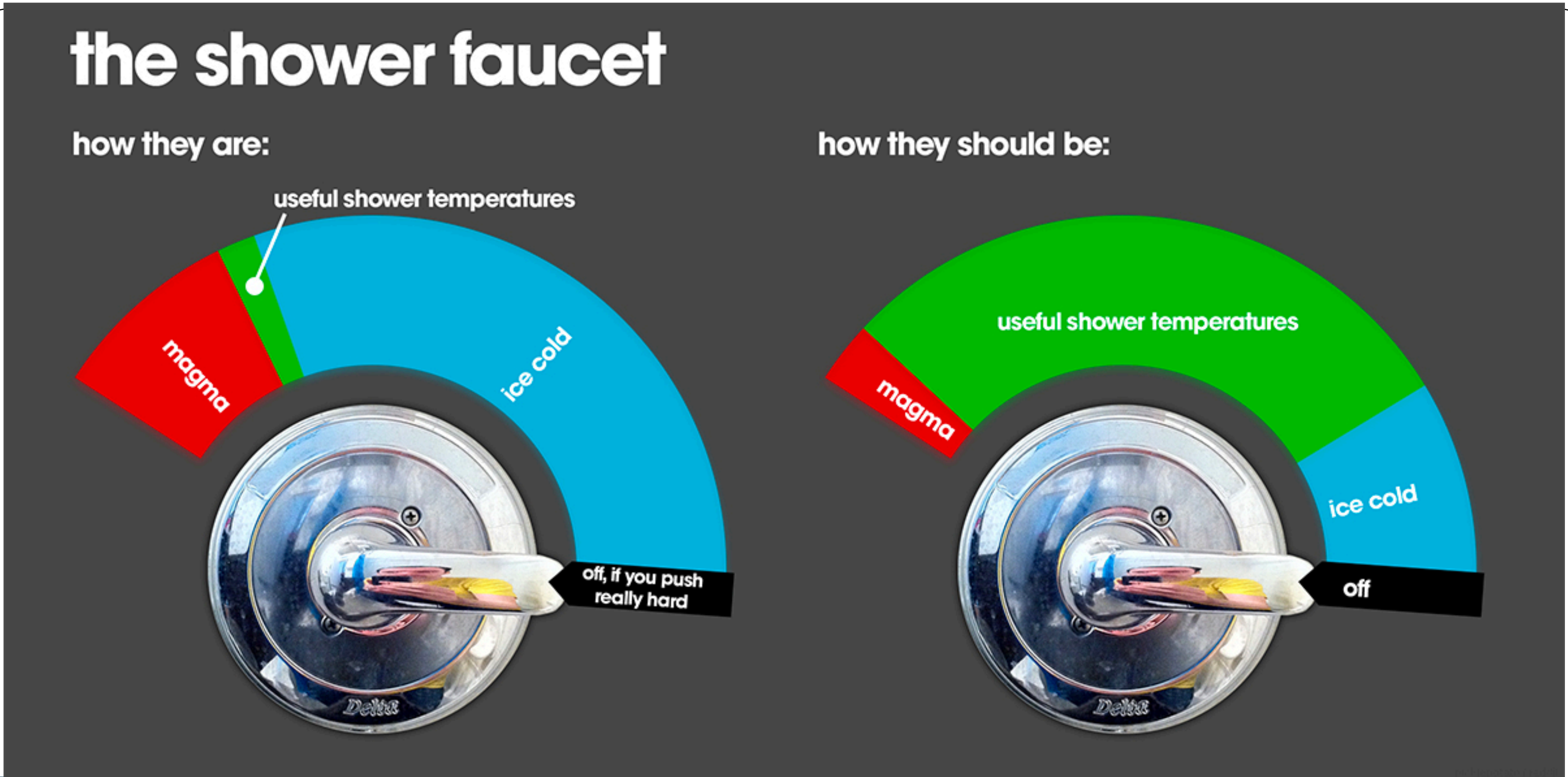
Linear System of Equations - Conditioning


the shower faucet
how they are:
useful shower temperatures
magma
ice cold
off, if you push really hard
how they should be:
useful shower temperatures
magma
ice cold
off


WHAT IT LOOKS LIKE
WHAT IT FEELS LIKE

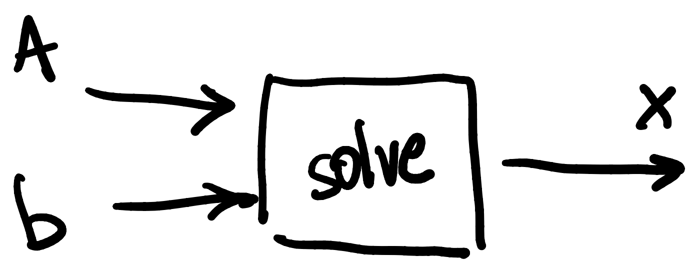
Numerical experiments

Input has uncertainties:

- Errors due to representation with finite precision
- Error in the sampling

Once you select your numerical method , how much error should you expect to see in your **output?**

Is your method sensitive to errors (perturbation) in the input?



