DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 02 | Part 1

Introduction

News

- Lab 01 released. Due Sunday @ 11:59 pm.
- HW 01 will be released today. Due Wednesday @ 11:59 pm.
  - LaTeX template available (optional).

Last Time

- We saw **nearest neighbor** predictors.
- They can work well.
- But they **memorize** the training data rather than **learning** a simpler underlying pattern.

The Rest of DSC 140A

- We'll explore three different paradigms for learning from data.
  - **Part 1:** Empirical Risk Minimization
  - **Part 2:** Probabilistic Modeling
  - **Part 3:** Tree-based Methods

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Probabilistic Modeling & Machine Learning

Lecture 02 | Part 2

Empirical Risk Minimization

Prediction

- Prediction is the most common task in ML:
  - given: a **feature vector**, $\vec{x}$
  - predict: an **output target**, y.

- Example:
  - given: years of experience and college GPA
  - predict: salary

Prediction Functions

- **Informally:** we think experience, GPA, etc., are predictive of salary.

- **Formally:** we think there is a function H that takes in (experience, GPA) and outputs a good prediction of the salary.

$$H(\text{experience}, \text{GPA}) \to \text{predicted salary}$$

Prediction Functions

- In general, a **prediction function**[1] H takes in a feature vector and outputs a predicted label.

$$H(\vec{x}) \to y$$

[1] Sometimes called a **hypothesis** function.

Example Prediction Function

$$
\begin{aligned}
H(\text{experience}, \text{GPA}) = {} & \$50{,}000 \\
& + \$10{,}000 \times \text{experience} \\
& + \$5{,}000 \times \text{GPA}
\end{aligned}
$$

Goal

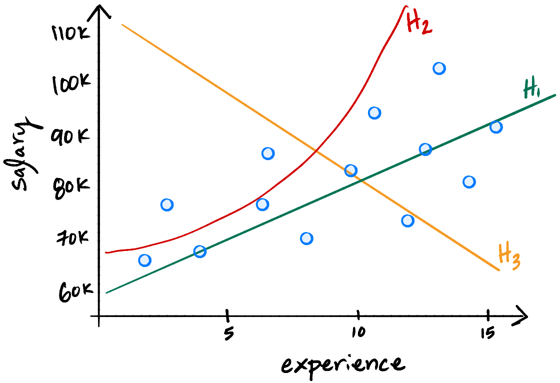
- There are many possible prediction functions.
- How do we pick a good one?
- One that **works well on unseen, future data**.
- **Problem**: we **don't know** the future.

Data

- **Assumption:** the future will be like the past.
- So a prediction function that works well on past data will likely work well on future data.
- **Idea:** can use past data to “measure” how a good prediction function is, select between them.

Example

- $H_1(x) = 60{,}000 + 10{,}000x$
- $H_2(x) = 70{,}000 + 200x^2$
- $H_3(x) = 110{,}000 - 15{,}000x$

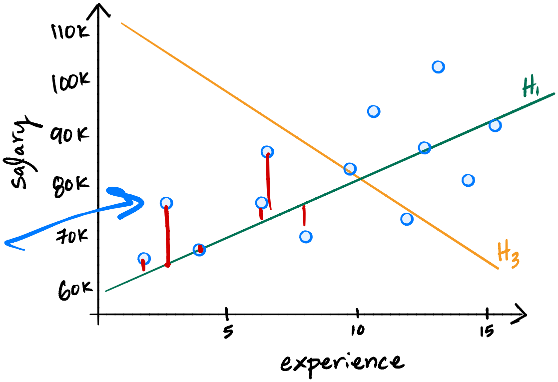


Fit

- We preferred H_1 over H_2 and H_3 because it “fit” the data better.
- How do we formally **quantify** how well a prediction function fits the data?

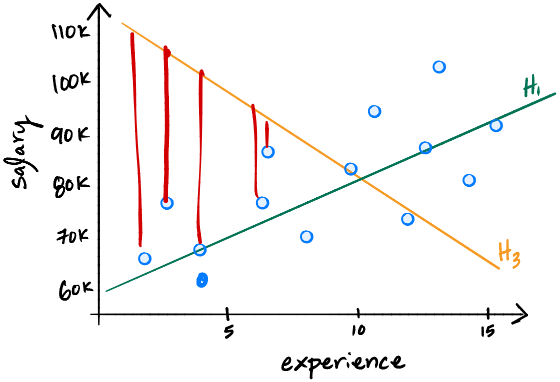
Measuring Errors

- **Idea:** measure the difference between the prediction and the correct label.



Measuring Errors

- **Idea:** measure the difference between the prediction and the correct label.



Loss Functions

- A **loss function** measures the difference between a prediction $H(\vec{x}^{(i)})$ and the "right answer" y_i.
- There are many different loss functions. For now, we'll consider two.
- **Absolute loss**: $\ell_{\text{abs}}(H(\vec{x}^{(i)}), y_i) = |H(\vec{x}^{(i)}) - y_i|$
- **Square loss**: $\ell_{\text{sq}}(H(\vec{x}^{(i)}), y_i) = (H(\vec{x}^{(i)}) - y_i)^2$

Quantifying Overall Fit

- A loss function measures the difference between a prediction and the correct label for a **single training point**.
- A good prediction function should make good predictions *on average* over the entire training set.
- That is, for a good H, the **average loss** should be small.

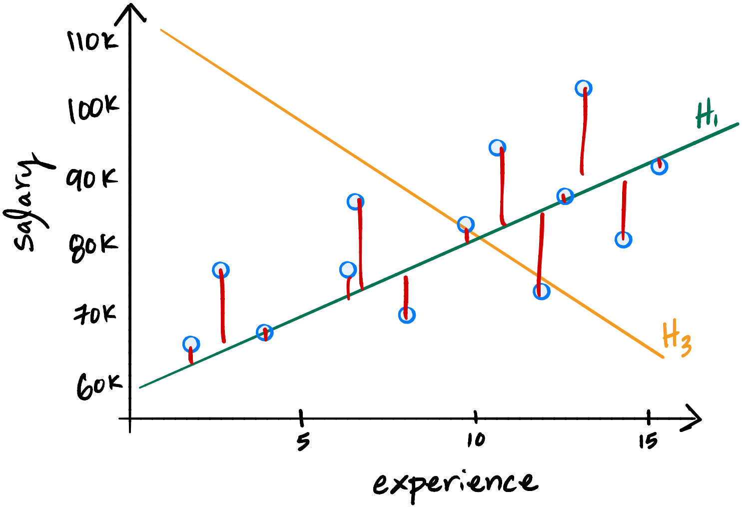
Empirical Risk

- The average loss on the training set, also called the **empirical risk**, is defined to be:

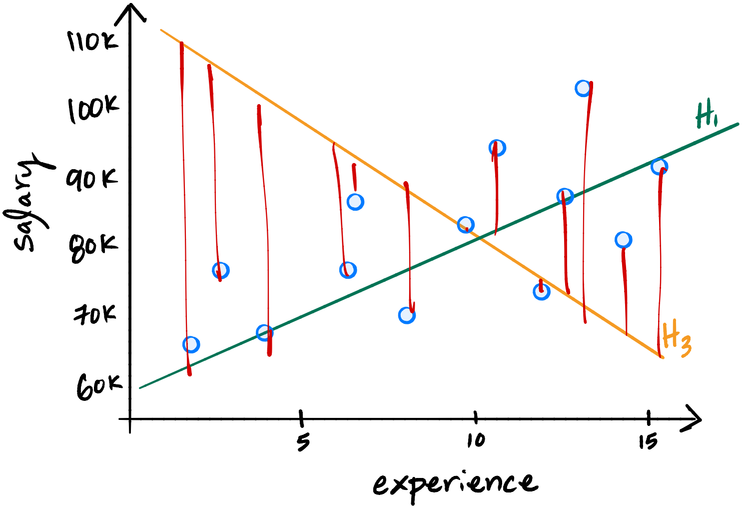
$$R(H) = \frac{1}{n}\sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}), y_i)$$

- It is a function of H, but it also depends on:
  - The training data, $\mathcal{X} = (\vec{x}^{(1)}, y_1), \dots, (\vec{x}^{(n)}, y_n)$
  - The particular choice of loss function ℓ

Example



Example



Terminology

- We might say: “the empirical risk with respect to absolute loss”. This means:

$$R(H) = \frac{1}{n}\sum_{i=1}^{n} |H(\vec{x}^{(i)}) - y_i|$$

- Or, “the empirical risk with respect to square loss”. This means:

$$R(H) = \frac{1}{n}\sum_{i=1}^{n} (H(\vec{x}^{(i)}) - y_i)^2$$

Terminology

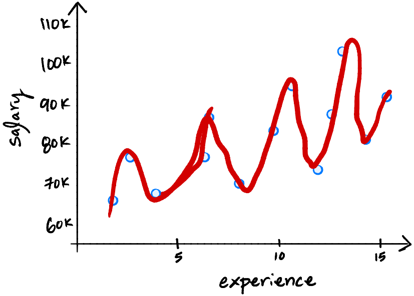
- We might be quick and say “risk” instead of “empirical risk”.

Minimizing Empirical Risk

- Empirical risk measures the “fit” of a prediction function to the training data.
- **Idea:** find a prediction function H that has the smallest empirical risk.

Exercise

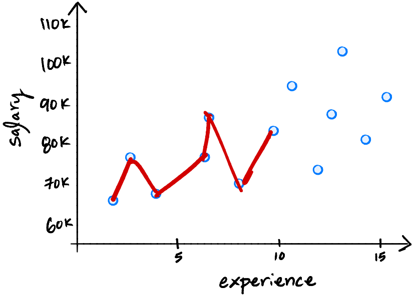
Consider the data shown below, and assume absolute loss.



Sketch a prediction function H that minimizes the empirical risk.

Exercise

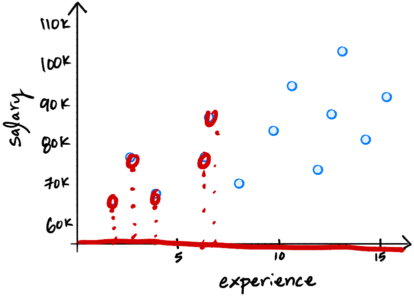
Consider the data shown below, and assume absolute loss.



Sketch a prediction function H that minimizes the empirical risk.

Exercise

Consider the data shown below, and assume absolute loss.



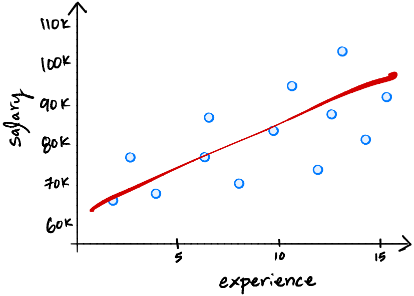
Sketch a prediction function *H* that minimizes the empirical risk.

Problem

- It is **too easy** to find a prediction function that has **zero** empirical risk.
  - Simply memorize the training data.
  - We want to learn a simpler pattern.
- Instead, we will restrict our search for prediction functions to a smaller set of (simple) functions.
- This set is called the **hypothesis class**.

Exercise

Consider the data shown below, and assume absolute loss.



Sketch a **linear** prediction function H that minimizes the empirical risk.

Empirical Risk Minimization

- The learning strategy we have just derived is called **empirical risk minimization (ERM)**.
- Step 1: choose a **hypothesis class**
  - for example, linear functions
- Step 2: choose a **loss function**
- Step 3: find H minimizing **empirical risk**

ERM is a Recipe

- By choosing different hypothesis classes and losses, we derive different learning algorithms.
- Some choices for Step 1 & 2 make Step 3 easier or harder.
- We’ll see different choices in the coming weeks.

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Linear Prediction Functions

A Simple Choice

- ERM asks us to choose a hypothesis class.
- Let's start with a simple one: **linear functions**.
- This choice will take us quite far.

Linear Functions

- A **linear prediction function** of one feature has the form:

$$H(x) = w_0 + w_1 x$$

- In general, a linear prediction function of d features has the form:

$$H(\vec{x}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

- $w_0, w_1, \ldots, w_d$ are the **parameters** or **weights**.

Interpreting Weights

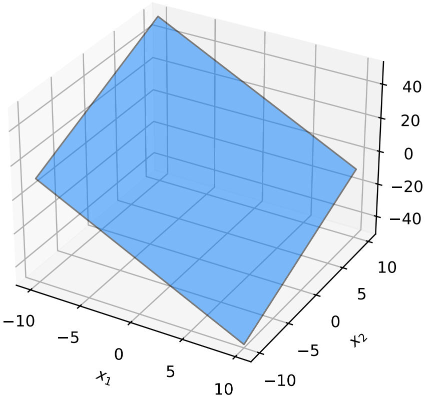
$$H(\vec{x}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

- w_0 (the **bias**) determines the prediction when all features are zero.
- w_1 determines how much the prediction changes when x_1 increases by one unit
- Similarly for $w_2, \ldots, w_d$

Interpreting Weights

- When plotted, linear prediction functions are:
  - straight lines when $\vec{x} \in \mathbb{R}^1$
  - planes when $\vec{x} \in \mathbb{R}^2$
  - hyperplanes when $\vec{x} \in \mathbb{R}^d$
- w_i is the **slope** of the hyperplane in the x_i direction.

