Least Squares, Uniqueness, and Regularization

Graduate Quantitative Economics and Datascience

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Overview

Motivation

- In this section we will use some of the previous tools and discuss concepts on the curvature of optimization problems
- Doing so, we will consider uniqueness in optimization problems in datascience, economics, and ML
- Our key optimization problems to consider will be the quadratic problems than come out of least squares regressions.
  → This will provide a foundation for understanding nonlinear objectives since we can think of Hessians are locally quadratic.

Extra Materials

- scikit-learn ridge regression

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
```

First and Second Order Conditions in Optimization

- For univariate unconstrained optimization $\min_x f(x)$
- The FONC was $f'(x) = 0$.
  - → But this might not be a valid solution! Or there might be many
- The second order condition gives us more information and provides sufficient conditions
  - → if $f''(x) > 0$, then x is a local minimum; if $f''(x) < 0$, then x is a local maximum.
  - → if $f''(x) = 0$ then there may be multiple solutions (locally)

Related Univariate Conceptsed

- Recall in your math prep that for a univariate function $f(x)$, we have:
  → $f(x)$ is **convex** if $f''(x) \geq 0$ for all x in the domain.
  → $f(x)$ is **concave** if $f''(x) \leq 0$ for all x in the domain.
  → $f(x)$ is **strictly convex** if $f''(x) > 0$ for all x in the domain.
  → $f(x)$ is **strictly concave** if $f''(x) < 0$ for all x in the domain.
- We will generalize these concepts for thinking about multivariate functions
  → Local behavior, x' such that $|x - x'| < \epsilon$, for some ϵ “balls”

Definiteness

Reminder: Positive Definite

```python
A = np.array([[3, 1],
              [1, 2]])
# 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}")
```

```
[1.38196601 3.61803399]
pos-def? True
pos-semi-def? True
```

Reminder: Positive Definite

```
A = np.array([[3, -0.5],
              [-0.1, 2]])
# 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}")
```

```
[1.99009805 3.00990195]
pos-def? True
pos-semi-def? True
```

Reminder: Positive Semi-Definite Matrices

- 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
```

Negative Definite Matrices

- Simply swap the inequality. Think of a convex vs. concave function

```
A = -1 * np.array([[3, -0.5],
                   [-0.1, 2]])
A_eigs = eigvalsh(A)
print(A_eigs)
is_negative_definite = np.all(A_eigs < 0)
is_negative_semi_definite = np.all(A_eigs <= 0) # or eigvals(A) >= -eps
print(f"neg-def? {is_negative_definite}, neg-semi-def? {is_negative_semi_definite}")
```

```
[-3.00990195 -1.99009805]
neg-def? True, neg-semi-def? True
```

Negative Semi-Definite Matrix

- Semi-definite, but not definite requires the matrix to not be full rank
- At least one zero eigenvalue is necessary and sufficient for a matrix to be singular

```
A = np.array([[-1, -1],
              [-1, -1]])
A_eigs = eigvalsh(A)
print(A_eigs)
is_negative_definite = np.all(A_eigs < 0)
is_negative_semi_definite = np.all(A_eigs <= 0) # or eigvals(A) >= -eps
print(f"neg-def? {is_negative_definite}, neg-semi-def? {is_negative_semi_definite}")
```

```
[-2.  0.]
neg-def? False, neg-semi-def? True
```

Quadratic Forms

Quadratic Functions in Higher Dimensions

- Recall univariate function $f(x) = \frac{a}{2}x^2 + bx + c$ for $x \in \mathbb{R}$.
- General quadratic for $x \in \mathbb{R}^N$ requires cross-terms ($a_{12}x_1x_2, a_{11}x_1^2$ etc.) and linear terms (e.g, b_1x_1, b_2x_2)
- Can be written as $f(x) = \frac{1}{2}x^\top Ax + b^\top x + c$ for some symmetric matrix A, vector b, and scalar c

