UNIVERSITY OF KWAZULU-NATAL ™
INYUVESI YAKWAZULU-NATALI

NITheCS
National Institute for Theoretical and Computational Sciences

Introduction to ML

The 15th CHPC & 7th NITheCS Coding Summer School

on Data Science and Computational Thinking

27 January - 7 February 2025

Based on Lecture Slides CIS 4190/5190: Applied Machine Learning, Penn Engineering, University of Pennsylvania

What is Machine Learning?

"Learning is any process by which a system improves performance from experience."

Herbert Simon

What is Machine Learning?

“Machine learning … gives computers the ability to learn without being explicitly programmed.”

Arthur Samuel

What is Machine Learning?

- **Tom Mitchell:** Algorithms that
  - improve their **performance** P
  - at **task** T
  - with **experience** E

- A well-defined machine learning task is given by (P, T, E)

Example: Game Playing

- **Tom Mitchell:** Algorithms that
  - improve their **performance** P
  - at **task** T
  - with **experience** E

- $T =$ playing Checkers
- $P =$ win rate against opponents
- $E =$ playing games against itself

Example: Prediction

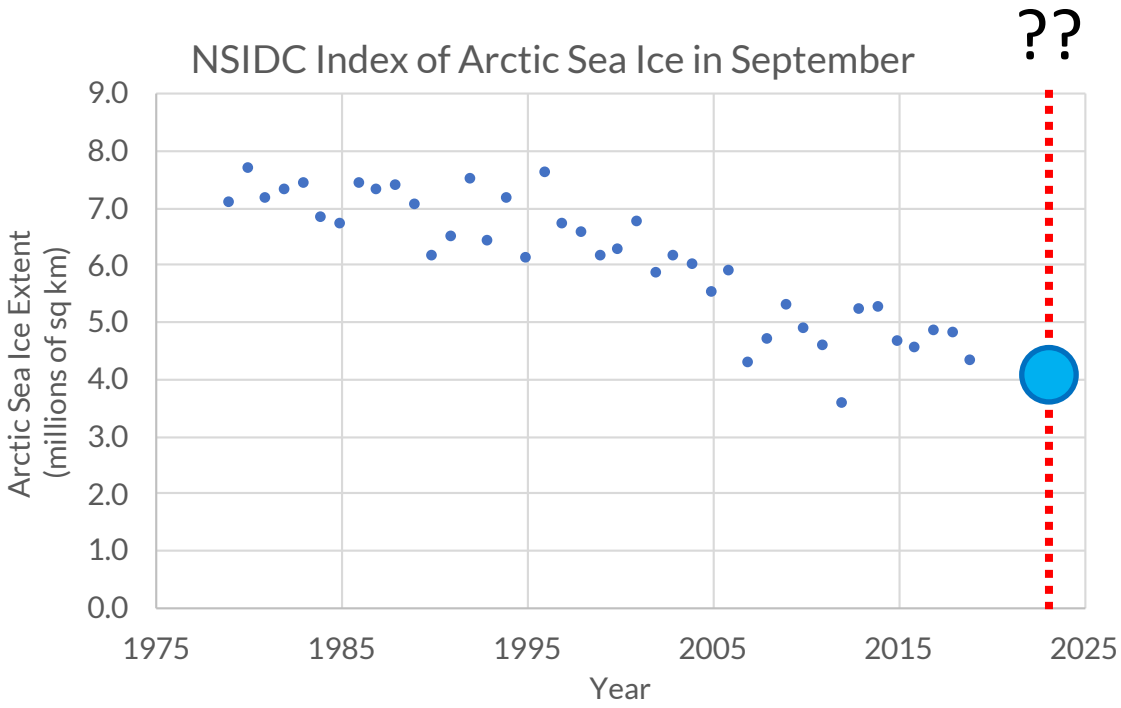
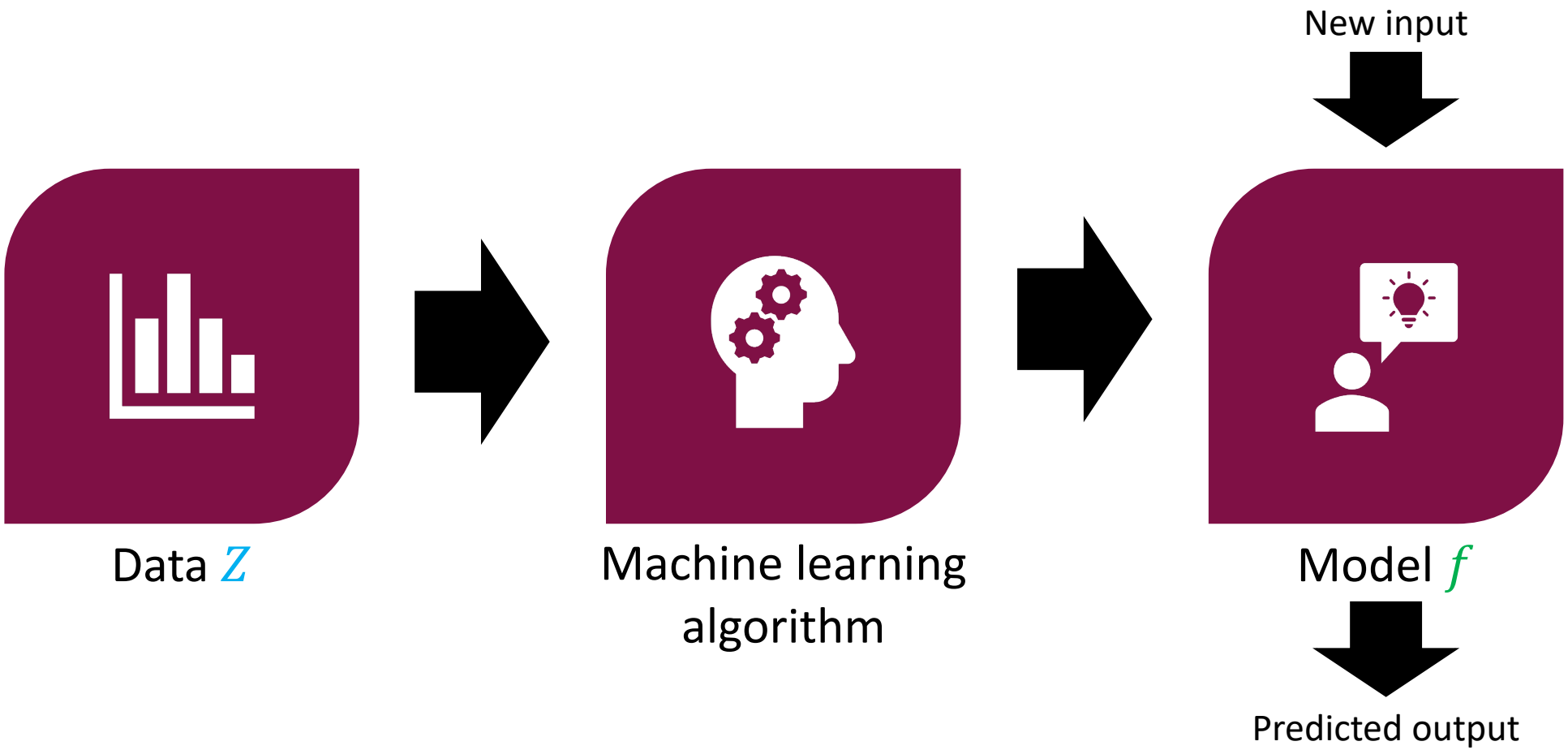