Demo “HilbertMatrix-ConditionNumber”

$$Ax = b$$

1. Defining A $(N \times N)$
   - A) random
   - B) Hilbert

2. Start with a know exact solution:

   $x_{true} = [1, 1, \ldots, 1]$ (np.ones(N))

3. Compute $b = A @ x_{true}$

4. Solve $\begin{matrix} A \longrightarrow \\ b \longrightarrow \end{matrix} \boxed{} \longrightarrow x_{solve}$

5. Compute error $\| x_{solve} - x_{true} \|$

Sensitivity of Solutions of Linear Systems

Suppose we start with a non-singular system of linear equations $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$.

We change the right-hand side vector $\boldsymbol{b}$ (input) by a small amount $\Delta\boldsymbol{b}$.

How much the solution $\boldsymbol{x}$ (output) changes, i.e., how large is $\Delta\boldsymbol{x}$?

$$\frac{\text{Output Relative error}}{\text{Input Relative error}} = \frac{\|\Delta\boldsymbol{x}\|/\|\boldsymbol{x}\|}{\|\Delta\boldsymbol{b}\|/\|\boldsymbol{b}\|} = \frac{\|\Delta\boldsymbol{x}\|\,\|\boldsymbol{b}\|}{\|\Delta\boldsymbol{b}\|\,\|\boldsymbol{x}\|}$$

$Ax = b \rightarrow$ exact

$A\hat{x} = \hat{b} \rightarrow$ pert

$\hat{x} = x + \Delta x \qquad \hat{b} = b + \Delta b$

$A(x+\Delta x) = b + \Delta b \longrightarrow \boxed{A\,\Delta x = \Delta b}$

Sensitivity of Solutions of Linear Systems

$$\boxed{Ax = b}$$

$$A\Delta x = \Delta b$$

$$\Delta x = A^{-1}\Delta b$$

$$\frac{\text{Output Relative error}}{\text{Input Relative error}} = \frac{\|\Delta \boldsymbol{x}\|/\|\boldsymbol{x}\|}{\|\Delta \boldsymbol{b}\|/\|\boldsymbol{b}\|} = \frac{\|\Delta \boldsymbol{x}\|\,\|\boldsymbol{b}\|}{\|\Delta \boldsymbol{b}\|\,\|\boldsymbol{x}\|}$$

$$\frac{\text{Output Relative error}}{\text{Input Relative error}} = \frac{\|A^{-1}\Delta b\|\,\|b\|}{\|\Delta b\|\,\|x\|} \leq \frac{\|A^{-1}\|\,\cancel{\|\Delta b\|}\,\|b\|}{\cancel{\|\Delta b\|}\,\|x\|} =$$

$$\|A^{-1}\Delta b\| \leq \|A^{-1}\|\,\|\Delta b\|$$

$$= \frac{\|A^{-1}\|\,\|b\|}{\|x\|} = \frac{\|A^{-1}\|\,\|Ax\|}{\|x\|} \leq \frac{\|A^{-1}\|\,\|A\|\,\cancel{\|x\|}}{\cancel{\|x\|}}$$

$$\|Ax\| \leq \|A\|\,\|x\|$$

$$\frac{\text{out}}{\text{inp}} \leq \|A^{-1}\|\,\|A\|$$

Sensitivity of Solutions of Linear Systems

$$\frac{\text{out}}{\text{inp}} \le \underline{\qquad\qquad}$$

$$\underbrace{\frac{\|\Delta \boldsymbol{x}\|}{\|\boldsymbol{x}\|}} \le \underbrace{\|\boldsymbol{A}^{-1}\|\,\|\boldsymbol{A}\|}_{\text{cond}(A)} \underbrace{\frac{\|\Delta \boldsymbol{b}\|}{\|\boldsymbol{b}\|}}$$

Sensitivity of Solutions of Linear Systems

We can also add a perturbation to the matrix $\boldsymbol{A}$ (input) by a small amount $\boldsymbol{E}$, such that

$$(\boldsymbol{A} + \boldsymbol{E})\,\widehat{\boldsymbol{x}} = \boldsymbol{b}$$

and in a similar way obtain:

$$\frac{\|\Delta \boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq \underbrace{\|\boldsymbol{A}^{-1}\|\,\|\boldsymbol{A}\|}_{\text{cond(A)}}\;\underbrace{\frac{\|\boldsymbol{E}\|}{\|\boldsymbol{A}\|}}$$

Condition number

The condition number is a measure of sensitivity of solving a linear system of equations to variations in the input.

