Announcements

- Homework 1 due **Wednesday at 8pm**
- Quiz 1 due **Thursday at 8pm**
- Office hours posted on Course Website (starting **today**!)
  - See announcement on Ed Discussion
  - Virtual office hours held via OHQ
- Waitlist update

Lecture 3: Linear Regression (Part 2)

CIS 4190/5190

Fall 2022

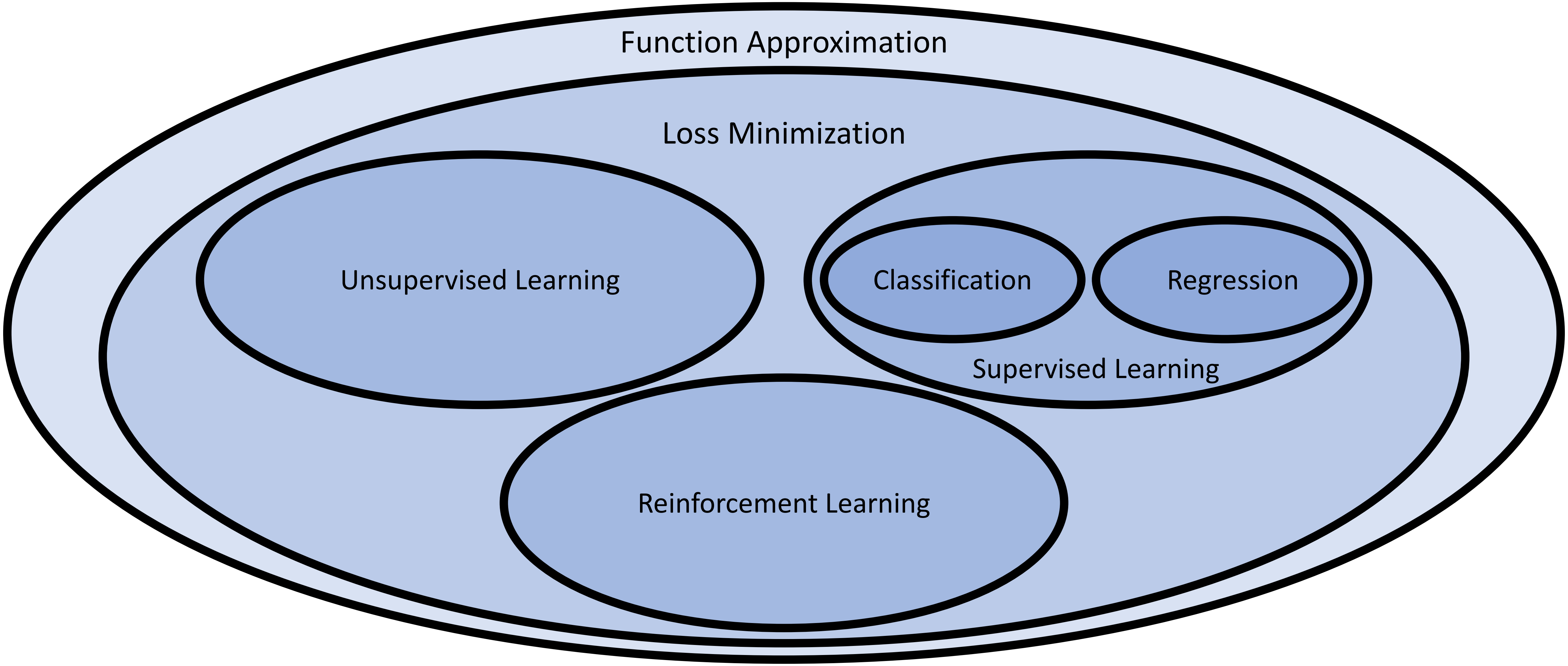
Recap: Linear Regression

- **Input:** Dataset $Z = \{(x_1, y_1), \dots, (x_n, y_n)\}$
- Compute

$$\hat{\beta}(Z) = \arg\min_{\beta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2$$

- **Output:** $f_{\hat{\beta}(Z)}(x) = \hat{\beta}(Z)^\top x$
- Discuss algorithm for computing the minimal β later today

Recap: Views of ML



Recap: Loss Minimization View of ML

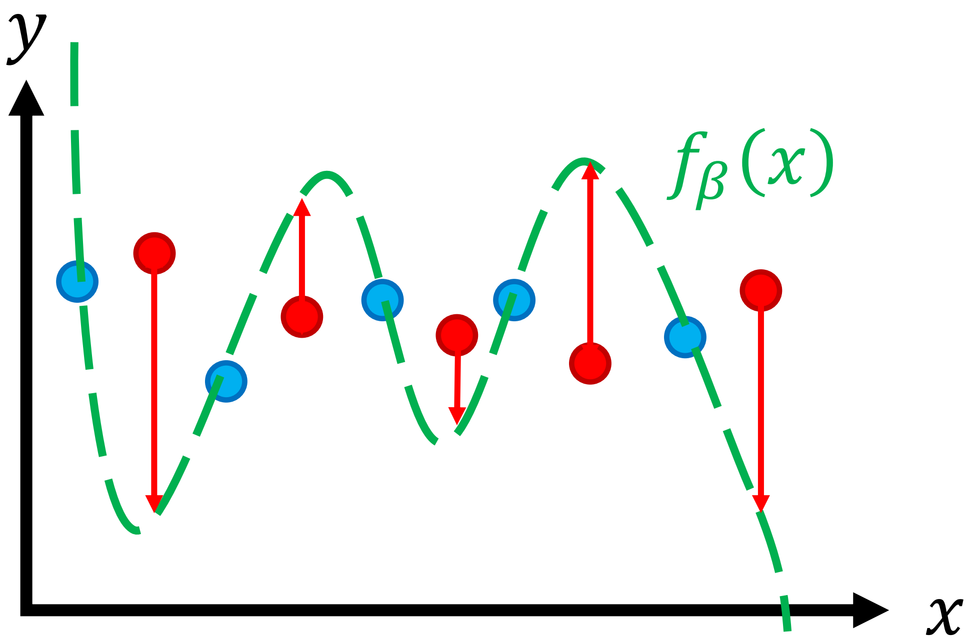
- **To design an ML algorithm:**
  - Choose model family $F = \{f_\beta\}_\beta$ (e.g., linear functions)
  - Choose loss function $L(\beta; Z)$ (e.g., MSE loss)

- **Resulting algorithm:**

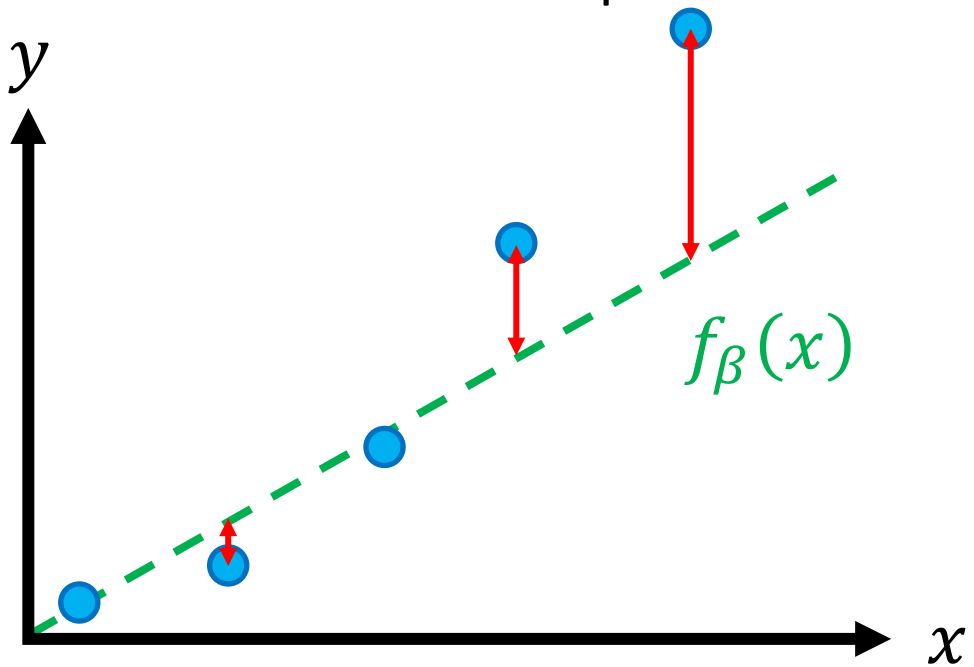
$$\hat{\beta}(Z) = \arg\min_{\beta} L(\beta; Z)$$

