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Manchester Numerical Analysis

The Nonlinear Eigenvalue Problem: Part II

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Outline

Two lectures:

- Part I: Mathematical properties of nonlinear eigenproblems (NEPs)
  - Definition and historical aspects
  - Examples and applications
  - Solution structure

- Part II: Numerical methods for NEPs
  - Solvers based on Newton's method
  - Solvers using contour integrals
  - Linear interpolation methods

S. GÜTTEL AND F. TISSEUR, *The nonlinear eigenvalue problem*. Acta Numerica 26:1–94, 2017.

Solvers Based on Newton's Method

- Newton's method is a natural approach to compute e'vals/e'vecs of NEPs provided good initial guesses are available. Local quadratic convergence.
- Initial guess is the only crucial parameter $\Rightarrow$ great advantage over other NEP eigensolvers.
- Two broad ways NEP $F(\lambda)v = 0$ can be tackled by a Newton-type method:
  - Apply Newton's method to a scalar equation $f(z) = 0$ whose roots are the wanted e'vals of F.
  - Apply Newton's method directly to the vector problem $F(\lambda)v = 0$ together with some normalization condition on v.

Newton's Method for Scalar Function

Most obvious approach: Find roots of $f(z) = \det F(z)$.

Combining Newton's method with Jacobi's formula

$$\lambda^{(k+1)} = \lambda^{(k)} - \frac{f(\lambda^{(k)})}{f'(\lambda^{(k)})}$$

$$f'(z) = \det F(z) \operatorname{trace}\big(F(z)^{-1} F'(z)\big),$$

we obtain the **Newton-trace iteration** [Lancaster 1966]

$$\lambda^{(k+1)} = \lambda^{(k)} - \frac{1}{\operatorname{trace}\big(F(\lambda^{(k)})^{-1} F'(\lambda^{(k)})\big)}.$$

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Potential problems:

- Inverse of nearly singular $F(\lambda^{(k)})$ as $\lambda^{(k)} \to \lambda$.
- Requires $F'(z)$ explicitly. Computationally expensive.
- Initialization?

Newton's Method for Scalar Function (Cont.)

Kublanovskaya $f(z) = r_{nn}(z)$, where $r_{nn}(z)$ is (n, n) entry of R in **rank-revealing QR** decomposition of $F(z)$,

$$F(z)\Pi(z) = Q(z)R(z).$$

This yields the **Newton-QR iteration** for a root of $r_{nn}(z)$,

$$\lambda^{(k+1)} = \lambda^{(k)} - 1/(e_n^T Q_k^* F'(\lambda^{(k)})\Pi_k R_k^{-1} e_n).$$

At convergence, we can take $x = \Pi_k R_k^{-1} e_n$, $y = Q_k e_n$ as approx for the right and left e'vecs of the converged e'val.

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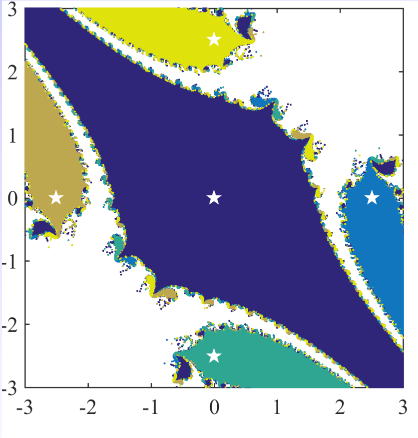
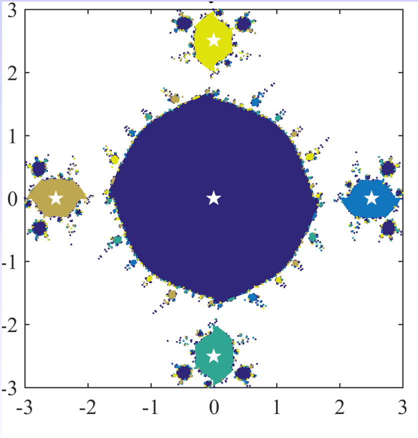
- Garret, Bai and Li (2016) propose an efficient implementation for large banded NEPs.
- MATLAB and C++ implementations including deflation are publicly available.