Example



$$w_0 = 1, \quad w_1 = -3, \quad w_2 = 2$$

$$H(\vec{x}) = 1 - 3x_1 + 2x_2$$

Parameter Vectors

- The parameters of a linear function can be packaged into a **parameter vector**, $\vec{w}$.
- **Example:** if $H(\vec{x}) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3$ then $\vec{w} = (w_0, \ldots, w_3)^T$.
- If $\vec{x} \in \mathbb{R}^d$, then $\vec{w} \in \mathbb{R}^{d+1}$.

Parameterization

- A linear function $H(\vec{x})$ is **completely specified** by its parameter vector.
  - Can work either with the function, H, or vector, $\vec{w}$.

- Sometimes write $H(\vec{x}; \vec{w})$.

- Example: $\vec{w} = (8, 3, 1, 5, -2, -7)^T$ specifies

$$H(\vec{x}; \vec{w}) = 8 + 3x_1 + 1x_2 + 5x_3 - 2x_4 - 7x_5$$

Compact Form

- Recall the **dot product** of vectors $\vec{a}$ and $\vec{b}$:

$$\vec{a} = (a_1, a_2, \dots, a_d)^T \qquad \vec{b} = (b_1, b_2, \dots, b_d)^T$$

$$\vec{a} \cdot \vec{b} = a_1 b_1 + a_2 b_2 + \dots + a_d b_d$$

- Observe:

$$\begin{aligned} H(\vec{x}; \vec{w}) &= w_0 + w_1 x_1 + \dots + w_d x_d \\ &= \underbrace{(w_0, w_1, \dots, w_d)^T}_{\vec{w}} \cdot \underbrace{(1, x_1, \dots, x_d)^T}_{?} \end{aligned}$$

Compact Form

- The **augmented feature vector** $\text{Aug}(\vec{x})$ is the vector obtained by adding a 1 to the front of $\vec{x}$:

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix} \qquad \text{Aug}(\vec{x}) = \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix}$$

- With augmentation, we can write:

$$\begin{aligned} H(\vec{x}) &= w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_d x_d \\ &= \vec{w} \cdot \text{Aug}(\vec{x}) \end{aligned}$$

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Lecture 02 | Part 4

ERM for Linear Predictors

Empirical Risk Minimization

To create a new ML algorithm:

- Step 1: choose a **hypothesis class**
  - We've chosen linear functions
- Step 2: choose a **loss function**
- Step 3: find H minimizing **empirical risk**

Loss Functions

- Next, we need to choose a loss function.
- Choice depends on the problem at hand.
- Let's focus on **regression** for now.
- The **absolute loss** is a natural first choice.

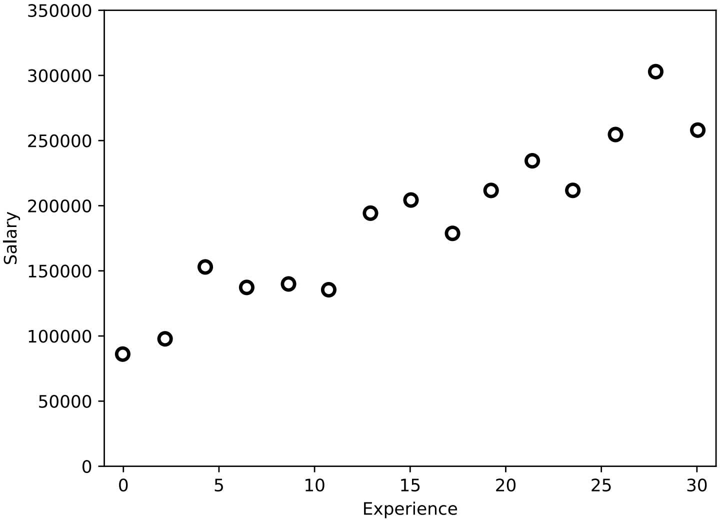
Empirical Risk w.r.t. Absolute Loss

- Now that we have assumed $H(\vec{x})$ is linear, we can write the empirical risk w.r.t. the absolute loss as:

$$
\begin{aligned}
R_{\text{abs}}(\vec{w}) &= \frac{1}{n}\sum_{i=1}^{n} |H(\vec{x}^{(i)}) - y_i| \\
&= \frac{1}{n}\sum_{i=1}^{n} |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i|
\end{aligned}
$$

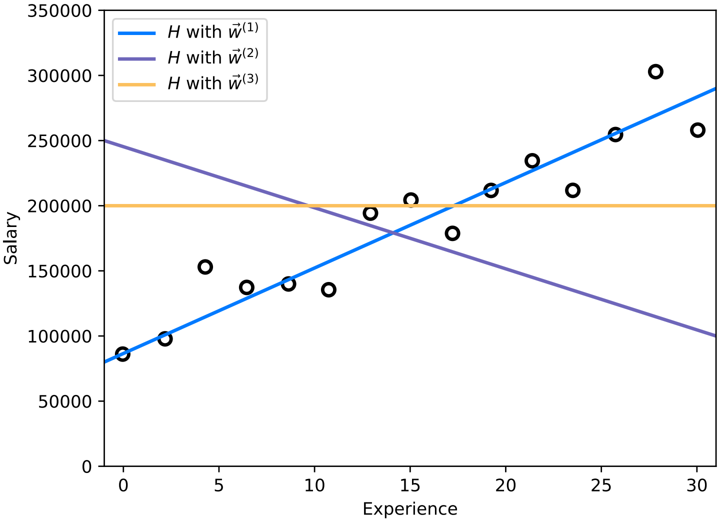
- A function of $\vec{w}$, since H is totally specified by $\vec{w}$.

Example



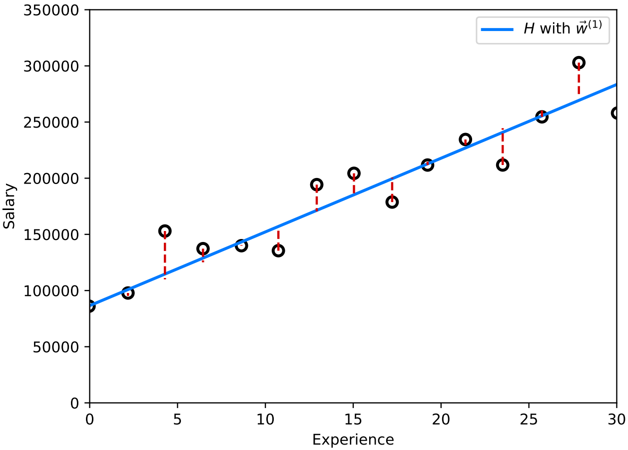
350000
300000
250000
200000
150000
100000
50000
0
Salary
0
5
10
15
20
25
30
Experience

