Numerical Linear Algebra
for Computational Science and Information Engineering
Floating-Point Arithmetic and Error Analysis

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Outline I

Number representation and arithmetic on digital computers

Section 3.2 in Darve & Wootters (2021)

Number representation on computers

- Computers store numbers with **finite memory**, leading to limitations:
  - **Representation errors**: Most real numbers cannot be exactly represented.
  - **Rounding errors**: Arithmetic operations result in quantities which cannot be exactly represented either.
  - **Overflow/Underflow**: Numbers may exceed their representable range.
- These limitations introduce challenges in numerical computations, such as maintaining
  - **Accuracy**: How close is the computed result to the true value? Affected by accumulation of representation and rounding errors, and by algorithmic choices.
  - **Stability**: Does the method prevent error growth for small input changes? Specific to both the problem and the algorithm together.
- **Error analysis** helps understand these challenges by focusing on
  - **Perturbation**: effect of small input changes on the true solution of a problem.
  - **Propagation**: cumulative effects of rounding errors through calculations.
- Understanding these concepts is essential to prevent unwanted behaviors when using numerical methods.

Bit representation of integers

- Digital computers represent integers using a fixed number b of bits, e.g., 8, 16, 32, or 64 bits.
- For every **unsigned integers** x ranging from 0 to $2^b - 1$,

$$\exists!\,(d_0, \dots, d_{b-1}) \in \{0,1\}^b \text{ s.t. } x = \sum_{i=0}^{b-1} d_i 2^i.$$

  We say that x is represented as $d_{b-1} \dots d_0$.

  Attempting to represent integers out of the range from 0 to $2^b - 1$, leads to **underflow** or **overflow**.

  Example: integers from 0 to 7 can be represented as follows using 3 bits:

integer	binary representation	decomposition
0	000	$0\times 1 + 0\times 2 + 0\times 4$
1	001	$1\times 1 + 0\times 2 + 0\times 4$
2	010	$0\times 1 + 1\times 2 + 0\times 4$
3	011	$1\times 1 + 1\times 2 + 0\times 4$
4	100	$0\times 1 + 0\times 2 + 1\times 4$
5	101	$1\times 1 + 0\times 2 + 1\times 4$
6	110	$0\times 1 + 1\times 2 + 1\times 4$
7	111	$1\times 1 + 1\times 2 + 1\times 4$

Bit representation of integers, cont'd

- Different systems exist in order to encode **signed integers** with bits. In particular, we consider the **two's complement representation**:

  For every integer x ranging from -2^{b-1} to 2^{b-1},

  $$\exists!\,(d_0,\ldots,d_{b-1})\in\{0,1\}^b \text{ s.t. } x=-d_{b-1}2^{b-1}+\sum_{i=0}^{b-2}d_i2^i.$$

  Example: integers from -4 to 3 can be represented as follows using 3 bits:

integer	binary representation	decomposition
0	000	$-0\times 4+0\times 1+0\times 2$
1	001	$-0\times 4+1\times 1+0\times 2$
2	010	$-0\times 4+0\times 1+1\times 2$
3	011	$-0\times 4+1\times 1+1\times 2$
-4	100	$-1\times 4+0\times 1+0\times 2$
-3	101	$-1\times 4+1\times 1+0\times 2$
-2	110	$-1\times 4+0\times 1+1\times 2$
-1	111	$-1\times 4+1\times 1+1\times 2$

  Clearly, the most significant bit d_{b-1} represents the sign (0 for +, 1 for -).

  Arithmetic operations on two's complement numbers follow the same rules as unsigned arithmetic.

Bit representation of floating-point numbers

- **Floating-point numbers** are used to represent a wide range of **real numbers**, including fractions and very large or small numbers.
- A **floating-point number** x is given by $x = (-1)^s \times m \times 2^{e-2^{b-p-1}}$ where
  - s is the **sign bit** (0 for +, 1 for -).
  - $m = 1 + \sum_{i=1}^{p-1} q_i 2^{-i} \in [1, 2)$ is the **significand** (or **mantissa**), encoded by $p-1$ **fraction bits**, where p is the **precision** of the numerical system.
  - $e - 2^{b-p-1}$ is the **exponent** represented by $b-p$ bits with $e = \sum_{i=0}^{b-p-1} d_i 2^i$.

