



# ECON526: Quantitative Economics with Data Science Applications

*Foundations of Numerical Linear Algebra*

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# Going Beyond “`reg y x, robust`”

- Data science, econometrics, and macroeconomics are built on linear algebra.
- Numerical linear algebra has all sorts of pitfalls, which become more critical as we scale up to larger problems.
- Speed differences in choosing better algorithms can be orders of magnitude.
- Crucial to know what goes on under-the-hood in Stata/R/python packages for applied work, even if you don't implement it yourself.
- Material here is related to
  - [QuantEcon Python](#)
  - [QuantEcon Data Science](#)
  - [A First Course in Quantitative Economics with Python](#)

# Packages

This section uses the following packages:

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 import scipy
4 from numpy.linalg import cond, matrix_rank, norm
5 from scipy.linalg import inv, solve, det, eig, lu, eigvals
6 from scipy.linalg import solve_triangular, eigvalsh, cholesky
```

# Basic Computational Complexity

## Big-O Notation

For a function  $f(N)$  and a positive constant  $C$ , we say  $f(N)$  is  $O(g(N))$ , if there exist positive constants  $C$  and  $N_0$  such that:

$$0 \leq f(N) \leq C \cdot g(N) \quad \text{for all } N \geq N_0$$

- Often crucial to know how problems scale asymptotically (as  $N \rightarrow \infty$ )
- Caution! This is only an asymptotic limit, and can be misleading for small  $N$ 
  - $f_1(N) = N^3 + N$  is  $O(N^3)$
  - $f_2(N) = 1000N^2 + 3N$  is  $O(N^2)$
  - For roughly  $N > 1000$  use  $f_2$  algorithm, otherwise  $f_1$

# Examples of Computational Complexity

- Simple examples:

→  $x \cdot y = \sum_{n=1}^N x_n y_n$  is  $O(N)$  since it requires  $N$  multiplications and additions

→  $Ax$  for  $A \in \mathbb{R}^{N \times N}$ ,  $x \in \mathbb{R}^N$  is  $O(N^2)$  since it requires  $N$  dot products, each  $O(N)$

# Numerical Precision

## Machine Epsilon

For a given datatype,  $\epsilon$  is defined as  $\epsilon = \min_{\delta > 0} \{\delta : 1 + \delta > 1\}$

- Computers have finite precision. 64-bit typical, but 32-bit on GPUs

```
1 print(f"machine epsilon for float64 = {np.finfo(float).eps}")
2 print(f"1 + eps/2 == 1? {1.0 + 1.1e-16 == 1.0}")
3 print(f"machine epsilon for float32 = {np.finfo(np.float32).eps}")
```

```
machine epsilon for float64 = 2.220446049250313e-16
```

```
1 + eps/2 == 1? True
```

```
machine epsilon for float32 = 1.1920928955078125e-07
```



# Basic Linear Algebra



# Norms

- Common measure of size is the Euclidean norm, or  $L^2$  norm for  $x \in \mathbb{R}^2$
- Complexity is  $O(N)$ , square  $N$  times then  $N$  additions

$$\|x\|_2 = \sqrt{\sum_{n=1}^N x_n^2}$$

```
1 x = np.array([1, 2, 3]) # Calculating different ways (in order of preference)
2 print(np.sqrt(sum(xval**2 for xval in x))) # manual with comprehensions
3 print(np.sqrt(np.sum(np.square(x)))) # broadcasts
4 print(norm(x)) # built-in to numpy norm(x, ord=2) alternatively
5 print(f"||x||_2^2 = {norm(x)**2} = {x.T @ x} = {np.dot(x, x)}")
```

3.7416573867739413

3.7416573867739413

3.7416573867739413

||x||\_2^2 = 14.0 = 14 = 14

# Solving Systems of Equations

- Solving  $Ax = b$  for  $x$  is equivalent  $A^{-1}Ax = A^{-1}b$
- Then since  $A^{-1}A = I$ , and  $Ix = x$ , we have  $x = A^{-1}b$
- Careful since matrix algebra is not commutative!

