Numerical Matrix Analysis

Notes #17 — Systems of Equations
Gaussian Elimination & Cholesky Factorization

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Outline

Student Learning Targets, and Objectives

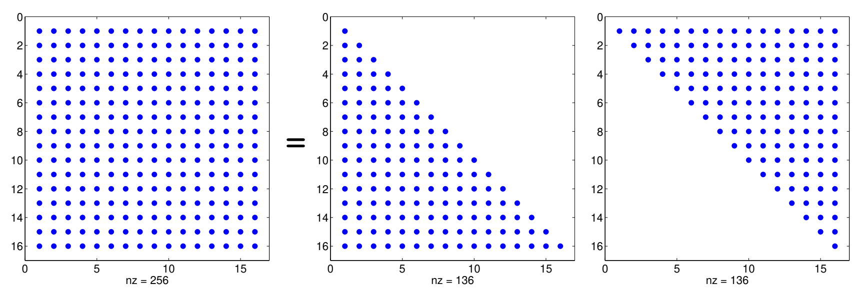
Target Gaussian Elimination
- **Objective** The Growth Factor, ρ as a measurement of (in)stability
- **Objective** Worst-case ρ for partial and complete pivoting vs. typical behavior

Target Gaussian Elimination — Special Case
- Hermitian Positive Definite Matrices
- Cholesky Factorization

Rewind: Last Time

We quickly reviewed a familiar algorithm — **Gaussian Elimination**.

If we save the multipliers generated by the elimination, we get the **LU-factorization** of A, *i.e.* $\mathbf{A} = \mathbf{LU}$, where L is lower triangular, and U is upper triangular.



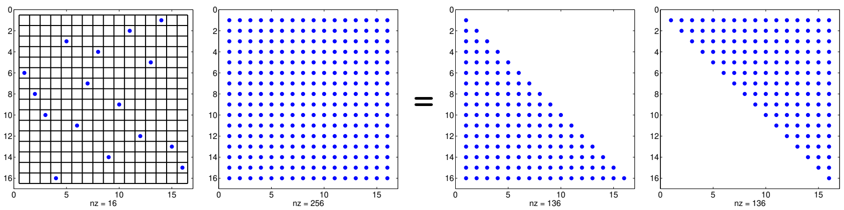
In this initial form, GE/LU is completely useless (unstable), we discussed a couple of fixes, some probably familiar, some new...

Rewind: Last Time

In **Partial Pivoting** we rearrange the rows of the matrix A (on the fly) in order to move the largest element in the "active" column to the diagonal entry — this way we can guarantee that the multiplier is bounded by one

$$\tilde{l}_{ji} = a_{ji} \oslash a_{ii} = \frac{a_{ji}}{a_{ii}}(1+\epsilon), \quad |\epsilon| \leq \varepsilon_{\text{mach}}, \qquad |\delta \tilde{\mathbf{l}}_{\mathbf{ji}}| \leq \varepsilon_{\text{mach}} \ell_{\mathbf{ji}}$$

We get $\mathbf{PA} = \mathbf{LU}$



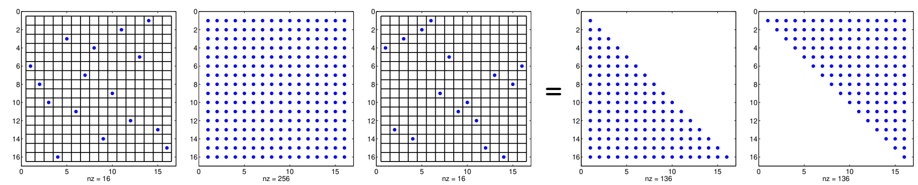
Rewind: Last Time

Partial Pivoting is stable "most of the time." We looked at enhancements taking scale into consideration: **Scaled Partial Pivoting**.

The overall work for GE/LU is $\sim \frac{2m^3}{3}$, and partial pivoting adds $\mathcal{O}(m^2)$ operations, which is a small cost.

Sometimes **Complete Pivoting** — rearrangement of both the rows and columns of A is necessary to achieve high accuracy. The cost is significant since the additional work adds $\mathcal{O}(m^3)$ operations.