Convergence basins

$F(z) = \begin{bmatrix} e^{iz^2} & 1 \\ 1 & 1 \end{bmatrix}$ has e'vals $0, \pm\sqrt{2\pi}, \pm i\sqrt{2\pi}$ in $\Omega = \{z \in \mathbb{C} : -3 \le \mathrm{Re}(z) \le 3, -3 \le \mathrm{Im}(z) \le 3\}$.



Newton-trace method



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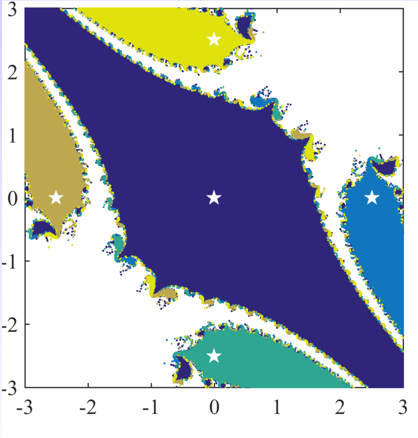

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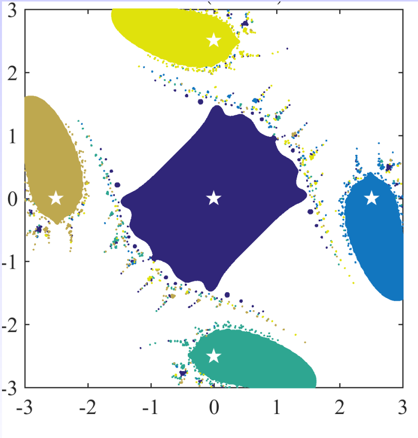


Newton-trace (secant) method

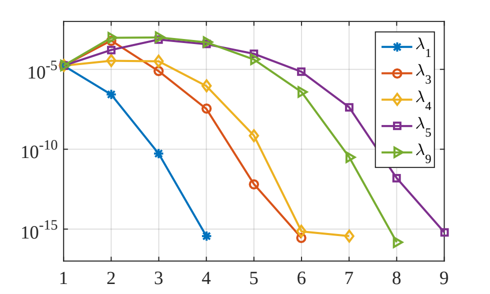
Newton-QR for Banded NEP

Consider the `loaded_string` problem defined by

$$F(\lambda)v = \left(C_1 - \lambda C_2 + \frac{\lambda}{\lambda - \sigma} C_3 \right) v = 0$$

with C_1, C_2 tridiagonal and $C_3 = e_n e_n^T$. $n = 100$.
Use `NQR4UB` [Garret and Li (2013)] to compute the 5 e'vals in $[4, 296]$ with `lambda0 = 4`.

Residuals $|r_{nn}(\lambda)|/||F(\lambda)||_F$ at each iter.



$$\eta_F(\lambda_i, v_i) = \frac{\|F(\lambda_i)v_i\|_2}{\|F(\lambda_i)\|_F \|v_i\|_2}$$

i	λ_i	$\eta_F(\lambda_i, v_i)$	$\eta_F(\lambda_i, w_i^*)$
1	4.482	3.5e-17	3.7e-16
3	63.72	3.1e-17	2.1e-16
4	123.0	2.7e-17	9.2e-17
5	202.2	4.9e-17	5.4e-16
9	719.4	3.5e-17	1.8e-16

Other Variants

Many variations based on **scalar root finding** exist:

- Newton-LU [Yang 1983, Wobst 1987]
- BDS (bordered, deletion, substitution) method [Andrew/Chu/Lancaster 1995]
- implicit determinant method [Spence/Poulton 2005]

Newton's Method for Vector Equation

Applying Newton's method to $\mathcal{N}\left[\begin{smallmatrix} v \\ \lambda \end{smallmatrix}\right] = 0$ where

$$\mathcal{N}\begin{bmatrix} v \\ \lambda \end{bmatrix} = \begin{bmatrix} F(\lambda)v \\ u^*v - 1 \end{bmatrix}$$

leads to the Newton's iteration

$$\begin{bmatrix} v^{(k+1)} \\ \lambda^{(k+1)} \end{bmatrix} = \begin{bmatrix} v^{(k)} \\ \lambda^{(k)} \end{bmatrix} - \begin{bmatrix} F(\lambda^{(k)}) & F'(\lambda^{(k)})v^{(k)} \\ u^* & 0 \end{bmatrix}^{-1} \begin{bmatrix} F(\lambda^{(k)})v^{(k)} \\ u^*v^{(k)} - 1 \end{bmatrix}.$$