  The associated bits are stored in the form $\boxed{s}\boxed{d_{b-p-1}\dots d_0}\boxed{q_1 \dots q_{p-1}}$.
- Example: Half precision (1 sign bit, 5 exponent bits, 10 fraction bits)
  - Then, the floating-point number fl(π), which best approximates $\pi = 3.1416...$, is represented as 0100001001001000 so that

$$s = 0 \qquad \begin{aligned} e &= 1 \times 2^4 \\ &= 16 \end{aligned} \qquad \begin{aligned} m &= 1 + 1 \times 2^{-1} + 1 \times 2^{-4} + 1 \times 2^{-7} \\ &= 1 + 0.5 + 0.0625 + 0.0078125 \\ &= 1.5703125 \end{aligned}$$

and fl$(\pi) = (-1)^0 \times 1.5703125 \times 2^{16-2^{4-1}} = 1.5703125 \times 2 = 3.140625.$

Bit repsentation of floating-point numbers, cont'd

- Most real numbers cannot be exactly represented due to the finite number of bits used for the mantissa. The **machine epsilon** and the **unit roundoff** are often used to characterize the rounding error of a numerical system.

Definition (Machine epsilon & unit roundoff)

- The (interval) **machine epsilon**, often denoted by ϵ_{mach}, is the distance between 1 and the next floating-point number.
- The **unit roundoff** u is half the machine precision, i.e., $u = \epsilon_{mach}/2$.

- Common floating-point formats:
  - **Half precision** (16 bits): 1 sign bit, 5 exponent bits, 10 significand bits and unit roundoff $u = 2^{-11} \approx 4.88 \times 10^{-4}$.
  - **Single precision** (32 bits): 1 sign bit, 8 exponent bits, 23 significand bits and unit roundoff $u = 2^{-24} \approx 5.96 \times 10^{-8}$.
  - **Double precision** (64 bits): 1 sign bit, 11 exponent bits, 52 significand bits and unit roundoff $u = 2^{-53} \approx 1.11 \times 10^{-16}$.
- The **distribution** of floating-point numbers is **not uniform** within the range of a numerical system.

Floating-point conversion and arithmetic

- For every number x within the range of a floating-point number system, it can be shown that the associated rounding $\mathsf{fl}(x)$ is such that

$$\mathsf{fl}(x) = (1+\delta)x \text{ for some } \delta \text{ s.t. } |\delta| \leq u.$$

- When performing arithmetic operations between floating-point numbers, i.e., $\mathsf{fl}(x) \circ \mathsf{fl}(y)$ with $\circ \in \{+, -, \times, \div\}$, the result is not necessarily a floating-point number, so that further rounding applies.

  Floating-point number systems follow the **standard model of arithmetic**, which states they must satisfy

$$\mathsf{fl}(\mathsf{fl}(x) \circ \mathsf{fl}(y)) = (1+\delta)(\mathsf{fl}(x) \circ \mathsf{fl}(y)) \text{ for some } \delta \text{ s.t. } |\delta| \leq u.$$

- Properties of floating-point arithmetic:
  - **Not associative**, e.g., $\mathsf{fl}(\mathsf{fl}(x) + \mathsf{fl}(y)) + \mathsf{fl}(z) \neq \mathsf{fl}(x) + \mathsf{fl}(\mathsf{fl}(y) + \mathsf{fl}(z))$.
  - **Not distributive**, e.g.,

$$\mathsf{fl}(x) \times \mathsf{fl}(\mathsf{fl}(y) + \mathsf{fl}(z)) \neq \mathsf{fl}(\mathsf{fl}(x) \times \mathsf{fl}(y)) + \mathsf{fl}(\mathsf{fl}(x) \times \mathsf{fl}(z)).$$

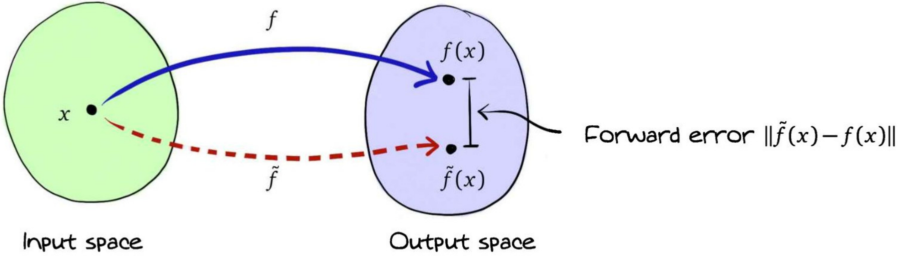
  - Subtraction of nearly equal numbers can lead to **catastrophic cancellation**.

