

Chapter 8: Factorizations and Sensitivity

1. Apply Gaussian elimination to obtain triangular system:

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \rightarrow \begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \\ & & & & \times \end{bmatrix} \quad \text{ca. } \frac{1}{3}n^3 \text{ LOps}$$

2. Back substitution

$$\begin{aligned} x_n &= b_n / a_{nn} \\ x_{n-1} &= (b_{n-1} - a_{n-1,n} \cdot x_n) / a_{n-1,n-1} \\ &\vdots \end{aligned} \quad \text{ca. } \frac{1}{2}n^2 \text{ LOps}$$

LU factorization

Another formulation of Gaussian elimination with pivoting:

$$\mathbf{P} \mathbf{A} = \mathbf{L} \mathbf{U},$$

where

- \mathbf{P} is a permutation matrix,
- \mathbf{U} is an upper triangular *after* Gaussian eliminationen, and
- \mathbf{L} is a unit lower triangular including elimination coefficients:

$$\ell_{ik} = f_{ik}, \quad k < i \quad \text{and} \quad \ell_{kk} = 1.$$

When we have LU factorization of \mathbf{A} , the solution of the linear system $\mathbf{A} \mathbf{x} = \mathbf{b}$ equals $\mathbf{x} = \mathbf{U}^{-1} \mathbf{L}^{-1} \mathbf{P} \mathbf{b}$, and it only costs n^2 LOps to obtain \mathbf{x} .

LDL^T factorization (page 367)

If the matrix \mathbf{A} is symmetric, then we have

$$\mathbf{L}\mathbf{U} = \mathbf{A} = \mathbf{A}^T = (\mathbf{L}\mathbf{U})^T = \mathbf{U}^T \mathbf{L}^T.$$

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Since the left-hand side is upper triangular and the right-hand side is lower triangular, both sides have to be diagonal, say, \mathbf{D} . Then, we have

$$\mathbf{U} (\mathbf{L}^T)^{-1} = \mathbf{D}$$

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Since the left-hand side is upper triangular and the right-hand side is lower triangular, both sides have to be diagonal, say, \mathbf{D} . Then, we have

$$\mathbf{U} (\mathbf{L}^T)^{-1} = \mathbf{D} \implies \mathbf{U} = \mathbf{D} \mathbf{L}^T \implies \mathbf{A} = \mathbf{L} \mathbf{D} \mathbf{L}^T.$$

Cholesky factorization (page 369–370)

The Matrix \mathbf{A} is *symmetric* and *positive definite* (SPD) when

$$\mathbf{A}^T = \mathbf{A} \quad \text{and} \quad \mathbf{x}^T \mathbf{A} \mathbf{x} > 0 \quad \text{for all } \mathbf{x} \neq 0.$$

An important example: normal equation in data-fitting.

Due to symmetry, we have $\mathbf{A} = \mathbf{L} \mathbf{D} \mathbf{L}^T$. Further, \mathbf{A} is SPD, so \mathbf{D} has a positive diagonal. Then, we have

$$\mathbf{A} = \mathbf{L} \sqrt{\mathbf{D}} \sqrt{\mathbf{D}}^T \mathbf{L}^T = \mathbf{L} \mathbf{L}^T, \quad \mathbf{L} = \mathbf{L} \sqrt{\mathbf{D}}$$

This is called as Cholesky factorization.

NB: In Cholesky factorization \mathbf{L} is lower triangular with a positive diagonal, which is different as \mathbf{L} in LU factorization!

We can derive the elements in \mathbf{L} by comparing the elements in $\mathbf{L} \mathbf{L}^T$ and \mathbf{A} . For example, in a 2×2 matrix:

$$\begin{bmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} \\ 0 & l_{22} \end{bmatrix} = \begin{bmatrix} l_{11}^2 & l_{11}l_{21} \\ l_{11}l_{21} & l_{21}^2 + l_{22}^2 \end{bmatrix} \Rightarrow$$
$$l_{11} = \sqrt{a_{11}}, \quad l_{21} = a_{21}/l_{11}, \quad l_{22} = \sqrt{a_{22} - l_{21}^2}.$$

Python-code for Cholesky factorization

This code is a bit different from the one in page 370:

```
for k in range(n):
    A[k, k] = np.sqrt(A[k, k])
    A[k+1:n, k] = A[k+1:n, k] / A[k, k]
    for j in range(k+1, n):
        A[j:n, j] = A[j:n, j] - A[j, k]*A[j:n, k]
L = np.tril(A) # lower triangle of A
```

Pivoting is not necessary in Cholesky factorization!