```
1 A = np.array([[0, 2], [3, 4]]) # or ((0, 2), (3, 4))
2 b = np.array([2, 1]) # Column vector
3 x = solve(A, b) # Solve Ax = b for x
4 x
```

```
array([-1.,  1.])
```

# Using the Inverse Directly

- Can replace the `solve` with a calculation of an inverse
- But it can be slower or less accurate than solving the system directly

```
1 A_inv = inv(A)
2 A_inv @ b # i.e, A^{-1} * b
```

```
array([-1.,  1.])
```

# Linear Combinations

We can think of solving a system as finding the linear combination of columns of  $A$  that equal  $b$

```
1 b_star = x[0] * A[:, 0] + x[1] * A[:, 1] # using x solution
2 print(f"b = {b}, b_star = {b_star}")
```

```
b = [2 1], b_star = [2. 1.]
```

# Column Space and Rank

- The column space of a matrix represents all possible linear combinations of its columns.
- It forms a basis for the space of solutions when solving systems of linear equations represented by the matrix
- The rank of a matrix is the dimension of its column space

```
1 A = np.array([[0, 2], [3, 4]])  
2 matrix_rank(A)
```

2

Hence, can solve  $Ax = b$  for any  $b \in \mathbb{R}^2$  since the column space is the entire space  $\mathbb{R}^2$

# Singular Matrices

On the other hand, note

```
1 A = np.array([[1, 2],  
2               [2, 4]])  
3 matrix_rank(A)
```

1

So we can only solve  $Ax = b$  for  $b \propto \begin{bmatrix} 1 \\ 2 \end{bmatrix} \propto \begin{bmatrix} 2 \\ 4 \end{bmatrix}$

# Checking Singularity

```
1 A = np.array([[1, 2], [2, 4]])
2 # An (expensive) way to check if A is singular is if det(A) = 0
3 print(det(A) == 0.0)
4 print(matrix_rank(A) != A.shape[0]) # or check rank
5 # Check before inverting or use exceptions
6 try:
7     inv(A)
8     print("Matrix is not singular (invertible).")
9 except np.linalg.LinAlgError:
10     print("Matrix is singular (non-invertible).")
```

True

True

Matrix is singular (non-invertible).

# Determinant is Not Scale Invariant

- Reminder: numerical precision in calculations makes it hard to compare to zero
- The determinate is useful but depends on the scale of the matrix
- A more robust alternative is the condition number (more next lecture)

```
1 eps, K = 1e-8, 100000
2 A = np.array([[1, 2], [1 + eps, 2 + eps]])
3 print(f"det(A)={det(A):.5g}, det(K*A)={det(K*A):.5g}")
4 print(f"cond(A)={cond(A):.5g}, cond(K*A)={cond(K*A):.5g},")
5 print(f"det(inv(A))={det(inv(A)):.5g}, cond(inv(A))={cond(inv(A)):.5g}")
```

```
det(A)=-1e-08, det(K*A)=-100
cond(A)=1e+09, cond(K*A)=1e+09,
det(inv(A))=-1e+08, cond(inv(A))=1e+09
```





# Solving Linear Systems of Equations

# Solving Systems with Multiple RHS

- Inverse is nice because you can reuse the  $A^{-1}$  to solve  $Ax = b$  for many  $b$
- However, you can do this with `solve` as well
- Or can reuse LR factorizations (discussed next)

```
1 A = np.array([[0, 2], [3, 4]])
2 B = np.array([[2,3], [1,2]]) # [2,1] and [3,2] as columns
3 # or: B = np.column_stack([np.array([2, 1]),np.array([3,2])])
4 X = solve(A, B) # Solve AX = B for X
5 print(X)
6 print(f"Checking: A*{X[:,0]} = {A@X[:, 0]} = {B[:,0]}, column of B")
```