We get $\mathbf{PAQ} = \mathbf{LU}$



Now...

— We look at the stability of Gaussian elimination.

— Gaussian Elimination for **Hermitian Positive Definite Matrices:**

  — Cholesky Factorization — The Hermitian (Symmetric) version of LU-factorization.

Stability of Gaussian Elimination: Introduction

"Gaussian Elimination with partial pivoting is ***explosively unstable*** *for certain matrices, yet stable in practice. This apparent paradox has a statistical explanation."*
[Trefethen-&-Bau, p.163]

The stability analysis of Gaussian Elimination with Partial Pivoting (GE w/PP) is complicated, consider the example $A = LU$

$$\begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix} \begin{bmatrix} 10^{-20} & 1 \\ 0 & 1-10^{20} \end{bmatrix}$$

The likely **naively computed** $\tilde{L}$ and $\tilde{U}$ are

$$\begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix} \begin{bmatrix} 10^{-20} & 1 \\ 0 & \mathbf{-10^{20}} \end{bmatrix} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & \mathbf{0} \end{bmatrix} \neq A$$

Stability of Gaussian Elimination: Introduction — 2 of 2

This behavior is quite generic — instability in Gaussian Elimination (with or without pivoting) can arise if the factors $\tilde{L}$ or $\tilde{U}$ are large compared with A.

In the previous example we have

$$\|A\|_F = 1.7321, \ \|\tilde{L}\|_F = 1.0000 \times 10^{20}, \ \|\tilde{U}\|_F = 1.0000 \times 10^{20}$$

i.e. the computed factors are 20 orders of magnitude larger than the initial matrix — no wonder we run into problems!

The purpose of pivoting — from the point of view of stability/accuracy — is to make sure that $\tilde{L}$ and $\tilde{U}$ are not too large.

Formal Result

Theorem (*LU*-Factorization without (explicit) Pivoting)

Let the factorization $A = LU$ of a non-singular matrix $A \in \mathbb{C}^{m\times m}$ be computed by Gaussian Elimination without pivoting in a floating point environment satisfying the floating point axioms. If A has an LU-factorization, then for ε_{mach} small enough, the factorization completes successfully in floating point arithmetic (no zero pivots $\tilde{a}_{ii}$ are encountered), and the computed matrices $\tilde{L}$, and $\tilde{U}$ satisfy

$$\tilde{L}\tilde{U} = A + \delta A, \quad \frac{\|\delta A\|}{\|L\|\,\|U\|} = \mathcal{O}(\varepsilon_{mach})$$

for some $\delta A \in \mathbb{C}^{m\times m}$.

Note that we can make the theorem apply to GE w/Pivoting by applying it to the "pre-pivoted matrix:" $A := PA[Q]$.

Formal Result: Comments

If we just flash by the previous slide, the result look just like all the other backward stability results... **BUT!!!** take a closer look... we have

$$\frac{\|\delta A\|}{\|L\|\,\|U\|} = \mathcal{O}(\varepsilon_{\text{mach}}).$$

Usually, the results contain something like

$$\frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\varepsilon_{\text{mach}}).$$

There is a **critical difference** here. If $\|L\|\,\|U\| = \mathcal{O}(\|A\|)$, then the theorem states that GE is backward stable. However (like in our previous example), if $\|L\|\,\|U\| \gg \mathcal{O}(\|A\|)$, all bets are off!

Quantifying Stability — The Growth Factor

Without pivoting, both $\|L\|$ and $\|U\|$ can be unbounded, and GE w/o Pivoting is unstable by any standard.

Consider GE w/PP. By construction $|\ell_{ij}| \le 1$, so that $\|L\| = \mathcal{O}(1)$ in any norm (this is true for all the pivoting schemes we have discussed). We now focus our attention to U; essentially GE w/PP is backward stable provided $\|U\| = \mathcal{O}(\|A\|)$.