Image: https://www.flickr.com/photos/gsfc/5937599688/
Data from https://nsidc.org/arcticseaicenews/sea-ice-tools/

Machine Learning for Prediction



Types of Learning

- **Supervised learning**
  - **Input:** Examples of inputs and outputs
  - **Output:** Model that predicts unknown output given a new input

- **Unsupervised learning**
  - **Input:** Examples of some data (no “outputs”)
  - **Output:** Representation of structure in the data

- **Reinforcement learning**
  - **Input:** Sequence of interactions with an environment
  - **Output:** Policy that performs a desired task

Supervised Learning

- Given $(x_1, y_1), \ldots, (x_n, y_n)$, learn a function that predicts y given x
- **Regression:** Labels y are real-valued

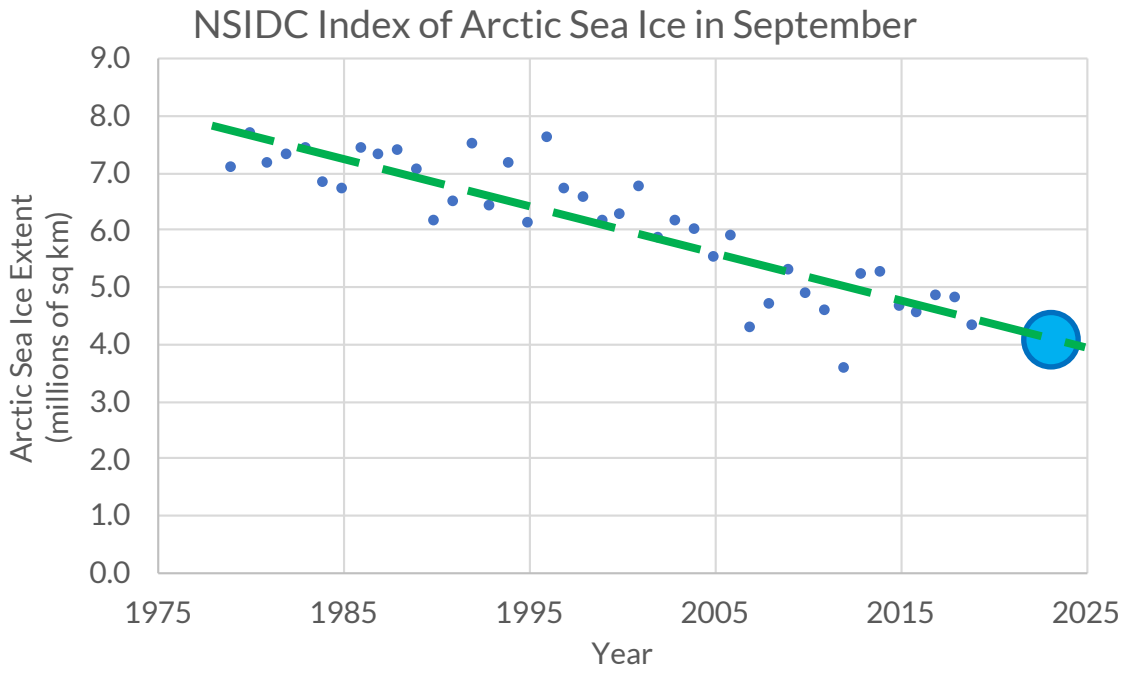
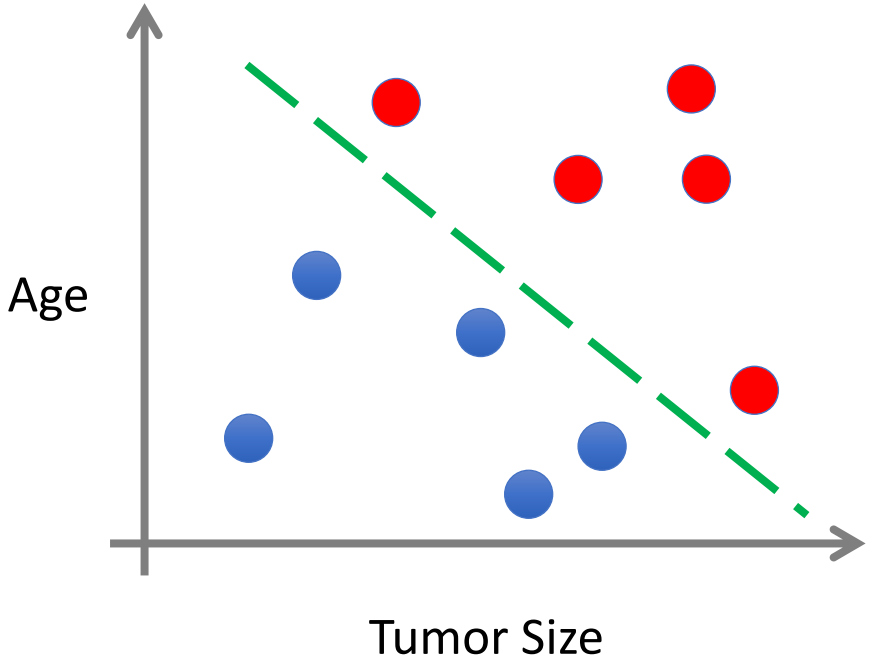


