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
```

Δ

Basic Computational Complexity

Definition (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 $N \to \infty$)
- \cdot Caution: $f_1(N) = N^3 + N$ is $O(N^3)$ and $f_2(N) = 1000N^2 + 3N$ is $O(N^2)$
 - · Asymptotically choose $f_2(N)$ algorithm, but choose $f_1(N)$ for small N
- · Simple examples:
 - $\cdot \ x \cdot y = \sum_{n=1}^N x_n y_n$ 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

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

Definition (Machine Epsilon)

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

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

- \cdot Common measure of "size" is the Euclidean norm, or L^2 norm for $x \in \mathbb{R}^2$
- \cdot Complexity is O(N): requires squaring N times then N additions to sum. Not nested

$$||x||_2 = \sqrt{\sum_{n=1}^N x_n^2}$$
 x = np.array([1, 2, 3]) # Calculating different ways (in order of preference)

- print(np.sqrt(sum(xval**2 for xval in x))) # manual with comprehensions
- print(np.sqrt(np.sum(np.square(x)))) # broadcasts
- print(norm(x)) # built-in to numpy norm(x, ord=2) alternatively
- 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

```
Then since A^{-1}A = I, and Ix = x, we have x = A^{-1}b. Careful since matrix algebra is not commutative!

A = np.array([[0, 2], [3, 4]]) # or ((0, 2), (3, 4))

b = np.array([2,1]) # Column vector

x = solve(A, b) # Solve Ax = b for x

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

· Solving Ax = b for x is equivalent $A^{-1}Ax = A^{-1}b$

Using the Inverse Directly

array([-1., 1.])

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

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

С

Linear Combinations

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

```
b_star = x[0] * A[:, 0] + x[1] * A[:, 1] # using x solution
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

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

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

True

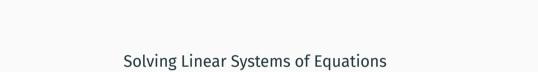
True

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)

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

```
A = np.array([[0, 2], [3, 4]])
B = np.array([[2,3], [1,2]]) # [2,1] and [3,2] as columns
# or: B = np.column stack([np.array([2, 1]),np.array([3,2])])
X = solve(A, B) \# Solve AX = B for X
print(X)
print(f"Checking: A*{X[:,0]} = {A@X[:,0]} = {B[:,0]}, column of B")
[[-1.
             -1.333333333
 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
- \cdot Singular matrices may not have full-rank L or U matrices

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

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

P, U, and L

The ${\cal P}$ matrix is a permutation matrix of "pivots" the others are triangular

```
print(f"P = n{P}")
print(f"L = \n{L}")
print(f"U =\n{U}")
P =
[[0. 1.]
 [1. 0.]]
I =
[[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)
- \cdot 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 ${\cal O}(N^2)$ (but LU itself ${\cal O}(N^3)$)
- Could be used to find inv
 - $\cdot A = LU$ 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

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

L, U, P

```
print(f"P = \n{P}")
print(f"L =\n{L}")
print(f"U = n\{U\}")
[[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 \boldsymbol{x}_1 , substituting for \boldsymbol{x}_2

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

Generalizes to many rows. For L it is "forward substitution"

Use Triangular Structure if Possible

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

Symmetric Matrix Structure

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

```
A = np.array([[1, 2], [2, 5]]) # also posdef, not singular
b = np.array([1,4])
print(f"Symmetric A? {scipy.linalg.issymmetric(A)}")
solve(A, b, assume_a="sym") # could also use "pos" since positive definite
Symmetric A? True
array([-3., 2.])
```

Positive Definite Matrices

- A symmetric matrix A is positive definite if $x^TAx>0$ 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

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

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

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Solving Positive Definite Systems

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

```
A = np.array([[1, 2], [2, 5]])
  b = np.arrav([1.4])
  print(solve(A, b, assume a="pos")) # uses cholesky internally
4
  L = cholesky(A, lower=True)
  v = solve triangular(L. b. lower=True)
  x = solve_triangular(L.T, y, lower=False)
  print(x)
```

Cholesky for Covariance Matrices

- · Covariance matrices are positive-definite, semi-definite if degenerate
- Key property of Gaussian random variables:

$$\cdot \ \, X \sim N(\mu, \Sigma) \mbox{ for } \mu \in \mathbb{R}^N, \Sigma \in \mathbb{R}^{N \times N}$$

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

 $\boldsymbol{\cdot}$ 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 $A\in\mathbb{R}^{M\times N}$ 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 $f^{-1}(y)=A^{-1}y$ transforms from \mathbb{R}^M to \mathbb{R}^N
 - If the matrix is square and invertible, this means we can go back and forth without losing information (i.e., it is bijective). Otherwise we may be projected onto a lower-dimensional "manifold" (e.g. a line in a plane or plane in a cube)
- \cdot 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 $||y-X\beta||_2$
- \cdot Matrix structure or decompositions of A help us better understand the f(x) mapping

Orthogonal Matrices

Definition (Orthogonal Matrices)

