{Re}(\lambda_2) \leq \cdots \leq \mathrm{Re}(\lambda_n)$$

- Let’s review standard approaches

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Standard approach

$$(\mathbf{A} - \mathbf{B}\sigma)^{-1}\mathbf{B}\mathbf{p} = \mathbf{p}(\lambda - \sigma)^{-1}$$

- Shift-invert spectral transformation (for eigenvalues near the shift σ)
- Inverse subspace iteration (simple but slow to converge)
- Shift-invert Arnoldi/Lanczos method (better convergence but not nearly as simple as inverse subspace iteration)

Computational bottleneck

- Solving the linear system at each iteration
- Sparse direct solves or preconditioned inner iterations required
- can we avoid an inner iteration altogether and just apply a preconditioner (including the identity)?

K-eigenvalue problem

- Determine whether there is self-sustaining time-independent chain reaction in neutron transport calculations (criticality problem)
- Smallest eigenvalue is the effective number of neutrons created; magnitude determines whether there is a self-sustaining reaction. Eigenvector represents the asymptotic power distribution
- Six dimensional Boltzman transport leads to huge non Hermitian eigenvalue problems (30,000,000)
- **Krylov Subspace Iterations for Deterministic k-Eigenvalue Calculations,** (J. S. Warsa, T. A. Warming, J. E. Morel and J. M. McGhee, L.), Nuclear Science and Engineering 2004

Some notation

$$\mathbf{A} \in \mathbb{C}^{n \times n}$$

$$(\mathbf{p}, \mathbf{q}) \in \mathbb{C}$$

$$\mathbf{p}, \mathbf{q} \in \mathbb{C}^{n}$$

$$(\mathbf{p}, \mathbf{q}) = \mathbf{q}^{H} \mathbf{p}$$

Dynamical system

$$\dot{\mathbf{p}} = \mathbf{p}\frac{(\mathbf{A}\mathbf{p}, \mathbf{p})}{(\mathbf{p}, \mathbf{p})} - \mathbf{A}\mathbf{p}, \quad \mathbf{p}(0) = \mathbf{p}_0$$

$$\mathbf{A}\mathbf{x}_i = \mathbf{x}_i \lambda_i, \quad \mathbf{p}(0) = \mathbf{x}_i$$

$$\Rightarrow \dot{\mathbf{p}} = 0 \Rightarrow \mathbf{p} = \mathbf{x}_i$$

Simple iteration

$$\dot{\mathbf{p}} = \mathbf{p}\frac{(\mathbf{A}\mathbf{p}, \mathbf{p})}{(\mathbf{p}, \mathbf{p})} - \mathbf{A}\mathbf{p}, \quad \mathbf{p}(0) = \mathbf{p}_0$$

$$\mathbf{p}_{j+1} = \mathbf{p}_j + h\left(\frac{(\mathbf{A}\mathbf{p}_j, \mathbf{p}_j)}{(\mathbf{p}_j, \mathbf{p}_j)} - \mathbf{A}\right)\mathbf{p}_j$$

First integral (or invariant)

$$\dot{\mathbf{p}} = \mathbf{p}\frac{(\mathbf{A}\mathbf{p},\mathbf{p})}{(\mathbf{p},\mathbf{p})} - \mathbf{A}\mathbf{p}, \quad \mathbf{p}(0) = \mathbf{p}_0$$

$$\begin{aligned} \frac{d}{dt}(\mathbf{p},\mathbf{p}) &= (\dot{\mathbf{p}},\mathbf{p}) + (\mathbf{p},\dot{\mathbf{p}}) \\ (\mathbf{p},\mathbf{p}) &= (\mathbf{p}_0,\mathbf{p}_0) \end{aligned}$$

Gradient flows

$$\begin{aligned} \mathbf{A} &= \mathbf{A}^{\star} \\ \phi(\mathbf{p}) &= \frac{(\mathbf{A}\mathbf{p},\mathbf{p})}{(\mathbf{p},\mathbf{p})} \\ \dot{\mathbf{p}} &= -\frac{(\mathbf{p},\mathbf{p})}{2}\nabla\phi(\mathbf{p}) \end{aligned}$$

- Dynamical systems community has studied gradient flows

Solutions of the dynamical system

- Apparently, the *flow* of the dynamical system must lie on a constant energy surface, or manifold
- Should the flow of the discrete dynamical system lie on the manifold? Does it matter?
- If so, how should we do this?