Example



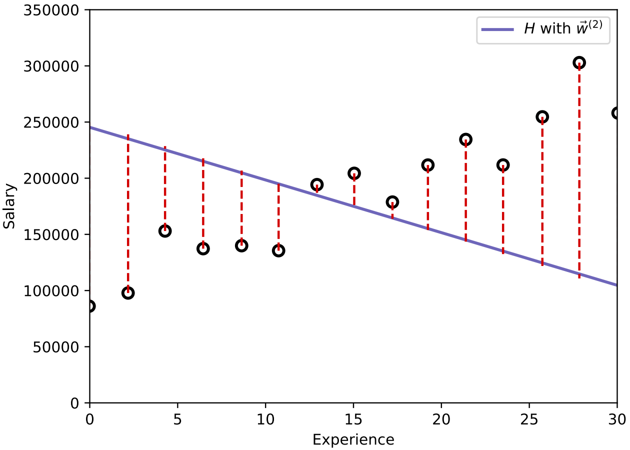
H with $\vec{w}^{(1)}$
H with $\vec{w}^{(2)}$
H with $\vec{w}^{(3)}$
Salary
Experience
350000
300000
250000
200000
150000
100000
50000
0
0
5
10
15
20
25
30

Example



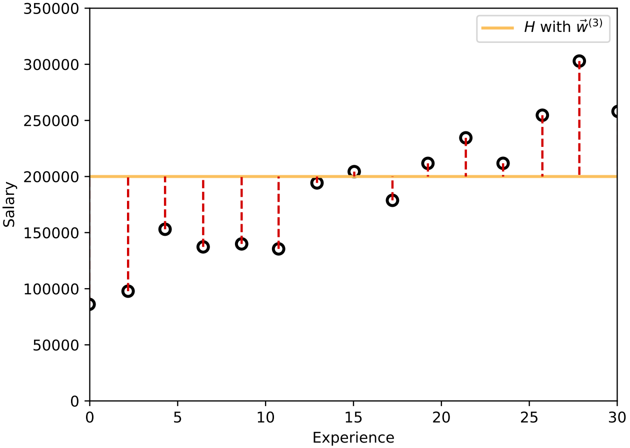
$$R_{\text{abs}}(\vec{w}^{(1)}) \approx 17{,}000$$

Example



$$R_{\text{abs}}(\vec{w}^{(2)}) \approx 90{,}000$$

Example



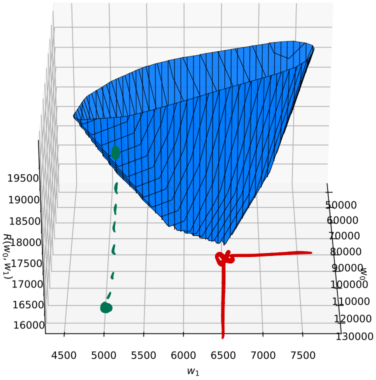
$$R_{\text{abs}}(\vec{w}^{(3)}) \approx 50{,}000$$

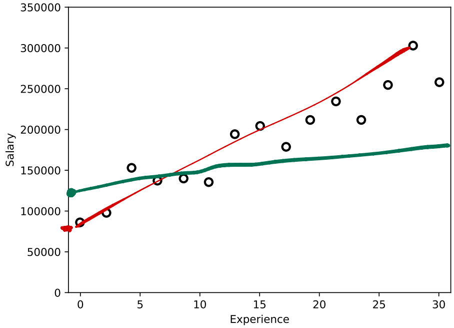
Risk Surface

- Can imagine plotting $R_{\text{abs}}(\vec{w})$ for all values of $\vec{w}$.
- This is called the **risk surface**.
- A $\vec{w}$ that makes the surface lowest minimizes the empirical risk.

Risk Surface

Plot of $R_{\text{abs}}(\vec{w})$





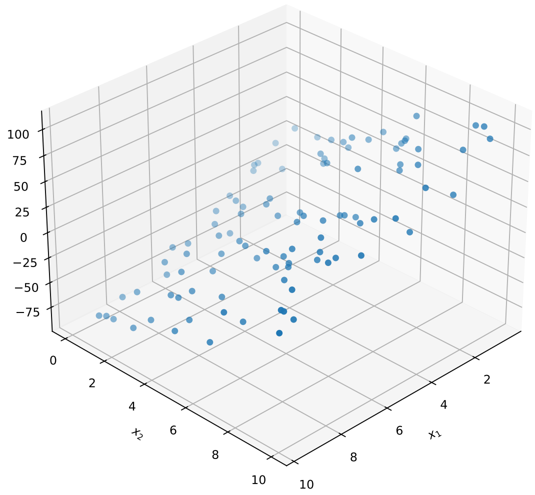
More Features

- With 2 features, we fit a plane instead of a line.
  - With ≥ 3 features, we fit a hyperplane.

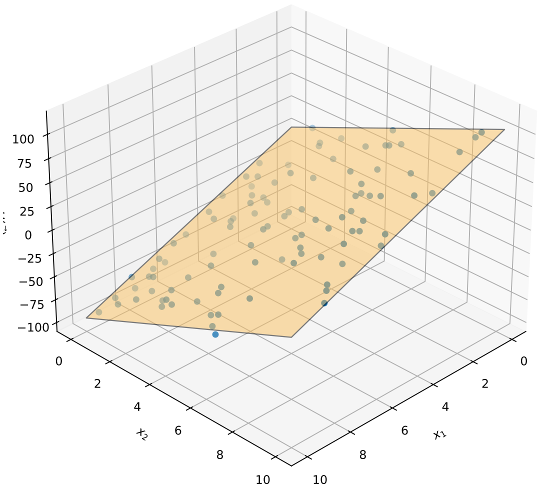
- We can no longer easily visualize the risk surface.

- But the idea is the same: find the $\vec{w}$ that minimizes the empirical risk.

Example

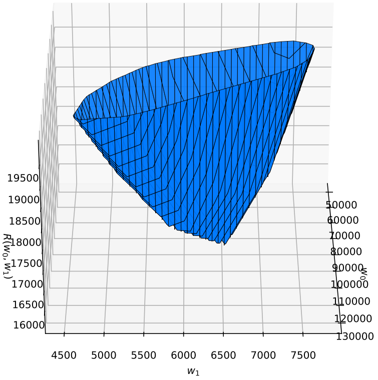


Example



Minimizing Empirical Risk

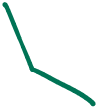
- How do we find the $\vec{w}$ that minimizes $R_{\text{abs}}(\vec{w})$ (the empirical risk with respect to the absolute loss)?