Recap: Bias-Variance Tradeoff

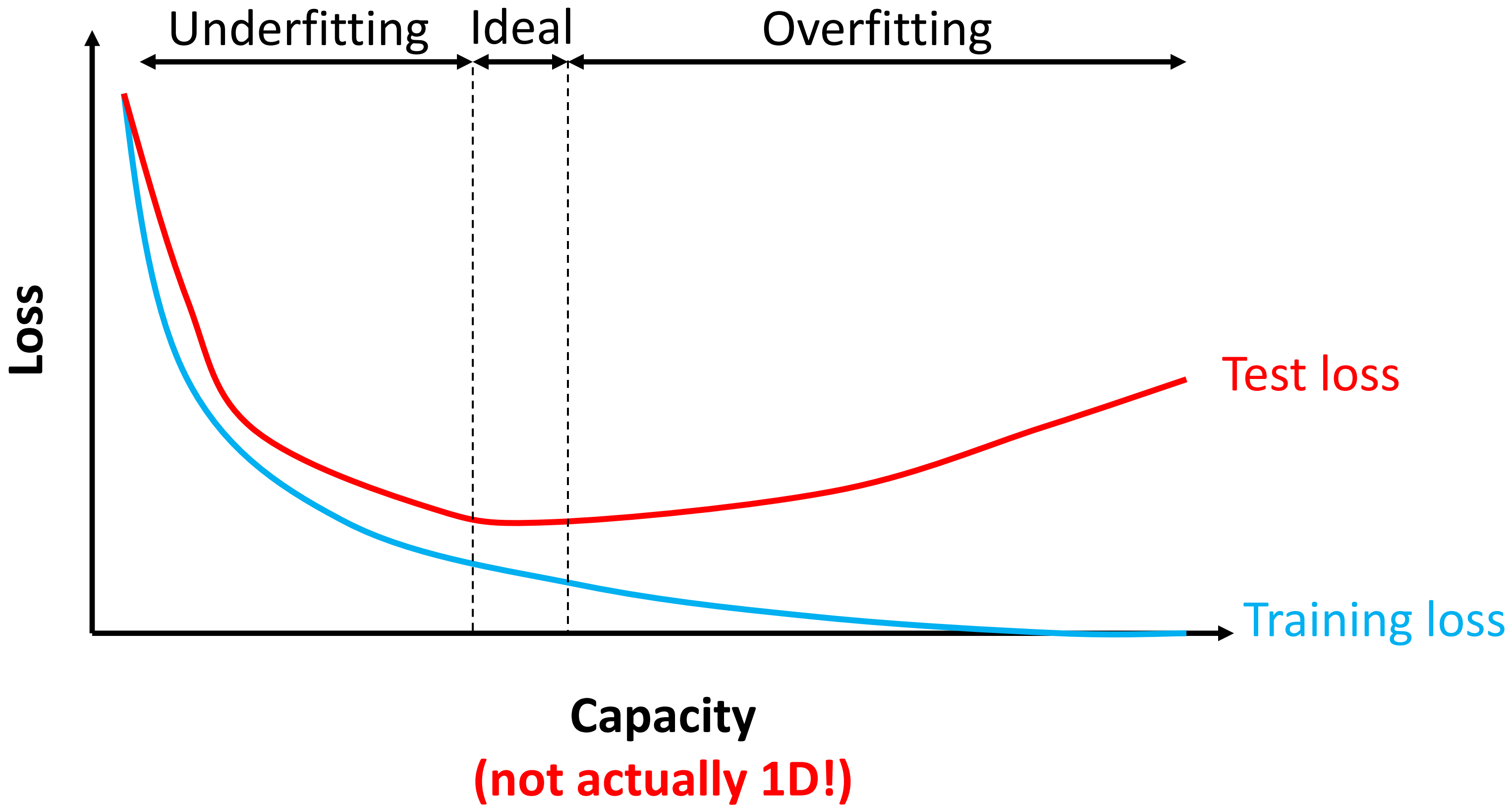
- **Overfitting (high variance)**
  - High capacity model capable of fitting complex data
  - Insufficient data to constrain it



- **Underfitting (high bias)**
  - Low capacity model that can only fit simple data
  - Sufficient data but poor fit