The algorithm overwrites the current element in **A**, which is saved in **L** in the end.

Only the lower triangular part of **A** is needed – so in the end we only need save a part of the matrix.

Operation count $\approx 1/6n^3$, i.e. *only half* as in LU factorization.

Cholesky factorization in Python with `np.linalg.cholesky`

```
>>> A = np.array([[6, 15, 55],  
                  [15, 55, 225],  
                  [55, 225, 979]], dtype=float)  
>>> L = np.linalg.cholesky(A)  
>>> print(L)
```

```
L =  
[[ 2.44948974  0.  0. ]  
 [ 6.12372436  4.18330013  0. ]  
 [22.45365598 20.91650066  6.11010093]]
```

Solve linear systems with Cholesky factorization

$$\begin{aligned}\mathbf{A}\mathbf{x} = \mathbf{b} &\Rightarrow \mathbf{L}\mathbf{L}^T\mathbf{x} = \mathbf{b} \\ &\Rightarrow \mathbf{L}^T\mathbf{x} = \mathbf{L}^{-1}\mathbf{b} \\ &\Rightarrow \mathbf{x} = (\mathbf{L}^T)^{-1}(\mathbf{L}^{-1}\mathbf{b})\end{aligned}$$

Solve linear systems with Cholesky factorization

$$\begin{aligned} \mathbf{A} \mathbf{x} = \mathbf{b} &\Rightarrow \mathbf{L} \mathbf{L}^T \mathbf{x} = \mathbf{b} \\ &\Rightarrow \mathbf{L}^T \mathbf{x} = \mathbf{L}^{-1} \mathbf{b} \\ &\Rightarrow \mathbf{x} = (\mathbf{L}^T)^{-1} (\mathbf{L}^{-1} \mathbf{b}) \end{aligned}$$

In Python, there are two ways to implement this procedure:

```
>>> tmp = scipy.linalg.solve_triangular(L,b,lower=True)
>>> x = scipy.linalg.solve_triangular(L.T, tmp, lower=False)
```

OR

```
>>> c, low = scipy.linalg.cho_factor(A)
>>> x = scipy.linalg.cho_solve((c, low), b)
```

Sensitivity analysis for $f(x) = 0$ (Motivation)

How much does the root change, when the function f is perturbed?

Relevant to: when f is described by noisy data – in this case, is the root affected by the data error?

Sensitivity analysis/error assessment:

How sensitive is the root to the perturbation of the function f ?

Error assessment of a simple root

When ξ is close to x^* we can always assume that $0 < M \leq |f'(\xi)|$.

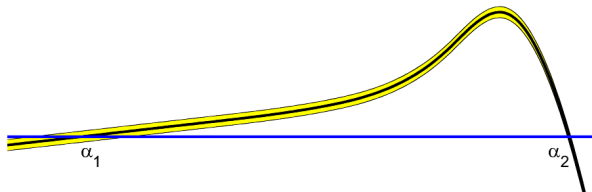
We want to calculate the root x^* of f , but we only have a *perturbed* function \tilde{f} and can calculate its root \tilde{x}^* . Assume that when ξ is close to x^* we have

$$|\tilde{f}(\xi) - f(\xi)| \leq \delta,$$

where δ is an upper bound for the absolute error of the function values. So we can obtain the upper bound for the absolute error:

$$|\tilde{x}^* - x^*| \leq \delta/M.$$

Smaller M (lower bound of the slope) is, more sensitive the root is to the error in \tilde{f} :



Sensitivity analysis for $\mathbf{A} \mathbf{x} = \mathbf{b}$

The rest of the lecture is about, how the solution \mathbf{x} of $\mathbf{A} \mathbf{x} = \mathbf{b}$ is affected by the perturbation in the data, i.e. the error in the right-hand side.

How much does \mathbf{x} change, when the right-hand side \mathbf{b} is perturbed?