```
[[-1.          -1.33333333]
 [ 1.           1.5       ]]
```

```
Checking: A*[-1.  1.] = [2. 1.] = [2 1], column of B
```

# LU(P) Decompositions

- We can “factor” any square  $A$  into  $PA = LU$  for triangular  $L$  and  $U$ . Invertible can have  $A = LU$ , called the LU decomposition. “P” is for partial-pivoting
- Singular matrices may not have full-rank  $L$  or  $U$  matrices

```
1 A = np.array([[1, 2], [2, 4]])
2 P, L, U = lu(A)
3 print(f"L*U =\n{L @ U}")
4 print(f"P*A =\n{P @ A}")
```

```
L*U =
[[2. 4.]
 [1. 2.]]
P*A =
[[2. 4.]
 [1. 2.]]
```

# P, U, and L

The  $P$  matrix is a permutation matrix of “pivots” the others are triangular

```
1 print(f"P =\n{P}")
2 print(f"L =\n{L}")
3 print(f"U =\n{U}")
```

```
P =
[[0.  1.]
 [1.  0.]]
L =
[[1.  0. ]
 [0.5 1. ]]
U =
[[2.  4.]
 [0.  0.]]
```

# LU Decompositions and Systems of Equations

- Pivoting is typically implied when talking about “LU”
- Used in the default **solve** algorithm (without more structure)
- Solving systems of equations with triangular matrices: for  $Ax = LUx = b$ 
  1. Define  $y = Ux$
  2. Solve  $Ly = b$  for  $y$  and  $Ux = y$  for  $x$
- Since both are triangular, process is  $O(N^2)$  (but LU itself  $O(N^3)$ )
- Could be used to find **inv**
  - $A = LU$  then  $AA^{-1} = I = LUA^{-1} = I$
  - Solve for  $Y$  in  $LY = I$ , then solve  $UA^{-1} = Y$
- Tight connection to textbook Gaussian elimination (including pivoting)

# LU for Non-Singular Matrices

```
1 A = np.array([[1, 2], [3, 4]])  
2 P, L, U = lu(A)  
3 print(f"L*U =\n{L @ U}")  
4 print(f"P*A =\n{P @ A}")
```

```
L*U =  
[[3. 4.]  
 [1. 2.]  
P*A =  
[[3. 4.]  
 [1. 2.]
```

# L, U, P

```
1 print(f"P =\n{P}")
2 print(f"L =\n{L}")
3 print(f"U =\n{U}")
```

```
P =
[[0. 1.]
 [1. 0.]]
L =
[[1.          0.          ]
 [0.33333333  1.          ]]
U =
[[3.          4.          ]
 [0.          0.66666667]]
```

# Backwards Substitution Example

$$Ux = b$$

$$U \equiv \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}, \quad b = \begin{bmatrix} 7 \\ 2 \end{bmatrix}$$

Solving bottom row for  $x_2$

$$2x_2 = 2, \quad x_2 = 1$$

Move up a row, solving for  $x_1$ , substituting for  $x_2$

$$3x_1 + 1x_2 = 7, \quad 3x_1 + 1 \times 1 = 7, \quad x_1 = 2$$

Generalizes to many rows. For  $L$  it is “forward substitution”



# Use Triangular Structure if Possible

- Triangular matrices of size  $N$  can be solved with back substitution in  $O(N^2)$
- Is  $O(N^2)$  good or bad? Beats,  $O(N^3)$  typical of general methods

```
1 U = np.array([[3, 1],
2               [0, 2]])
3 b = np.array([7, 2])
4 solve(U, b) # works, but internally does an LU which is  $O(N^3)$ 
5 solve_triangular(U, b, lower=False) # fast  $O(N^2)$ 
```

```
array([2., 1.])
```

# Symmetric Matrix Structure

Another common matrix type are symmetric,  $A = A^T$

```
1 A = np.array([[1, 2], [2, 5]]) # also posdef, not singular
2 b = np.array([1,4])
3 # With scipy 1.11.3 check with scipy.linalg.issymmetric(A)
4 solve(A, b, assume_a="sym") # could also use "pos" since positive definite
```