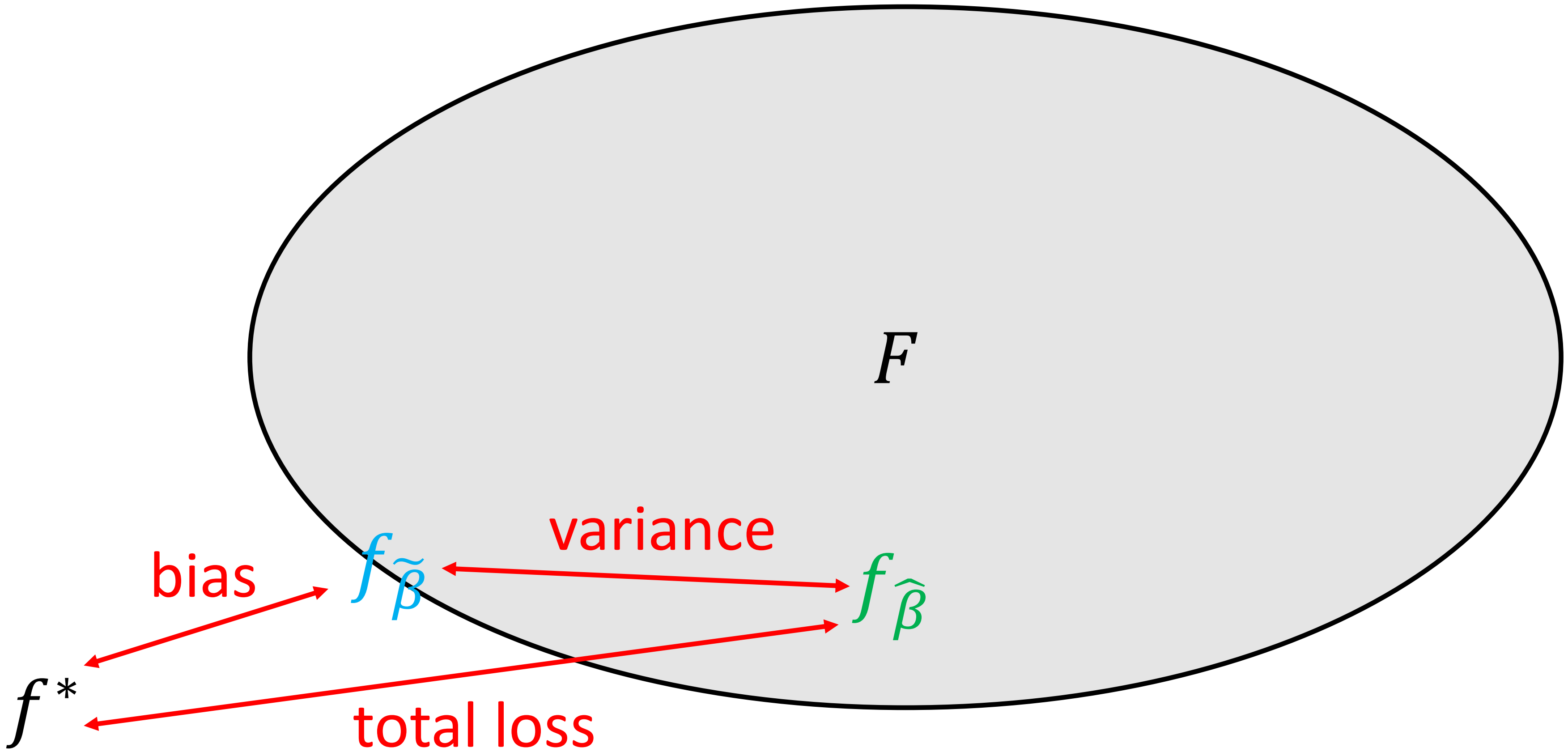


Recap: Bias-Variance Tradeoff

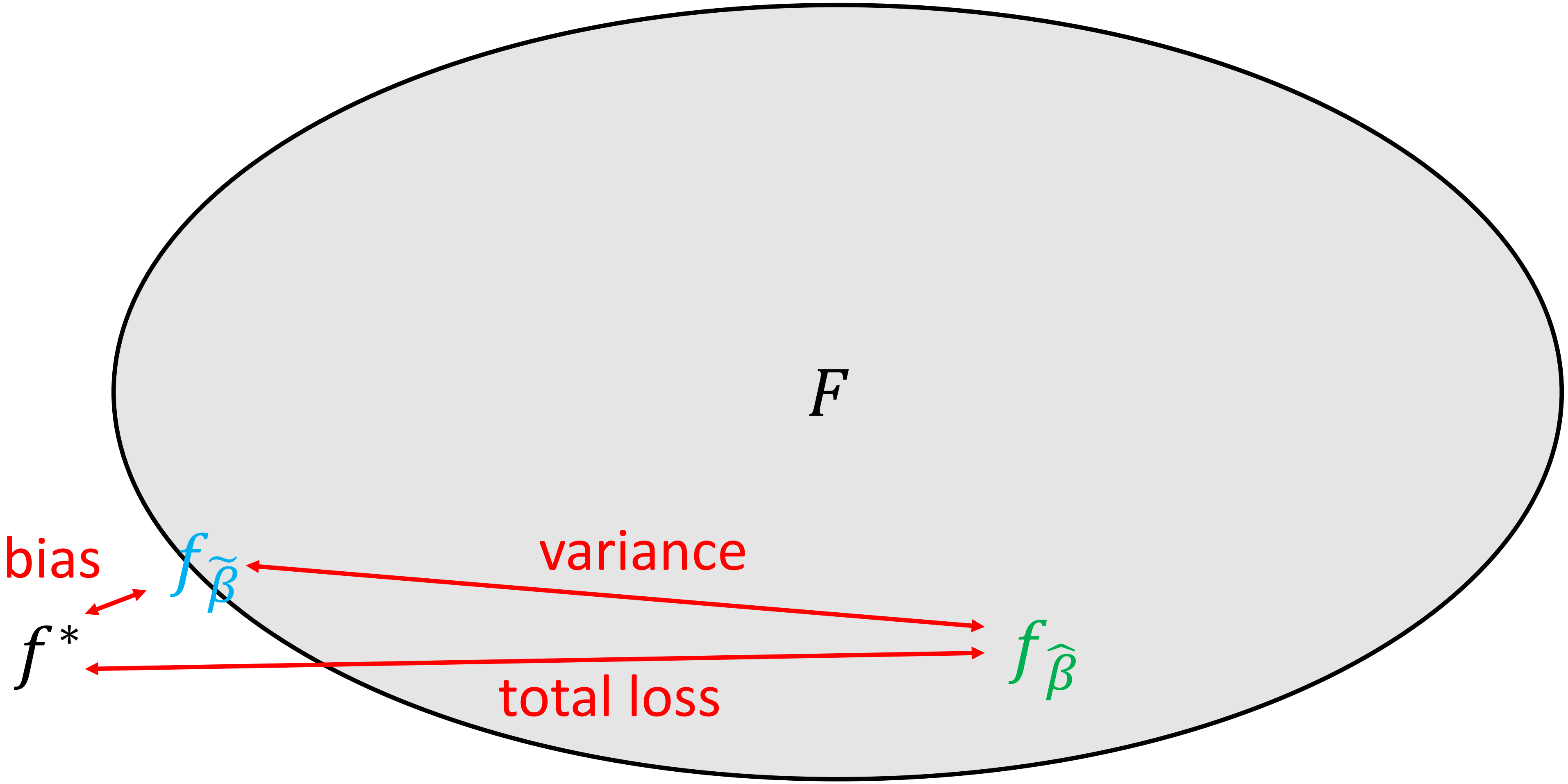


Slide by Padhraic Smyth, UCIrvine

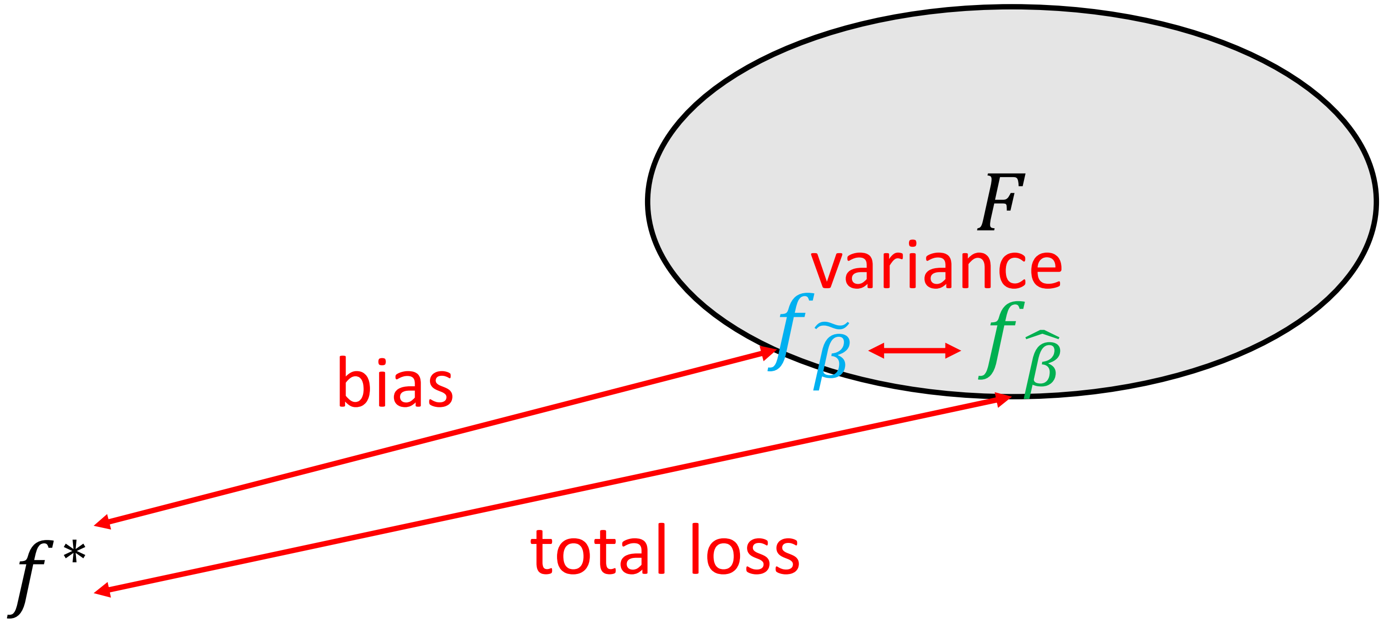
Recap: Bias-Variance Tradeoff



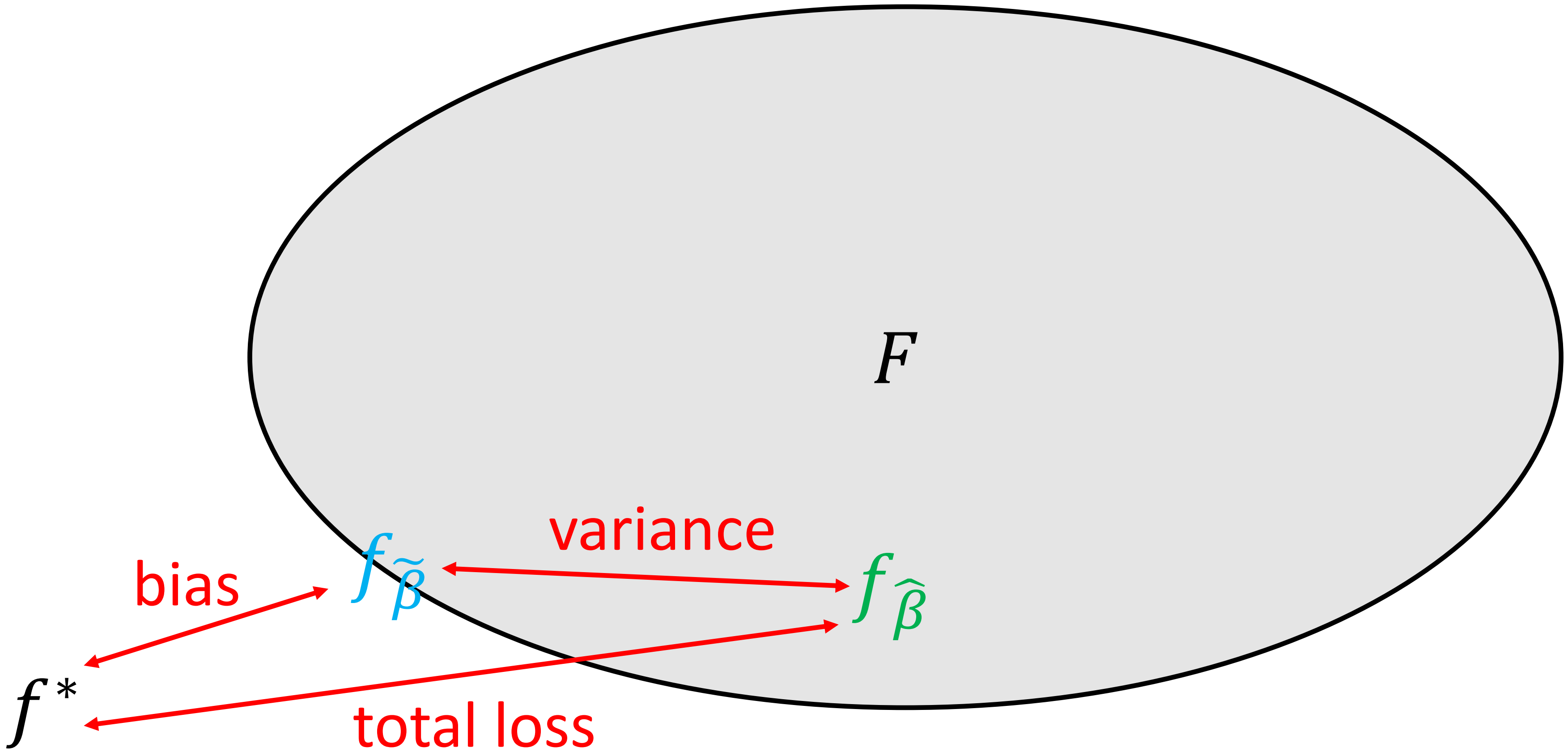
Recap: Bias-Variance Tradeoff (Overfitting)



Recap: Bias-Variance Tradeoff (Underfitting)



Recap: Bias-Variance Tradeoff (Ideal)



Agenda

- **Regularization**
  - Strategy to address bias-variance tradeoff
  - **By example:** Linear regression with L_2 regularization

- **Minimizing the MSE Loss**
  - Closed-form solution
  - Gradient descent

Recall: Mean Squared Error Loss

- Mean squared error loss for linear regression:

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$$

Linear Regression with L_2 Regularization

- **Original loss** + **regularization**:

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \cdot \|\beta\|_2^2$$

$$= \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{j=1}^{d}\beta_j^2$$

- λ is a **hyperparameter** that must be tuned (satisfies $\lambda \geq 0$)

Intuition on $\boldsymbol{L_2}$ Regularization

- Equivalently the L_2 norm of β:

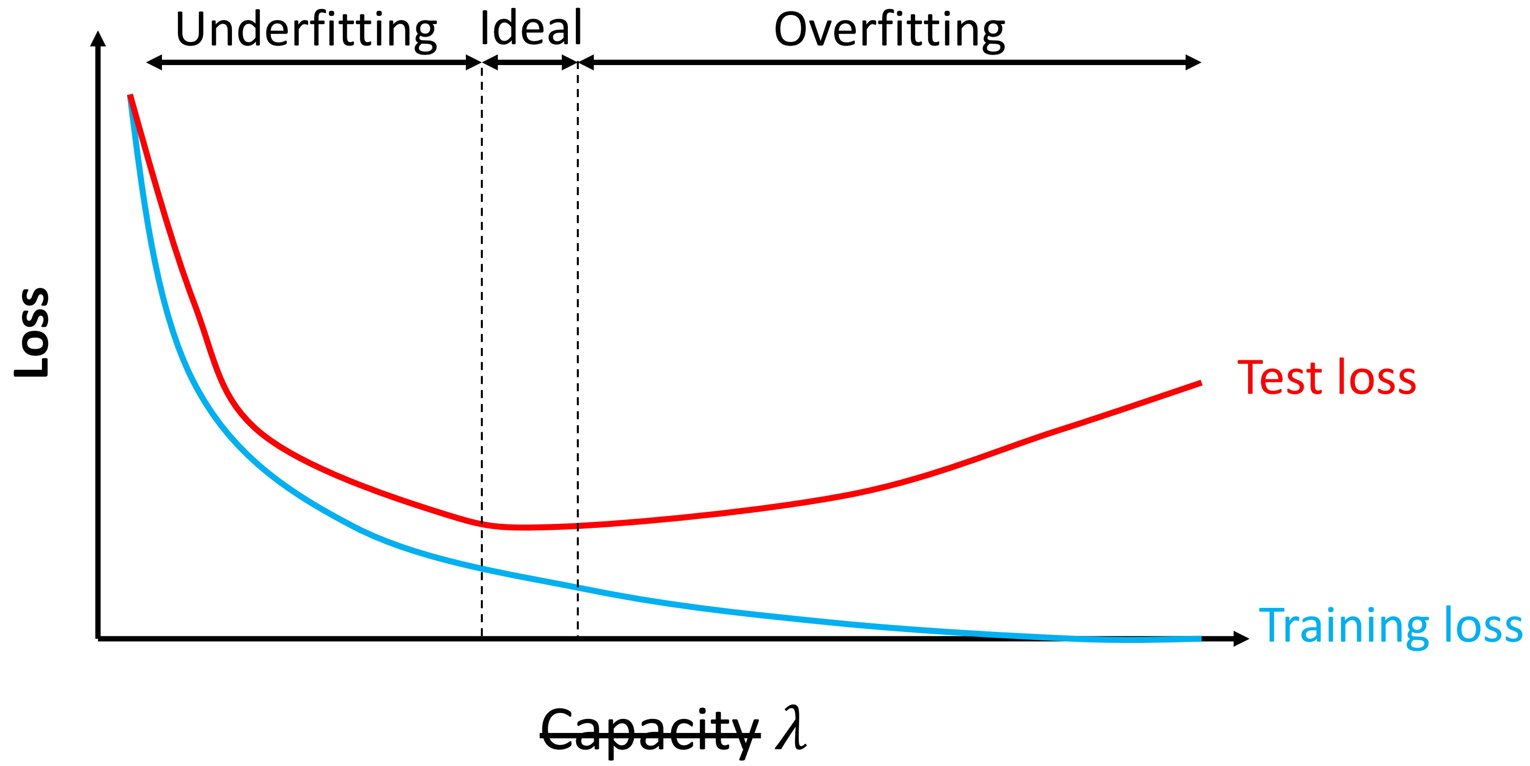
$$\sum_{j=1}^{d} \beta_j^2 = \|\beta\|_2^2 = \|\beta - 0\|_2^2$$

- I.e., “pulling” β to zero
  - “Pulls” more as λ becomes larger

Intuition on $\boldsymbol{L_2}$ Regularization

- **Why does it help?**
  - Encourages "simple" functions
  - E.g., as $\lambda \to \infty$, obtain $\beta = 0$
  - Use λ to tune bias-variance tradeoff

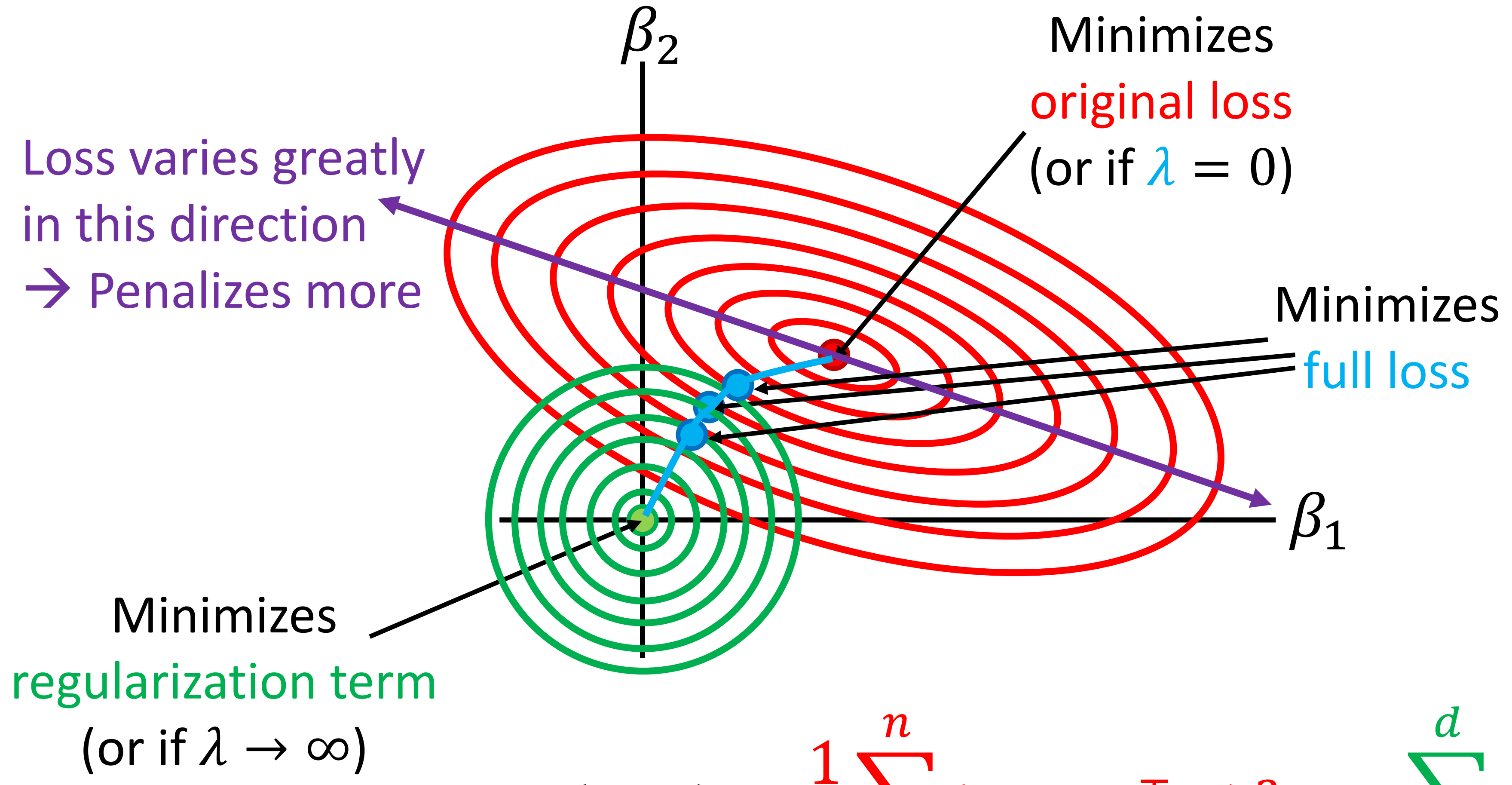
Bias-Variance Tradeoff for Regularization



Intuition on $\boldsymbol{L_2}$ Regularization

- **More precisely:** Restricts directions of β with little variation in data
  - Little variation in data → highly varying loss
- **Example:**
  - Suppose that $x_{ij} = 0.36$ for all training examples x_i
  - Then, we cannot learn what would happen if $x_j = 1.29$ (for a new input x)
  - I.e., hard to estimate β_j
- How does L_2 regularization help?