Example: the right-hand side $\tilde{\mathbf{b}}$ includes measurement error

$$\tilde{\mathbf{b}} = \mathbf{b} + \text{error} = \begin{bmatrix} 1.3 \\ 2.4 \\ 3.5 \end{bmatrix} = \begin{bmatrix} 1.2 \\ 2.5 \\ 3.3 \end{bmatrix} + \begin{bmatrix} 0.1 \\ -0.1 \\ 0.2 \end{bmatrix}.$$

How can we measure the difference between $\mathbf{x} = \mathbf{A}^{-1} \mathbf{b}$ and $\tilde{\mathbf{x}} = \mathbf{A}^{-1} \tilde{\mathbf{b}}$.

Content:

- ➊ Vector and matrix norm.
- ➋ Sensitivity analysis and condition number.

Review: absolute and relative error (page 5–6)

Absolute error

When we say the error in a is ± 0.01 , we mean

$$-0.01 \leq a - \bar{a} \leq 0.01, \quad \bar{a} = \text{exact value.}$$

Relative error

If we say a has a *relative* error 0.01 (or 1%), we mean

$$\frac{|a - \bar{a}|}{|\bar{a}|} \leq 0.01 .$$

But what can we say when we talk about the error in the vectors \mathbf{x} and \mathbf{b} ?

Vector norm (page 405)

For a vector, we define vector norm:

$$\|\mathbf{x}\|_2 = (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2}.$$

It is in fact an Euclidean distance in 2 and 3 dimensions.

Example:

$$\mathbf{x} = \begin{bmatrix} -1 \\ 2 \\ 3 \end{bmatrix}, \quad \|\mathbf{x}\|_2 \approx 3.74 \quad \text{Python: } \text{np.linalg.norm}(\mathbf{x}).$$

We can show that: $\max_i |x_i| \leq \|\mathbf{x}\|_2 \leq \sqrt{n} \max_i |x_i|$.

- If $\|\mathbf{x}\|_2$ is large, \mathbf{x} has at least one large element (because $\max_i |x_i| \geq \|\mathbf{x}\|_2 / \sqrt{n}$).
- If $\|\mathbf{x}\|_2$ is small, \mathbf{x} only has small elements (because $\max_i |x_i| \leq \|\mathbf{x}\|_2$).

An application of norm: error in vectors

Assume that $\tilde{\mathbf{x}}$ is an approximation of \mathbf{x} . With the difference

$$\delta\mathbf{x} = \tilde{\mathbf{x}} - \mathbf{x}$$

it is not practical to be used for measuring the error, since we need observe all elements in the vector $\delta\mathbf{x}$.

By using the vector norm, we can define the **absolute error**

$$\|\delta\mathbf{x}\|_2 = \|\tilde{\mathbf{x}} - \mathbf{x}\|_2$$

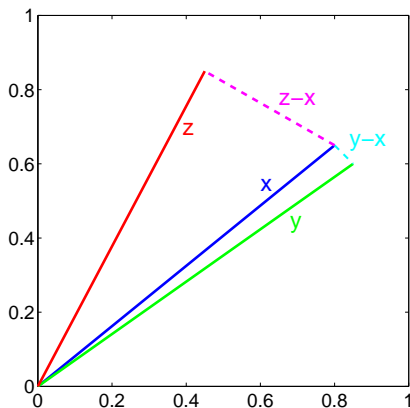
and the **relative error**

$$\frac{\|\delta\mathbf{x}\|_2}{\|\mathbf{x}\|_2} = \frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|_2}{\|\mathbf{x}\|_2}.$$

If the norm $\|\delta\mathbf{x}\|_2$ is small, then all elements in $\delta\mathbf{x} = \tilde{\mathbf{x}} - \mathbf{x}$ are small, then we can say that $\tilde{\mathbf{x}}$ is close to \mathbf{x} . \rightarrow In the end of the lecture, we will show how to *estimate* these errors without known \mathbf{x} .

Example to use vector norm

Which vector is close to \mathbf{x} ? \mathbf{y} or \mathbf{z} ?



Relative error: $\|\mathbf{y} - \mathbf{x}\|_2 / \|\mathbf{x}\|_2 = 0.07$ and $\|\mathbf{z} - \mathbf{x}\|_2 / \|\mathbf{x}\|_2 = 0.20$.