A square matrix Q is orthogonal if $Q^{-1}=Q^T$, and hence $Q^TQ=QQ^T=I$

- \cdot For orthogonal Q, f(x)=Qx is interpreted as rotating x without stretching it
- Similarly if y=f(x)=Qx then $f^{-1}(y)=Q^{-1}y=Q^Ty$ is rotating y back
- · Columns are orthonormal: $Q=\begin{bmatrix}q_1|&\dots&|q_N| \end{bmatrix}$ then $\cdot q_i\cdot q_i=0$ 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, machine learning, and economics especially with high-dimensional data

Eigenvalues and Eigenvectors

Eigenvalues and Eigenvectors

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

$$Ax = \lambda x$$

- \cdot $A \in \mathbb{R}^{N imes N}$ 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:
 - 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

```
A = np.array([[3, 1], [2, 1]])
# A eigs = np.real(eigvals(A)) # symmetric matrices have real eigenvalues
A eigs = eigvalsh(A) # specialized for symmetric/hermitian matrices
print(A eigs)
is positive definite = np.all(A eigs > 0)
is_positive_semi_definite = np.all(A_eigs >= 0) # or eigvals(A) >= -eps
print(f"pos-def? {is positive definite}")
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

```
A_eigs = eigvalsh(np.array([[1, 0], [0, 0]]))
print(A eigs)
is positive definite = np.all(A eigs > 0)
is positive semi definite = np.all(A eigs >= 0) # or eigvals(A) >= -eps
print(f"pos-def? {is positive definite}")
print(f"pos-semi-def? {is_positive semi definite}")
[0, 1,]
pos-def? False
pos-semi-def? True
```

Eigen Decomposition (i.e., Spectral Decomposition)

 \cdot For square, symmetric, non-singular matrix A factor into

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

- $\cdot \; Q$ is a matrix of eigenvectors, Λ is a diagonal matrix of paired eigenvalues (in order)
- \cdot 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)
- With symmetric A, an interpretation of Ax is that we can first rotate x into the Q basis, then stretch by Λ , then rotate back
- \cdot Can be used to find A^t for large t (e.g. for Markov chains)
 - $\cdot P^t$, i.e. $P \cdot P \cdot \dots \cdot P$ for t times
 - $\cdot \ P = Q \Lambda Q^{-1}$ then $P^t = Q \Lambda^t Q^{-1}$ where Λ^t is just the pointwise power

Eigenvalue Decomposition of Symmetric Matrix Example

```
A = np.array([[2, 1], [1, 3]])
   Lambda. 0 = eig(A)
2
   print(f"eigenvectors are column-by-column in Q = \ln\{Q\}")
   print(f"eigenvalues are in Lambda = {Lambda}")
  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.i 3.61803399+0.i]
  O Lambda O^T =
   \lceil \lceil 2. 1. \rceil
    [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 $\boldsymbol{x}_{t+1} = A\boldsymbol{x}_t$ from a \boldsymbol{x}_0 explodes

Definition (Spectral Radius)

The spectral radius of matrix A is $\rho(A) = \max_{\lambda \in \Lambda} |\lambda|$

Equations

Least Squares and the Normal

Least Squares

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

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

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

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

$$(X^TX)\beta = X^Ty$$

Solving the Normal Equations

- \cdot The X is often referred to as the "design matrix". X^TX as the Gram matrix
- · Can form $A=X^TX$ and $b=X^Ty$ and solve $A\beta=b$.
 - Or invert X^TX to get $\beta = (X^TX)^{-1}X^Ty$
 - Note that X^TX is symmetric and, if X is full-rank, positive definite
- 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
 - \cdot There, X=QR for Q orthogonal and R upper triangular. See QR Decomposition for more
- · We are exploring linear algebra in this lecture
 - For applied work use higher-level libraries like statsmodels (integrated well with pandas and seaborn)
 - See statsmodels docs for R-style notation
 - · See QuantEcon OLS NOtes for more.

Example of LLS using Scipy

```
N. M = 100.5
X = np.random.randn(N. M)
beta = np.random.randn(M)
y = X \otimes beta + 0.05 * np.random.randn(N)
beta hat, residuals, rank, s = scipy.linalg.lstsq(X, y)
print(f"beta =\n {beta}\nbeta hat =\n{beta hat}")
beta =
 [ 0.31773836 -0.04933223 -0.62369336 -1.13882456 -1.41336433]
beta hat =
[ 0.32336752 -0.04733509 -0.622372 -1.13952362 -1.41707406]
```

Solving using the Normal Equations

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

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

beta =
   [ 0.31773836 -0.04933223 -0.62369336 -1.13882456 -1.41336433]
beta_hat =
   [ 0.32336752 -0.04733509 -0.622372 -1.13952362 -1.41707406]
```

Collinearity in "Tall" Matrices

- \cdot 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
- \cdot 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

 \cdot If X is not full rank, then X^TX is not invertible. For example:

```
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
- \cdot The rule-of-thumb with condition numbers is that if it is 1×10^k then you lose about k digits of precision. So this effectively means it is singular
- \cdot 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 ${\tt solve(X.T@X, y)}$
- 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

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

```
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 $\beta \in \mathbb{R}^{M-{\rm rank}(X)}$ 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}")
5  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

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

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