∇f

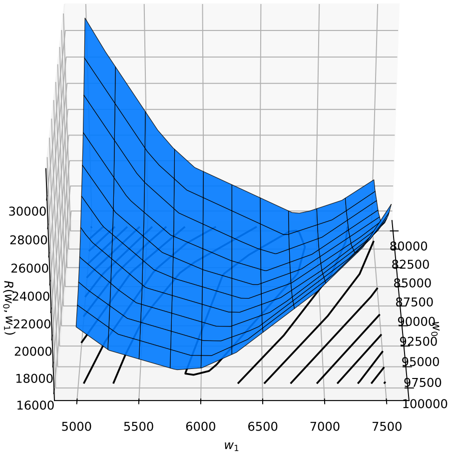
Calculus

- We know how to use calculus to find the minimum of a function:
  1. Find the **gradient** $\frac{d}{d\vec{w}} R_{\text{abs}}(\vec{w})$.
  2. Set it equal to zero, solve for $\vec{w}$.
  3. This finds places where $R_{\text{abs}}(\vec{w})$ is flat; check that it is a minimum (and not a maximum or saddle point).



Problem

- $R_{\text{abs}}(\vec{w})$ is **not differentiable**.
- There are places where the gradient (slope) is not defined.
- These appear as "cusps" or "sharp creases" in the risk surface.



$R(w_0, w_1)$
30000
28000
26000
24000
22000
20000
18000
16000
5000
5500
6000
6500
7000
7500
w_1
80000
82500
85000
87500
90000
92500
95000
97500
100000
w_0

Another Loss?

- We cannot use the usual calculus approach to minimize $R_{\text{abs}}(\vec{w})$.
  - We'll come back to this in a later lecture.

- Instead, let's see if the square loss is any better.

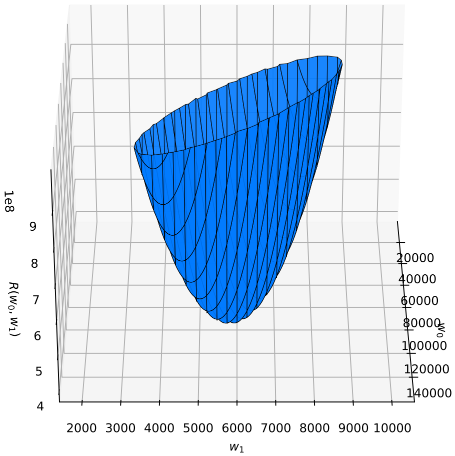
Empirical Risk w.r.t. Square Loss

- Assuming $H(\vec{x})$ is linear, we can write the empirical risk w.r.t. the square loss as:

$$\begin{aligned} R_{\text{sq}}(\vec{w}) &= \frac{1}{n} \sum_{i=1}^{n} (H(\vec{x}^{(i)}) - y_i)^2 \\ &= \frac{1}{n} \sum_{i=1}^{n} (\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i)^2 \end{aligned}$$

- $R_{\text{sq}}(\vec{w})$ is called the **mean squared error (MSE)**.

Risk Surface



Good News!

- The mean squared error is **differentiable**.
- Now, we'll try to find the $\vec{w}$ that minimizes $R_{\text{sq}}(\vec{w})$ with calculus.

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Lecture 02 | Part 5

Least Squares

Minimizing the MSE

- **Goal**: minimize $R_{\text{sq}}(\vec{w})$ with respect to $\vec{w}$.
- **Calculus Approach**: Find **gradient** of $R_{\text{sq}}(\vec{w})$; set to zero; solve for $\vec{w}$.
- We'll rely on results from vector calculus.

First Step: Rewrite Risk

- Step one: rewrite R_{sq} in vector form.
- We will find:

$$
\begin{aligned}
R_{\text{sq}}(\vec{w}) &= \frac{1}{n} \sum_{i=1}^{n} \left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)^2 \\
&= \frac{1}{n} \|X\vec{w} - \vec{y}\|^2
\end{aligned}
$$

Recall

- If $\vec{u} = (u_1, u_2, \ldots, u_k)^T$, then:

$$\|\vec{u}\|^2 = \vec{u} \cdot \vec{u} = \sum_{i=1}^{k} u_i^2$$

- So, if $\vec{a} = (a_1, \ldots, a_k)^T$ and $\vec{b} = (b_1, \ldots, b_k)^T$:

$$\begin{aligned} \|\vec{a} - \vec{b}\|^2 &= (\vec{a} - \vec{b}) \cdot (\vec{a} - \vec{b}) \\ &= \sum_{i=1}^{k} (a_i - b_i)^2 \end{aligned}$$

First Step: Rewrite Risk

- Define $p_i = \text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}$, and let $\vec{p} = (p_1, \ldots, p_n)^T$.
  - $\vec{p}$ is a vector of the predictions on training set.
  - Note: $\vec{p} \in \mathbb{R}^n$, not $\mathbb{R}^d$!

- Then:

$$
\begin{aligned}
R_{\text{sq}}(\vec{w}) &= \frac{1}{n} \sum_{i=1}^{n} \left(\overbrace{\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}}^{p_i} - y_i \right)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \left(p_i - y_i \right)^2 \\
&= \frac{1}{n} \|\vec{p} - \vec{y}\|^2
\end{aligned}
$$

First Step: Rewrite Risk

- Define the (augmented) **design matrix**, X:

$$X = \begin{pmatrix} \text{Aug}(\vec{x}^{(1)}) \longrightarrow \\ \text{Aug}(\vec{x}^{(2)}) \longrightarrow \\ \vdots \qquad\qquad \vdots \\ \text{Aug}(\vec{x}^{(n)}) \longrightarrow \end{pmatrix} = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \dots & x_d^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \dots & x_d^{(2)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_1^{(n)} & x_2^{(n)} & \dots & x_d^{(n)} \end{pmatrix}$$

First Step: Rewrite Risk

- **Observe:** $\vec{p} = X\vec{w}$.

$$\underbrace{\begin{pmatrix} \text{Aug}(\vec{x}^{(1)}) & \longrightarrow & \\ \text{Aug}(\vec{x}^{(2)}) & \longrightarrow & \\ \vdots & & \vdots \\ \text{Aug}(\vec{x}^{(n)}) & \longrightarrow & \end{pmatrix}}_{X} \underbrace{\begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{pmatrix}}_{\vec{w}} = \underbrace{\begin{pmatrix} \text{Aug}(\vec{x}^{(1)}) \cdot \vec{w} \\ \text{Aug}(\vec{x}^{(2)}) \cdot \vec{w} \\ \vdots \\ \text{Aug}(\vec{x}^{(n)}) \cdot \vec{w} \end{pmatrix}}_{\vec{p}}$$

First Step: Rewrite Risk

- Therefore, the MSE can be written:

$$
\begin{aligned}
R_{\text{sq}}(\vec{w}) &= \frac{1}{n} \sum_{i=1}^{n} \left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i \right)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \left(p_i - y_i \right)^2 \\
&= \frac{1}{n} \|\vec{p} - \vec{y}\|^2 \\
&= \frac{1}{n} \|X\vec{w} - \vec{y}\|^2
\end{aligned}
$$

Goal

- Find $\vec{w} \in \mathbb{R}^{d+1}$ minimizing:

$$R_{\text{sq}}(\vec{w}) = \frac{1}{n} \|X\vec{w} - \vec{y}\|^2$$

- **Step Two:** find gradient, set to zero, solve.