Gradients of Quadratic Forms

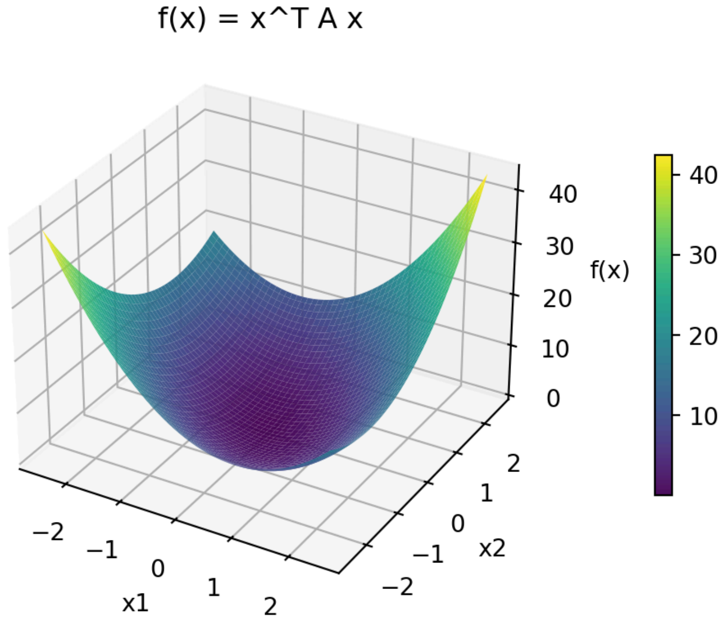
- Univariate: $f'(x) \equiv \nabla f(x) = ax + b$ and $f''(x) \equiv \nabla^2 f(x) = a$
- Multivariate: $\nabla f(x) = Ax + b$ and $\nabla^2 f(x) = A$
  - → $\nabla f(x)$ is the gradient vector at x
  - → $\nabla^2 f(x)$ is the Hessian matrix at x

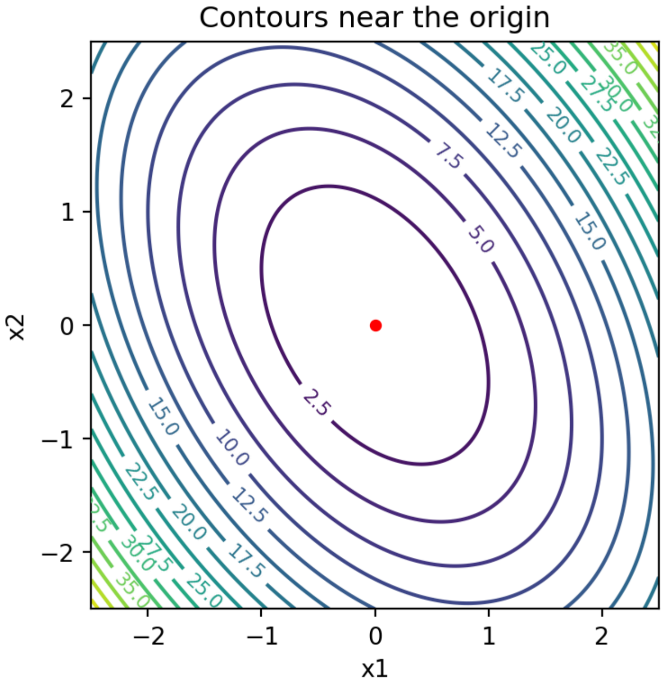
Strict Concavity/Convexity

- Quadratic functions have the same curvature everywhere, so not x dependent
- Univariate:
  - → $a > 0$ is strict convexity
  - → $a < 0$ is strict concavity
  - → $a = 0$ is linear (neither)
- Multivariate:
  - → A is positive definite is strict convexity, A is negative definite is strict concavity.
  - → A is semi-definite weakly convex (maybe strictly in some "directions")
  - → And vice-versa for concavity
- Recall that the univariate is nested: $A = [a]$ with eigenvalue a