Intuition on L_2 Regularization



- At this point, the gradients are **equal** (with opposite sign)
- Tradeoff depends on choice of λ

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{j=1}^{d} \beta_j^2$$

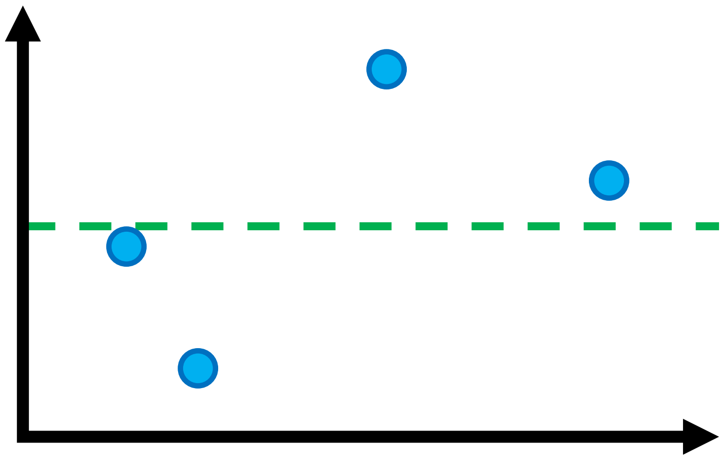
Regularization and Intercept Term

- If using intercept term ($\phi(x) = [1 \quad x_1 \quad \cdots \quad x_d]^\top$), no penalty on β_1:

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{j=2}^{d} \beta_j^2$$

← Sum from $j = 2$

- As $\lambda \to \infty$, we have $\beta_2 = \cdots = \beta_d = 0$
  - I.e., only fit β_1 (which yields $\hat{\beta}_1(Z) = \mathrm{mean}(\{y_i\}_{i=1}^n)$)



Feature Standardization

- **Unregularized linear regression is invariant to feature scaling**
  - Suppose we scale $x_{ij} \leftarrow 2x_{ij}$ for all examples x_i
  - Without regularization, simply use $\beta_j \leftarrow \beta_j/2$ to obtain equivalent solution
  - In particular, $\frac{\beta_j}{2} \cdot 2x_{ij} = \beta_j \cdot x_{ij}$

- Not true for regularized regression!
  - Penalty $\left(\beta_j/2\right)^2$ is scaled by 1/4 (not cancelled out!)

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{j=2}^{d} \beta_j^2$$

Feature Standardization

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$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda\left(\beta_2^2 + \cdots + \beta_j^2 + \cdots + \beta_d^2\right)$$

Feature Standardization

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  - Suppose we scale $x_{ij} \leftarrow 2x_{ij}$ for all examples x_i
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$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda\left(\beta_2^2 + \cdots + \frac{\beta_j^2}{4} + \cdots + \beta_d^2\right)$$

Feature Standardization

- **Solution:** Rescale features to zero mean and unit variance

$$x_{i,j} \leftarrow \frac{x_{i,j}-\mu_j}{\sigma_j} \qquad \mu_j = \frac{1}{N}\sum_{i=1}^{N} x_{i,j} \qquad \sigma_j = \frac{1}{N}\sum_{i=1}^{N}\left(x_{i,j} - \mu_j\right)^2$$

  - **Note:** When using intercept term, do not rescale $x_1 = 1$
  - Can be sensitive to outliers (fix by dropping outliers)

- **Must use same transformation during training and for prediction**
  - Compute on standardization on training data and use on test data

General Regularization Strategy

- **Original loss** + **regularization**:

$$L_{\text{new}}(\beta; Z) = L(\beta; Z) + \lambda \cdot R(\beta)$$

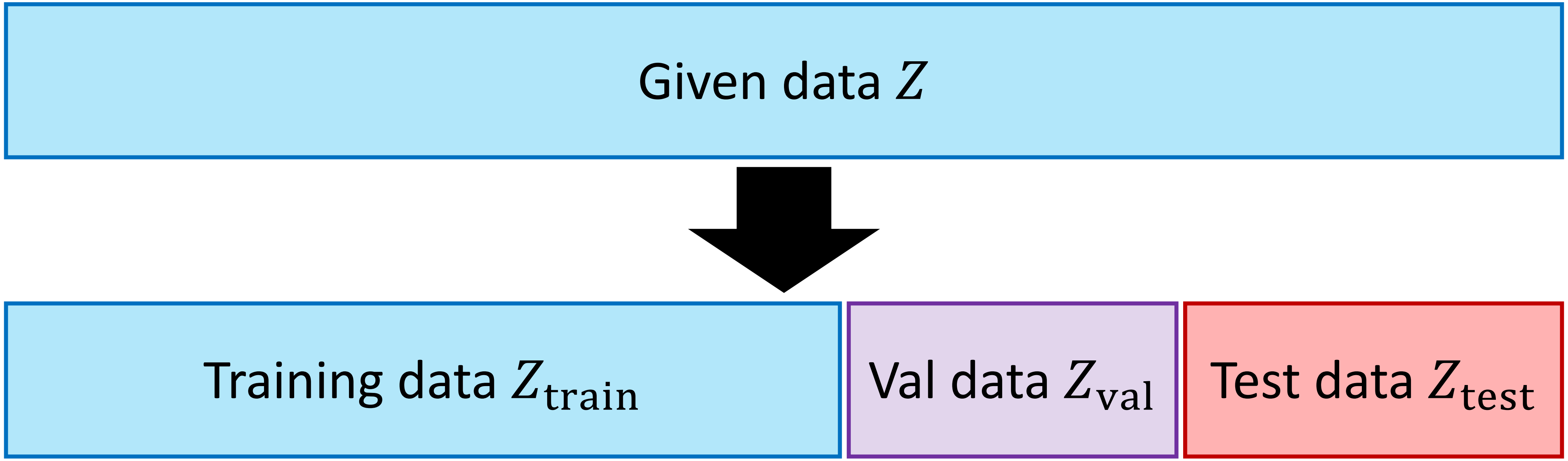
  - Offers a way to express a preference "simpler" functions in family
  - Typically, regularization is independent of data

Hyperparameter Tuning

- λ is a **hyperparameter** that must be tuned (satisfies $\lambda \geq 0$)
- **Naïve strategy:** Try a few different candidates λ_t and choose the one that minimizes the test loss
- **Problem:** We may overfit the test set!
  - Major problem if we have more hyperparameters

Training/Val/Test Split

- **Goal:** Choose best hyperparameter λ
  - Can also compare different model families, feature maps, etc.
- **Solution:** Optimize λ on a **held-out validation data**
  - **Rule of thumb:** 60/20/20 split



Basic Cross Validation Algorithm

- **Step 1:** Split Z into Z_{train}, Z_{val}, and Z_{test}

- **Step 2:** For $t \in \{1, \ldots, h\}$:
  - **Step 2a:** Run linear regression with Z_{train} and λ_t to obtain $\hat{\beta}(Z_{\text{train}}, \lambda_t)$
  - **Step 2b:** Evaluate validation loss $L_{\text{val}}^t = L\left(\hat{\beta}(Z_{\text{train}}, \lambda_t); Z_{\text{val}}\right)$

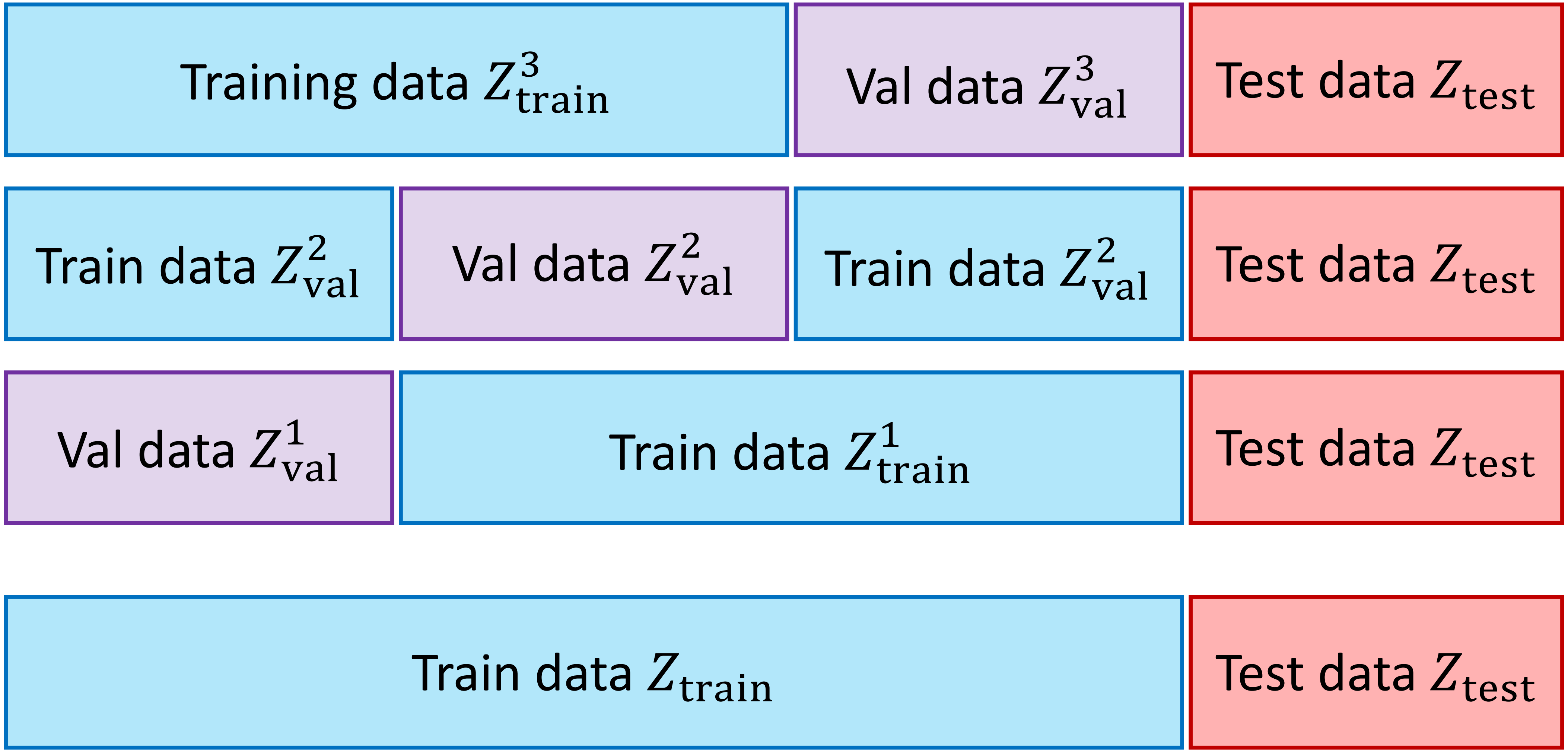
- **Step 3:** Use best λ_t
  - Choose $t' = \arg\min_t L_{\text{val}}^t$ with lowest validation loss
  - Re-run linear regression with Z_{train} and $\lambda_{t'}$ to obtain $\hat{\beta}(Z_{\text{train}}, \lambda_{t'})$