Principles of error analysis

Section 3.3 in Darve & Wootters (2021)

Forward error

- **Error analysis** is crucial for understanding the accuracy and stability of numerical algorithms.
- Let f be a function and $\tilde{f}$ be its computed approximation for an input x.
- The **forward error** $\|f(x) - \tilde{f}(x)\|$ measures the **distance between** the **true value** $f(x)$ and the **computed approximation** $\tilde{f}(x)$.



Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

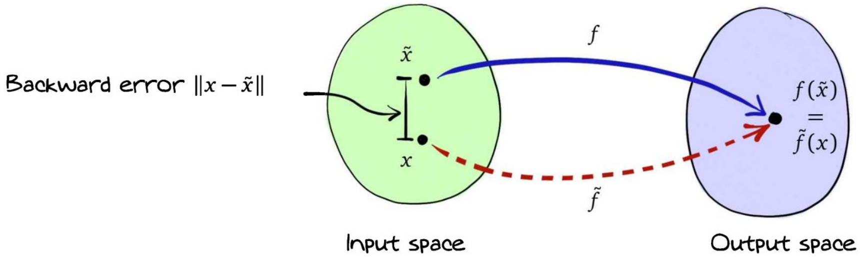
- The **relative forward error** is given by $\|f(x) - \tilde{f}(x)\|/\|f(x)\|$.
- In practice, we often do not know $f(x)$, which makes the forward error **difficult to evaluate**.

Backward error

- For an approximation $y := \tilde{f}(x)$ of a true quantity $f(x)$ for some input x, the **backward error** $\eta(x, y)$ is the **smallest perturbation to the input** whose exact map equates the approximation, i.e.,

$$\eta(x, y) = \min_{\tilde{x}}\{\|x - \tilde{x}\| \text{ s.t. } f(\tilde{x}) = y\}.$$

  This can be represented as



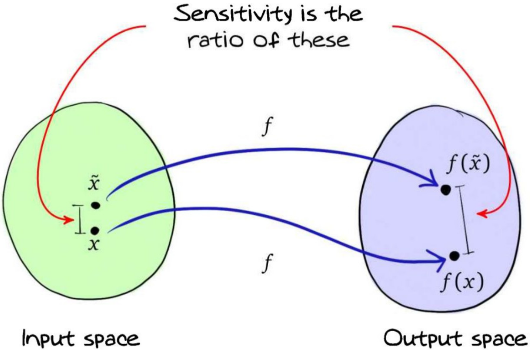
  Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

- The **relative backward error** is given by $\eta(x, y)/\|x\|$.

Sensitivity of a problem

- **Sensitivity** measures how much the output of a function changes relative to small changes in the input:

$$\text{sensitivity} = \frac{\text{forward error}}{\text{backward error}} = \frac{\|f(x) - f(\tilde{x})\|}{\|x - \tilde{x}\|}.$$



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- The **relative sensitivity** is given by $\dfrac{\|f(x) - f(\tilde{x})\|/\|f(x)\|}{\|x - \tilde{x}\|/\|x\|}$.

Conditioning of a problem

- The (relative) **condition number** $\kappa(x)$ of a problem $x \mapsto f(x)$ bounds the **relative sensitivity for small perturbations in the input data**:

$$\kappa(x) = \lim_{\varepsilon \to 0} \sup_{\|\delta x\| \leq \varepsilon} \frac{\|f(x+\delta x) - f(x)\| / \|f(x)\|}{\|\delta x\| / \|x\|}.$$

- A fundamental result of numerical analysis states

$$\begin{array}{c} \text{relative} \\ \text{forward error} \end{array} \lesssim \begin{array}{c} \text{condition} \\ \text{number} \end{array} \times \begin{array}{c} \text{relative} \\ \text{backward error} \end{array}$$

also written as $\dfrac{\|f(x) - y\|}{\|f(x)\|} \lesssim \kappa(x) \dfrac{\eta(x, y)}{\|x\|}$ for any approximation y of $f(x)$.

- A problem $x \mapsto f(x)$ with a large condition number $\kappa(x)$ is **ill-conditioned**.
- The **approximation** $\tilde{f}(x)$ of an **ill-conditioned problem can have a large forward error**, even if $\tilde{f}(x)$ has a small backward error.
- The condition number is **problem-dependent**, i.e., it is specifically defined for linear system solving, least-squares solving, eigenvalue solving, ...
- The condition number **does not depend on the algorithm**.