The following quantity turns out to be very useful:

Definition (Growth Factor)

The **growth factor** of A (and the algorithm) is defined as the ratio

$$\rho = \frac{\max_{i,j} |u_{ij}|}{\max_{i,j} |a_{ij}|}$$

The Growth Factor... and Stability

If $\rho \sim 1$, there is little growth, and the elimination process is stable. When ρ is large, we expect loss of accuracy and/or instability of the algorithm... We make this precise: —

Theorem

Let the factorization $PA = LU$ of a non-singular matrix $A \in \mathbb{C}^{m\times m}$ be computed by GE w/PP in a floating point environment satisfying the floating point axioms. The computed matrices $\tilde{P}$, $\tilde{L}$, and $\tilde{U}$ satisfy

$$\tilde{L}\tilde{U} = \tilde{P}A + \delta A, \quad \frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\rho\,\varepsilon_{mach})$$

for some $\delta A \in \mathbb{C}^{m\times m}$, where ρ is the growth factor of A. If $|\ell_{ij}| < 1$ for $i > j$, then $P = \tilde{P}$ for ε_{mach} small enough.

Backward Stability for GE w/PP? 1 of 3

If $\rho = \mathcal{O}(1)$ uniformly for all matrices of a given dimension m, then GE w/PP is backward stable; otherwise it is not.

Let the mathematical hair-splitting begin!

Consider the worst-case scenario

$$\begin{bmatrix} 1 & & & & & 1 \\ -1 & 1 & & & & 1 \\ -1 & -1 & 1 & & & 1 \\ \vdots & \vdots & \ddots & \ddots & & \vdots \\ -1 & -1 & \dots & -1 & 1 & 1 \\ -1 & -1 & \dots & -1 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & & & & \\ -1 & 1 & & & & \\ -1 & -1 & 1 & & & \\ \vdots & \vdots & \ddots & \ddots & & \\ -1 & -1 & \dots & -1 & 1 & \\ -1 & -1 & \dots & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & & & 1 \\ & 1 & & & & 2 \\ & & 1 & & & 4 \\ & & & \ddots & & \vdots \\ & & & & 1 & 2^{m-2} \\ & & & & & 2^{m-1} \end{bmatrix}$$

Here $\rho = 2^{m-1}$, which is the maximal value ρ can take for GE w/PP.

Backward Stability for GE w/PP? 2 of 3

A growth factor of 2^{m-1} corresponds to a loss of $\sim (m-1)$ bits of information (Recall: we have at most 52 binary digits in IEEE-754-1985 double precision floating point computations).

According the worst-case estimate we cannot safely operate on matrices of dimension larger than (52×52), and in that case only have one bit of information! This is an intolerable state of affairs for practical computations!!!

Backward Stability for GE w/PP? 3 of 3

On the other hand... We have a uniform bound (2^{m-1}) on the growth factor for $(m \times m)$-matrices, thus according to our previous definitions of backward stability; **GE w/PP is backward stable.**

Clearly, **for practical purposes**, this is an absurd conclusion. In this context, let's put the previous formal definition of backward stability aside; and say that the worst-case scenario indicates that **GE w/PP can be unstable.**

Practical Stability of Gaussian Elimination

Now... If GE w/PP is so unstable, why is it so famous and popular?!?

> *"Despite worst-case examples, GE w/PP is utterly stable in practice. Large factors U like the one in the worst-case scenario never seem to appear in real applications. In 50 years of computing no matrix problems that excite explosive instability are known to have arisen under natural circumstances."*
> [Trefethen-&-Bau (1997), p.166]

In "Matrix Computations" by Golub & Van-Loan, the upper bounds for the growth factors for partial and complete pivoting are given as

$$\rho_{\text{PP}} \leq 2^{m-1}, \quad \rho_{\text{CP}} \leq 1.8 m^{\left(\frac{\ln m}{4}\right)}.$$

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Curious...

The number of matrices with large growth factors is very small — if we select a random matrix in $\mathbb{C}^{m\times m}$ it turns out that a practical bound on ρ_{PP} is given by $\sqrt{m}$. This is illustrated below.