Matrix norm (page 406)

We can also define the 2-norm for a matrix to measure its “magnitude”:

$$\|\mathbf{A}\|_2 = \sup\{\|\mathbf{Ax}\|_2 : \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_2 = 1\} \quad (1)$$

$$= (\text{the largest eigenvalue of } \mathbf{A}^T \mathbf{A})^{1/2} = \text{np.linalg.norm(A)} \quad (2)$$

Example:

$$\mathbf{A} = \begin{bmatrix} 1 & -0.01 & 0 \\ 0.02 & -5 & 3 \\ -4 & 1 & -0.01 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0.01 & -0.02 & 0 \\ 0.03 & -0.01 & 0.05 \\ -0.04 & 0 & 0.03 \end{bmatrix}$$

$$\|\mathbf{A}\|_2 = 5.95, \quad \|\mathbf{B}\|_2 = 0.060.$$

If the norm of $\|\mathbf{B}\|_2$ is small, then we can conclude that there are only small elements in \mathbf{B} .

Continue: vector and matrix norm (page 405–406)

Some important properties of vector and matrix norm:

$$\|\mathbf{x}\|_2 = 0 \Leftrightarrow \mathbf{x} = \mathbf{0} , \quad \|\mathbf{A}\|_2 = 0 \Leftrightarrow \mathbf{A} = \mathbf{0}$$

$$\|\alpha \mathbf{x}\|_2 = |\alpha| \|\mathbf{x}\|_2 , \quad \|\alpha \mathbf{A}\|_2 = |\alpha| \|\mathbf{A}\|_2$$

$$\|\mathbf{x} + \mathbf{y}\|_2 \leq \|\mathbf{x}\|_2 + \|\mathbf{y}\|_2 , \quad \|\mathbf{A} + \mathbf{B}\|_2 \leq \|\mathbf{A}\|_2 + \|\mathbf{B}\|_2 .$$

Very important properties:

$$\|\mathbf{A} \mathbf{x}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{x}\|_2 , \quad \|\mathbf{A} \mathbf{B}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{B}\|_2 .$$

Any properties with “−”?

$$\|\mathbf{y} + (\mathbf{x} - \mathbf{y})\|_2 \leq \|\mathbf{y}\|_2 + \|\mathbf{x} - \mathbf{y}\|_2 \implies \|\mathbf{x}\|_2 - \|\mathbf{y}\|_2 \leq \|\mathbf{x} - \mathbf{y}\|_2$$

Python example with perturbation in the right-hand side

True solution \mathbf{x} , perturbation solution \mathbf{x}_t , and $\mathbf{x}-\mathbf{x}_t$:

5.5090e+00	5.4010e+00	1.0810e-01
3.2564e+00	3.3586e+00	1.0214e-01
1.6696e+00	1.6794e+00	9.8571e-03

$\|\mathbf{b}-\mathbf{b}_t\|_2$:

1.5684e+00

$\|\mathbf{x}-\mathbf{x}_t\|_2$:

1.4905e-01

Is there any relation between $\|\mathbf{b}-\tilde{\mathbf{b}}\|_2$ and $\|\mathbf{x}-\tilde{\mathbf{x}}\|_2$?

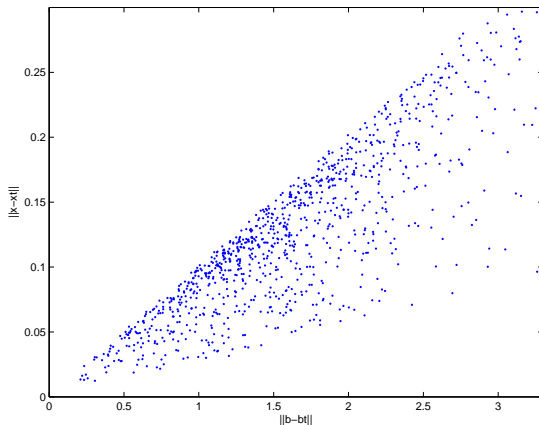
Let's test on 1000 different perturbation on $\mathbf{b} \rightarrow$ next slide.