Image: https://www.flickr.com/photos/gsfc/5937599688/
Data from https://nsidc.org/arcticseaicenews/sea-ice-tools/

Supervised Learning

- Given $(x_1, y_1), \ldots, (x_n, y_n)$, learn a function that predicts y given x
- Inputs x can be multi-dimensional



- Patient age
- Clump thickness
- Tumor Color
- Cell type
- …

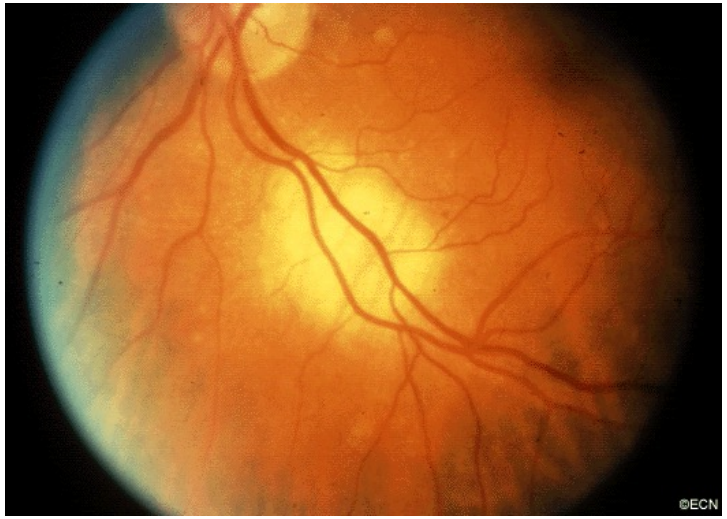
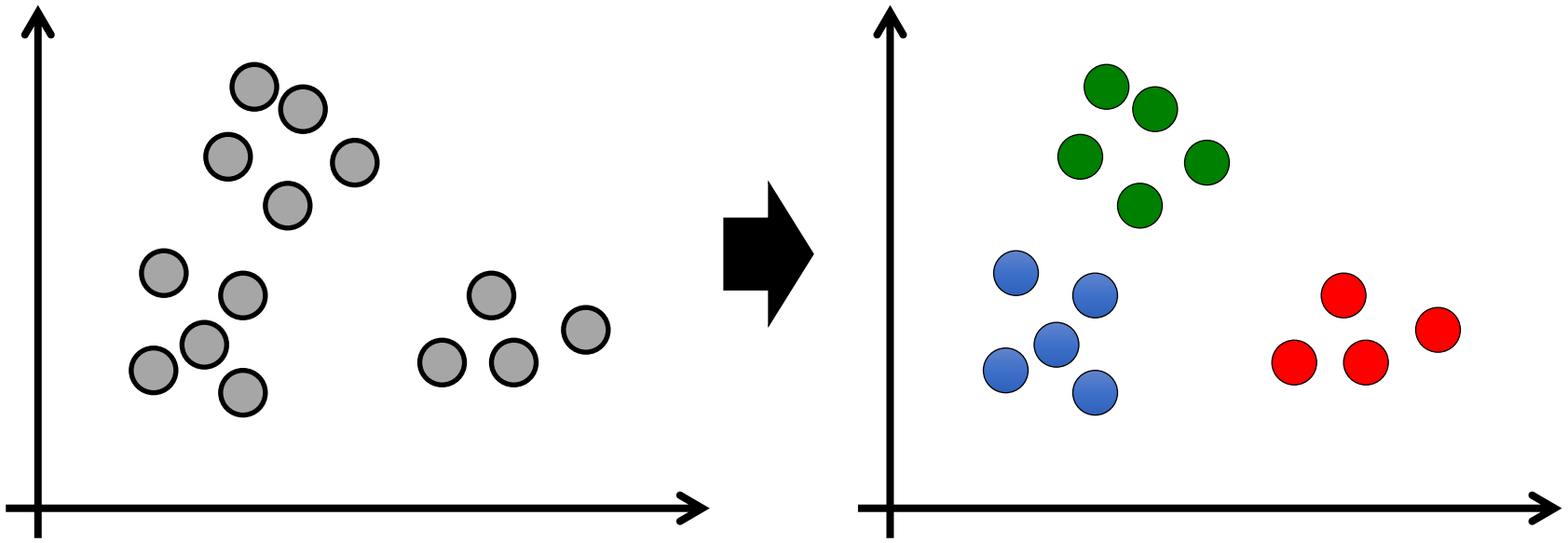