Related work

- Others have observed the connection of the eigenvalue problem with a dynamical system

1. Chu (1988) considered continuous realizations of iterative process
2. Symes (1982) and Nanda (1985) drew relationships between the QR algorithm and differential equations
3. See survey paper by Absil (2006)
4. Optimization and Dynamical systems, Helmke and Moore
5. The simple iteration forms the basis of gradient based preconditioned eigensolvers when applied to a symmetric positive definite eigenvalue problems (Knyazev (1998))
6. Car-Parrinello use a second order ODE for computing ground-states

Our contribution

- Non-Hermitian eigenvalue problems
- Convergence analysis for the continuous and discrete dynamical system
- Role of preconditioning
- Exploit the quadratic invariant

Continuous flow (Nanda 1985)

$$\dot{\mathbf{p}} = \mathbf{p}\frac{\left(\mathbf{Ap},\mathbf{p}\right)}{\left(\mathbf{p},\mathbf{p}\right)} - \mathbf{Ap}, \;\; \mathbf{A} \in \mathbb{R}^{n\times n}, \; \mathbf{p}(0) = \mathbf{p}_0$$

$$\mathbf{p}(t) = e^{-\mathbf{A}t}\mathbf{p}_0\omega(t)$$

$$\omega^2(t) = \frac{\left(\mathbf{p}_0,\mathbf{p}_0\right)}{\left(e^{-\mathbf{A}t}\mathbf{p}_0, e^{-\mathbf{A}t}\mathbf{p}_0\right)}$$

$$\left(\mathbf{p}(t),\mathbf{p}(t)\right) = \left(\mathbf{p}_0,\mathbf{p}_0\right)$$

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Convergence rate

$$\mathrm{Re}(\lambda_1) < \mathrm{Re}(\lambda_2) \le \cdots \le \mathrm{Re}(\lambda_n)$$

$$\begin{aligned}
\sin\angle(\mathbf{p},\mathbf{x}_1) &= \min_{\alpha\in\mathbb{C}} \|\alpha\mathbf{p}-\mathbf{x}_1\|, \quad \mathbf{A}\mathbf{x}_1 = \mathbf{x}_1\lambda_1 \\
&= \min_{\alpha\in\mathbb{C}} \|\alpha\mathbf{X}e^{-\mathbf{\Lambda}t}\mathbf{X}^{-1}\mathbf{p}_0-\mathbf{x}_1\|, \quad \mathbf{A}\mathbf{X} = \mathbf{X}\mathbf{\Lambda} \\
&\le \left\|\frac{e^{\lambda_1 t}}{\mathbf{y}_1^*\mathbf{p}_0}\mathbf{X}e^{-\mathbf{\Lambda}t}\mathbf{X}^{-1}\mathbf{p}_0-\mathbf{x}_1\right\| \\
&\le \|\mathbf{X}\|\,\|\mathbf{X}^{-1}\|\frac{\|\mathbf{p}_0\|}{|\mathbf{y}_1^*\mathbf{p}_0|}e^{\mathrm{Re}(\lambda_1-\lambda_2)t}
\end{aligned}$$

$\mathrm{Re}(\lambda_1 - \lambda_2)$ determines the convergence rate

Preconditioned iteration

$$\dot{\mathbf{p}} = \mathbf{N}^{-1}\left(\mathbf{p}\frac{(\mathbf{Ap},\mathbf{p})}{(\mathbf{p},\mathbf{p})} - \mathbf{Ap}\right)$$

$$\mathbf{p}_{j+1} \quad = \quad \mathbf{p}_j + h\mathbf{N}^{-1}\left(\frac{(\mathbf{Ap}_j,\mathbf{p}_j)}{(\mathbf{p}_j,\mathbf{p}_j)} - \mathbf{A}\right)\mathbf{p}_j$$

$$\frac{\left(\mathbf{NN}^{-1}\mathbf{Ap},\mathbf{p}\right)}{\left(\mathbf{NN}^{-1}\mathbf{p},\mathbf{p}\right)} = \frac{\left(\mathbf{Ap},\mathbf{p}\right)}{\left(\mathbf{p},\mathbf{p}\right)}$$

Why simple preconditioned iterations?

$$\begin{aligned} \mathbf{N} &= h\mathbf{A} \\ \mathbf{p}_{j+1} &= \mathbf{A}^{-1}\mathbf{p}_j \frac{(\mathbf{A}\mathbf{p}_j, \mathbf{p}_j)}{(\mathbf{p}_j, \mathbf{p}_j)} \end{aligned}$$

- Inverse iteration results when the preconditioner is selected judiciously
- We'll established convergence rates