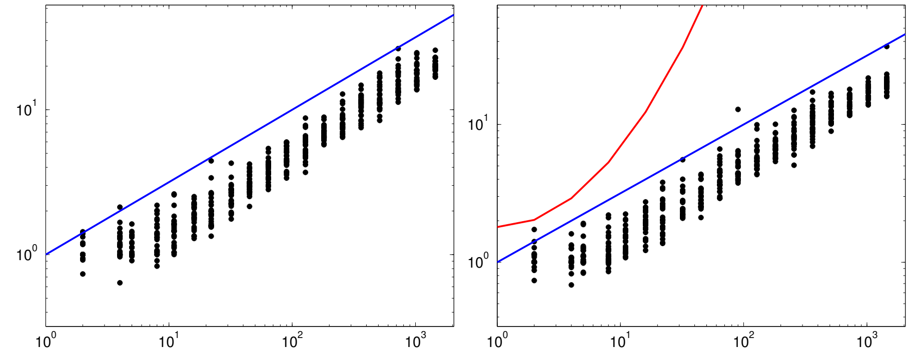

Figure: The growth factors for GE w/PP for 500 random matrices ranging in size from (2×2) to (1448×1448). The **blue** line (left panel) corresponds to the practical bound $\sqrt{m}$; and the **red line** (right panel only) corresponds to the worst-case bound for **complete pivoting**, ρ_{cp}.

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Curious... Where is the ρ_{pp} line?! Pt. 2

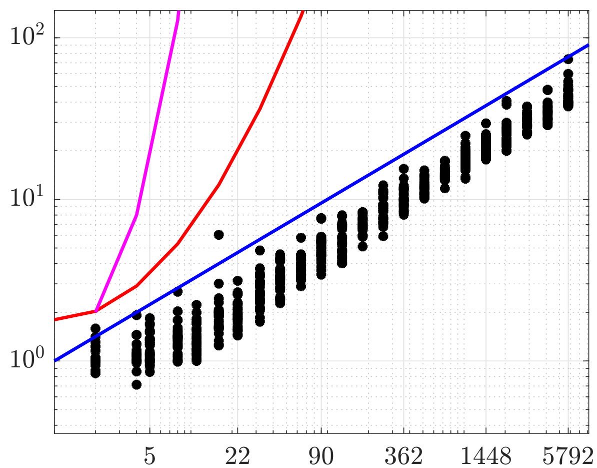

Figure: The corresponding values for ρ_{pp} are $\geq$ { 2, 8, 16, 128, 10^3, 10^4, 10^6, 10^9, 10^{13}, 10^{18}, 10^{26}, 10^{38}, 10^{54}, 10^{76}, 10^{108}, 10^{153}, 10^{217}, 10^{307}, 10^{435}, 10^{616}, 10^{871}, 10^{1232}, 10^{1743} }, whereas in this ($m \in \{2, \ldots, 5792\}$) range, $\rho_{cp} < 2.6 \cdot 10^8$; and $\sqrt{m} \leq 77$.

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GE w/PP Bottom Line

The bottom line is that GE w/PP works well "almost always."

It is almost impossible to prove any useful result in this context.

Vigorous hand-waving and numerical recovery of the probability density functions for the growth-factor vs. the matrix size can be used to get indications that the number of matrices with large growth factors is exponentially small in a probabilistic sense.

See *e.g.* Trefethen-&-Bau pp.166–170, for some discussion.

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Cholesky Factorization — Hermitian Positive Definite Matrices

We now turn our attention to application of Gaussian Elimination / LU-Factorization to a special class of matrices —

Definition (Hermitian Positive Definite)

$A \in \mathbb{C}^{m\times m}$ is **Hermitian Positive Definite** if $A = A^*$, and

$$\vec{x}^* A \vec{x} > 0, \quad \forall \vec{x} \in \mathbb{C}^m - \{\vec{0}\}.$$

This type of matrices show up **many** applications — due to symmetry (reciprocity) in physical systems.