Image: https://eyecancer.com/uncategorized/choroidal-metastasis-test/

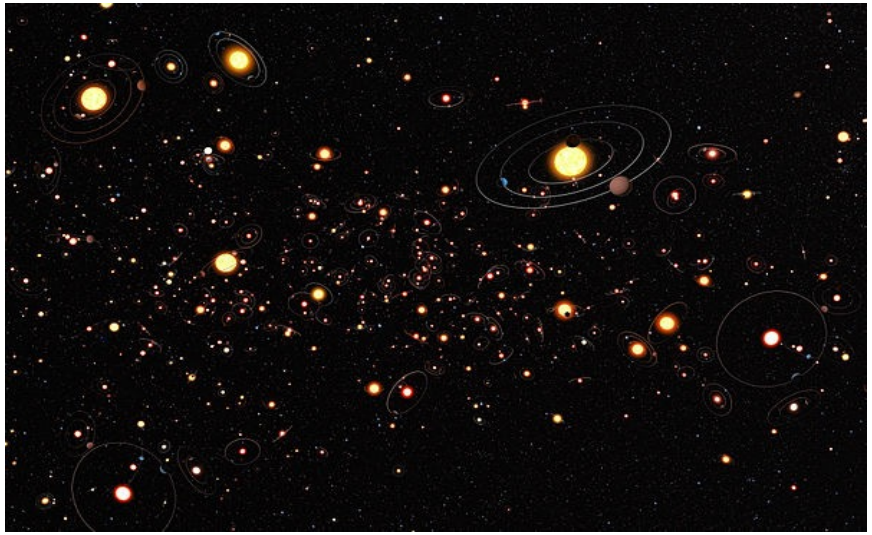
Unsupervised Learning

- Given $x_1, \ldots, x_n$ (no labels), output hidden structure in x's
  - E.g., clustering

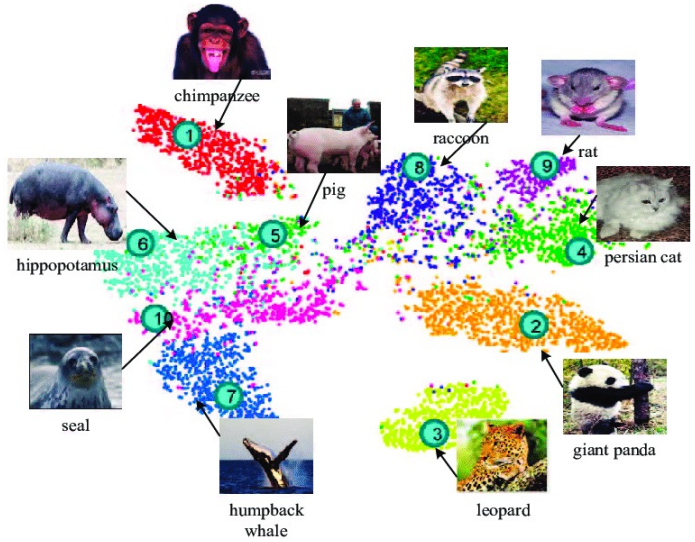


Unsupervised Learning

Find Subgroups in Social Networks



Identify Types of Exoplanets



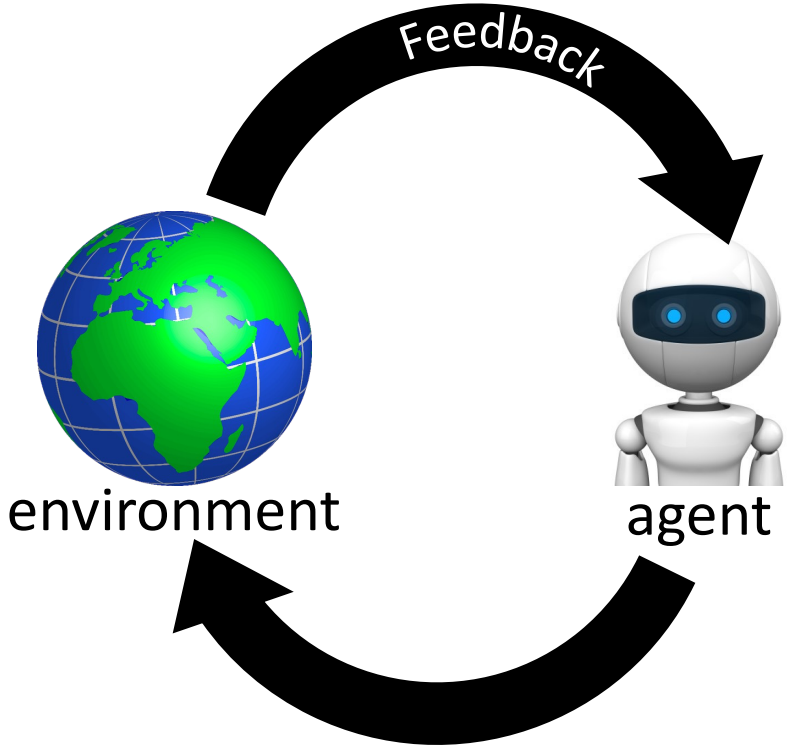
Visualize Data

Image Credits:
https://medium.com/graph-commons/finding-organic-clusters-in-your-complex-data-networks-5c27e1d4645d
https://arxiv.org/pdf/1703.08893.pdf
https://en.wikipedia.org/wiki/Exoplanet