Difference in Rayleigh-quotients

$$\begin{aligned}\mathbf{A}\mathbf{p} &= \mathbf{p}\lambda \\ \mathbf{N}^{-1}\mathbf{A}\mathbf{N}\hat{\mathbf{p}} &= \hat{\mathbf{p}}\lambda, \quad \mathbf{N}\hat{\mathbf{p}} = \mathbf{p} \\ \frac{(\mathbf{N}^{-1}\mathbf{A}\mathbf{N}\hat{\mathbf{p}}, \hat{\mathbf{p}})}{(\hat{\mathbf{p}}, \hat{\mathbf{p}})} &\neq \frac{(\mathbf{A}\mathbf{p}, \mathbf{p})}{(\mathbf{p}, \mathbf{p})}\end{aligned}$$

- Transforming the eigenvalue problem does not give the simple Rayleigh quotient.
- Hence we can't simply used previous analysis

Stability analysis for the one-sided preconditioned dynamical system

- We cannot derive a solution operator (unlike the unpreconditioned iteration)
- Resort to a non-linear stability analysis on a manifold—Center Manifold theorem
- If the dynamical system is sufficiently close to a stable steady-state, then the system converges to the left-most eigenpair

Center Manifold Theorem gives

$$\dot{\mathbf{p}} = \mathbf{N}^{-1}\mathbf{p}\frac{(\mathbf{A}\mathbf{p},\mathbf{p})}{(\mathbf{p},\mathbf{p})} - \mathbf{A}\mathbf{p}$$

$$\mathbf{A}\mathbf{x}_1 = \mathbf{x}_1\lambda_1, \quad \mathbf{p}(0) = \mathbf{x}_1$$

$$\Rightarrow \dot{\mathbf{p}} = 0 \Rightarrow \mathbf{p} = \mathbf{x}_1$$

$$\left\|\mathbf{p}(t) - \xi\mathbf{x}_1\right\| = O(e^{-\gamma t}), \quad \gamma > 0, t > 0$$

Need only assume that the Jacobian of the steady-state has a simple zero eigenvalue

$$\mathbf{N}^{-1}(\mathbf{I} - \mathbf{x}_1\mathbf{x}_1^*)(\lambda_1 - \mathbf{A})$$

What about the forward Euler (FE) discretization?

- FE does NOT preserve quadratic invariants and so we bound the departure
- Determine a critical time step
- Theorem on the global convergence of FE
- Assume real matrix A, Euclidean inner product

Departure from the manifold

$$0 \leq \frac{\mathbf{p}_{j+1}^T \mathbf{N} \mathbf{p}_{j+1} - \mathbf{p}_0^T \mathbf{N} \mathbf{p}_0}{\mathbf{p}_0^T \mathbf{N} \mathbf{p}_0} \leq (1 + h^2 M \|\mathbf{N}^{-1}\|^2)^{j+1} - 1,$$

the upper bound being asymptotic to $(j+1)h^2\|\mathbf{N}^{-1}\|^2 M$ *as* $h \to 0$.

$$M := \inf_{s \in \mathbb{R}} 4\|\mathbf{A} - s\|_{\mathbf{N}}^2$$

Critical time step

$$h\sqrt{j+1} \lesssim \frac{1}{\|\mathbf{N}^{-1}\|\sqrt{M}}$$

$$M := \inf_{s \in \mathbb{R}} 4\|\mathbf{A} - s\|_{\mathbf{N}}^2$$

FE convergence analysis

$$\mathbf{A} = \begin{bmatrix} \lambda_1 & \mathbf{d}^T \\ \mathbf{0} & \mathbf{C} \end{bmatrix}, \quad \mathbf{N} = \begin{bmatrix} \eta & \mathbf{0}^T \\ \mathbf{0} & \mathbf{M} \end{bmatrix}^{-1}$$

$$\gamma = \left\| (\mathbf{I} - \mathbf{x}_1 \mathbf{x}_1^*)(\mathbf{I} + h\mathbf{N}(\lambda_1 - \mathbf{A})) \right\| \in [0, \frac{1}{\sqrt{\kappa(\mathbf{N})}})$$

$$\kappa(\mathbf{N}) \equiv \left\| \mathbf{N} \right\| \left\| \mathbf{N}^{-1} \right\|$$

$$\sin(\angle(\mathbf{p}_j, \mathbf{x}_1)) = O(\gamma^j) = \left| \theta_j - \lambda_1 \right|$$

$$\mathbf{d} = \mathbf{0} \Rightarrow \left| \theta_j - \lambda_1 \right| = O(\gamma^{2j})$$

Summary of the proof

- Determine a Lipshitz constant so that FE gets close enough to the flow of the dynamical system
- Show that once we're close enough, then the iterates *remain* close
- Monotonic drift from the quadratic constraint is essential