Step Two: Find Gradient

- We want to compute:

$$\frac{d}{d\vec{w}}\left[R_{\text{sq}}(\vec{w})\right] = \frac{d}{d\vec{w}}\left[\frac{1}{n}\|X\vec{w} - \vec{y}\|^2\right]$$

- $\frac{dR_{\text{sq}}}{d\vec{w}}$ is the **gradient** of R_{sq}.

- It is the vector of partial derivatives:

$$\frac{dR_{\text{sq}}}{d\vec{w}} = \left(\frac{\partial R_{\text{sq}}}{\partial w_0}, \frac{\partial R_{\text{sq}}}{\partial w_1}, \dots, \frac{\partial R_{\text{sq}}}{\partial w_d}\right)^T$$

Good to know...

$$(A + B)^T = A^T + B^T$$

$$(AB)^T = B^T A^T$$

$$\vec{u} \cdot \vec{v} = \vec{v} \cdot \vec{u} = \vec{u}^T \vec{v} = \vec{v}^T \vec{u}$$

$$(\vec{u} + \vec{v}) \cdot (\vec{w} + \vec{z}) = \vec{u} \cdot \vec{w} + \vec{u} \cdot \vec{x} + \vec{v} \cdot \vec{w} + \vec{v} \cdot \vec{z}$$

$$\|\vec{u}\|^2 = \vec{u} \cdot \vec{u}$$

Step Two: Find Gradient

- Expand norm to make gradient easier.

$$
\begin{aligned}
\|X\vec{w} - \vec{y}\|^2 &= (X\vec{w} - \vec{y}) \cdot (X\vec{w} - \vec{y}) \\
&= (X\vec{w} - \vec{y})^T (X\vec{w} - \vec{y}) \\
&= (\vec{w}^T X^T - \vec{y}^T)(X\vec{w} - \vec{y}) \\
&= \vec{w}^T X^T X \vec{w} - \vec{w}^T X^T \vec{y} \\
&\quad - \vec{y}^T X \vec{w} \\
&\quad + \vec{y}^T \vec{y}
\end{aligned}
$$

Exercise

Consider:

$$\vec{w}^T X^T X \vec{w} - 2\vec{y}^T X \vec{w} + \vec{y}^T \vec{y}$$

1. What type of object *should* it be?
   - Scalar, vector, or matrix?

2. What type of object *is* it?

Step Two: Find Gradient

$$\frac{d}{d\vec{w}}\left[R_{\text{sq}}(\vec{w})\right] = \frac{1}{n}\frac{d}{d\vec{w}}\left[\vec{w}^T X^T X\vec{w} - 2\vec{y}^T X\vec{w} + \vec{y}^T\vec{y}\right]$$

$$= ?$$

Idea

- While we could compute each of: $\frac{\partial R_{\text{sq}}}{\partial w_0}, \frac{\partial R_{\text{sq}}}{\partial w_1}, \ldots.$
- there's an easier way using matrix-vector calculus.

$$\frac{d}{dx} ax^2 = 2ax$$

Exercise

If you had to guess, which of the following is equal to $\frac{d}{d\vec{w}}\left[\vec{w}^T X^T X \vec{w}\right]$?

$x^2 w^2 = 2x^2 w$

1. $\cancel{X}$
2. $\vec{w}$
3. $2X^T X\vec{w}$
4. $2X\vec{w}$

Claims

- $\frac{d}{d\vec{w}}\left[\vec{w}^T X^T X \vec{w}\right] = 2X^T X \vec{w}$
- $\frac{d}{d\vec{w}}\left[\vec{y}^T X \vec{w}\right] = X^T \vec{y}$
- $\frac{d}{d\vec{w}}\left[\vec{y}^T \vec{y}\right] = 0$

How?

- General procedure: expand, differentiate, gather
    1. Expand $\vec{v}^T\vec{u}$ until coordinates $u_1, \ldots, u_k$ are visible.
    2. Compute $\partial d / \partial u_1$, $\partial d / \partial u_2$, ..., $\partial d / \partial u_k$.
    3. Gather result in vector form.

Step Two: Find Gradient

- We claimed

$$\frac{d}{d\vec{w}}\left[\vec{w}^T X^T X \vec{w}\right] = 2X^T X\vec{w} \qquad \frac{d}{d\vec{w}}\left[\vec{y}^T X \vec{w}\right] = X^T\vec{y} \qquad \frac{d}{d\vec{w}}\left[\vec{y}^T\vec{y}\right] = 0$$

- So:

$$\frac{d}{d\vec{w}}\left[R_{\text{sq}}(\vec{w})\right] = \frac{1}{n}\frac{d}{d\vec{w}}\left[\vec{w}^T X^T X\vec{w} - 2\vec{y}^T X\vec{w} + \vec{y}^T\vec{y}\right]$$

$$= 2X^T X\vec{w} - 2X^T\vec{y} + 0$$

Solution

- We have found:

$$\frac{d}{d\vec{w}}\left[R_{\text{sq}}(\vec{w})\right] = \frac{1}{n}\left(2X^TX\vec{w} - 2X^T\vec{y}\right)$$

- To minimize $R_{\text{sq}}(\vec{w})$, set gradient to zero, solve:

$$2X^TX\vec{w} - 2X^T\vec{y} = 0 \implies X^TX\vec{w} = X^T\vec{y}$$

- This is a system of equations in matrix form, called the **normal equations**.

The Normal Equations

- The least squares solutions for $\vec{w}$ are found by solving the **normal equations**:

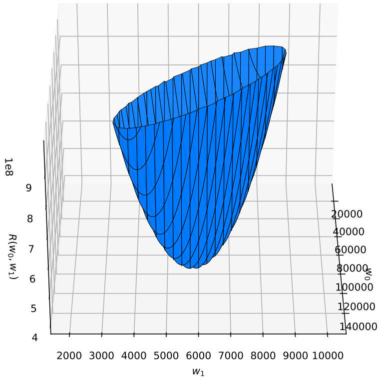
$$X^T X \vec{w} = X^T \vec{y}$$

- Mathematically, solved by:

$$\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$$

A Direct Solution

- $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$ is exactly at the bottom of the risk surface.