The condition number of a matrix $\boldsymbol{A}$:

$$cond(\boldsymbol{A}) = \|\boldsymbol{A}^{-1}\| \, \|\boldsymbol{A}\|$$

Recall that the induced matrix norm is given by

$$\|\boldsymbol{A}\|_p = \max_{\|\boldsymbol{x}\|=1} \|\boldsymbol{A}\boldsymbol{x}\|_p$$

And since the condition number is relative to a given norm, we should be precise and for example write:

$$cond_2(\boldsymbol{A}) \text{ or } cond_\infty(\boldsymbol{A})$$

Demo "HilbertMatrix-ConditionNumber"

Condition number

$A \to$ sing

$\text{cond}(A) = \infty$

$$\frac{\|\Delta \boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq cond(\boldsymbol{A}) \frac{\|\Delta \boldsymbol{b}\|}{\|\boldsymbol{b}\|}$$

Small condition numbers mean not a lot of error amplification. Small condition numbers are good!

But how small?

$\text{cond}(A) = \|A\| \|A^{-1}\|$

1) $\|X\| > 0 \longrightarrow \text{cond}(A) > 0$

2) $\|XY\| \leq \|X\| \|Y\| \to \|\underbrace{AA^{-1}}\| \leq \|A\| \|A^{-1}\|$

$\|A\| \|A^{-1}\| > \|I\|$

$\|I\| = \max\limits_{\|x\|=1} \|Ix\| = 1$

$\boxed{\|A\| \|A^{-1}\| \geq 1}$

Condition number

$$\frac{||\Delta\boldsymbol{x}\,||}{||\boldsymbol{x}||} \leq cond(\boldsymbol{A})\ \frac{||\Delta\boldsymbol{b}||}{||\boldsymbol{b}||}$$

Small condition numbers mean not a lot of error amplification. Small condition numbers are good!

Recall that

$$||\boldsymbol{I}|| = \max_{||\boldsymbol{x}||=1} ||\boldsymbol{I}\ \boldsymbol{x}|| = 1$$

Which provides with a lower bound for the condition number:

$$cond(\boldsymbol{A}) = ||\boldsymbol{A}^{-1}||\ ||\boldsymbol{A}|| \geq ||\boldsymbol{A}^{-1}\boldsymbol{A}|| = ||\boldsymbol{I}|| = 1$$

If $\boldsymbol{A}^{-1}$ does not exist, then $cond(\boldsymbol{A}) = \infty$ (by convention)

Recall Induced Matrix Norms

$$\|\boldsymbol{A}\|_1 = \max_j \sum_{i=1}^{n} |A_{ij}|$$

Maximum absolute column sum of the matrix $\boldsymbol{A}$

$$\|\boldsymbol{A}\|_\infty = \max_i \sum_{j=1}^{n} |A_{ij}|$$

Maximum absolute row sum of the matrix $\boldsymbol{A}$

$$\|\boldsymbol{A}\|_2 = \max_k \sigma_k$$

σ_k are the singular value of the matrix $\boldsymbol{A}$

Condition Number of a Diagonal Matrix

What is the 2-norm-based condition number of the diagonal matrix

$$A = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 13 & 0 \\ 0 & 0 & 0.5 \end{bmatrix}?$$

$\{100, 13, 0.5\}$

$$A^{-1} = \begin{bmatrix} 1/100 & & \\ & 1/13 & \\ & & 1/0.5 \end{bmatrix}$$

$\left\{\frac{1}{100}, \frac{1}{13}, \frac{1}{0.5}\right\}$

$\|A\|_2 = 100$

$\|A^{-1}\|_2 = 2$

$\text{cond}(A) = 100 \times 2 = 200$ //

Condition Number of Orthogonal Matrices

What is the 2-norm condition number of an orthogonal matrix A?

$$cond(\boldsymbol{A}) = \|\boldsymbol{A}^{-1}\|_2 \ \|\boldsymbol{A}\|_2 = \left\|\boldsymbol{A}^T\right\|_2 \|\boldsymbol{A}\|_2 = 1$$

That means orthogonal matrices have optimal conditioning.