Python example with perturbation in the right-hand side

```
import numpy as np
import matplotlib.pyplot as plt
E = np.empty(1000)
D = np.empty(1000)
for i in range(1000):
    e = np.random.randn(3) # vector with 3 samples from  $N(0,1)$ 
    E[i] = np.linalg.norm(e)
    d = np.linalg.solve(A, b) - np.linalg.solve(A, b+e)
    D[i] = norm(d)
end
```

Python example with perturbation in the right-hand side

```
plt.figure()  
plt.plot(E, D, linewidth=0, marker='.')  
plt.show()
```



Analysis of a perturbation in the right-hand side (page 407)

Let \mathbf{x} denote the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$.

Now we *perturb* the right-hand side with a vector $\delta\mathbf{b}$ and obtain $\tilde{\mathbf{b}} = \mathbf{b} + \delta\mathbf{b}$, and compute

$$\mathbf{A}\tilde{\mathbf{x}} = \tilde{\mathbf{b}} \quad \Rightarrow \quad \tilde{\mathbf{x}} = \mathbf{A}^{-1}\tilde{\mathbf{b}}.$$

We want to measure the error $\delta\mathbf{x} = \tilde{\mathbf{x}} - \mathbf{x}$ in the solution, i.e. find the relation between $\|\delta\mathbf{x}\|_2$ and the perturbation $\|\delta\mathbf{b}\|_2$. We can easily get

$$\mathbf{A}\delta\mathbf{x} = \mathbf{A}(\tilde{\mathbf{x}} - \mathbf{x}) = \mathbf{A}\tilde{\mathbf{x}} - \mathbf{A}\mathbf{x} = \tilde{\mathbf{b}} - \mathbf{b} = \delta\mathbf{b} \quad \Leftrightarrow \quad \delta\mathbf{x} = \mathbf{A}^{-1}\delta\mathbf{b}.$$

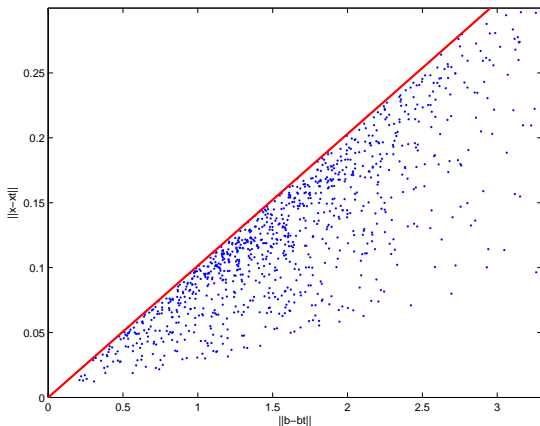
Now based on the properties of vector and matrix norm, we obtain

$$\|\delta\mathbf{x}\|_2 = \|\mathbf{A}^{-1}\delta\mathbf{b}\|_2 \leq \|\mathbf{A}^{-1}\|_2 \|\delta\mathbf{b}\|_2.$$

This is an upper bound (a “worst-case”) for the absolute error.

```
t = np.array([0, np.max(E)])  
upp_bound = np.linalg.norm(np.linalg.inv(A))*t  
plt.plot(t, upp_bound, color='red', linewidth=2)
```

$$\|\mathbf{A}^{-1}\|_2 = 0.1054.$$



Relative error – condition number (page 406–407)

Now we want to measure the *relative* error $\|\tilde{\mathbf{x}} - \mathbf{x}\|_2 / \|\mathbf{x}\|_2 = \|\delta\mathbf{x}\|_2 / \|\mathbf{x}\|_2$.

From the original linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$, we have

$$\|\mathbf{b}\|_2 = \|\mathbf{A}\mathbf{x}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{x}\|_2 \quad \Leftrightarrow \quad \frac{1}{\|\mathbf{x}\|_2} \leq \frac{\|\mathbf{A}\|_2}{\|\mathbf{b}\|_2} .$$

Then combining with the former result on absolute error, we get

$$\frac{\|\delta\mathbf{x}\|_2}{\|\mathbf{x}\|_2} = \frac{1}{\|\mathbf{x}\|_2} \|\delta\mathbf{x}\|_2 \leq \frac{\|\mathbf{A}\|_2}{\|\mathbf{b}\|_2} \|\mathbf{A}^{-1}\|_2 \|\delta\mathbf{b}\|_2 = \kappa(\mathbf{A}) \frac{\|\delta\mathbf{b}\|_2}{\|\mathbf{b}\|_2} .$$

We define the **condition number**:

$$\kappa(\mathbf{A}) = \|\mathbf{A}\|_2 \|\mathbf{A}^{-1}\|_2 = \text{np.linalg.cond}(\mathbf{A}) .$$

Larger the condition number is, larger the relative error can be.