Backward stability of an algorithm

- In practice, we develop algorithms of the form $x \mapsto \tilde{f}(x)$ to approximate the solution of the problem $x \mapsto f(x)$, and that minimize the associated backward error $\eta(x, \tilde{f}(x))$.
- In particular, an algorithm is **backward stable** if the associated backward error remains small, i.e.,

$$\frac{\eta(x, \tilde{f}(x))}{\|x\|} = \mathcal{O}(u)$$

  irrespective of x, where u is, typically, the unit roundoff of the floating-point number system.
- For **well-conditioned problems**, a **backward stable algorithm** ensures **small forward errors**.
- But, for **ill-conditioned problems**, **even backward stable algorithms** may produce **large forward errors**.

Analysis of linear systems

Section 3.3 in Darve & Wootters (2021)

Perturbation of linear systems

- Consider the problem of solving for x such that $Ax = b$ for some invertible matrix A and non-zero vector b.
- Let us assume $\tilde{x} := x + \delta x$ is the true solution of a non-singular perturbed problem $(A + \delta A)\tilde{x} = b + \delta b$. Then, the following remainder is obtained

$$\begin{array}{rl} & (A+\delta A)(x+\delta x) = b + \delta b \\ - & \qquad\qquad\qquad Ax = b \\ \hline & A\delta x + \delta A x + \delta A \delta x = \delta b \end{array}$$

Multiplying the remainder by A^{-1}, we get

$$\delta x + A^{-1}\delta A x + A^{-1}\delta A \delta x = A^{-1}\delta b.$$

Then, assuming the matrix norm is consistent with the vector norm:

$$\|\delta x\| \leq \|A^{-1}\| \cdot \|\delta A\| \cdot \|x\| + \|A^{-1}\| \cdot \|\delta A\| \cdot \|\delta x\| + \|A^{-1}\| \cdot \|\delta b\|.$$

Dividing by $\|x\|$, and neglecting the 2nd order term $\|\delta A\| \cdot \|\delta x\|$, we get

$$\frac{\|\delta x\|}{\|x\|} \lesssim \|A^{-1}\| \cdot \|\delta A\| + \frac{\|A^{-1}\| \cdot \|\delta b\|}{\|x\|}.$$

Perturbation of linear systems, cont'd

We can then factor by $\|A^{-1}\| \cdot \|A\|$, which leads to

$$\frac{\|\delta x\|}{\|x\|} \lesssim \|A^{-1}\| \cdot \|A\| \cdot \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|A\| \cdot \|x\|} \right).$$

But since $Ax = b$ implies $\|b\| \leq \|A\| \cdot \|x\|$, we obtain

$$\frac{\|\delta x\|}{\|x\|} \lesssim \|A^{-1}\| \cdot \|A\| \cdot \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right).$$

where the relative forward error $\|\delta x\|/\|x\|$ is measured by $\|A^{-1}\| \cdot \|A\|$ as a multiple of the relative input perturbations $\|\delta A\|/\|A\|$ and $\|\delta b\|/\|b\|$.

- Therefore, the **condition number** of the linear system solving problem $A \mapsto x := A^{-1}b$ is given by $\kappa(A) = \|A^{-1}\| \cdot \|A\|$.
- When using the 2-norm, we have $\kappa(A) = \sigma_{max}(A)/\sigma_{min}(A)$, in which $\sigma_{max}(A)$ and $\sigma_{min}(A)$ are the maximal and minimal singular values of A, respectively.

Backward errors of linear systems

- Let $\tilde{x}$ be an approximation of the solution x of the linear system $Ax = b$, and define the associate residual $r := b - A\tilde{x}$.
- Then, we are interested in the backward error $\eta_{A,b}(x)$ defined as

$$\eta_{A,b}(\tilde{x}) = \min\{\varepsilon \text{ s.t. } (A + \delta A)\tilde{x} = b + \delta b,\ \|\delta A\| \leq \varepsilon\|A\|,\ \|\delta b\| \leq \varepsilon\|b\|\}.$$

- To find $\eta_{A,b}(x)$, we first rearrange the perturbed system as follows:

$$\begin{aligned}(A + \delta A)\tilde{x} &= b + \delta b \\ \delta A\tilde{x} &= b - A\tilde{x} + \delta b \\ \delta A\tilde{x} &= r + \delta b.\end{aligned}$$