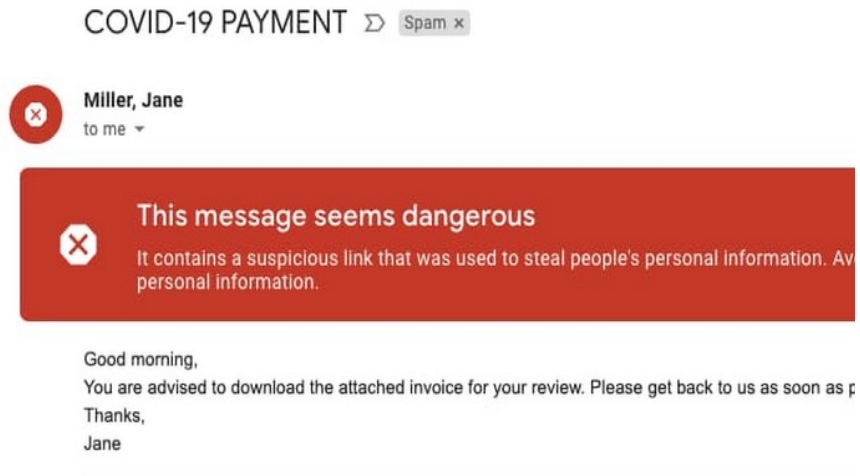
Reinforcement Learning

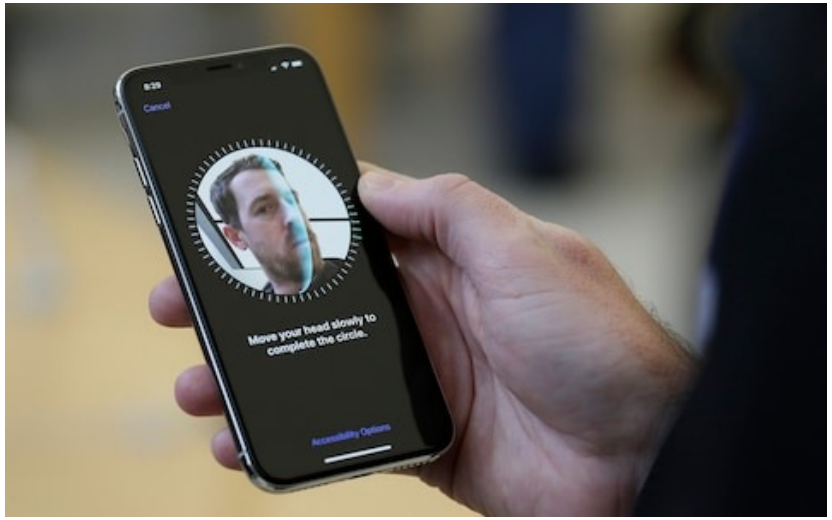
- Learn how to perform a task from interactions with the **environment**

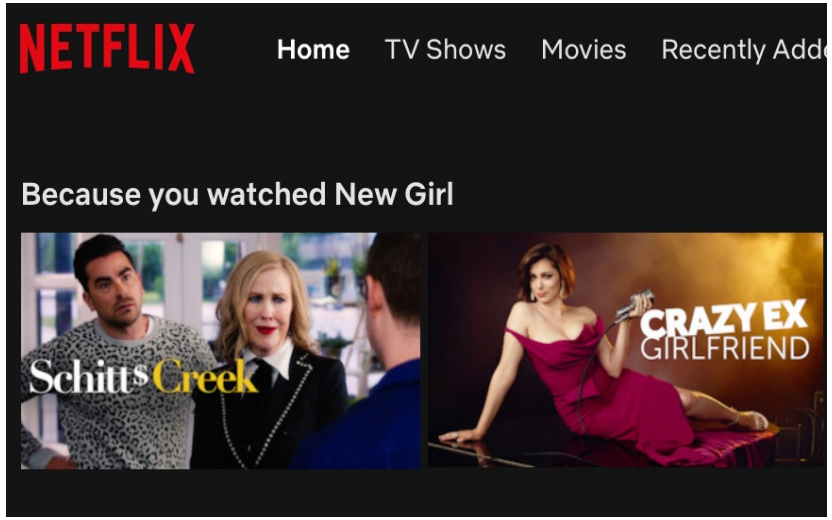
- **Examples:**
  - Playing chess (interact with the game)
  - Robot grasping an object (interact with the object/real world)
  - Optimize inventory allocations (interact with the inventory system)