Other variants include

- nonlinear inverse iteration [Unger 1950, Ruhe 1973]
- two-sided Rayleigh functional iteration [Schreiber 2008]
- residual inverse iteration [Neumaier 1985]

Iterative Projection Methods for NEPs

Let $U \in \mathbb{C}^{n\times k}$ with $k \ll n$ and $U^*U = I_k$ (**search space**) and $Q \in \mathbb{C}^{n\times k}$, $Q^*Q = I_k$ (test space). Instead of solving $F(\lambda)v = 0$, solve $k \times k$ projected NEP $Q^*F(\vartheta)Ux = 0 \qquad (\star)$

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Let (ϑ, x) be an e'pair of $(\star)$.

- If $\|F(\vartheta)Ux\|$ is small enough, accept (ϑ, Ux) as an approximate e'pair for F.
- If not, extend search space into $\mathrm{span}\{U, \Delta v\}$ by one step of Newton iteration with initial guess (ϑ, Ux). Δv solves the **Jacobi–Davidson correction eqn**:

$$(I_n - F'(\vartheta)vq^*)F(\vartheta)(I_n - vv^*)\Delta v = -F(\vartheta)v.$$

(Does not need to be solved accurately.)

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Variations of Jacobi–Davidson for NEPs are proposed by [Hochstenbach and Sleijpen (2003)], [Betcke and Voss (2004)], [Voss (2007)] and [Effenberger (2013)].

Deflation of Computed Eigenpairs

- Prevent the iteration from converging to already computed eigenpairs.
- Maps the already computed eigenvalues to infinity.

Suppose we have computed ℓ simple e'vals of F, $\lambda_1, \dots, \lambda_\ell$ and let $x_i, y_i \in \mathbb{C}^n$ be s.t. $y_i^* x_i = 1$, $i = 1, \dots, \ell$. Let

$$\widetilde{F}(z) = F(z) \prod_{i=1}^{\ell} \left(I - \frac{z - \lambda_i - 1}{z - \lambda_i} y_i x_i^* \right).$$

Then $\Lambda(\widetilde{F}) = \Lambda(F) \cup \{\infty\} \setminus \{\lambda_1, \dots, \lambda_\ell\}$.

If $\widetilde{v}$ is an e'vec of $\widetilde{F}$ with e'val λ then

$$v = \prod_{i=1}^{\ell} \left(I - \frac{z - \lambda_i - 1}{z - \lambda_i} y_i x_i^* \right) \widetilde{v}$$

is an e'vec of F associated with the e'val λ.

[Ferng et al. (2001)], [Huang et al. (2016)].

Robust Succesive Computation of Eigenpairs

- Suppose we have already computed a **minimal invariant pair** $(V, M) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$ for F.
- Extend (V, M) into one size larger minimal invariant pair

$$(\widehat{V}, \widehat{M}) = \left([\, V \quad x \,], \begin{bmatrix} M & b \\ 0 & \lambda \end{bmatrix} \right) \in \mathbb{C}^{n\times(m+1)} \times \mathbb{C}^{(m+1)\times(m+1)}.$$

[Effenberger (2013)] shows that $\left(\lambda, \left[\begin{smallmatrix} x \\ b \end{smallmatrix}\right]\right)$ is an eigenpair of an $(n+m)\times(n+m)$ NEP $\widetilde{F}(\lambda)\left[\begin{smallmatrix} x \\ b \end{smallmatrix}\right] = 0$.

- Solve $\widetilde{F}(\lambda)\left[\begin{smallmatrix} x \\ b \end{smallmatrix}\right] = 0$ by any of the previous methods.