FE convergence analysis: special case

$$\mathbf{A} = \begin{bmatrix} \lambda_1 & \mathbf{d}^T \\ \mathbf{0} & \mathbf{C} \end{bmatrix}, \quad \mathbf{C}\mathbf{C}^* = \mathbf{C}^*\mathbf{C}, \quad \mathbf{N} = \begin{bmatrix} \eta & \mathbf{0}^T \\ \mathbf{0} & \mathbf{I} \end{bmatrix}$$

$$\delta = \frac{\lambda_2 - \lambda_1}{\lambda_n - \lambda_1}, \quad \gamma = \frac{1-\delta}{1+\delta} < 1$$

$$\sin(\angle(\mathbf{p}_j, \mathbf{x}_1)) = O(\gamma^j) = \left|\theta_j - \lambda_1\right|$$

$$\mathbf{d} = \mathbf{0} \Rightarrow \left|\theta_j - \lambda_1\right| = O(\gamma^{2j})$$

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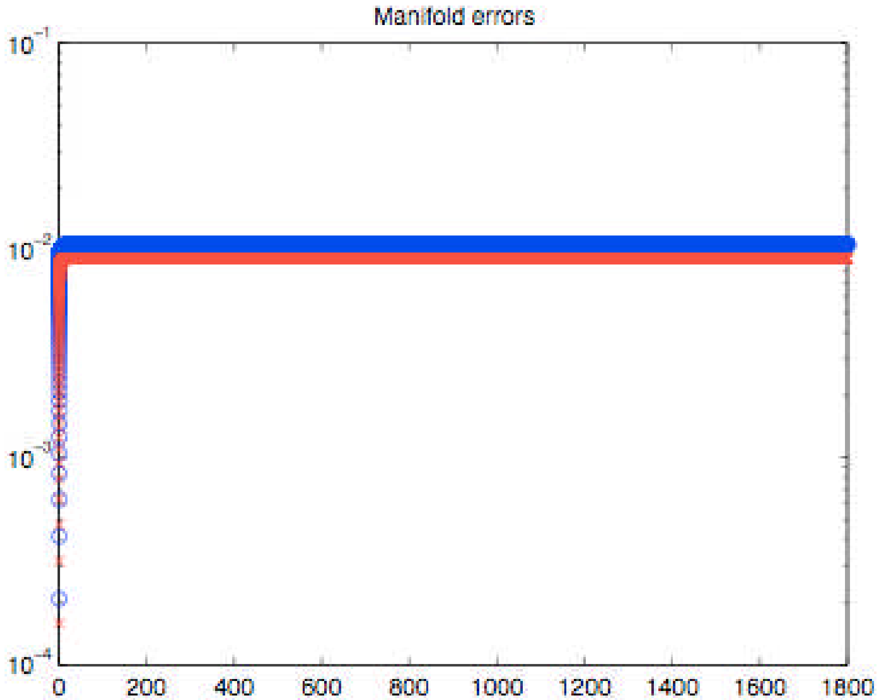
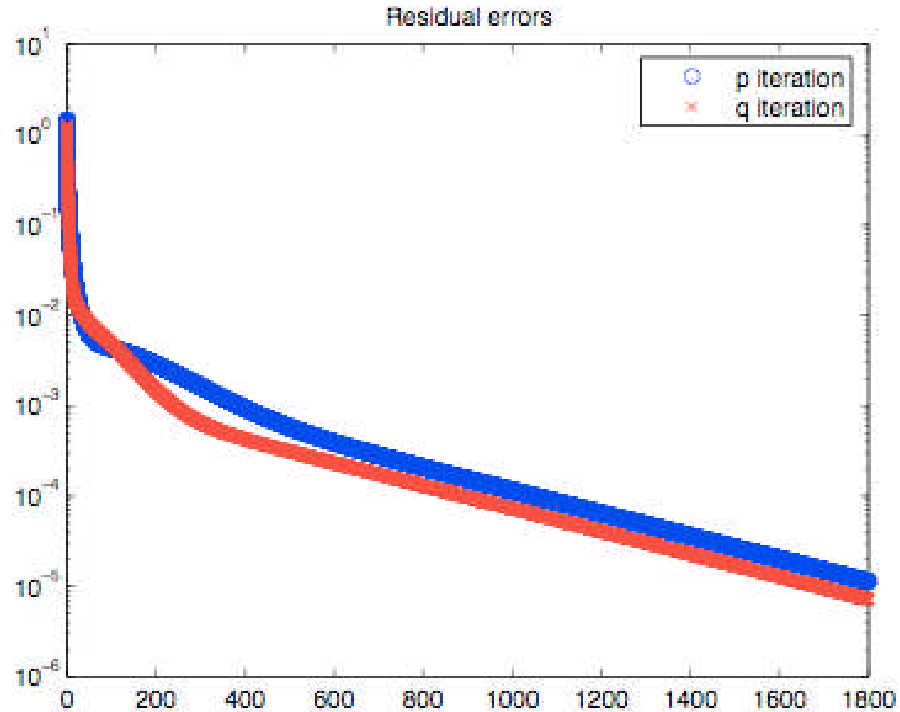
Sample problem

$$\mathbf{T}_\rho^n \equiv \begin{pmatrix} 2 & -1+\rho & & 0 \\ -1-\rho & 2 & \ddots & \\ & \ddots & \ddots & -1+\rho \\ 0 & & -1-\rho & 2 \end{pmatrix} \in \mathbb{R}^{n\times n}$$