My favorite application is **optimization** [MATH 693A], where we constantly build second order models

$$m_k(\vec{p}) = f(\vec{x}_k) + \vec{p}\nabla f(\vec{x}_k) + \frac{1}{2}\vec{p}^* B_k \vec{p}_k$$

where the matrix $B_k \approx \nabla^2 f(\vec{x}_k)$ is symmetric (Hermitian) positive definite.

Hermitian Positive Definite (HPD) Matrices: Properties

Let $A \in \mathbb{C}^{m\times m}$ be HPD.

- $\lambda(A) \in \mathbb{R}^+$.
- Eigenvectors that correspond to **distinct** eigenvalues of a Hermitian matrix are **orthogonal** (For general matrixes we only get linear independence).
- $\forall X \in \mathbb{C}^{m\times n}$, $m \geq n$, $\mathrm{rank}(X) = n$; X^*AX is also HPD.
- By selecting $X \in \mathbb{C}^{m\times n}$ to be a matrix with a 1 in each column, and zeros everywhere else, we can write any $(n \times n)$ principal sub-matrix of A in the form X^*AX. It follows that every principal sub-matrix of A must be HPD, and in particular $a_{ii} \in \mathbb{R}^+$.

Cholesky R^*R-factorization — 1 of 4

We now turn to the main task at hand — decomposing a HPD matrix into triangular factors, R^*R...

We assume that A is an HPD matrix, and write it in the form

$$\begin{bmatrix}\alpha & \vec{w}^* \\ \vec{w} & \boxed{B}\end{bmatrix} = \begin{bmatrix}\beta & \vec{0}^* \\ \vec{w}/\beta & \boxed{I(n-1)}\end{bmatrix}\begin{bmatrix}1 & \vec{0}^* \\ \vec{0} & \boxed{B - ww'/a}\end{bmatrix}\begin{bmatrix}\beta & \vec{w}^*/\beta \\ \vec{0} & \boxed{I(n-1)}\end{bmatrix}$$

Where

$\beta = \sqrt{\alpha}$, $\vec{0}$ is the zero-vector, (B - ww'/a) $\equiv (B - \vec{w}\vec{w}^*/\alpha)$,

`I(n-1)` is the $(n-1)\times(n-1)$-identity matrix

Before moving forward, we check the matrix identity...

Cholesky R^*R-factorization — 2 of 4

We have

$$\begin{bmatrix}\beta & \vec{0}^* \\ \vec{w}/\beta & \boxed{I(n-1)}\end{bmatrix}\begin{bmatrix}1 & \vec{0}^* \\ \vec{0} & \boxed{B - ww'/a}\end{bmatrix}\begin{bmatrix}\beta & \vec{w}^*/\beta \\ \vec{0} & \boxed{I(n-1)}\end{bmatrix}$$

Multiplying the first two matrices, and then third together gives

$$\begin{bmatrix}\beta & \vec{0}^* \\ \vec{w}/\beta & \boxed{B - ww'/a}\end{bmatrix}\begin{bmatrix}\beta & \vec{w}^*/\beta \\ \vec{0} & \boxed{I(n-1)}\end{bmatrix} = \begin{bmatrix}\alpha & \vec{w}^* \\ \vec{w} & \boxed{B}\end{bmatrix}$$

as desired.

Cholesky R^*R-factorization

It can be shown (see slides 31–32) that the sub-matrix $(B - \vec{w}\vec{w}^*/\alpha)$ is also HPD.

We can now define the Cholesky Factorization recursively:

$$R^{(n)} = \begin{bmatrix} \beta & \vec{w}^*/\beta \\ \vec{0} & \boxed{\mathrm{R(n{-}1)}} \end{bmatrix}$$

Where $\mathtt{R(n-1)} = R^{(n-1)}$ is the Cholesky factor R associated with $(B - \vec{w}\vec{w}^*/\alpha)$, *i.e.* $[R^{(n-1)}]^*[R^{(n-1)}] = (B - \vec{w}\vec{w}^*/\alpha)$.

A note on the implementation (next slide): Since we only need to compute one of the triangular parts (it's Hermitian, remember?!?) of the factorization, the Cholesky factorization uses about 1/2 the operations of a general LU-factorization.