Alternative Cross-Validation Algorithms

- If Z is small, then splitting it can reduce performance
  - Can use $Z_{\text{train}} \cup Z_{\text{val}}$ in Step 3

- **Alternative:** k-fold cross-validation (e.g., $k = 3$)
  - Split Z into Z_{train} and Z_{test}
  - Split Z_{train} into k disjoint sets Z_{val}^s, and let $Z_{\text{train}}^s = \bigcup_{s' \neq s} Z_{\text{val}}^s$
  - Use λ' that works best on average across $s \in \{1, \dots, k\}$ with Z_{train}
  - Chooses better λ' than above strategy

Example: 3-Fold Cross Validation



k-Fold Cross-Validation

- If Z is small, then splitting it can reduce performance
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- **Alternative:** k-fold cross-validation (e.g., $k = 3$)
  - Split Z into Z_{train} and Z_{test}
  - Split Z_{train} into k disjoint sets Z_{val}^s, and let $Z_{\text{train}}^s = \bigcup_{s' \neq s} Z_{\text{val}}^s$
  - Use λ' that works best on average across $s \in \{1, \ldots, k\}$ with Z_{train}
  - Chooses better λ' than above strategy

- **Compute vs. accuracy tradeoff**
  - As $k \to N$, the model becomes more accurate
  - But algorithm becomes more computationally expensive

Housing Dataset

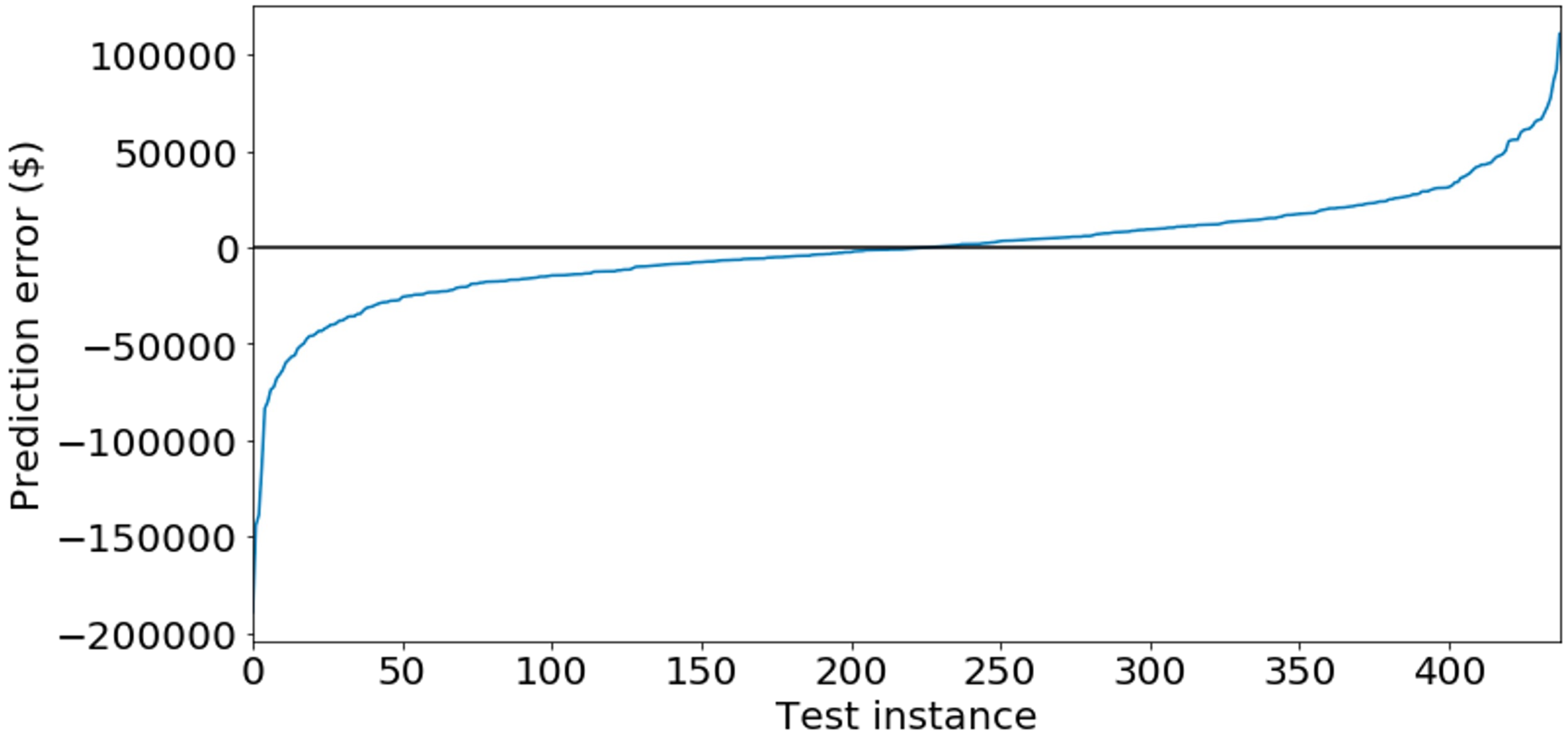
- Sales of residential property in Ames, Iowa from 2006 to 2010
  - **Examples:** 1,022
  - **Features:** 79 total (real-valued + categorical), some are missing!
  - **Label**: Sales price

MSSubClass	MSZoning	LotFrontage	LotArea	Street	Alley	LotShape	...	MoSold	YrSold	SaleType	SaleCondition	SalePrice
20	RL	80.0	10400	Pave	NaN	Reg	...	5	2008	WD	Normal	174000
180	RM	35.0	3675	Pave	NaN	Reg	...	5	2006	WD	Normal	145000
60	FV	72.0	8640	Pave	NaN	Reg	...	6	2010	Con	Normal	215200
20	RL	84.0	11670	Pave	NaN	IR1	...	3	2007	WD	Normal	320000
60	RL	43.0	10667	Pave	NaN	IR2	...	4	2009	ConLw	Normal	212000
80	RL	82.0	9020	Pave	NaN	Reg	...	6	2008	WD	Normal	168500
60	RL	70.0	11218	Pave	NaN	Reg	...	5	2010	WD	Normal	189000
80	RL	85.0	13825	Pave	NaN	Reg	...	12	2008	WD	Normal	140000
60	RL	NaN	13031	Pave	NaN	IR2	...	7	2006	WD	Normal	187500