```
array([-3.,  2.])
```

# Positive Definite Matrices

- A symmetric matrix  $A$  is positive definite if  $x^T A x > 0$  for all  $x \neq 0$
- Useful in many areas, such as covariance matrices. Example

```
1 A = np.array([[1, 2], [2, 5]])
2 x = np.array([0, 1]) # can't really check for all x
3 print(f"x^T A x = {x.T @ A @ x}")
```

$x^T A x = 5$

- Example of a symmetric matrix that is not positive definite

```
1 A = np.array([[1, 2], [2, 0]])
2 print(f"x^T A x = {x.T @ A @ x}") # one counterexample is enough
```

$x^T A x = 0$

- We can check these with eigenvalues

# Cholesky Decomposition

- For symmetric positive definite matrices:  $L = U^T$ ,
- Called a Cholesky decomposition:  $A = LL^T$  for a lower triangular matrix  $L$ .
- Equivalently, could find  $A = U^T U$  for an upper triangular matrix  $U$

```
1 A = np.array([[1, 2], [2, 5]])
2 L = cholesky(A, lower=True) # cholesky also defined for upper=True
3 print(L)
4 print(f"L*L^T =\n{L @ L.T}")
```

```
[[1. 0.]
 [2. 1.]]
L*L^T =
[[1. 2.]
 [2. 5.]]
```

# Solving Positive Definite Systems

```
1 A = np.array([[1, 2], [2, 5]])
2 b = np.array([1, 4])
3 print(solve(A, b, assume_a="pos")) # uses cholesky internally
4
5 L = cholesky(A, lower=True)
6 y = solve_triangular(L, b, lower=True)
7 x = solve_triangular(L.T, y, lower=False)
8 print(x)
```

```
[-3.  2.]
[-3.  2.]
```

# Cholesky for Covariance Matrices

- Covariance matrices are positive-definite, semi-definite if degenerate
- Key property of Gaussian random variables:
  - $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  for  $\boldsymbol{\mu} \in \mathbb{R}^N, \boldsymbol{\Sigma} \in \mathbb{R}^{N \times N}$
  - $\mathbf{X} = \boldsymbol{\mu} + \mathbf{A}\mathbf{Z}$  for  $\mathbf{Z} \sim \mathcal{N}(\mathbf{0}_N, \mathbf{I}_N)$  where  $\mathbf{A}\mathbf{A}^T = \boldsymbol{\Sigma}$
- That is,  $\mathbf{A}$  is the Cholesky decomposition of the covariance matrix

# Matrices as Linear Transformations

- Recall: for  $x \in \mathbb{R}^N$  we should think of a  $f(x) = Ax$  for  $A \in \mathbb{R}^{M \times N}$  as a linear transformation from  $\mathbb{R}^N$  to  $\mathbb{R}^M$ 
  - Definition of Linear:  $f(ax_1 + bx_2) = af(x_1) + bf(x_2)$  for scalar  $a, b$
- Similarly, the  $y = f(x) = Ax$  then  $f^{-1}(y) = A^{-1}y$  goes from  $\mathbb{R}^M$  to  $\mathbb{R}^N$ 
  - If the matrix is square and invertible, we can go back and forth without losing information (i.e., bijective). Otherwise we may be projected onto a lower-dimensional “manifold”.

# Norms and Linear Transformations

- The vector norm  $||x||_2$  is an important feature in many applications
  - Hence  $||f(x)||_2 = ||Ax||_2$  frequently comes up in economics and datascience
  - e.g. linear regression is written as minimizing a vector norm

$$\min_{\beta} ||y - X\beta||_2$$

- Matrix structure or decompositions of  $A$  help us better understand the  $f(x)$  mapping



# Orthogonal Matrices

- A square matrix  $Q$  is **orthogonal** if:  $Q^{-1} = Q^T$ , and hence  $Q^T Q = Q Q^T = I$ 
  - For orthogonal  $Q$ ,  $f(x) = Qx$  is interpreted as rotating  $x$  without stretching
  - $y = f(x) = Qx$  then  $f^{-1}(y) = Q^{-1}y = Q^T y$  is rotating  $y$  back
  - Columns are orthonormal:  $Q = [q_1 | \dots | q_N]$  then
    - $q_i \cdot q_j = 0$  for  $i \neq j$  and  $q_i \cdot q_i = 1$
  - Rotation means the length doesn't change:  $\|Qx\|_2 = \|x\|_2$
  - Transformations which preserve norms are central in many applications within data science, ML, and economics - especially in high-dimensions



# Eigenvalues and Eigenvectors

# Eigenvalues and Eigenvectors

- For a square  $A$ , an eigenvector  $x$  and eigenvalue  $\lambda$  satisfy

$$Ax = \lambda x$$

- $A \in \mathbb{R}^{N \times N}$  has  $N$  eigenvalue/eigenvector pairs, possible multiplicity of  $\lambda$
- Intuition:  $x$  is a direction  $Ax \propto x$  and  $\lambda$  says how much it “stretches”

# Properties of Eigenvalues and Eigenvectors

- For any eigenvector  $x$  and scalar  $c$  then  $cx \propto Ax$  as well
- Symmetric matrices have real eigenvalues and orthogonal eigenvectors. i.e.  $x_1 \cdot x_2 = 0$  for  $x_1 \neq x_2$  eigenvectors. Complex in general
- Singular if and only if it has an eigenvalue of zero
- Positive (semi)definite if and only if all eigenvalues are strictly (weakly) positive
- Diagonal matrix has eigenvalues as its diagonal
- Triangular matrix has eigenvalues as its diagonal

# Positive Definite and Eigenvalues

You cannot check  $x^T A x > 0$  for all  $x$ . Check if “stretching” is positive