Everyday Applications

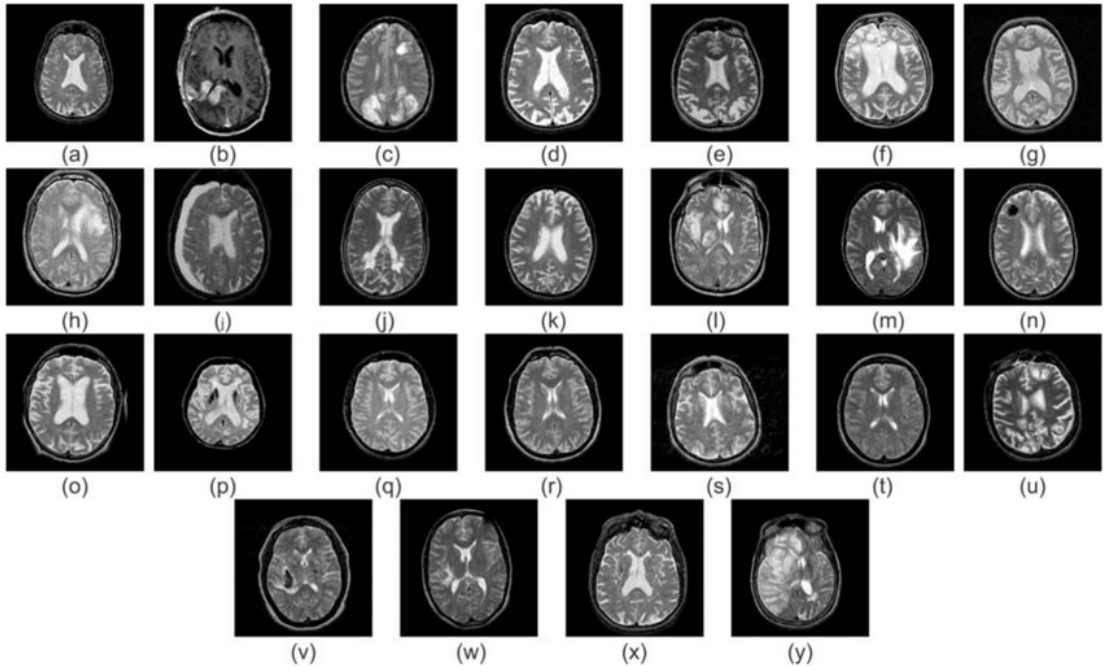






Radiology and Medicine

Input: Brain scans



Output: Neurological disease labels

Machine learning studies on major brain diseases: 5-year trends of 2014–2018

Koji Sakai[1] · Kei Yamada[1]

Applications of machine learning in drug discovery and development

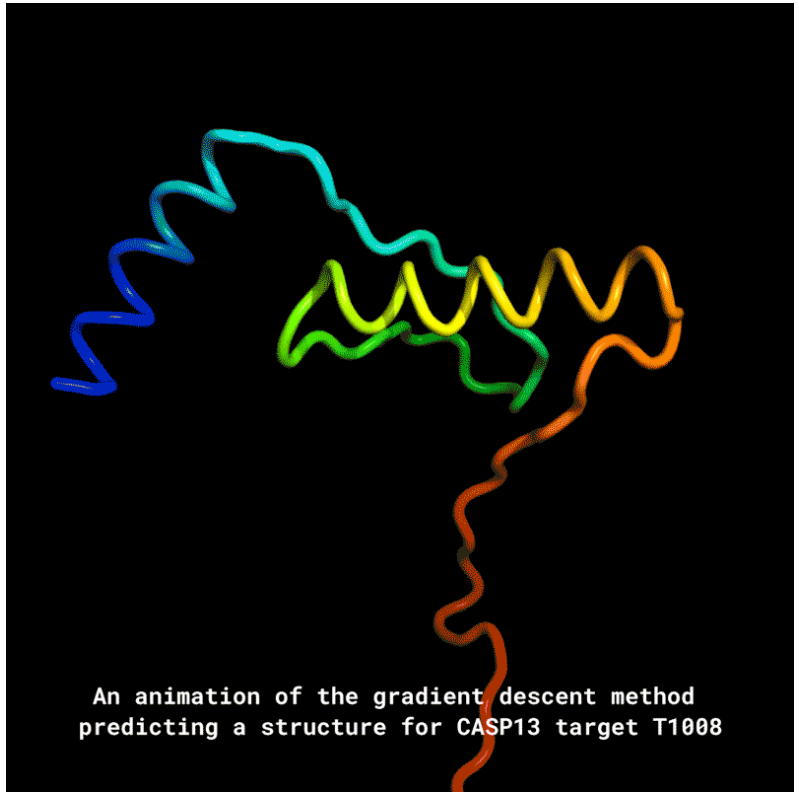
https://www.nature.com/articles/s41573-019-0024-5

Deep learning-enabled medical computer vision

Andre Esteva ✉, Katherine Chou, Serena Yeung, Nikhil Naik, Ali Madani, Ali Mottaghi, Yun Liu, Eric Topol, Jeff Dean & Richard Socher

https://www.nature.com/articles/s41746-020-00376-2

Scientific Discovery



https://deepmind.com/blog/article/AlphaFold-Using-AI-for-scientific-discovery

https://www.jpl.nasa.gov/edu/news/2019/4/19/how-scientists-captured-the-first-image-of-a-black-hole/

Creating Images & Text

https://thispersondoesnotexist.com/

SYSTEM PROMPT (HUMAN-WRITTEN)

Recycling is good for the world.