Block-Newton Method

$(V, M) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$ is an invariant pair for $F \in H(\Omega, \mathbb{C}^{n\times n})$ if

$$\mathcal{F}(V, M) = C_1 V f_1(\Lambda) + C_2 V f_2(\Lambda) + \cdots + C_\ell V f_\ell(\Lambda) = 0_{n\times m}.$$

Add normalization condition:

$$\mathcal{N}(V, M) = 0_{m\times m}.$$

[Kressner (2009)] showed that (V, M) is complete iff Jacobian

$$\begin{aligned} \mathcal{M} : \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m} &\to \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m} \\ (\Delta V, \Delta M) &\mapsto \big(L_{\mathcal{F}}(\Delta V, \Delta M), L_{\mathcal{N}}(\Delta V, \Delta M)\big) \end{aligned}$$

is invertible. Newton correction $(\Delta V, \Delta M)$ satisfies

$$\mathcal{M}(\Delta V, \Delta M) = -\big(\mathcal{F}\big(V, M\big), O_{m\times m}\big).$$

Safeguarded Iteration for Hermitian NEPs

Assume $F(\bar{z}) = F(z)^*$ for all $z \in \mathbb{C}$ and that if λ_k is a kth eigenvalue of $F(z)$ (i.e., $\mu = 0$ is the kth largest eigenvalue of the Hermitian matrix $F(\lambda_k)$), then (see Part I)

$$\lambda_k = \min_{\substack{V \in \mathbb{S}_k \\ V \cap \mathbb{K}(p) \neq \emptyset}} \; \max_{\substack{x \in V \cap \mathbb{K}(p) \\ x \neq 0}} p(x) \in \mathbb{I}.$$

