

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:

```
import numpy as np
import matplotlib.pyplot as plt
import scipy
from numpy.linalg import cond, matrix_rank, norm
from scipy.linalg import inv, solve, det, eig, lu, eigvals
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:

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

- ullet Often crucial to know how problems scale asymptotically (as $N o\infty$)
- ullet Caution! This is only an asymptotic limit, and can be misleading for small N

$$ightarrow f_1(N) = N^3 + N$$
 is $O(N^3)$

$$ightarrow f_2(N) = 1000N^2 + 3N$$
 is $O(N^2)$

ightarrow For roughly N>1000 use f_2 algorithm, otherwise f_1



Examples of Computational Complexity

- Simple examples:
 - $o x \cdot y = \sum_{n=1}^N x_n y_n$ is O(N) since it requires N multiplications and additions
 - o Ax for $A\in \mathbb{R}^{N imes N}, x\in \mathbb{R}^N$ is $O(N^2)$ since it requires N dot products, each O(N)



Numerical Precision

Machine Epsilon

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

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

- ullet Common measure of size is the Euclidean norm, or L^2 norm for $x\in \mathbb{R}^2$
- ullet 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 $A^{-1}Ax=A^{-1}b$
- ullet 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 $oldsymbol{A}$ that equal $oldsymbol{b}$

```
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)
```

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

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



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(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

- ullet 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)



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
- ullet 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
- ullet Since both are triangular, process is $O(N^2)$ (but LU itself $O(N^3)$)
- Could be used to find inv
 - ightarrow A = LU then $AA^{-1} = I = LUA^{-1} = I$
 - ightarrow 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



Backwards Substitution Example

$$Ux=b \ U\equivegin{bmatrix} 3 & 1 \ 0 & 2 \end{bmatrix}, \quad b=egin{bmatrix} 7 \ 2 \end{bmatrix}$$

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

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

Generalizes to many rows. For $oldsymbol{L}$ it is "forward substitution"



Use Triangular Structure if Possible

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



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

- ullet A symmetric matrix A is positive definite if $x^TAx>0$ for all x
 eq 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

- ullet For symmetric positive definite matrices: $L=U^{T}$
- ullet Called a Cholesky decomposition: $A=LL^T$ for a lower triangular matrix L.
- ullet 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:

$$o X \sim N(\mu, \Sigma)$$
 for $\mu \in \mathbb{R}^N, \Sigma \in \mathbb{R}^{N imes N}$

$$ightarrow X = \mu + AZ$$
 for $Z \sim N(0_N, I_N)$ where $AA^T = \Sigma$

ullet That is, 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 $A\in\mathbb{R}^{M imes N}$ as a linear transformation from \mathbb{R}^N to \mathbb{R}^M
 - ightarrow Definition of Linear: $f(ax_1+bx_2)=af(x_1)+bf(x_2)$ for scalar a,b
- ullet 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
 - ightarrow Hence $||f(x)||_2 = ||Ax||_2$ frequently comes up in economics and datascience
 - → e.g. linear regression is written as minimizing a vector norm

$$\min_{eta} ||y - Xeta||_2$$

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



Orthogonal Matrices

- ullet A square matrix Q is **orthogonal** if: $Q^{-1}=Q^T$, and hence $Q^TQ=QQ^T=I$
 - ightarrow For orthogonal Q, f(x)=Qx is interpreted as rotating x without stretching
 - ightarrow y = f(x) = Qx then $f^{-1}(y) = Q^{-1}y = Q^Ty$ is rotating y back
 - ightarrow Columns are orthonormal: $Q=[q_1| \ \dots \ |q_N]$ then
 - $ightarrow q_i \cdot q_j = 0$ for i
 eq j and $q_i \cdot q_i = 1$
 - ightarrow 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

ullet For a square A, an eigenvector x and eigenvalue λ satisfy

$$Ax = \lambda x$$

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



Properties of Eigenvalues and Eigenvectors

- ullet 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 $x^TAx > 0$ 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 (i.e., Spectral Decomposition if Symmetric)

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

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

- ullet Q is a matrix of eigenvectors, Λ is a diagonal matrix of paired eigenvalues (in order)
- For symmetric matrices, the eigenvectors are orthogonal and $Q^{-1}Q=Q^TQ=I$, and we can think of them as forming an orthonormal basis
- Orthogonal matrices can be thought of as rotations without stretching
- More general matrices all have a Singular Value Decomposition (SVD)



Eigendecompositions and Matrix Powers

- Can be used to find A^t for large t (e.g. for Markov chains)
 - $ightarrow P^t$, i.e. $P \cdot P \cdot \ldots \cdot P$ for t times
 - ightarrow $P=Q\Lambda Q^{-1}$ then $P^t=Q\Lambda^tQ^{-1}$ where Λ^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^T =
[[2. 1.]
[1. 3.]]
```



Spectral Radius is Maximum Absolute Eigenvalue

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

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



Least Squares and the Normal Equations



Least Squares

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

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

$$\min_{eta} \sum_{n=1}^N rac{1}{N} (y_n - X_n \cdot eta)^2$$

Where X_n is n'th row. Take FOCS and rearrange to get

$$(X^T X)\beta = X^T y$$



Solving the Normal Equations

- ullet The X is often referred to as the "design matrix". X^TX as the Gram matrix
- ullet Can form $A=X^TX$ and $b=X^Ty$ and solve Aeta=b.
 - \rightarrow Or invert X^TX to get

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

ightharpoonup Note that X^TX 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
 - ightarrow There, X=QR for Q orthogonal and 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 =
[-0.13457084 -0.07290219 -0.13819097 -0.98573991  0.37165065]
beta_hat =
[-0.14107132 -0.06679078 -0.14203432 -0.98971531  0.37720416]
```



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 =
[-0.13457084 -0.07290219 -0.13819097 -0.98573991  0.37165065]
beta_hat =
[-0.14107132 -0.06679078 -0.14203432 -0.98971531  0.37720416]
```



Collinearity in "Tall" Matrices

- ullet Tall $\mathbb{R}^{N imes M}$ "design matrices" have N>M and are "overdetermined"
- The rank of a matrix is full rank if all columns are linearly independent
- ullet 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 X is not full rank, then X^TX 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)=2819.3329786399063, cond(X_col'*X_col)=1.2999933999712892e+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 $1 imes 10^k$ then you lose about k digits of precision. So this effectively means it is singular
- ullet Given the singular matrix, this means a continuum of eta 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

- ullet Fat $\mathbb{R}^{N imes M}$ "design matrices" have N < M and are "underdetermined"
- Less common in econometrics, but useful to understand the structure
- ullet A continuum $eta \in \mathbb{R}^{M-\mathrm{rank}(X)}$ 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

$$\min_{eta} ||eta||_2^2 ext{ s.t. } Xeta = y$$

- i.e., the "smallest" coefficients which interpolate the data exactly
- ullet Which trivially fulfills the OLS objective: $\min_eta ||y-Xeta||_2^2$



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."