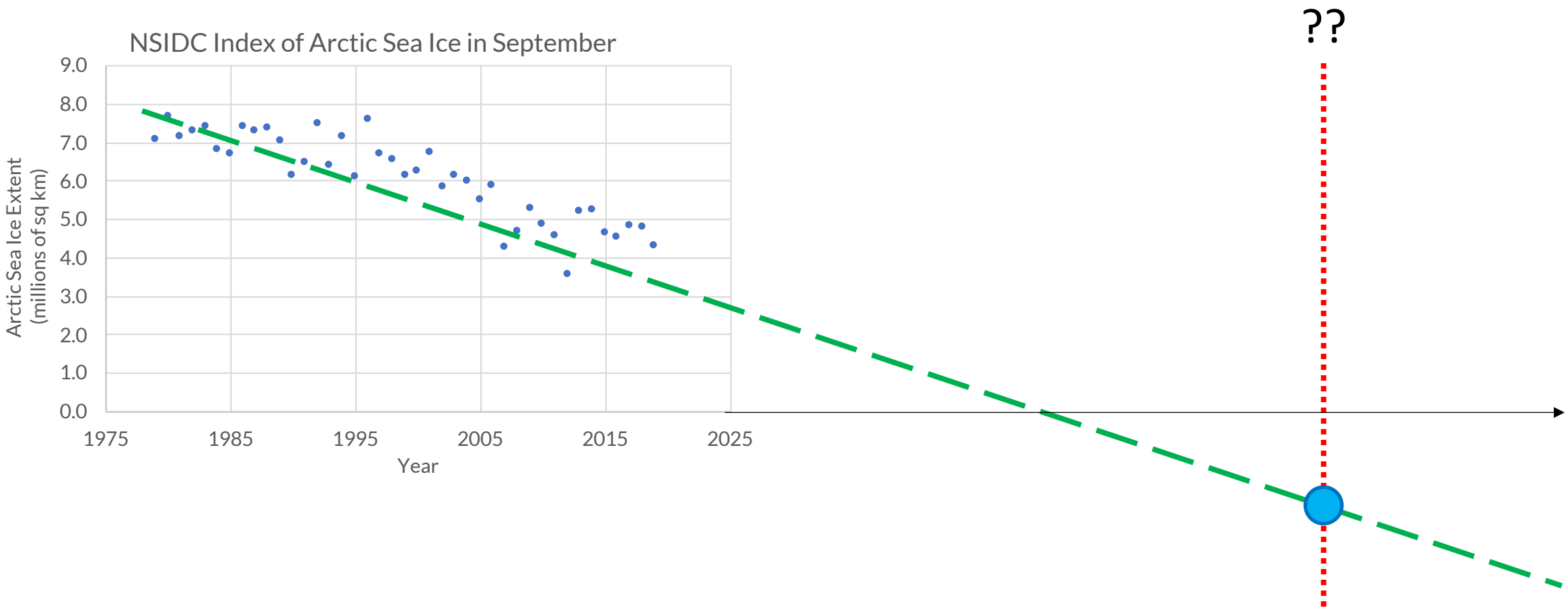
NO! YOU COULD NOT BE MORE WRONG!!

MODEL COMPLETION (MACHINE-WRITTEN, 25 TRIES)

Recycling is NOT good for the world. It is bad for the environment, it is bad for our health, and it is bad for our economy. I'm not kidding. Recycling is not good for the environment. It is destructive to the earth and it is a major contributor to global warming. Recycling is not good for our health. It contributes to obesity and diseases like heart disease and cancer. Recycling is bad for our economy. It increases the cost of a product, and in turn, the price of everything that is made with that product. Recycling is not good for our nation. We pay a

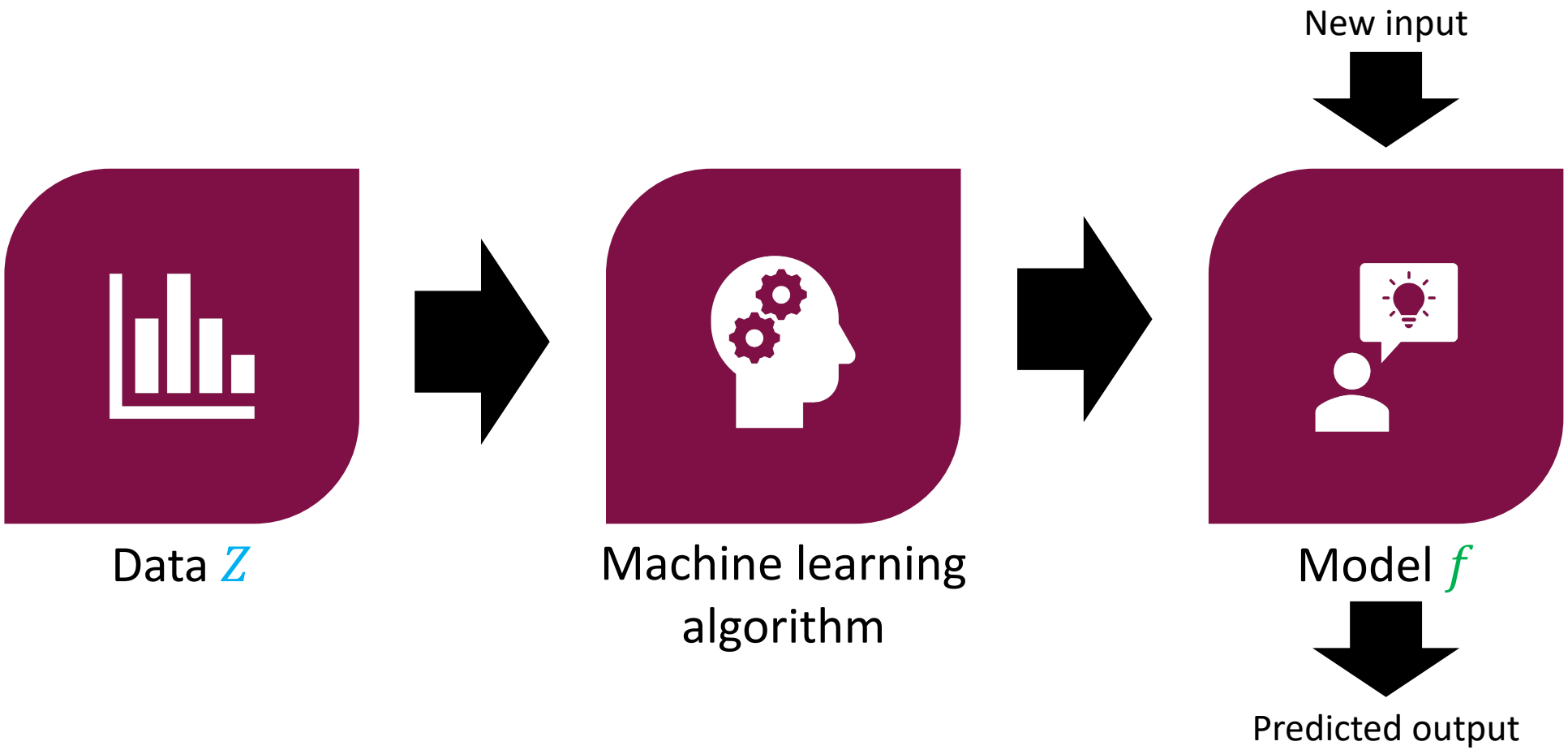
https://transformer.huggingface.co/doc/gpt2-large