Data from: De Cock. Journal of Statistics Education 19(3), 2011

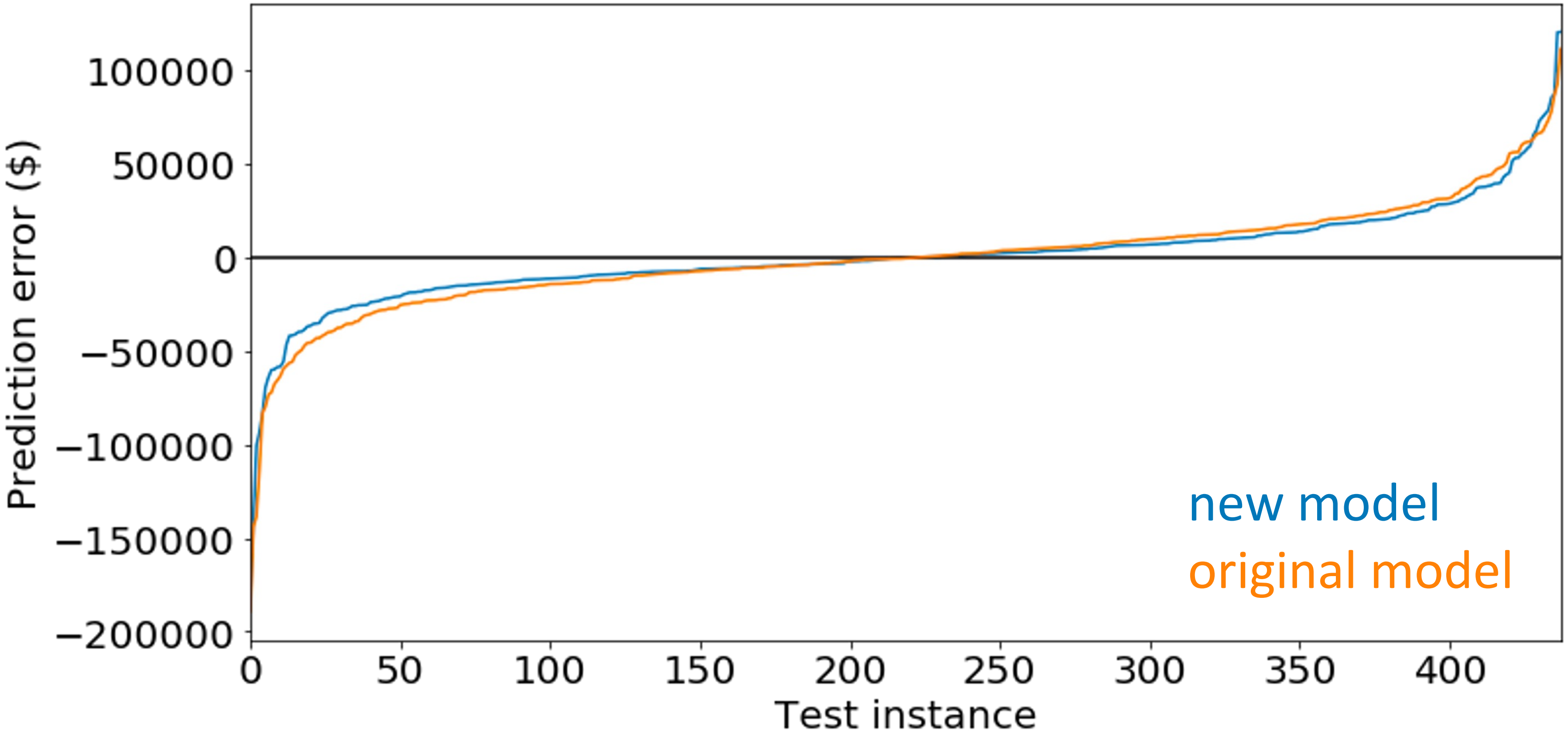
Housing Dataset

- 438 test examples, **preprocessed same as training data**
- Sorted by prediction error



Housing Dataset

- Quadratic features, feature standardization, L_2 regularization



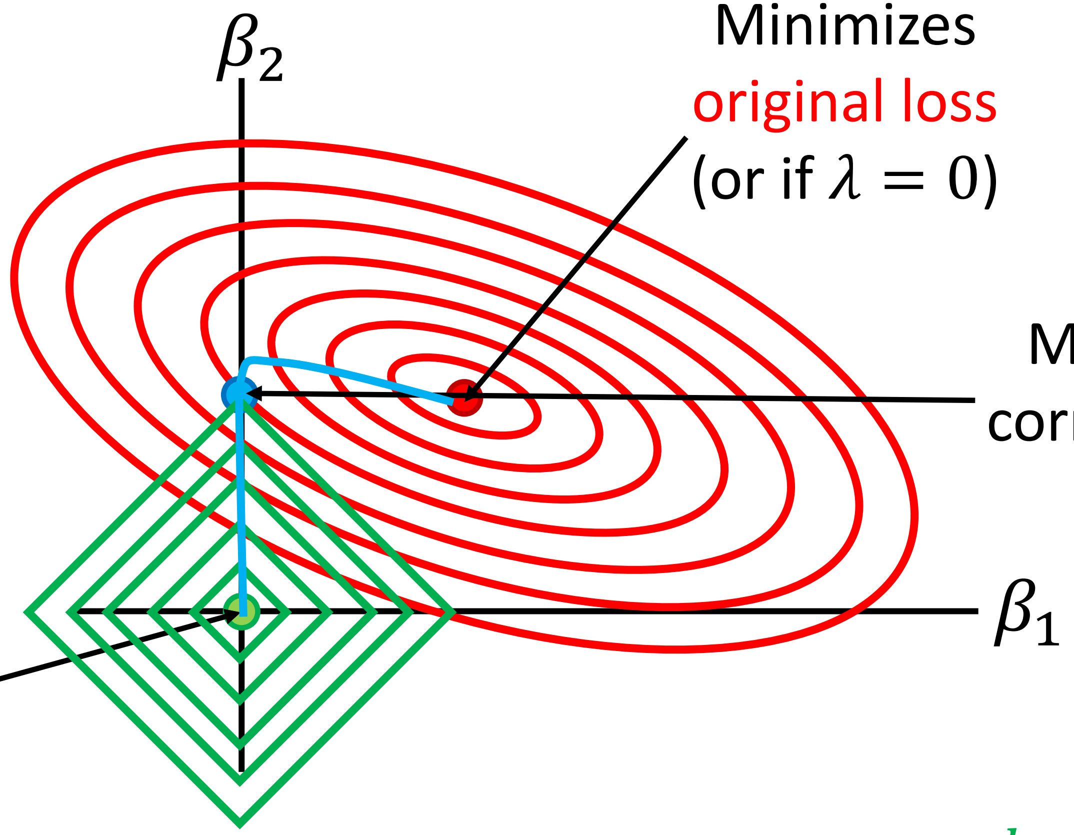
$\boldsymbol{L_1}$ Regularization

- **Sparsity:** Can we minimize $\|\beta\|_0 = |\{ j \mid \beta_j \neq 0 \}|$?
  - That is, the number of nonzero components of β
  - Improves interpretability (automatic **feature selection**!)
  - Also serves as a **strong** regularizer ($n \sim s \log d$, where $s = \|\beta\|_0$)

- **Challenge:** $\|\beta\|_0$ is not differentiable, making it hard to optimize

- **Solution**
  - We can instead use an L_1 norm as the regularizer!
  - Still harder to optimize than L_2 norm, but at least it is convex

Intuition on L_1 Regularization



$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{j=1}^{d} |\beta_j|$$

L_1 Regularization for Feature Selection

- **Step 1:** Construct a lot of features and add to feature map
- **Step 2:** Use L_1 regularized regression to "select" subset of features
  - I.e., coefficient $\beta_j \neq 0$ → feature j is selected)
- **Optional:** Remove unselected features from the feature map and run vanilla linear regression (a.k.a. ordinary least squares)

Agenda

- **Regularization**
  - Strategy to address bias-variance tradeoff
  - **By example:** Linear regression with L_2 regularization

- **Minimizing the MSE Loss**
  - Closed-form solution
  - Stochastic gradient descent

Minimizing the MSE Loss

- Recall that linear regression minimizes the loss

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$$

- **Closed-form solution:** Compute using matrix operations
- **Optimization-based solution:** Search over candidate β

Vectorizing Linear Regression

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix}$$

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix} = \begin{bmatrix} \beta^\top x_1 \\ \vdots \\ \beta^\top x_n \end{bmatrix}$$

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix} = \begin{bmatrix} \beta^\top x_1 \\ \vdots \\ \beta^\top x_n \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{d} \beta_j x_{1,j} \\ \vdots \\ \sum_{j=1}^{d} \beta_j x_{n,j} \end{bmatrix}$$

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix} = \begin{bmatrix} \beta^\top x_1 \\ \vdots \\ \beta^\top x_n \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{d} \beta_j x_{1,j} \\ \vdots \\ \sum_{j=1}^{d} \beta_j x_{n,j} \end{bmatrix} = \begin{bmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_d \end{bmatrix}$$

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix} = \begin{bmatrix} \beta^\top x_1 \\ \vdots \\ \beta^\top x_n \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{d} \beta_j x_{1,j} \\ \vdots \\ \sum_{j=1}^{d} \beta_j x_{n,j} \end{bmatrix} = \begin{bmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_d \end{bmatrix}$$

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Vectorizing Linear Regression

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$$\approx$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix} = \begin{bmatrix} \beta^\top x_1 \\ \vdots \\ \beta^\top x_n \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{d} \beta_j x_{1,j} \\ \vdots \\ \sum_{j=1}^{d} \beta_j x_{n,j} \end{bmatrix} = \begin{bmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_d \end{bmatrix} = X\beta$$

$$\approx$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = Y$$

Summary: $Y \approx X\beta$

Vectorizing Linear Regression

$$Y \approx X\beta$$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad X = \begin{bmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{bmatrix} \qquad \beta = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_d \end{bmatrix}$$

Vectorizing Mean Squared Error

Vectorizing Mean Squared Error

$$L(\beta; Z)$$

Vectorizing Mean Squared Error

$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2$$

Vectorizing Mean Squared Error

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad \begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix}$$

$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 = \frac{1}{n} \|Y - X\beta\|_2^2$$