Shape of Positive Definite Function

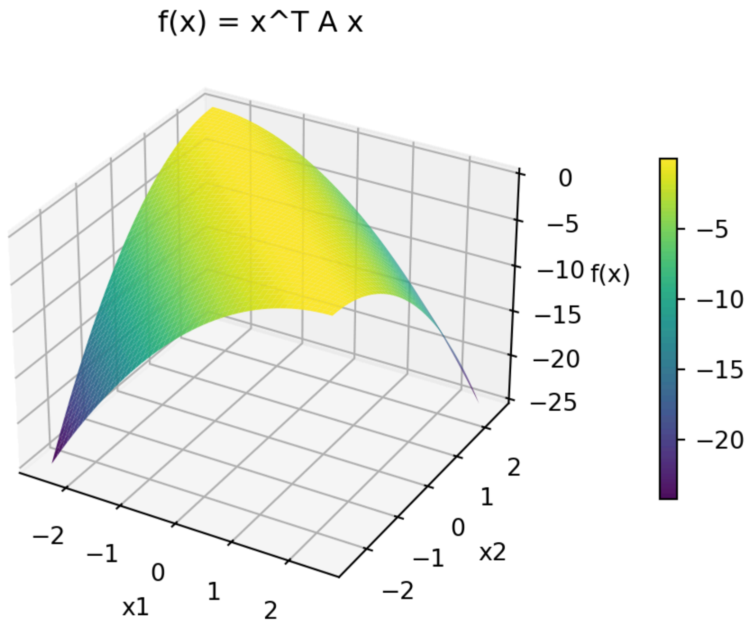
- For $A = \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix}$
- This has a **unique minima** (at $(0, 0)$, since no “affine” term, b)

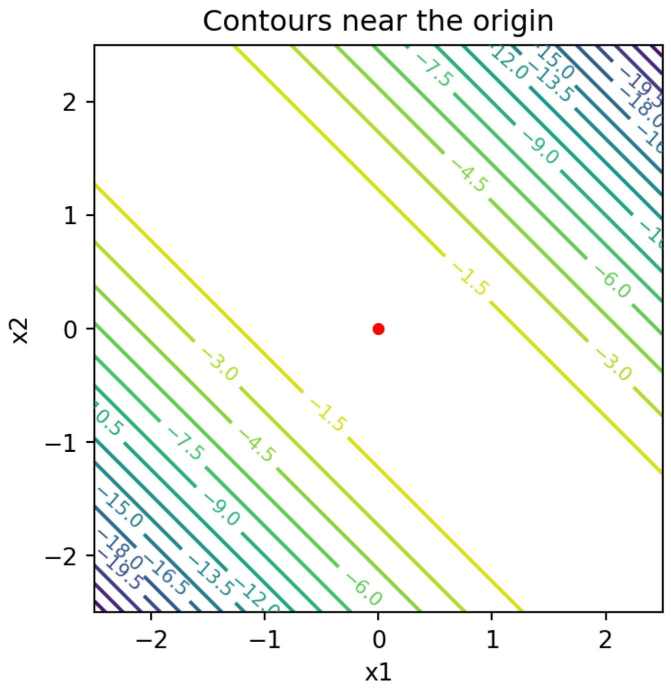




Shape of Negative Semi-Definite Function

- For our $A = \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix}$
- Note that this **does not** have a unique maximum! All values along a line hold
- Minima rather than maxima since negative rather than positive semi-definite





Least Squares and the Normal Equations

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

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

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

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

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

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, $X = QR$ 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

```python
N, M = 100, 5
X = np.random.randn(N, M)
beta = np.random.randn(M)
y = X @ 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 =
 [ 1.15674413 -0.58803774 -0.03466201  0.2684993  -1.62037615]
beta_hat =
[ 1.15794374 -0.58378157 -0.03528741  0.26587567 -1.61866435]
```

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 =
 [ 1.15674413 -0.58803774 -0.03466201  0.2684993  -1.62037615]
beta_hat =
[ 1.15794374 -0.58378157 -0.03528741  0.26587567 -1.61866435]
```

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