They are very well-behaved in computation.

$$cond(A) \begin{cases} \text{small} \rightarrow \text{well-conditioned} \\ \text{large} \rightarrow \text{ill-conditioned} \end{cases}$$

About condition numbers

1. For any matrix $\boldsymbol{A}$, $cond(\boldsymbol{A}) \geq 1$
2. For the identity matrix $\boldsymbol{I}$, $cond(\boldsymbol{I}) = 1$
3. For any matrix $\boldsymbol{A}$ and a nonzero scalar γ, $cond(\gamma\boldsymbol{A}) = cond(\boldsymbol{A})$
4. For any diagonal matrix $\boldsymbol{D}$, $cond(\boldsymbol{D}) = \dfrac{\boldsymbol{max}|d_i|}{\boldsymbol{min}|d_i|}$
5. The condition number is a measure of how close a matrix is to being singular: a matrix with large condition number is nearly singular, whereas a matrix with a condition number close to 1 is far from being singular
6. The determinant of a matrix is NOT a good indicator is a matrix is near singularity

$\det(A) = 0 \longrightarrow$ sing

Demo “HilbertMatrix-ConditionNumber”

Residual versus error

Our goal is to find the solution $\boldsymbol{x}$ to the linear system of equations $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$

Let us recall the solution of the perturbed problem

$$\widehat{\boldsymbol{x}} = (\boldsymbol{x} + \Delta\boldsymbol{x})$$

which could be the solution of

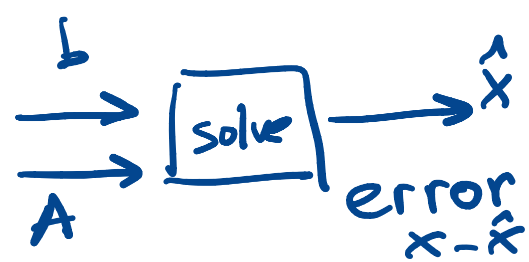
$$\boldsymbol{A}\,\widehat{\boldsymbol{x}} = (\boldsymbol{b} + \Delta\boldsymbol{b}), \qquad (\boldsymbol{A} + \boldsymbol{E})\widehat{\boldsymbol{x}} = \boldsymbol{b}, \qquad (\boldsymbol{A} + \boldsymbol{E})\,\widehat{\boldsymbol{x}} = (\boldsymbol{b} + \Delta\boldsymbol{b})$$

And the **error vector** as

$$\boldsymbol{e} = \Delta\boldsymbol{x} = \widehat{\boldsymbol{x}} - \boldsymbol{x}$$

We can write the **residual vector** as

$$\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\,\widehat{\boldsymbol{x}}$$



Relative residual: $\frac{\|\boldsymbol{r}\|}{\|\boldsymbol{A}\|\|\boldsymbol{x}\|}$

(How well the solution satisfies the problem)

Relative error: $\frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}\|}$

(How close the approximated solution is from the exact one)

Residual versus error

It is possible to show that the residual satisfy the following inequality:

$$\frac{||\boldsymbol{r}||}{||\boldsymbol{A}||\,||\widehat{\boldsymbol{x}}||} \leq c\,\epsilon_m$$

Where c is “large” constant when LU/Gaussian elimination is performed without pivoting and “small” with partial pivoting.

Therefore, Gaussian elimination with partial pivoting yields **small relative residual regardless of conditioning of the system**.

When solving a system of linear equations via LU with partial pivoting, the relative residual is guaranteed to be small!

Residual versus error

$$Ax = b \Rightarrow x = A^{-1}b$$

Let us first obtain the norm of the error:

$$\|\Delta x\| = \|\hat{x} - x\| = \|\underbrace{A^{-1}A}_{I}\hat{x} - A^{-1}b\| = \|A^{-1}\underbrace{(A\hat{x} - b)}_{r}\|$$

$$\frac{\|\Delta x\|}{\|x\|} = \underbrace{\frac{\|A^{-1}r\|}{\|x\|}} \leq \frac{\|A^{-1}\|\,\|r\|}{\|x\|}\,\frac{\|A\|}{\|A\|}$$

$$\frac{\|\Delta x\|}{\|x\|} \leq \underbrace{\|A^{-1}\|\,\|A\|}_{\text{cond}(A)}\,\frac{\|r\|}{\|x\|\,\|A\|}$$

$$\boxed{\frac{\|\Delta x\|}{\|x\|} \leq \text{cond}(A)\,\frac{\|r\|}{\|x\|\,\|A\|}}$$

Rule of thumb for conditioning

Suppose we want to find the solution $\boldsymbol{x}$ to the linear system of equations $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$ using LU factorization with partial pivoting and backward/forward substitutions.

Suppose we compute the solution $\hat{\boldsymbol{x}}$.

$$e_r = \frac{\|\Delta b\|}{\|b\|} \leq 10^{-S}$$

If the entries in $\boldsymbol{A}$ and $\boldsymbol{b}$ are accurate to S decimal digits,

and $cond(\boldsymbol{A}) \approx \mathbf{10}^{W}$,

$$e_r = \frac{\|\Delta x\|}{\|x\|} \leq cond(A)\frac{\|\Delta b\|}{\|b\|}$$

then the elements of the solution vector $\hat{\boldsymbol{x}}$ will be accurate to about

$S - W$

$$e_r \leq 10^{W}\,10^{-S}$$
$$= 10^{-(S-W)}$$

decimal digits