Conditioning and Backward Errors for Eigenvector Nonlinearities

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Introduction

- **Eigenvector nonlinearities (NEPv)** arise in several important applications, for instance in quantum chemistry [1]. We consider symmetric problems of the form

$$A(v)v = \lambda v, \quad \text{where} \quad A(\alpha v) = A(v),\ \alpha \in \mathbb{R}, \tag{1}$$

  which naturally generalizes the familiar linear eigenvalue problem
- **Conditioning and backward errors** are well studied for a large number of problem classes [2], and are **fundamental in numerical analysis**

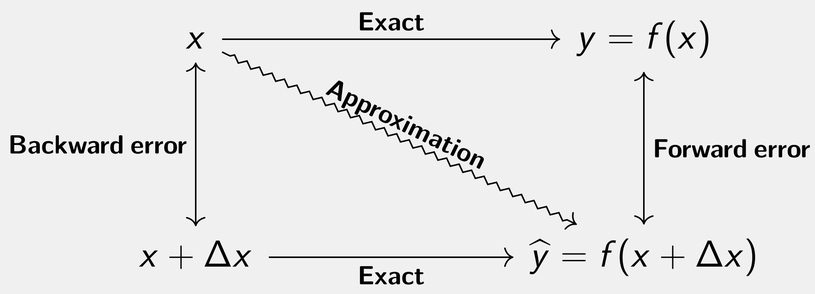


Figure: Illustration of forward and backward error for computing $y = f(x)$.

- **Often impossible** to determine forward error $\rightarrow$ **study backward error**
- **Backward and forward error** are related by the **condition number**

$$\text{Forward error} \lesssim \text{condition number} \times \text{backward error}$$

- **We study conditioning and backward errors** for the NEPv (1)

Definitions

- **Define the Jacobian** $J(v) := \frac{\partial}{\partial v}(A(v)v)$
- **Fact:** if (λ, v) is an eigenpair, then $A(v)v = J(v)v = \lambda v$
- **We consider a perturbation** to (1), **with a magnitude parameter** ε, and define

$$(A(v) + \Delta A(v, \varepsilon))v := \left(A(v) + \sum_{i=1}^{m} f_i(v)\varepsilon E_i\right) v = \lambda v, \tag{2}$$

  where $f_i(v) : \mathbb{R}^n \rightarrow \mathbb{R}$ are scaling invariant functions

Definition (Condition number)

View λ as a function of the perturbation size ε, and for weights w_i, define

$$\kappa(\lambda) = \sup\left\{\frac{|\lambda'|}{|\lambda|} \ :\ \|E_i\| \leq w_i,\ i = 1, \ldots, m\right\}. \tag{3}$$

Definition (Backward error)

Let $(\tilde{\lambda}, \tilde{v})$ be an approximate eigenpair of (1), and for weights w_i, define

$$\eta(\tilde{\lambda}, \tilde{v}) = \min\left\{|\varepsilon| \ :\ (A(\tilde{v}) + \Delta A(\tilde{v}, \varepsilon))\,\tilde{v} = \tilde{\lambda}\tilde{v},\ \|E_i\| \leq w_i\right\}. \tag{4}$$

Main results

Theorem

Let (λ, v) be an eigenpair of (1). Let u be the left eigenvector of $J(v)$ corresponding to λ. The we have

$$\kappa(\lambda) = \frac{\left(\sum_{i=1}^{m} |f_i(v)| w_i\right) \|u\| \|v\|}{|\lambda| |u^T v|}. \tag{5}$$

Furthermore, if $(\tilde{\lambda}, \tilde{v})$ be an approximate eigenpair of (1), then we have

$$\eta(\tilde{\lambda}, \tilde{v}) = \frac{\|A(\tilde{v})\tilde{v} - \tilde{\lambda}\tilde{v}\|}{\sum_{i=1}^{m} |f_i(\tilde{v})| w_i \|\tilde{v}\|}. \tag{6}$$