```python
X = np.array([[1, 2], [2, 5], [3, 7]]) # 3 observations, 2 variables
X_col = np.array([[1, 2], [2, 4], [3, 6]]) # all proportional
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 $X^T X$ 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
- 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
- Given the singular matrix, this means a continuum of β 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

```python
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(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 $\beta \in \mathbb{R}^{M - \mathrm{rank}(X)}$ solve this problem

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

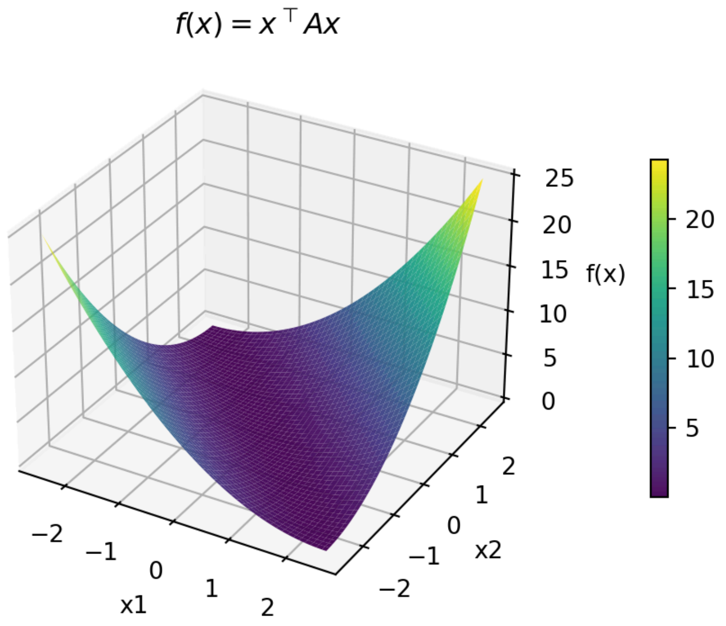
- Useful and common in ML, but be **very** careful when interpreting for economics
  - → Tight connections to Bayesian versions of statistical tests
  - → But until you understand econometrics and "identification" well, **stick to full-rank matrices**
  - → **Advanced topics:** search for "Regularization",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

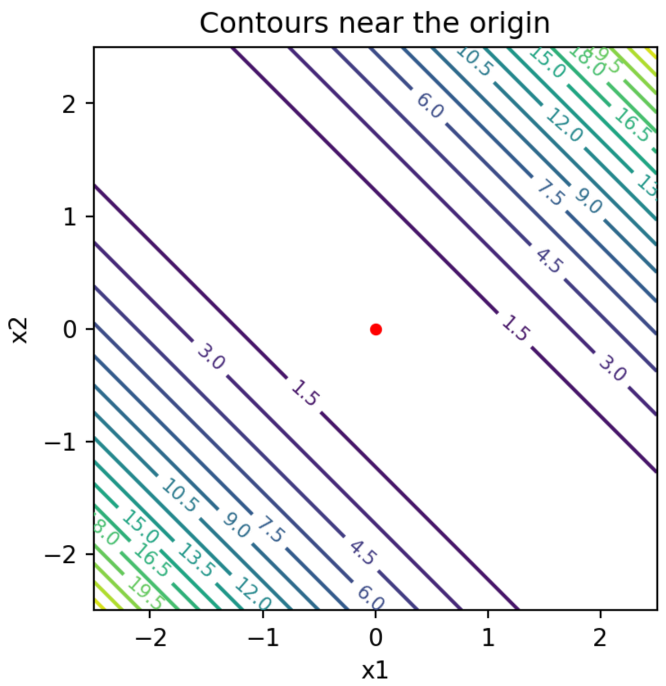
Regularization

Recall a Positive Semi-Definite Function

- For our $A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$. Multiple minima along a line!