Cholesky R^*R-factorization


```
% Cholesky Factorization of an m-by-m matrix A
for i = 1:m
  %
  % compute w*/β
  %
  A(i, i)        = sqrt(A(i, i));
  A(i, (i+1):m) = A(i, (i+1):m) / A(i, i);
  %
  % compute the upper triangular part of B − ww*/α
  %
  for j = (i+1):m
    A(j, j:m) = A(j, j:m) - A(i, j:m) * A(i, j)';
  end
  %
  % We zero out the sub-diagonal elements, since
  % the answer is an upper triangular matrix.
  %
  A((i+1):m, i) = zeros(m-i, 1);
end
```


Cholesky Factorization: Existence, Uniqueness, and Work

Theorem

Every HPD matrix $A \in \mathbb{C}^{m\times m}$ has a unique Cholesky factorization.

The existence follows from the argument on slides 31–32, and uniqueness from the algorithm. □

Compared with standard Gaussian elimination / LU-factorization we are saving about half the operations since we only form the upper triangular part R

Cholesky R^*R Factorization	$\frac{m^3}{3}$
LU-Factorization	$\frac{2m^3}{3}$
QR: Householder	$\frac{4m^3}{3}$
QR: Gram-Schmidt	$2m^3$
SVD	$13m^3$

Cholesky Factorization: Stability

Usually when we see this table

Cholesky R^*R Factorization	$\frac{m^3}{3}$
LU-Factorization	$\frac{2m^3}{3}$
QR: Householder	$\frac{4m^3}{3}$
QR: Gram-Schmidt	$2m^3$
SVD	$13m^3$

we note that with increased cost comes increased stability. The Cholesky factorization is the one pleasant exception!

All the subtle things that can go wrong in general LU-factorization (Gaussian elimination) are safe in the Cholesky factorization context!

Cholesky factorization is always backward stable!
(For HPD matrices, that is.)

Cholesky Factorization: Stability

In the 2-norm we have $\|R\| = \|R^*\| = \sqrt{\|A\|}$, thus the growth factor cannot be large. We also note that we can safely compute the Cholesky factorization **without pivoting**.

Theorem

Let $A \in \mathbb{C}^{m\times m}$ be HPD, and let $R^*R = A$ be computed using the Cholesky factorization algorithm in a floating point environment satisfying the floating point axioms. For sufficiently small ε_{mach}, this process is guaranteed to run to completion (no zero or negative entries r_{kk} will arise), generating a computed factor $\tilde{R}$ that satisfies

$$\tilde{R}^*\tilde{R} = A + \delta A, \qquad \frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\varepsilon_{mach})$$

for some $\delta A \in \mathbb{C}^{m\times m}$.

Solving $A\vec{x} = \vec{b}$ using Cholesky Factorization

If A is HPD, the standard (best) way to solve $A\vec{x} = \vec{b}$ is by Cholesky decomposition.

Once we have $R^*R\vec{x} = \vec{b}$, we get the solution by solving $R^*\vec{y} = \vec{b}$ (by forward substitution), followed by $R\vec{x} = \vec{y}$ (by backward substitution). Each triangular solve requires $\sim m^2$ operations, so the total work is $\sim \frac{1}{3}m^3$.

Solving $A\vec{x} = \vec{b}$ using Cholesky Factorization

We have the following important result

Theorem

The solution of an HPD system $A\vec{x} = \vec{b}$ via Cholesky factorization is backward stable, generating a computed solution $\tilde{x}$ that satisfies

$$(A + \Delta A)\tilde{x} = \vec{b}, \qquad \frac{\|\Delta A\|}{\|A\|} = \mathcal{O}(\varepsilon_{mach})$$

for some $\Delta A \in \mathbb{C}^{m\times m}$.

One More Comment

If we have a Hermitian matrix $A \in \mathbb{C}^{m\times m}$ the best way to **check** if it is also Positive Definite is to try to compute the Cholesky factorization.