  Then, considering a matrix norm consistent with the vector norm, we have

$$\|\delta A\| \cdot \|\tilde{x}\| \geq \|r + \delta b\| \geq \|r\| - \|\delta b\|.$$

  Applying the prescribed bounds $\|\delta A\| \leq \varepsilon\|A\|$ and $\|\delta b\| \leq \varepsilon\|b\|$, we get

$$\varepsilon\|A\| \cdot \|\tilde{x}\| \geq \|r\| - \varepsilon\|b\|$$

Backward errors of linear systems, cont'd$_1$

which we re-order as

$$\varepsilon \geq \frac{\|r\|}{\|A\| \cdot \|\tilde{x}\| + \|b\|}$$

and whose minimum, i.e., the backward error $\eta_{A,b}(\tilde{x})$, is

$$\eta_{A,b}(\tilde{x}) = \frac{\|r\|}{\|A\| \cdot \|\tilde{x}\| + \|b\|}.$$

When using 2-norms, the bound is attained for

$$\delta A = \frac{\|A\|_2}{\|\tilde{x}\|_2 \cdot (\|A\|_2 \cdot \|\tilde{x}\|_2 + \|b\|_2)}\, r\tilde{x}^T \;\text{ and }\; \delta b = -\frac{\|b\|_2}{\|A\|_2 \cdot \|\tilde{x}\|_2 + \|b\|_2}\, r.$$

- Note that $r\tilde{x}^T$ is a matrix of rank 1, so that the approximate solution $\tilde{x}$ to the linear system $Ax = b$ is the exact solution to a linear system whose matrix is a rank-1 perturbation of A.
- $\eta_{A,b}(\tilde{x})$ is sometimes referred to as the **normwise relative backward error**, so as to be distinguished from other definitions of backward error.

Backward errors of linear systems, cont'd$_2$

- In practice, evaluating $\eta_{A,b}(\tilde{x})$ can be challenging due to the need of $\|A\|$.
- Then, the backward error $\eta_b(\tilde{x})$ is considered, where only b is perturbed:

$$\eta_b(\tilde{x}) = \min\{\varepsilon \text{ s.t. } A\tilde{x} = b + \delta b,\ \|\delta b\| \leq \varepsilon\|b\|\}.$$

  Since we then have $\|\delta b\| = \|A\tilde{x} - b\| = \|r\|$, the backward error is

$$\eta_b(\tilde{x}) = \frac{\|r\|}{\|b\|}.$$

- Note that $\eta_b(\tilde{x}) \geq \eta_{A,b}(\tilde{x})$ for all A, b and $\tilde{x}$, so that the design of a stopping criteria on the basis of $\eta_b(\tilde{x})$ is **conservative**, and **good practice**.
- Some implementations of iterative linear solvers monitor the convergence of iterates $x_0, \ldots, x_k$ through $\|r_k\|/\|r_0\|$. But, if $x_0 \neq 0$ and $\|r_0\| \gg \|b\|$, we have

$$\eta_b(x_k) = \frac{\|r_k\|}{\|b\|} = \frac{\|r_k\|}{\|r_0\|}\frac{\|r_0\|}{\|b\|}$$

  so that, even if $\|r_k\|/\|r_0\| \leq \varepsilon$, we actually have $\eta_b(x_k) \gg \varepsilon$.
  Thus, this practice is **not recommended**, especially for ill-conditioned systems with poor non-zero initial guess.

Analysis of eigenvalue problems

Backward error of an eigenpair

- Let $(\tilde{\lambda}, \tilde{u})$ be an approximation of the eigenpair (λ, u) such that $Au = \lambda u$.
- Then, the associated normwise backward error $\eta_A(\tilde{\lambda}, \tilde{u})$ is given as

$$\eta_A(\tilde{\lambda}, \tilde{u}) = \min\{\varepsilon \text{ s.t. } (A + \delta A)\tilde{u} = \tilde{\lambda}\tilde{u},\ \|\delta A\| \leq \varepsilon \|A\|\}.$$

To find $\eta_A(\tilde{\lambda}, \tilde{u})$, we reorder the perturbed eigenvalue problem as

$$\begin{aligned}(A + \delta A)\tilde{u} &= \tilde{\lambda}\tilde{u} \\ \delta A\tilde{u} &= \tilde{\lambda}\tilde{u} - A\tilde{u}.\end{aligned}$$

Assuming consistent matrix and vector norms, we obtain

$$\varepsilon \|A\| \|\tilde{u}\| \geq \|\delta A\| \|\tilde{u}\| \geq \|\tilde{\lambda}\tilde{u} - A\tilde{u}\|$$

so that $\eta_A(\tilde{\lambda}, \tilde{u}) = \dfrac{\|r\|}{\|A\| \cdot \|\tilde{u}\|}$, where $r = A\tilde{u} - \tilde{\lambda}\tilde{u}$ is the eigen-residual.