Linear Least Squares Regression

- **To train:**
  - Given a training set $\{(\vec{x}^{(1)}, y_1), \ldots, (\vec{x}^{(n)}, y_n)\}$...
  1. Construct $n \times (d+1)$ augmented **design matrix**, X.
  2. Solve the **normal equations**: $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$.

- **To predict:**
  - Given a new $\vec{x}$, compute $H(\vec{x}) = \text{Aug}(\vec{x}) \cdot \vec{w}^*$.

Linear Least Squares Regression

The first algorithm we've derived from the ERM framework:

- Step 1: choose a **hypothesis class**
  - We've chosen linear functions
- Step 2: choose a **loss function**
  - We've chosen the square loss
- Step 3: find H minimizing **empirical risk**
  - We've found a direct solution: $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$

Compare to k-Nearest Neighbors

- **Then:** k-NN did not learn the relative importance of features.
- **Now:** Linear least squares learns a weight for *each* feature.

DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 02 | Part 6

From Theory to Practice

Implementation

- `sklearn.linear_model.LinearRegression`
- But linear least squares is very simple to implement in numpy:

```
> # training
> w = np.linalg.solve(X.T @ X, X.T @ y)
> # prediction on a new example, x
> # (you'll need to define augment)
> augment(x) @ w
```

Augmentation

- One easy way to implement `augment`:

```
def augment(x):
    return np.array([1, *x])
```

- This code only works for a single example.
- To augment an array of examples, use `np.ones` and `np.column_stack`.

Don't Invert!

- Don't actually compute $(X^T X)^{-1}$.
- That is, avoid `np.linalg.inv`
- Inverting a matrix can be **slow** and **numerically unstable**.

Practical Issues

- You’ll sometimes run into technical issues when using least squares.
- But we have the theoretical tools to understand and address them.

Issue: “Singular Matrix” Error

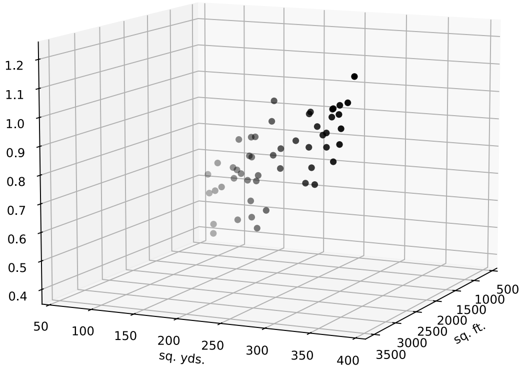
- You’re training a regression model to predict house prices.
- Two of your features are 1) size in square feet and 2) size in square yards.

```
np.linalg.solve(X.T @ X, X.T @ y)
```

```
---------------------------------------------------------------------------
LinAlgError                               Traceback (most recent call last)
Cell In[69], line 1
----> 1 np.linalg.solve(X.T @ X, X.T @ y)

File /nix/store/jmldnh8fda65lps694qff2yn9c4fnawp-python3-3.11.8-env/lib/python3.11/site-
b)
    407 signature = 'DD->D' if isComplexType(t) else 'dd->d'
    408 extobj = get_linalg_error_extobj(_raise_linalgerror_singular)
--> 409 r = gufunc(a, b, signature=signature, extobj=extobj)
    411 return wrap(r.astype(result_t, copy=False))

File /nix/store/jmldnh8fda65lps694qff2yn9c4fnawp-python3-3.11.8-env/lib/python3.11/site-
inalgerror_singular(err, flag)
    111 def _raise_linalgerror_singular(err, flag):
--> 112     raise LinAlgError("Singular matrix")

LinAlgError: Singular matrix
```

Issue: “Singular Matrix” Error

- Let’s look at the data.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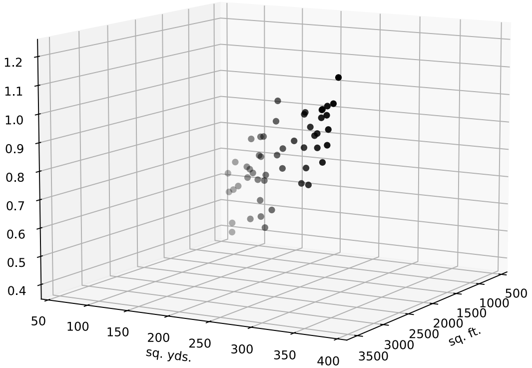
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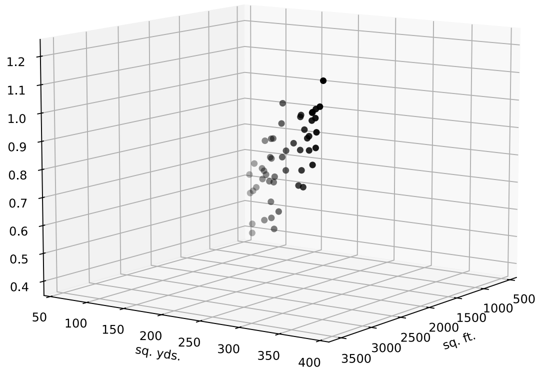
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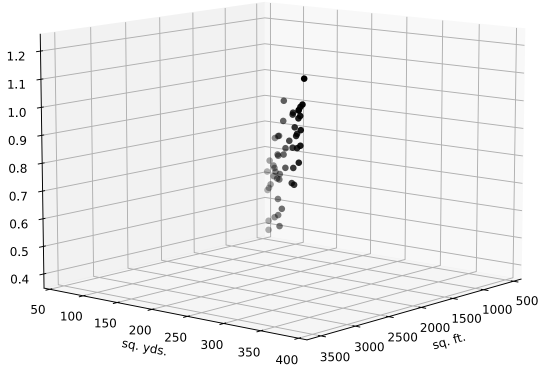
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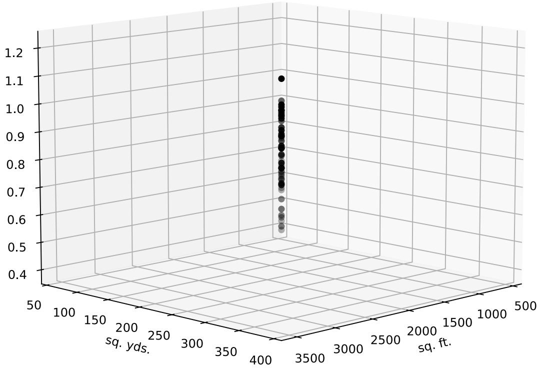