One-sided FE, h=.1





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One versus two-sided flows

$$\begin{aligned}\dot{\mathbf{p}} &= \mathbf{p}\theta - \mathbf{A}\mathbf{p}, \quad \mathbf{p}(0) = \mathbf{p}_0 \\ \dot{\mathbf{q}} &= \mathbf{q}\tilde{\theta} - \mathbf{A}^\star\mathbf{q}, \quad \mathbf{q}(0) = \mathbf{q}_0\end{aligned}$$

- One sided equations are uncoupled

$$\begin{aligned}\theta &= \frac{(\mathbf{A}\mathbf{p}, \mathbf{p})}{(\mathbf{p}, \mathbf{p})} \\ \tilde{\theta} &= \frac{(\mathbf{A}\mathbf{q}, \mathbf{q})}{(\mathbf{q}, \mathbf{q})}\end{aligned}$$

- Two sided equations are coupled via the Rayleigh-quotients

$$\begin{aligned}\theta &= \frac{(\mathbf{A}\mathbf{p}, \mathbf{q})}{(\mathbf{p}, \mathbf{q})} \\ \tilde{\theta} &= \bar{\theta} = \frac{(\mathbf{q}, \mathbf{A}\mathbf{p})}{(\mathbf{q}, \mathbf{p})}\end{aligned}$$

Flows

- Two sided flow has the invariants

$$
\begin{aligned}
(\mathbf{p}, \mathbf{q}) &= (\mathbf{p}_0, \mathbf{q}_0) \\
(\mathbf{q}, \mathbf{p}) &= (\mathbf{q}_0, \mathbf{p}_0)
\end{aligned}
$$