This suggests the **safeguarded iteration** [Werner 1970]:

```
Choose an initial approx λ^(0) to jth e'val of F.
 For k = 0, 1, ... until convergence
       Compute e'vec x^(k) of jth largest e'val of F(λ^(k)).
       Compute real root ρ of x^(k)* F(ρ) x^(k) = 0 closest to λ^(k)
       set λ^(k+1) = ρ.
 end
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1 Choose an initial approx $\lambda^{(0)}$ to jth e'val of F.
2 For $k = 0, 1, \ldots$ until convergence
3 Compute e'vec $x^{(k)}$ of jth largest e'val of $F\left(\lambda^{(k)}\right)$.
4 Compute real root ρ of $x^{(k)*} F(\rho) x^{(k)} = 0$ closest to $\lambda^{(k)}$
5 set $\lambda^{(k+1)} = \rho$.
6 end

Local quadratic convergence [Niendorf and Voss (2010)].

Methods Based on Contour Integration

Given $F \in H(\Omega, \mathbb{C}^{n\times n})$. By Keldysh's theorem we have

$$F(z)^{-1} = V(zI - J)^{-1}W^* + R(z)$$

on some closed set $\Sigma \subset \Omega$, where J is an $m \times m$ Jordan block matrix containing all the eigenvalues $\Lambda(F) \cap \Sigma$.

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Let $\Gamma \subset \Omega$ be a contour enclosing the eigenvalues of J, let $X \in \mathbb{C}^{n\times r}$ be a “probing matrix”, and $f \in H(\Omega, \mathbb{C})$ (**filter function**). Then

$$\begin{aligned} A_f := & \frac{1}{2\pi \mathrm{i}} \int_\Gamma f(z) F(z)^{-1} X \delta z \\ = & \frac{1}{2\pi \mathrm{i}} \int_\Gamma f(z) V(zI - J)^{-1} W^* X \delta z \\ = & V f(J) W^* X. \end{aligned}$$

Beyn's Integral Approach

Construct

$$\begin{aligned} A_0 &:= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma} F(z)^{-1} X \delta z = V\, W^* X \\ A_1 &:= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma} z\, F(z)^{-1} X \delta z = V\, J\, W^* X. \end{aligned}$$

Assuming that V, W, and $W^* X$ are of full rank m,
can show that e'vals of $\lambda A_0 - A_1$ are e'vals of F inside Γ.
[Asakura 2009] [Beyn 2012] [Yokota/Sakurai 2013]

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$$A_0 := \frac{1}{2\pi i}\int_{\Gamma} F(z)^{-1} X \delta z = V\,W^*\,X$$

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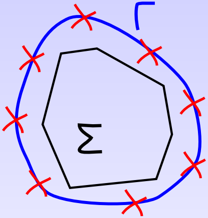
Other filter functions f can be used via $A_f = \frac{1}{2\pi i}\int_{\Gamma} f(z)F(z)^{-1}X\delta z$ leading to **higher-order moments.**

[Murakami '10] [Güttel et al '15] [Austin/Trefethen '15] [Van Barel '16]

Quadrature

The contour integrals involved in A_0 and A_1 are approximated by numerical quadrature.

Let $\gamma : [0,1] \to \Gamma$ be a parameterization, then



$$A_{j,n_c} = \sum_{\ell=1}^{n_c} \omega_\ell z^j F(\gamma(t_\ell))^{-1} X \approx A_j$$