```
1 A = np.array([[3, 1], [2, 1]])
2 # A_eigs = np.real(eigvals(A)) # symmetric matrices have real eigenvalues
3 A_eigs = eigvalsh(A) # specialized for symmetric/hermitian matrices
4 print(A_eigs)
5 is_positive_definite = np.all(A_eigs > 0)
6 is_positive_semi_definite = np.all(A_eigs >= 0) # or eigvals(A) >= -eps
7 print(f"pos-def? {is_positive_definite}")
8 print(f"pos-semi-def? {is_positive_semi_definite}")
```

```
[-0.23606798  4.23606798]
```

```
pos-def? False
```

```
pos-semi-def? False
```

# Positive Semi-Definite Matrices **May** Have a Zero Eigenvalue

The simplest positive-semi-definite (but not posdef) matrix is

```
1 A_eigs = eigvalsh(np.array([[1, 0], [0, 0]]))
2 print(A_eigs)
3 is_positive_definite = np.all(A_eigs > 0)
4 is_positive_semi_definite = np.all(A_eigs >= 0) # or eigvals(A) >= -eps
5 print(f"pos-def? {is_positive_definite}")
6 print(f"pos-semi-def? {is_positive_semi_definite}")
```

```
[0. 1.]
pos-def? False
pos-semi-def? True
```

# Eigen Decomposition

- For square, symmetric, non-singular matrix  $A$  factor into

$$A = Q\Lambda Q^{-1}$$

- $Q$  is a matrix of eigenvectors,  $\Lambda$  is a diagonal matrix of paired eigenvalues
- For symmetric matrices, the eigenvectors are orthogonal and  $Q^{-1}Q = Q^T Q = I$  which form an orthonormal basis
- Orthogonal matrices can be thought of as rotations without stretching
- More general matrices all have a Singular Value Decomposition (SVD)
- With symmetric  $A$ , an interpretation of  $Ax$  is that we can first rotate  $x$  into the  $Q$  basis, then stretch by  $\Lambda$ , then rotate back

# Eigendecompositions and Matrix Powers

- Can be used to find  $A^t$  for large  $t$  (e.g. for Markov chains)
  - $P^t$ , i.e.  $P \cdot P \cdot \dots \cdot P$  for  $t$  times
  - $P = Q\Lambda Q^{-1}$  then  $P^t = Q\Lambda^t Q^{-1}$  where  $\Lambda^t$  is just the pointwise power
- Related tools such as SVD can help with dimensionality reduction



# Spectral/Eigendecomposition of Symmetric Matrix Example