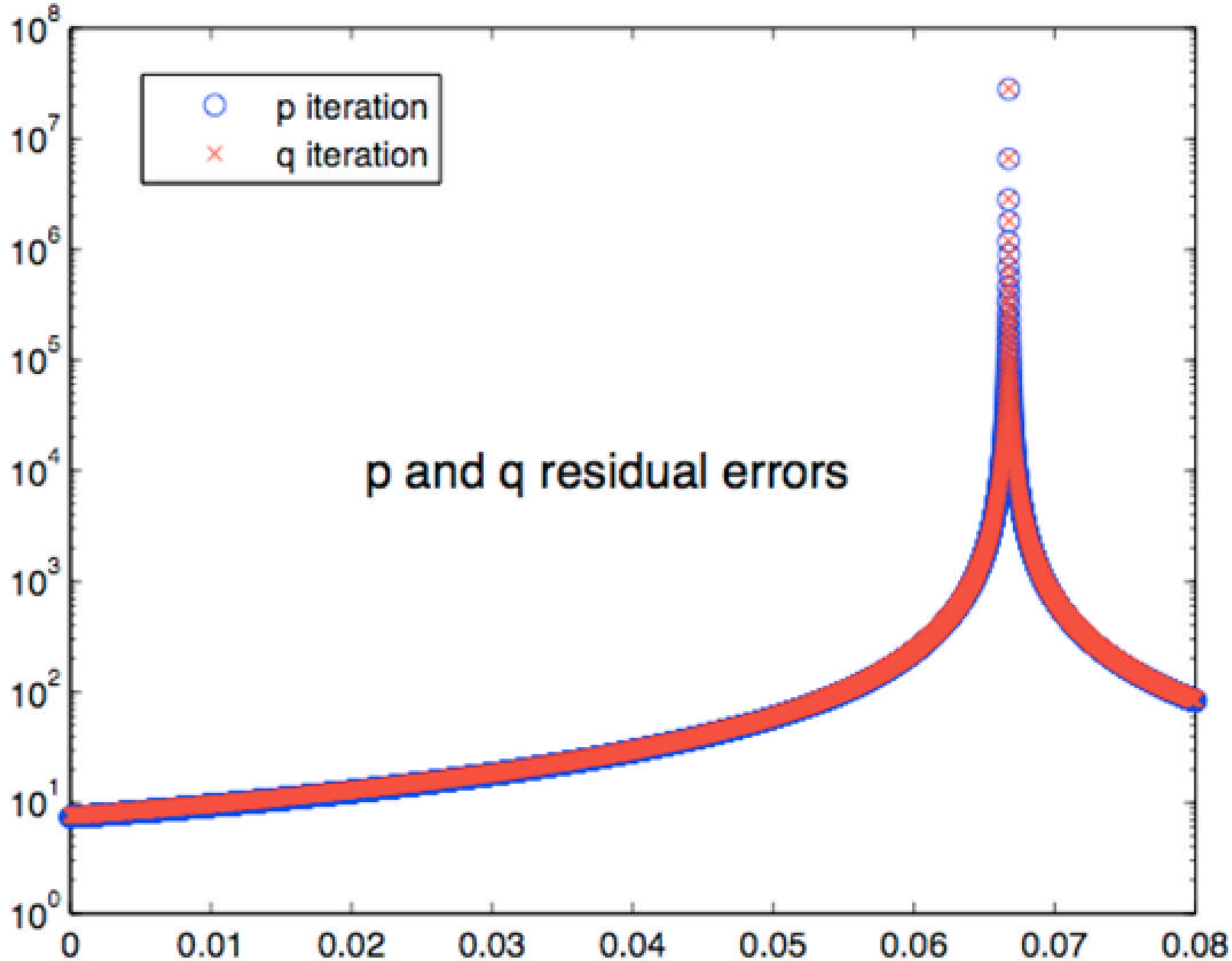
Two-sided flow

$$\begin{aligned}\dot{\mathbf{p}} &= \mathbf{p}\theta - \mathbf{A}\mathbf{p} \\ \dot{\mathbf{q}} &= \mathbf{q}\bar{\theta} - \mathbf{A}^{\star}\mathbf{q}\end{aligned} \qquad \theta = \frac{(\mathbf{A}\mathbf{p},\mathbf{q})}{(\mathbf{p},\mathbf{q})}, \quad \mathbf{p},\mathbf{q} \in \mathbb{C}^n$$

$$\mathbf{p} = e^{-\mathbf{A}t}\mathbf{p}_0\pi, \quad \mathbf{q} = e^{-\mathbf{A}^{\star}t}\mathbf{q}_0\bar{\pi}$$

$$\pi\bar{\pi} = \frac{(\mathbf{p}_0,\mathbf{q}_0)}{(e^{\mathbf{A}t}\mathbf{p}_0, e^{\mathbf{A}^{\star}t}\mathbf{q}_0)} \qquad (\mathbf{p},\mathbf{q}) = (\mathbf{p}_0,\mathbf{q}_0)$$

Sample the two-sided flow, n=100,



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Scaling of the two-sided flow

$$\pi\bar{\pi} = \frac{(\mathbf{p}_0, \mathbf{q}_0)}{(e^{\mathbf{A}t}\mathbf{p}_0, e^{\mathbf{A}^\star t}\mathbf{q}_0)}$$

- Experiments reveal that the denominator changes sign. Hence, the denominator is zero at some intermediate time.
- This finite time blow up of the ODE has the numerical linear algebra interpretation of ***incurable breakdown***
- Incurable breakdown is, roughly, defined to be that the inner product of two vectors is zero yet neither vector is the zero vector. Purely algebraic notion that has (now) and interesting interpretation.

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Two-sided Forward Euler (FE)

$$\begin{aligned}\dot{\mathbf{p}} &= \mathbf{p}\frac{\mathbf{q}^T\mathbf{A}\mathbf{p}}{\mathbf{q}^T\mathbf{p}} - \mathbf{A}\mathbf{p} \equiv \mathbf{f}(\mathbf{p},\mathbf{q}) \\ \dot{\mathbf{q}} &= \mathbf{q}\frac{\mathbf{p}^T\mathbf{A}^T\mathbf{q}}{\mathbf{p}^T\mathbf{q}} - \mathbf{A}^T\mathbf{q} \equiv \mathbf{g}(\mathbf{p},\mathbf{q})\end{aligned}$$

$$\begin{aligned}\mathbf{p}_{j+1} &= \mathbf{p}_j + h\mathbf{f}_j \\ \mathbf{q}_{j+1} &= \mathbf{q}_j + h\mathbf{g}_j\end{aligned}$$