Example with a small perturbation on the right-hand side

$$\mathbf{b} = \begin{bmatrix} 0.582 \\ 0.294 \end{bmatrix}, \quad \tilde{\mathbf{b}} = \begin{bmatrix} 0.583 \\ 0.293 \end{bmatrix}, \quad \frac{\|\delta \mathbf{b}\|_2}{\|\mathbf{b}\|_2} = \frac{\|\tilde{\mathbf{b}} - \mathbf{b}\|_2}{\|\mathbf{b}\|_2} = 0.00218$$

$$\mathbf{A} = \begin{bmatrix} 0.333 & 0.250 \\ 0.200 & 0.100 \end{bmatrix}, \quad \kappa(\mathbf{A}) = 13.3$$

$$\mathbf{x} = \begin{bmatrix} 0.916 \\ 1.108 \end{bmatrix}, \quad \tilde{\mathbf{x}} = \begin{bmatrix} 0.895 \\ 1.140 \end{bmatrix}, \quad \frac{\|\delta \mathbf{x}\|_2}{\|\mathbf{x}\|_2} = \frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|_2}{\|\mathbf{x}\|_2} = 0.0266.$$

The upper bound of the relative error:

$$\kappa(\mathbf{A}) \frac{\|\delta \mathbf{b}\|_2}{\|\mathbf{b}\|_2} = 13.3 \cdot 0.00218 = 0.0289.$$

The upper bound (“worst-case”) of the relative error usually is only a little bit larger.

Summary

- **Simple LU factorization.**

$\mathbf{A} = \mathbf{L} \mathbf{U}$ where \mathbf{L} is a unit lower triangular (with 1 on the diagonal) and \mathbf{U} is an upper triangular. It is direct from Gaussian elimination.

- **LU factorization with pivoting.**

$\mathbf{P} \mathbf{A} = \mathbf{L} \mathbf{U}$ where \mathbf{P} is a permutation matrix, which is from pivoting in Gaussian elimination.

- **Use LU factorization.**

```
P, L, U = scipy.linalg.lu(A)
```

```
x = np.linalg.solve(U, np.linalg.solve(L, P@b))
```

- **Cholesky factorization.**

For a symmetric positive definite matrix, we have $\mathbf{A} = \mathbf{L} \mathbf{L}^T$ and pivoting is not necessary.

- **Properties of vector and matrix norm.**

$$\|\mathbf{A} \mathbf{x}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{x}\|_2, \quad \|\mathbf{A} \mathbf{B}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{B}\|_2$$

- **Upper bound of the relative error for the solution.**

$$\frac{\|\delta \mathbf{x}\|_2}{\|\mathbf{x}\|_2} \leq \kappa(\mathbf{A}) \frac{\|\delta \mathbf{b}\|_2}{\|\mathbf{b}\|_2}, \quad \kappa(\mathbf{A}) = \|\mathbf{A}\|_2 \|\mathbf{A}^{-1}\|_2 = \text{np.linalg.cond}(\mathbf{A})$$

How about the residual? (not in the book)

We have an *approximated* solution $\tilde{\mathbf{x}}$ and calculate the *residual*:

$$\mathbf{r} = \mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}.$$

But can we use it to check if $\tilde{\mathbf{x}}$ is a good approximation of the true solution?

Theorem. The relative error of $\tilde{\mathbf{x}}$ is upper bounded by

$$\frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|_2}{\|\mathbf{x}\|_2} \leq \kappa(\mathbf{A}) \frac{\|\mathbf{r}\|_2}{\|\mathbf{b}\|_2}.$$

If the condition number $\kappa(\mathbf{A})$ is large, we can still have a large error on $\tilde{\mathbf{x}}$ even with small residual \mathbf{r} !



Reminders

Final evaluation is open until **Nov. 29**.

Next week will be 4-hour exercises in databars.

Homework assignment for Block 4 should be handed in before **Dec. 5 10pm**.

Dec. 6: mock exam from 8am to 11am, then the evaluation will start at 11:15am at B208 A054.

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Thank you for attending the course!