Backward error of an eigenpair, cont'd

- When using 2-norms, the minimal norm perturbation is achieved with
$$\delta A = -\frac{r\tilde{u}^H}{\|A\|_2 \cdot \|\tilde{u}\|_2^2}$$
which, again, is a rank-1 perturbation.
- So, computing an approximation $(\tilde{\lambda}, \tilde{u})$ of the eigenpair (λ, u) such that
$$\frac{\|r\|}{\|A\| \cdot \|\tilde{u}\|} \leq \varepsilon$$
for a small value of ε should ensure the good quality approximation, **if the problem is well-conditioned**.

  But, **what is the conditioning of solving for an eigenpair** (λ, u) of A?
- In practice, convergence is often monitored with the criterion
$$\frac{\|r\|}{|\tilde{\lambda}| \cdot \|\tilde{u}\|} \leq \varepsilon$$
which, for larger eigenvalues of the spectrum, is generally not an issue.

Perturbation of the normal eigenvalue problem

- Let λ be a simple eigenvalue of a matrix A with normalized right-eigenvector u and left-eigenvector v, i.e.,

$$Au = \lambda u\ , \quad v^H A = \lambda v^H \ \text{ and } \ \|u\|_2 = \|v\|_2 = 1.$$

We consider the approximate eigenpair $(\tilde{\lambda}(\varepsilon), \tilde{u}(\varepsilon))$ of A with the linear perturbation $\tilde{A}(\varepsilon) := A + \varepsilon E$ along a matrix E s.t. $(\tilde{\lambda}(0), \tilde{u}(0)) = (\lambda, u)$ and

$$\tilde{A}(\varepsilon)\tilde{u}(\varepsilon) = \tilde{\lambda}(\varepsilon)\tilde{u}(\varepsilon).$$

Multiplying both sides of this expression by the left-eigenvector v^H associated with λ, we obtain:

$$\begin{aligned} v^H \tilde{A}(\varepsilon)\tilde{u}(\varepsilon) &= \tilde{\lambda}(\varepsilon) v^H \tilde{u}(\varepsilon) \\ v^H A\tilde{u}(\varepsilon) + \varepsilon v^H E\tilde{u}(\varepsilon) &= \tilde{\lambda}(\varepsilon) v^H \tilde{u}(\varepsilon) \\ (v^H A = \lambda v^H) \qquad \lambda v^H \tilde{u}(\varepsilon) + \varepsilon v^H E\tilde{u}(\varepsilon) &= \tilde{\lambda}(\varepsilon) v^H \tilde{u}(\varepsilon) \end{aligned}$$

so that $(\tilde{\lambda}(\varepsilon) - \lambda)/\varepsilon = v^H E\tilde{u}(\varepsilon)/(v^H \tilde{u}(\varepsilon))$.

Perturbation of the normal eigenvalue problem, cont'd

- The rate of change in $\tilde{\lambda}$ induced by the linear perturbation of A along E is then given by:

$$\lim_{\varepsilon \to 0} \frac{\tilde{\lambda}(\varepsilon) - \lambda}{\varepsilon} = \frac{v^H E \tilde{u}(0)}{v^H \tilde{u}(0)} = \frac{v^H E \tilde{u}}{v^H \tilde{u}}.$$

  Using the Cauchy-Schwartz inequality, we obtain $|v^H E u| \leq \|E\|_2$ and

$$|\tilde{\lambda} - \lambda| \lesssim \frac{\|E\|_2}{|v^H u|},$$

  so that solving for the simple eigenvalue λ of A has conditioning given by $\kappa(A, \lambda) = 1/|v^H u|$.
- **Normal** (and thus **symmetric**) **matrices** have aligned right- and left-eigenvectors, which implies $\kappa(\lambda, A) = 1$, i.e., **solving for a simple eigenvalue of a normal matrix is a well-conditioned problem**.
- For general matrices, if u and v are nearly orthogonal, we have $\kappa(\lambda, A) \gg 1$, and **solving for the eigenvalue λ is an ill-conditioned problem**.