Two-sided FE and quadratic invariants

$$
\begin{aligned}
(\mathbf{q}_{j+1})^T \mathbf{p}_{j+1} &= \mathbf{q}_0^T \mathbf{p}_0 + h\left((\mathbf{q}_j)^T \mathbf{f}_j + (\mathbf{g}_j)^T \mathbf{p}_j\right) + h^2 (\mathbf{g}_j)^T \mathbf{f}_j \\
&= \mathbf{q}_0^T \mathbf{p}_0 + h^2 (\mathbf{g}_j)^T \mathbf{f}_j
\end{aligned}
$$

$$
\begin{aligned}
\frac{|(\mathbf{q}_{j+1})^T \mathbf{p}_{j+1} - \mathbf{q}_0^T \mathbf{p}_0|}{|\mathbf{q}_0^T \mathbf{p}_0|} &\leq h^2 \frac{\|\mathbf{f}_j\| \, \|\mathbf{g}_j\|}{|\mathbf{q}_0^T \mathbf{p}_0|} \\
&\leq h^2 \frac{\|\mathbf{A}\|^2}{|\mathbf{q}_0^T \mathbf{p}_0|} \left(1 + \frac{\|\mathbf{q}_j\| \, \|\mathbf{p}_j\|}{|\mathbf{q}_j^T \mathbf{p}_j|}\right)^2 \|\mathbf{q}_j\| \, \|\mathbf{p}_j\|
\end{aligned}
$$

Incurable breakdown rears its head

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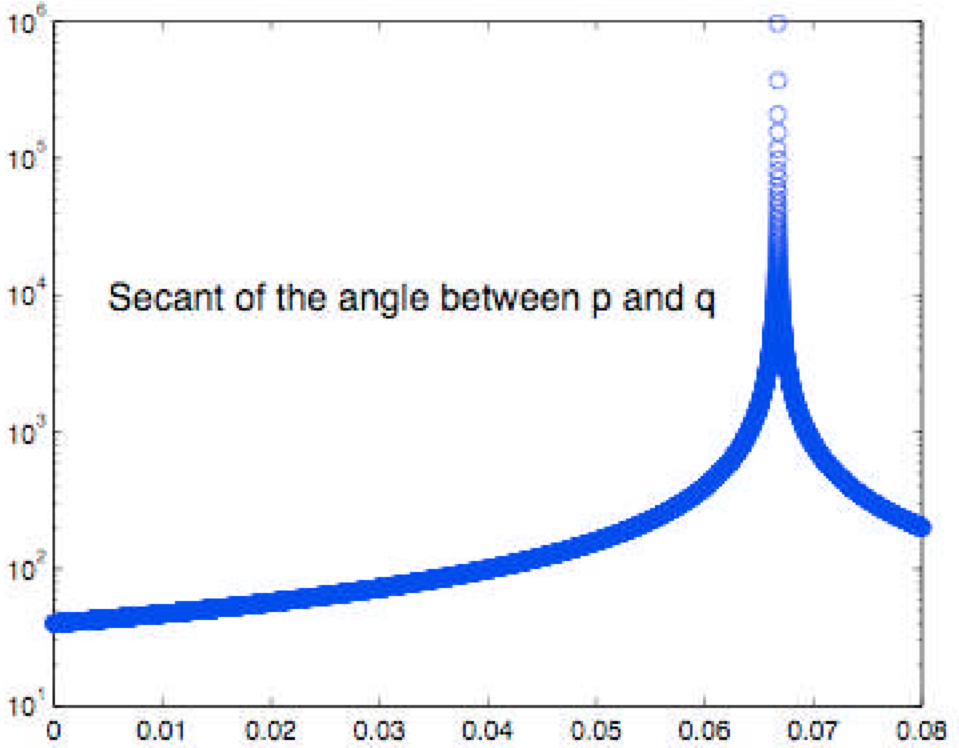
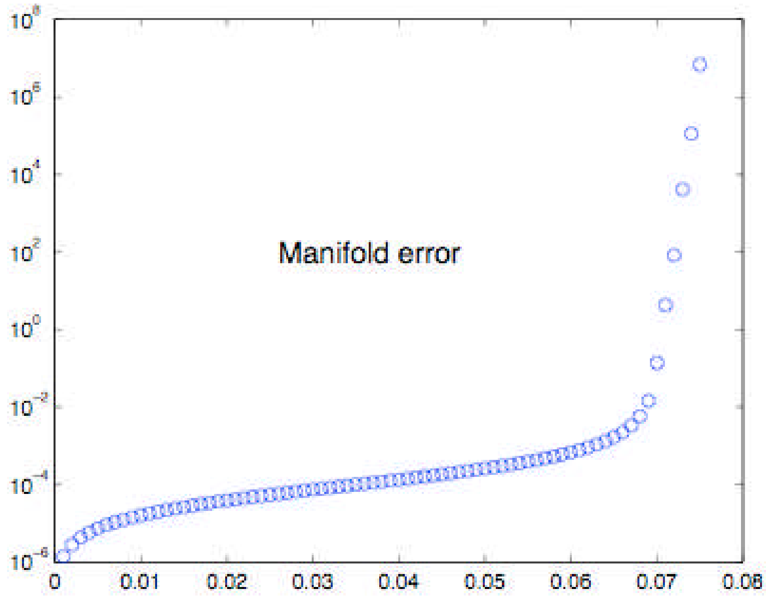