```
eigenvalues of A: [2. 0.]
```

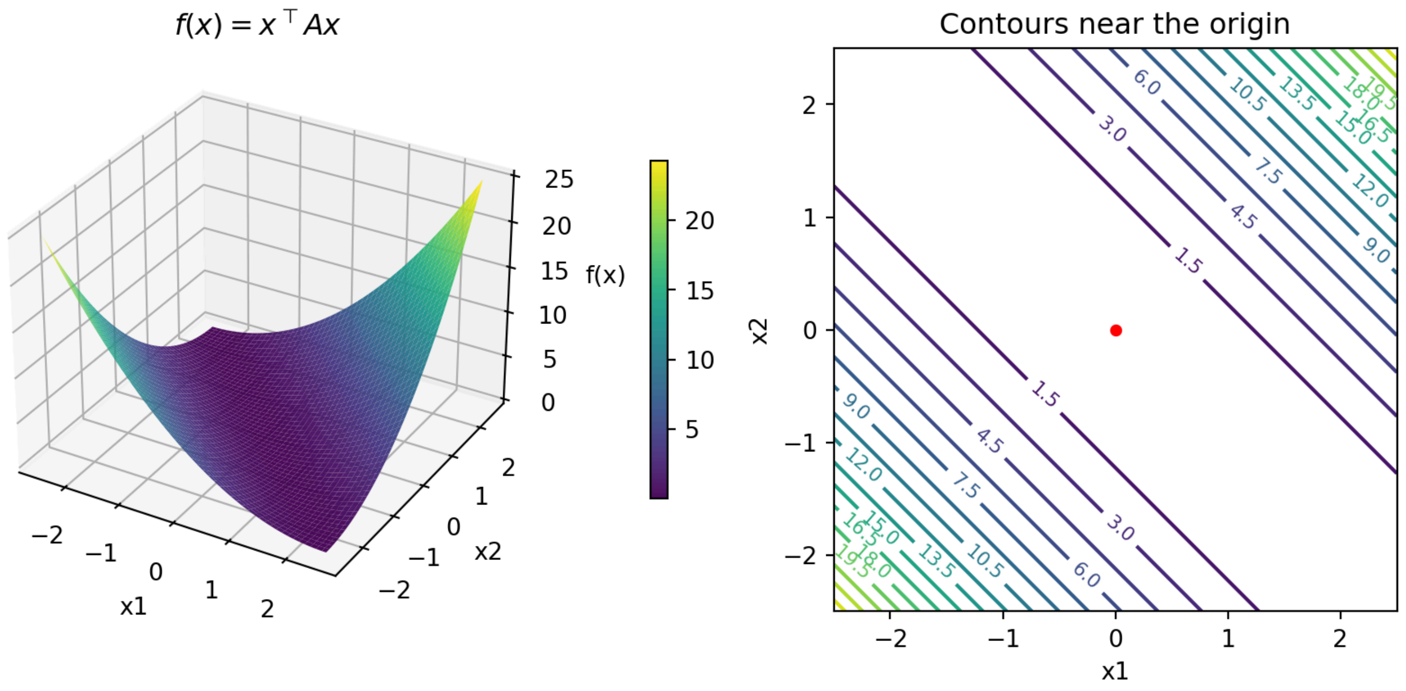




Fudge the Diagonal?

- Replace with $A = A + \lambda I$ for λ very small (e.g., $1E-5$)
- Now unique minima at $(0, 0)$

```
eigenvalues of A: [2.00001e+00 1.00000e-05]
```



Motivating this Fudge

- Previously solved $\mathbf{min}_x \{x^\top Ax\}$, which only has a unique solution if A is positive definite.
- Replace with

$$\min_x \{x^\top Ax + \lambda||x||_2^2\}$$

  - → i.e., penalize solutions by the euclidean length of x, called a "ridge" term
  - → Could instead penalize by different norms, e.g. $||x||_1$ is called LASSO
- What are the first order conditions? Lets look at least squares

Ridge Regression

- More generally, for OLS think of the following

$$\min_{\beta} \{||y - X\beta||_2^2 + \lambda||\beta||_2^2\}$$

- Take the FOCs and rearrange to get

$$(X^\top X + \lambda I)\beta = X^\top y$$

  → Note: if $X^\top X$ is not full rank (i.e., has a zero eigenvalue) then the addition of the λ term helps make things strictly positive definite

  → Sometimes you need to do this to overcome nearly collinear data or numerical approximations, even when it should be technically positive definite

Ridgeless Regression

- Recall statement that `lstsq` will return **some** solution even if not full rank.
- We said that in the case where the data could be fit exactly
  - → One can interpret the solution as $\min_\beta ||\beta||_2^2 \text{ s.t. } X\beta = y$
  - → Interpretation: this is the **min-norm** solution which fits the data with the “smallest” β
- Can show this is the limit of a ridge regression (i.e., “ridgeless”)

$$\lim_{\lambda \to 0} \min_\beta \{||y - X\beta||_2^2 + \lambda||\beta||_2^2\}$$

Regularization in ML

- In ML, with rich data sources there are often many possible ways to explain the data
- Economists often avoid this like the plague, and make assumptions to ensure perfect identification
  - → Identification arguments ensure positive definiteness of OLS, etc.
- As data becomes richer, it becomes hard to write down models with only a single explanation
  - → Regularization lets you bias your solution towards ones with certain properties
- There are Bayesian interpretations of all of these approaches