If A is not HPD, then the Cholesky factorization will break down in the sense that

$\sqrt{r_{kk}}$ **or, if you want** `sqrt(A(i, i))`

will fail (if $r_{kk} < 0$) or the subsequent division by $\sqrt{r_{kk}}$ will fail (if $r_{kk} = 0$).

Usually, in applications (such as optimization) we require A to be **sufficiently HPD**, meaning that we must have $r_{kk} \geq \delta > 0$ for some δ. Quite possibly $\delta \in \{\sqrt{\varepsilon_{\text{mach}}}, \sqrt[3]{\varepsilon_{\text{mach}}}\}$.

Homework #6.5 — Due Date in Canvas/Gradescope

Use Gaussian Elimination with Partial Pivoting, create plots like TB-Figure-22.1, and TB-Figure-22.2

- For matrices with random, normally distributed $N(0,1)$ entries:
  - 6.5.1 Growth factor ρ for GE w/PP. (TB-Figure-22.1) — Use at least 1,024 matrices with varying sizes (up to at least 2,048×2,048 matrices)
  - 6.5.2 Probability density of ρ. (TB-Figure-22.2) — Use at least **1,048,576** matrices of each $(m \times m)$ size, $m \in \{8, 16, 32, 64\}$.
- For matrices with random, uniformly distributed in $[0,1]$ entries:
  - 6.5.3 Growth factor ρ for GE w/PP. (variant of TB-Figure-22.1) — Use at least 1,024 matrices with varying size (up to at least 2,048×2,048 matrices)
  - 6.5.4 Probability density of ρ. (variant of TB-Figure-22.2) — Use at least **1,048,576** matrices of each $(m \times m)$ size, $m \in \{8, 16, 32, 64\}$.
- 6.5.5 Comment on similarities / differences of normally vs. uniformly distributed matrix entries.

Hint: For computational efficiency, use built-in/library *LU*-factorizations with partial pivoting — `lu()` or `scipy.linalg.lu()` — *read the fine documentation.*

Reference: Proof that $B - \vec{w}\vec{w}^*/\alpha$ is HPD — 1 of 2

If A is HPD, and X is a non-singular matrix, then $B = X^*AX$ is also HPD: since X is non-singular $\vec{x} \neq 0 \Rightarrow X\vec{x} \neq 0$, hence

$$\forall \vec{x} \neq 0, \quad \vec{x}^* B \vec{x} = \vec{x}^* X^* A X \vec{x} = (X\vec{x})^* A (X\vec{x}) > 0$$

Now, with the representation

$$A = \begin{bmatrix} \beta^2 & \vec{w}^* \\ \vec{w} & B \end{bmatrix}$$

We select

$$X = \begin{bmatrix} 1/\beta & -\vec{w}^*/\beta^2 \\ \vec{0} & I(n-1) \end{bmatrix}, \quad X^* = \begin{bmatrix} 1/\beta & \vec{0}^* \\ -\vec{w}/\beta^2 & I(n-1) \end{bmatrix}$$

Reference: Proof that $B - \vec{w}\vec{w}^*/\alpha$ is HPD — 2 of 2

Now,

$$X^*AX = \begin{bmatrix} 1/\beta & \vec{0}^* \\ -\vec{w}/\beta^2 & I(n-1) \end{bmatrix} \begin{bmatrix} \beta^2 & \vec{w}^* \\ \vec{w} & B \end{bmatrix} \begin{bmatrix} 1/\beta & -\vec{w}^*/\beta^2 \\ \vec{0} & I(n-1) \end{bmatrix}$$

$$= \begin{bmatrix} \beta & \vec{w}^*/\beta \\ \vec{0} & B - ww'/a \end{bmatrix} \begin{bmatrix} 1/\beta & -\vec{w}^*/\beta^2 \\ \vec{0} & I(n-1) \end{bmatrix} = \begin{bmatrix} 1 & \vec{0} \\ \vec{0} & B - ww'/a \end{bmatrix}$$

It now follows from the definition (use $\vec{x} \neq 0$ such that $x_1 = 0$) that $B - \vec{w}\vec{w}^*/\beta^2$ is also HPD.