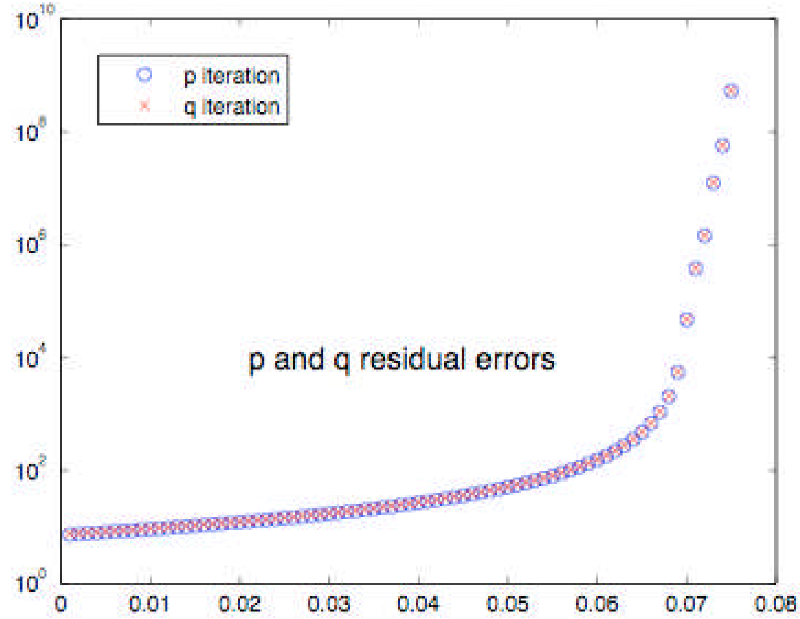
Secant of the angle (two-sided flow)

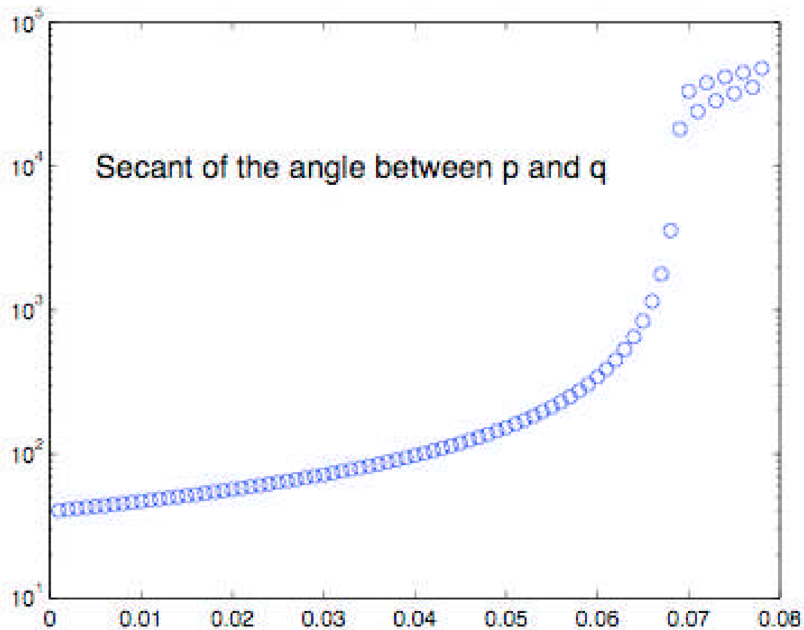
$$(\pi\bar{\pi})^{-1} = \left(\frac{e^{\mathbf{A}t}\mathbf{p}_0}{\sqrt{(\mathbf{p}_0,\mathbf{q}_0)}}, \frac{e^{\mathbf{A}^\star t}\mathbf{q}_0}{\sqrt{(\mathbf{q}_0,\mathbf{p}_0)}}\right)$$

$$\cos(\mathbf{p},\mathbf{q}) = \left(\frac{e^{\mathbf{A}t}\mathbf{p}_0}{\|e^{\mathbf{A}t}\mathbf{p}_0\|}, \frac{e^{\mathbf{A}^\star t}\mathbf{q}_0}{\|e^{\mathbf{A}^\star t}\mathbf{q}_0\|}\right)$$

Two-sided FE, h=.01







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Summary

- The continuous dynamical system represents an idealization and so useful for *algorithm analysis and design*
- One sided iterations are robust and stable
- Two-sided iterations suffer incurable breakdown
- Role of preconditioning
- Convergence analysis of the one-sided preconditioned flow