is a quadrature approximation with n_c nodes ($j = 1, 2$).

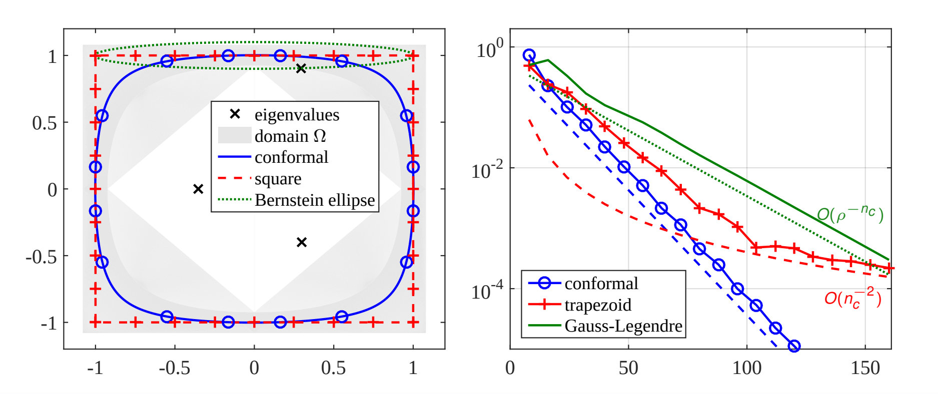
Note that the n_c solves $F(\gamma(t_\ell))^{-1} X$ are completely decoupled and can be assigned to different processors.

$\Longrightarrow$ Great potential for parallelization!

Care has to be taken with the quadrature rule

The quality of the quadrature approximation determines the accuracy of the computed e'vals [Beyn 2012] [Güttel/T. 2017].

Example: Quadrature errors $\|A_j - A_{j,n_c}\|$ as n_c increases (right) with different quadrature rules on (almost) square contour (left).



Methods based on linear interpolation

Instead of solving $F(\lambda)v = 0$ directly, we may approximate $F \approx R_m$ on $\Sigma \subseteq \mathbb{C}$ by simpler NEP and solve $R_m(\lambda)v = 0$.

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Practical approach: Rational form

$$R_m(z) = b_0(z)D_0 + b_1(z)D_1 + \cdots + b_m(z)D_m$$

where $D_j \in \mathbb{C}^{n\times n}$ are fixed and b_j are rational functions.

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Particularly useful: (scaled) rational Newton basis

$$b_0(z) \equiv 1, \quad b_{j+1}(z) = \frac{z - \sigma_j}{\beta_{j+1}(1 - z/\xi_{j+1})} b_j(z)$$

with interpolation points $\sigma_j \in \Sigma$ and poles $\xi_j \in \overline{\mathbb{C}} \setminus \Sigma$.

Choice of σ_j, ξ_j, β_j by NLEIGS sampling [Güttel et al 2014].

NLEIGS sampling

Assume F is holomorphic on $\Omega = \mathbb{C} \setminus \Xi$ and we target the eigenvalues in $\Sigma \subseteq \Omega$.

Assume we have chosen nodes $\sigma_0, \sigma_1, \ldots, \sigma_m \in \Sigma$ and poles $\xi_1, \ldots, \xi_m \in \Xi$. Define $s_m(z) := (z - \sigma_m) b_m(z)$.

By the **Hermite–Walsh formula** we have

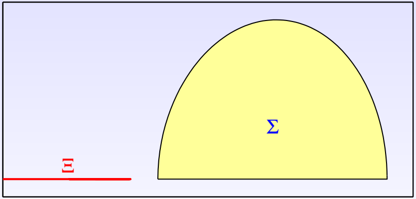
$$F(z) - R_m(z) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{s_m(z)}{s_m(\zeta)} \frac{F(\zeta)}{\zeta - z} \, \mathrm{d}\zeta,$$

and so the **uniform approximation error on Σ** satisfies

$$\|F - R_m\|_\Sigma := \max_{z \in \Sigma} \|F(z) - R_m(z)\|_2 \leq C \|s_m\|_\Sigma \cdot \|s_m^{-1}\|_\Gamma$$

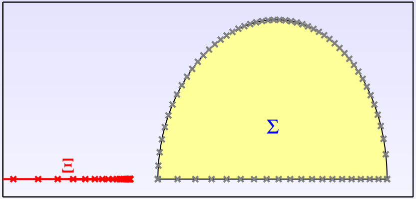
Aim: Make s_m small on Σ and large on Γ.

NLEIGS sampling of F on Σ



NLEIGS sampling of F on Σ

1. Discretize boundaries of Σ and Ξ sufficiently fine.



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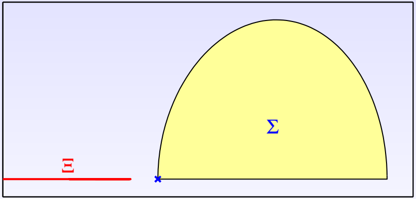

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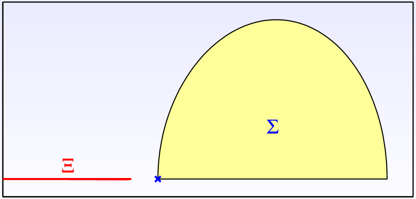

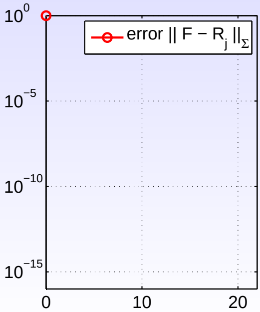

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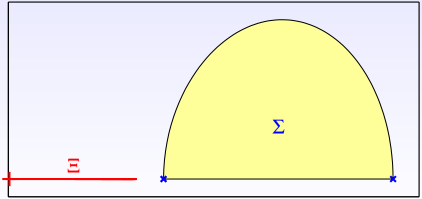