$$\|z\|_2^2 = \sum_{i=1}^{n} z_i^2$$

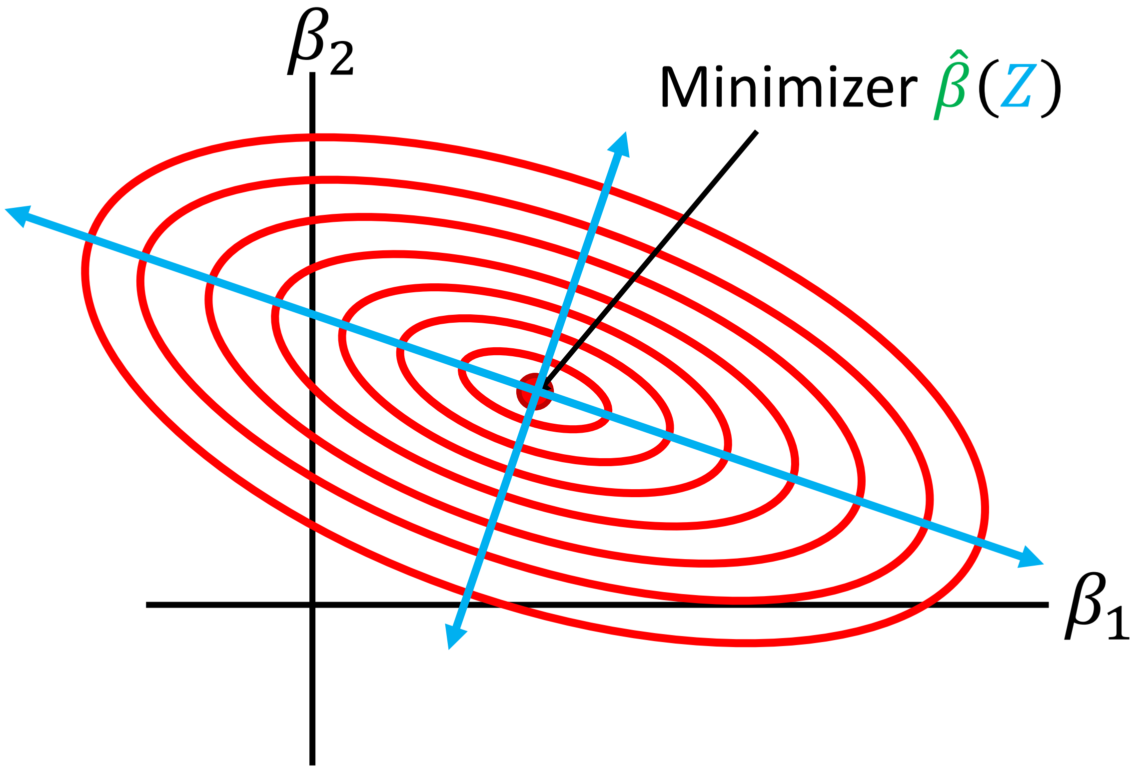
Intuition on Vectorized Linear Regression

- Rewriting the vectorized loss:

$$n \cdot L(\beta; Z) = \|Y - X\beta\|_2^2 = \|Y\|_2^2 - 2Y^\top X\beta + \|X\beta\|_2^2$$
$$= \|Y\|_2^2 - 2Y^\top X\beta + \beta^\top(X^\top X)\beta$$

- Quadratic function of β with leading "coefficient" $X^\top X$
  - In one dimension, "width" of parabola $ax^2 + bx + c$ is a^{-1}
  - In multiple dimensions, "width" along direction v_i is λ_i^{-1}, where v_i is an eigenvector of $X^\top X$ with eigenvalue λ_i

Intuition on Vectorized Linear Regression



Directions/magnitudes are given by eigenvectors/eigenvalues of $X^\top X$

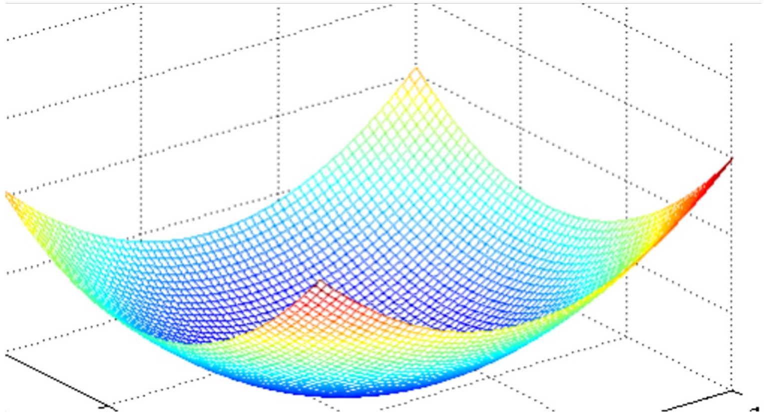
Strategy 1: Closed-Form Solution

- Recall that linear regression minimizes the loss

$$L(\beta; Z) = \frac{1}{n} \|Y - X\beta\|_2^2$$

- Minimum solution has gradient equal to zero:

$$\nabla_\beta L\left(\hat{\beta}(Z); Z\right) = 0$$



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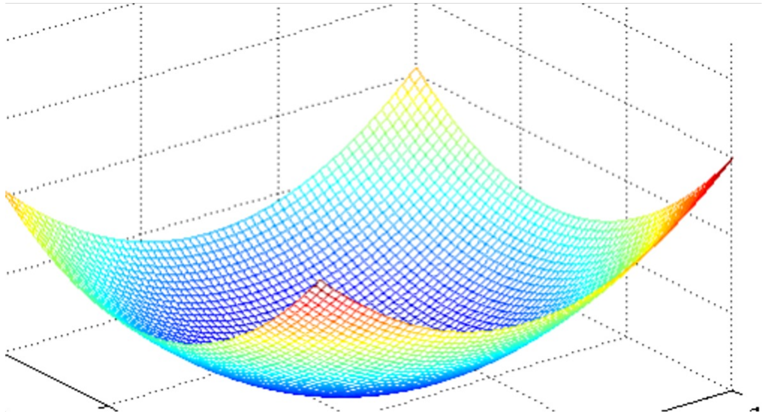
$$\nabla_\beta L(\hat{\beta}; Z) = 0$$



Strategy 1: Closed-Form Solution

- The gradient is

$$\nabla_{\beta} L(\beta; Z)$$

Strategy 1: Closed-Form Solution

- The gradient is

$$\nabla_{\beta} L(\beta; Z) = \nabla_{\beta} \frac{1}{n} \|Y - X\beta\|_2^2$$

Strategy 1: Closed-Form Solution

- The gradient is

$$\begin{aligned}
\nabla_\beta L(\beta; Z) = \nabla_\beta \frac{1}{n} \|Y - X\beta\|_2^2 &= \nabla_\beta \frac{1}{n} (Y - X\beta)^\top (Y - X\beta) \\
&= \frac{2}{n} \left[\nabla_\beta (Y - X\beta)^\top\right] (Y - X\beta) \\
&= -\frac{2}{n} X^\top (Y - X\beta) \\
&= -\frac{2}{n} X^\top Y + \frac{2}{n} X^\top X\beta
\end{aligned}$$

Aside: Intuition on Computing Gradients

- **Warning:** Intuitive but **easy to make mistakes**
- The loss is

$$
\begin{aligned}
L(\beta + d\beta; Z) &= \frac{1}{n}\|Y - X(\beta + d\beta)\|_2^2 \\
&= \frac{1}{n}\|(Y - X\beta) - Xd\beta\|_2^2 \\
&= \frac{1}{n}\|Y - X\beta\|_2^2 - \frac{2}{n}(Y - X\beta)^\top X d\beta + \frac{1}{n}\|Xd\beta\|_2^2 \\
&= L(\beta; Z) \underbrace{- \frac{2}{n}(Y - X\beta)^\top X}_{= \nabla_\beta L(\beta; Z)^\top} d\beta + O(\|d\beta\|_2^2)
\end{aligned}
$$

Coefficient of $d\beta$ term

Intuition on the Gradient

- By linearity of the gradient, we have

$$\nabla_{\beta} L(\beta; Z) = \sum_{i=1}^{n} \nabla_{\beta} (y_i - \beta^\top x_i)^2 = \sum_{i=1}^{n} 2(y_i - \beta^\top x_i) x_i$$

- The gradient for a single term is

$$\nabla_{\beta} (y_i - \beta^\top x_i)^2 = 2(y_i - \beta^\top x_i) x_i$$

- I.e., the current error $y_i - \beta^\top x_i$ times the feature x_i

Strategy 1: Closed-Form Solution

- The gradient is

$$\nabla_{\beta} L(\beta; Z) = \nabla_{\beta} \frac{1}{n} \|Y - X\beta\|_2^2 = -\frac{2}{n} X^{\top} Y + \frac{2}{n} X^{\top} X\beta$$

- Setting $\nabla_{\beta} L(\hat{\beta}; Z) = 0$, we have $X^{\top} X\hat{\beta} = X^{\top} Y$

Strategy 1: Closed-Form Solution

- Setting $\nabla_\beta L(\hat{\beta}; Z) = 0$, we have $X^\top X\hat{\beta} = X^\top Y$
- Assuming $X^\top X$ is invertible, we have

$$\hat{\beta}(Z) = (X^\top X)^{-1} X^\top Y$$

Note on Invertibility

- Closed-form solution only **unique** if $X^\top X$ is invertible
  - Otherwise, **multiple solutions exist** to $X^\top X\hat{\beta} = X^\top Y$
  - **Intuition:** Underconstrained system of linear equations

- **Example:**

$$\begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$$

  - In this case, any $\hat{\beta}_2 = 2 - \hat{\beta}_1$ is a solution

When Can this Happen?

- **Case 1**
  - Fewer data examples than feature dimension (i.e., $n < d$)
  - **Solution:** Remove features so $d \leq n$
  - **Solution:** Collect more data until $d \leq n$

- **Case 2:** Some feature is a linear combination of the others
  - **Special case (duplicated feature):** For some j and j', $x_{i,j} = x_{i,j'}$ for all i
  - **Solution:** Remove linearly dependent features
  - **Solution:** Use L_2 regularization

Shortcomings of Closed-Form Solution

- Computing $\hat{\beta}(Z) = (X^\top X)^{-1} X^\top Y$ can be challenging
- **Computing $(\boldsymbol{X}^\top \boldsymbol{X})^{-1}$ is $\boldsymbol{O}(\boldsymbol{d}^3)$**
  - $d = 10^4$ features → $O(10^{12})$
  - Even storing $X^\top X$ requires a lot of memory
- **Numerical accuracy issues due to "ill-conditioning"**
  - $X^\top X$ is "barely" invertible
  - Then, $(X^\top X)^{-1}$ has large variance along some dimension
  - Regularization helps (more on this later)