```
1 A = np.array([[2, 1], [1, 3]])
2 Lambda, Q = eig(A)
3 print(f"eigenvectors are column-by-column in Q =\n{Q}")
4 print(f"eigenvalues are in Lambda = {Lambda}")
5 print(f"Q Lambda Q^T =\n{Q @ np.diag(np.real(Lambda)) @ Q.T}")
```

eigenvectors are column-by-column in Q =

```
[[-0.85065081 -0.52573111]
 [ 0.52573111 -0.85065081]]
```

eigenvalues are in Lambda = [1.38196601+0.j 3.61803399+0.j]

Q Lambda Q<sup>T</sup> =

```
[[2. 1.]
 [1. 3.]]
```

# Spectral Radius is Maximum Absolute Eigenvalue

- If any  $\lambda \in \Lambda$  are  $> 1$  can see this would explode
- Useful for seeing if iteration  $x_{t+1} = Ax_t$  from a  $x_0$  explodes
- The **spectral radius** of matrix  $A$  is

$$\rho(A) = \max_{\lambda \in \Lambda} |\lambda|$$

# Least Squares and the Normal Equations

# Least Squares

Given a matrix  $\mathbf{X} \in \mathbb{R}^{N \times M}$  and a vector  $\mathbf{y} \in \mathbb{R}^N$ , we want to find  $\beta \in \mathbb{R}^M$  such that

$$\min_{\beta} ||\mathbf{y} - \mathbf{X}\beta||^2, \text{ that is,}$$

$$\min_{\beta} \sum_{n=1}^N \frac{1}{N} (y_n - \mathbf{X}_n \cdot \beta)^2$$

Where  $\mathbf{X}_n$  is n'th row. Take FOCs and rearrange to get

$$(\mathbf{X}^T \mathbf{X})\beta = \mathbf{X}^T \mathbf{y}$$

# Solving the Normal Equations

- The  $X$  is often referred to as the “design matrix”.  $X^T X$  as the Gram matrix
- Can form  $A = X^T X$  and  $b = X^T y$  and solve  $A\beta = b$ .
  - Or invert  $X^T X$  to get

$$\beta = (X^T X)^{-1} X^T y$$

- Note that  $X^T X$  is symmetric and, if  $X$  is full-rank, positive definite

# Solving Regression Models in Practice

- In practice, use the `lstsq` function in scipy
  - It uses better algorithms using eigenvectors. More stable (see next lecture on conditioning)
  - One algorithm uses another factoring, the QR decomposition
  - There,  $\mathbf{X} = \mathbf{Q}\mathbf{R}$  for  $\mathbf{Q}$  orthogonal and  $\mathbf{R}$  upper triangular. See [QR Decomposition](#) for more
- Better yet, for applied work use higher-level libraries like `statsmodels` (integrates well with `pandas` and `seaborn`)
  - See [statsmodels docs](#) for R-style notation
  - See [QuantEcon OLS Notes](#) for more.

# Example of LLS using Scipy

```
1 N, M = 100, 5
2 X = np.random.randn(N, M)
3 beta = np.random.randn(M)
4 y = X @ beta + 0.05 * np.random.randn(N)
5 beta_hat, residuals, rank, s = scipy.linalg.lstsq(X, y)
6 print(f"beta =\n {beta}\nbeta_hat =\n{beta_hat}")
```

```
beta =
[ 1.27699654  1.24976206 -0.02314793 -0.1603755  -1.71006662]
beta_hat =
[ 1.26798224  1.24374081 -0.02376603 -0.16370129 -1.72027267]
```

# Solving using the Normal Equations

Or we can solve it directly. Provide matrix structure (so it can use a Cholesky)

```
1 beta_hat = solve(X.T @ X, X.T @ y, assume_a="pos")
2 print(f"beta =\n {beta}\nbeta_hat =\n{beta_hat}")
```