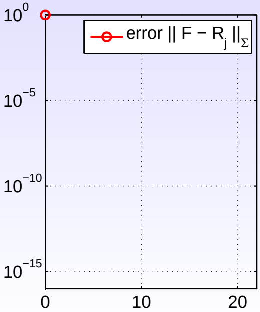
3. For $j = 1, 2, \ldots, m$ choose σ_j and ξ_j such that

$$\max_{z\in\Sigma} |s_{j-1}(z)| = |s_{j-1}(\sigma_j)| \quad \text{and} \quad \min_{z\in\Xi} |s_{j-1}(z)| = |s_{j-1}(\xi_j)|.$$





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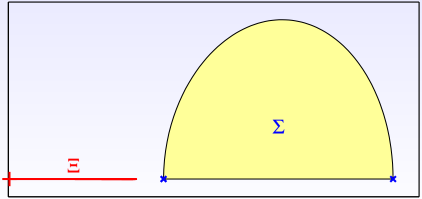
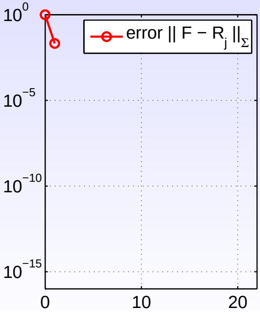
Choose β_j such that $\|s_j\|_\Sigma = 1$ and set $D_j = \frac{F(\sigma_j) - R_{j-1}(\sigma_j)}{b_j(\sigma_j)}$.





NLEIGS sampling of F on Σ

1. Discretize boundaries of Σ and Ξ sufficiently fine.
2. Choose interpolation node $\sigma_0 \in \Sigma$ and set $R_0(z) \equiv F(\sigma_0)$.
3. For $j = 1, 2, \dots, m$ choose σ_j and ξ_j such that

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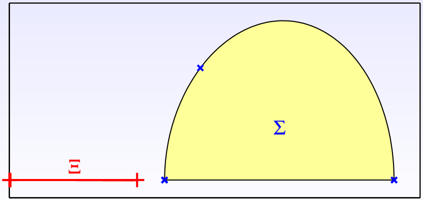

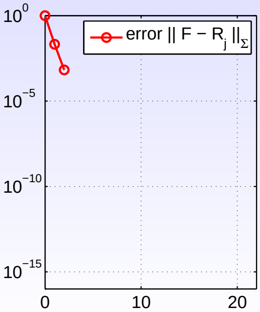

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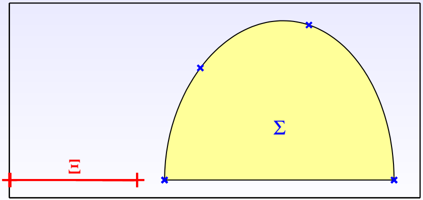

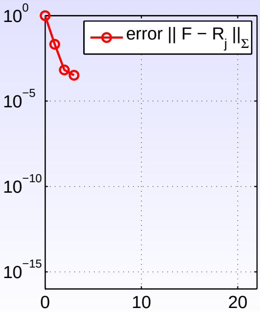

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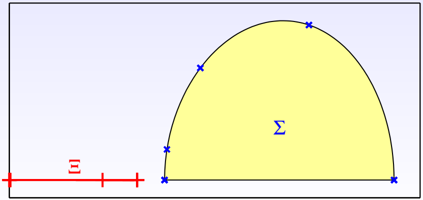

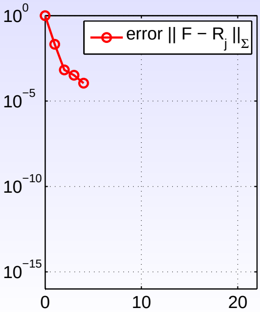

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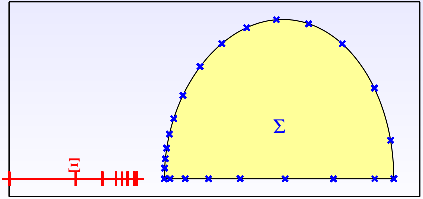

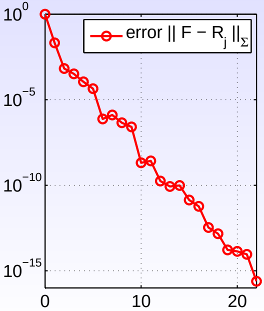

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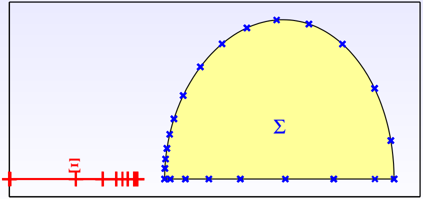

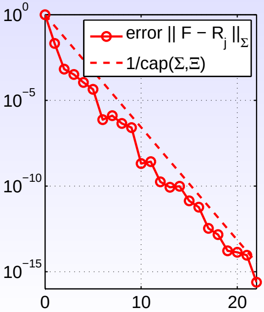

Krylov solution

Interpolation techniques can be combined with

- linearization of $R_m \Rightarrow$ structured GEP $A_m x = \lambda B_m x$
- rational Krylov algorithms for solving GEP
- dynamic increase of degree m during Krylov iteration
  $\Longrightarrow$ infinite Arnoldi method [Jarlebring et al 2012]
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NLEIGS implementations are available in the

- SLEPc library version 3.7 [Campos & Roman 2016]
- Rational Krylov Toolbox [Berljafa & Güttel 2015].

Concluding Remarks

NEPs have interesting mathematical properties. They arise in many applications and their efficient solution requires ideas from numerical linear algebra, complex analysis, and approximation theory (among other fields).

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NEPs have interesting mathematical properties. They arise in many applications and their efficient solution requires ideas from numerical linear algebra, complex analysis, and approximation theory (among other fields).

There is more to be said, e.g.,

- Structured NEPs?
- Higher-order integral moments
- Preconditioning/scaling of linearizations
- Implementation, software packages

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