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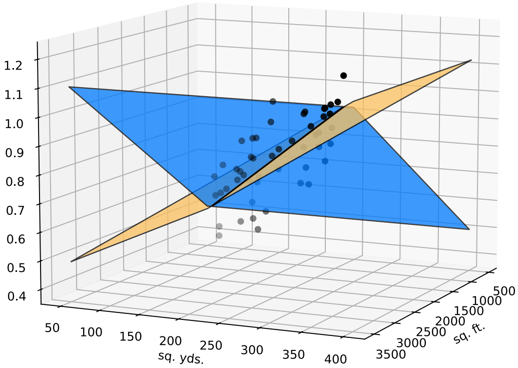
Issue: “Singular Matrix” Error

- The data aren’t truly 3-dimensional.
- There are **infinitely many** planes with the same empirical risk.
- That is, there are infinitely many solutions to the normal equations.
  - This is why the matrix is singular.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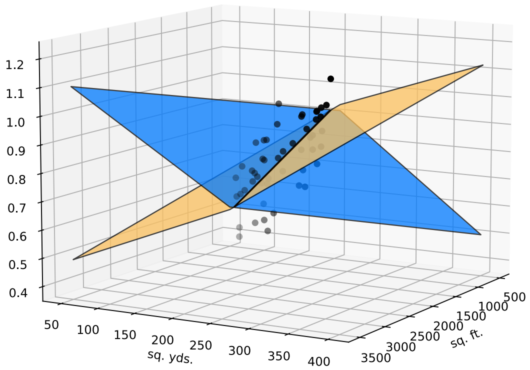
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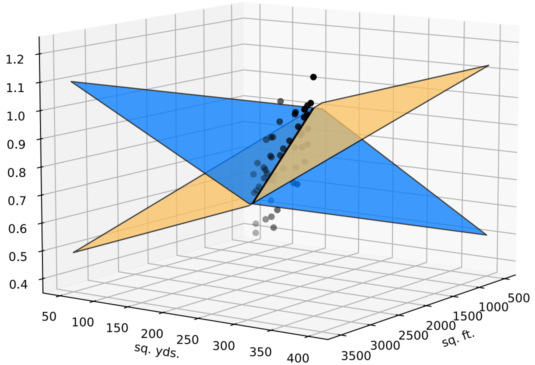

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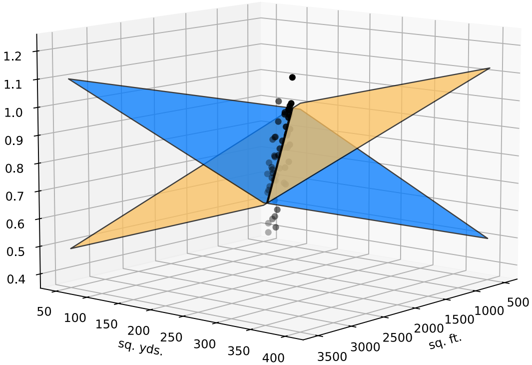
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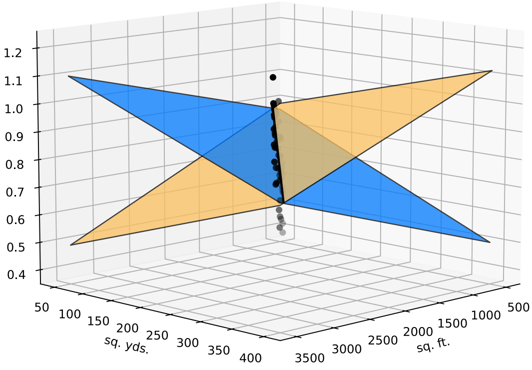

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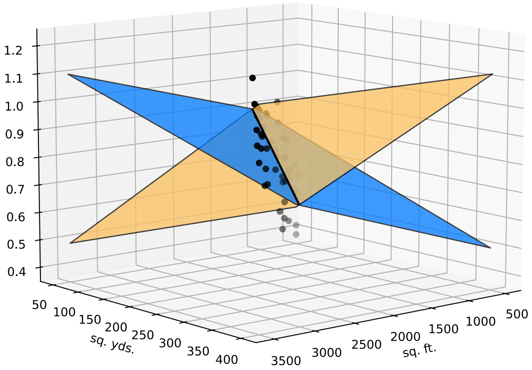
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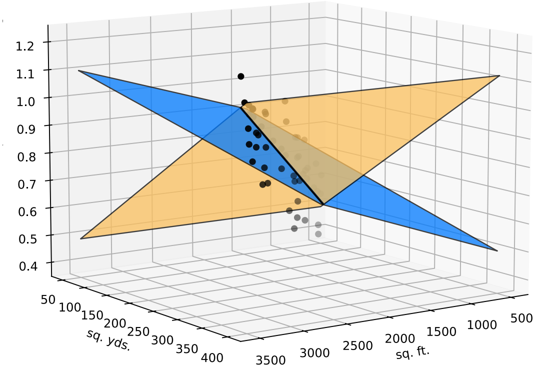
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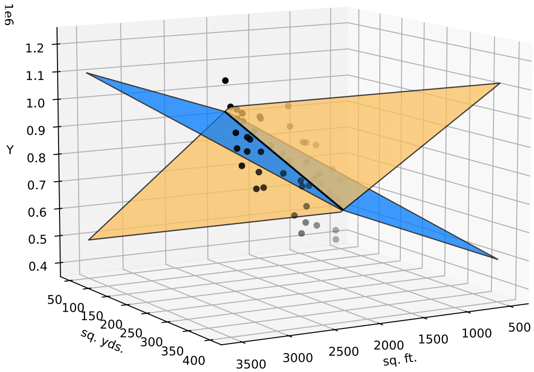
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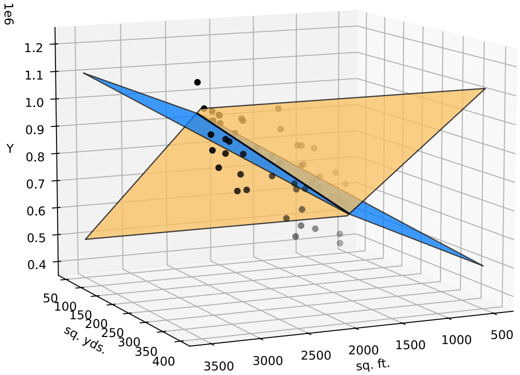

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Multicollinearity

- The situation where one feature is a linear combination of others is called **multicollinearity**.
- Can happen because the features are redundant, or because of chance.
- One fix: remove one of the redundant features.
  - We'll see another fix in lecture on **regularization**.

Issue: Time

```
[*]: np.linalg.solve(X.T @ X, X.T @ y)
```

- Solving a linear system in d unknowns takes $\Theta(d^3)$ time.
- Fine for small number of features, but can be slow when using many features.
- Next time: an approach for efficiently minimizing risk when data is very large.