```
beta =
[ 1.27699654  1.24976206 -0.02314793 -0.1603755  -1.71006662]
beta_hat =
[ 1.26798224  1.24374081 -0.02376603 -0.16370129 -1.72027267]
```



# Collinearity in “Tall” Matrices

- Tall  $\mathbb{R}^{N \times M}$  “design matrices” have  $N > M$  and are “overdetermined”
- The rank of a matrix is full rank if all columns are linearly independent
- You can only identify  $M$  parameters with  $M$  linearly independent columns

```
1 X = np.array([[1, 2], [2, 5], [3, 7]]) # 3 observations, 2 variables
2 X_col = np.array([[1, 2], [2, 4], [3, 6]]) # all proportional
3 print(f"rank(X) = {matrix_rank(X)}, rank(X_col) = {matrix_rank(X_col)}")
```

rank(X) = 2, rank(X\_col) = 1

# Collinearity and Estimation

- If  $\mathbf{X}$  is not full rank, then  $\mathbf{X}^T \mathbf{X}$  is not invertible. For example:

```
1 print(f"cond(X'*X)={cond(X.T@X)}, cond(X_col'*X_col)={cond(X_col.T@X_col)}")
```

```
cond(X'*X)=2819.332978639814, cond(X_col'*X_col)=1.1014450683078442e+16
```

- Note that when you start doing operations on matrices, numerical error creeps in, so you will not get an exact number
- The rule-of-thumb with condition numbers is that if it is  $1 \times 10^k$  then you lose about  $k$  digits of precision. So this effectively means it is singular
- Given the singular matrix, this means a continuum of  $\beta$  will solve the problem

# lstsq Solves it? Careful on Interpretation!

- Since  $X_{col}^T X_{col}$  is singular, we cannot use `solve(X.T@X, y)`
- But what about `lstsq` methods?
- As you will see, this gives an answer. Interpretation is hard
- The key is that in the case of non-full rank, you cannot identify individual parameters
  - Related to “Identification” in econometrics
  - Having low residuals is not enough

```
1 y = np.array([5.0, 10.1, 14.9])
2 beta_hat, residuals, rank, s = scipy.linalg.lstsq(X_col, y)
3 print(f"beta_hat_col = {beta_hat}")
4 print(f"rank={rank}, cols={X.shape[1]}, norm(X*beta_hat_col-y)={norm(residuals)}")
```

```
beta_hat_col = [0.99857143 1.99714286]
rank=1, cols=2, norm(X*beta_hat_col-y)=0.0
```

# Fat Design Matrices

- Fat  $\mathbb{R}^{N \times M}$  “design matrices” have  $N < M$  and are “underdetermined”
- Less common in econometrics, but useful to understand the structure
- A continuum  $\beta \in \mathbb{R}^{M - \text{rank}(X)}$  solve this problem

```
1 X = np.array([[1, 2, 3], [0, 5, 7]]) # 2 rows, 3 variables
2 y = np.array([5, 10])
3 beta_hat, residuals, rank, s = scipy.linalg.lstsq(X, y)
4 print(f"beta_hat = {beta_hat}, rank={rank}, ? residuals = {residuals}")
```

```
beta_hat = [0.8 0.6 1. ], rank=2, ? residuals = []
```

# Which Solution?

- Residuals are zero here because there are enough parameters to fit perfectly (i.e., it is underdetermined)
- Given the multiple solutions, the **lstsq** is giving

$$\min_{\beta} ||\beta||_2^2 \text{ s.t. } X\beta = y$$

- i.e., the “smallest” coefficients which interpolate the data exactly
- Which trivially fulfills the OLS objective:  $\min_{\beta} ||y - X\beta||_2^2$

# Careful Interpreting Underdetermined Solutions

- Useful and common in ML, but be **very** careful when interpreting for economics
  - Tight connections to Bayesian versions of statistical tests
  - But until you understand econometrics and “identification” well, **stick to full-rank matrices**
  - **Advanced topics:** search for “Regularization”, “Ridgeless Regression” and “Benign Overfitting in Linear Regression.”