- **Consequence:** conditioning depends on left and right eigenvectors of $J(v) \rightarrow$ often nonnormal $\rightarrow$ even **symmetric problems can become arbitrarily ill-conditioned!**

Numerical illustration

- Consider a specific instance of (1), defined by

$$A(v) = A_0 + \frac{v^T B v}{v^T v} A_1,$$

  where we choose the matrices to be

$$A_0 = \begin{bmatrix} 1+\delta & 1 & 1 \\ 1 & -2 & -2 \\ 1 & -2 & 0 \end{bmatrix}, \ A_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & -1 \\ 0 & -1 & 5 \end{bmatrix}, \ B = \begin{bmatrix} 0 & -1 & 2 \\ -1 & 2 & 1 \\ 2 & 1 & 1 \end{bmatrix}$$

- Here, δ is a perturbation parameter
- We vary δ and compute the eigenvalues using [3], as well as the eigenvalue condition number

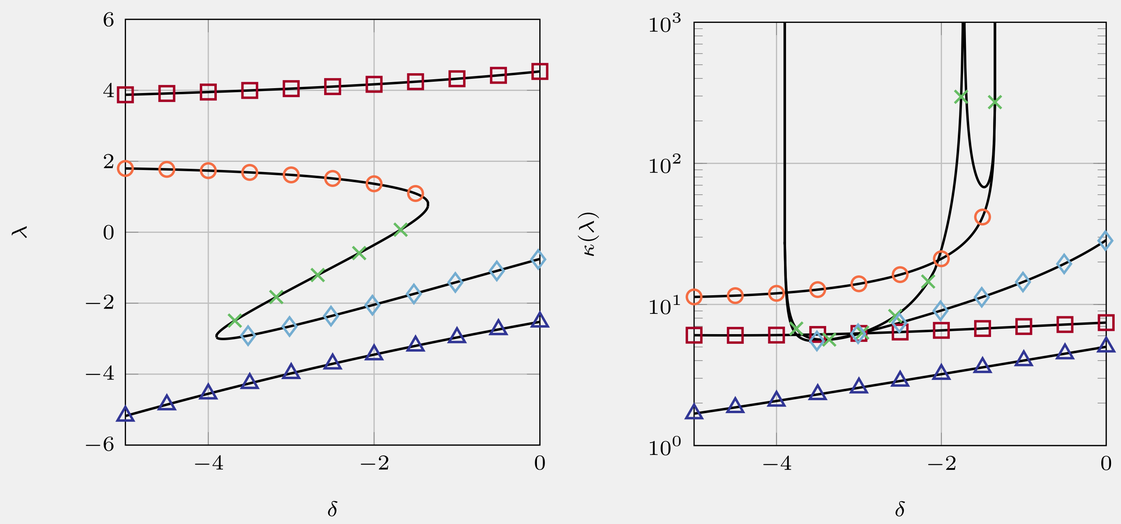


Figure: **Left:** Eigenvalues as function of the parameter δ. The different markers indicate different branches of the eigenvalues. **Right:** Corresponding eigenvalue condition numbers.

- **Small symmetric** example gives **severe ill-conditioning**
- **This behavior** never occurs for symmetric linear problems
- **Cause of ill-conditioning:** left and right eigenvectors of $J(v)$ become orthogonal

Additional results and future work

- **We also consider** the condition number when the perturbations are restricted to be symmetric $\rightarrow$ **essentially same expression for conditioning and backward error**
- **Consider what happens** when measuring the perturbations with different norms (spectral, Frobenius) $\rightarrow$ **introduces additional dependence on inner product** of left and right eigenvectors of $J(v)$
- **We derive expressions** for the conditioning of eigenvectors, $\kappa(v) \rightarrow$ **generalizes linear results**
- **Many problems appearing** in applications are **highly structured** $\rightarrow$ future work could consider structured or componentwise condition numbers and backward errors

References

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