Danger of Out-of-Domain Machine Learning



Any time you are evaluating on data “far” from your training data, beware!

Machine Learning for Prediction



Question: What **model family** (a.k.a. **hypothesis class**) to consider?

Linear Functions

- Consider the space of linear functions $f_\beta(x)$ defined by

$$f_\beta(x) = \beta^\top x$$

Linear Functions

- Consider the space of linear functions $f_\beta(x)$ defined by

$$f_\beta(x) = \beta^\top x = [\beta_1 \quad \cdots \quad \beta_d] \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} = \beta_1 x_1 + \cdots + \beta_d x_d$$

- $x \in \mathbb{R}^d$ is called an **input** (a.k.a. **features** or **covariates**)
- $\beta \in \mathbb{R}^d$ is called the **parameters** (a.k.a. **parameter vector**)
- $y = f_\beta(x)$ is called the **label** (a.k.a. **output** or **response**)

Linear Regression Problem

- **Input:** Dataset $Z = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$
- **Output:** A linear function $f_\beta(x) = \beta^\top x$ such that $y_i \approx \beta^\top x_i$

- **Typical notation**
  - Use i to index examples (x_i, y_i) in data Z
  - Use j to index components x_j of $x \in \mathbb{R}^d$
  - x_{ij} is component j of input example i

- **Goal:** Estimate $\beta \in \mathbb{R}^d$

Linear Regression Problem

What does this mean?

- **Input:** Data $Z = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$
- **Output:** A linear function $f_\beta(x) = \beta^\top x$ such that $y_i \approx \beta^\top x_i$

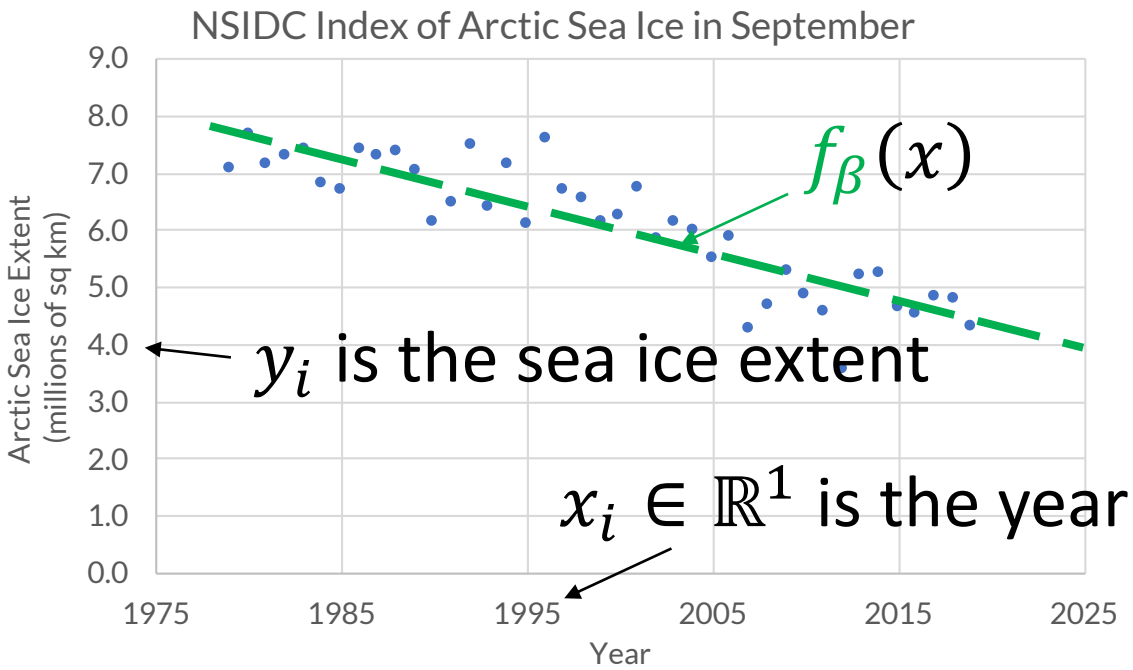


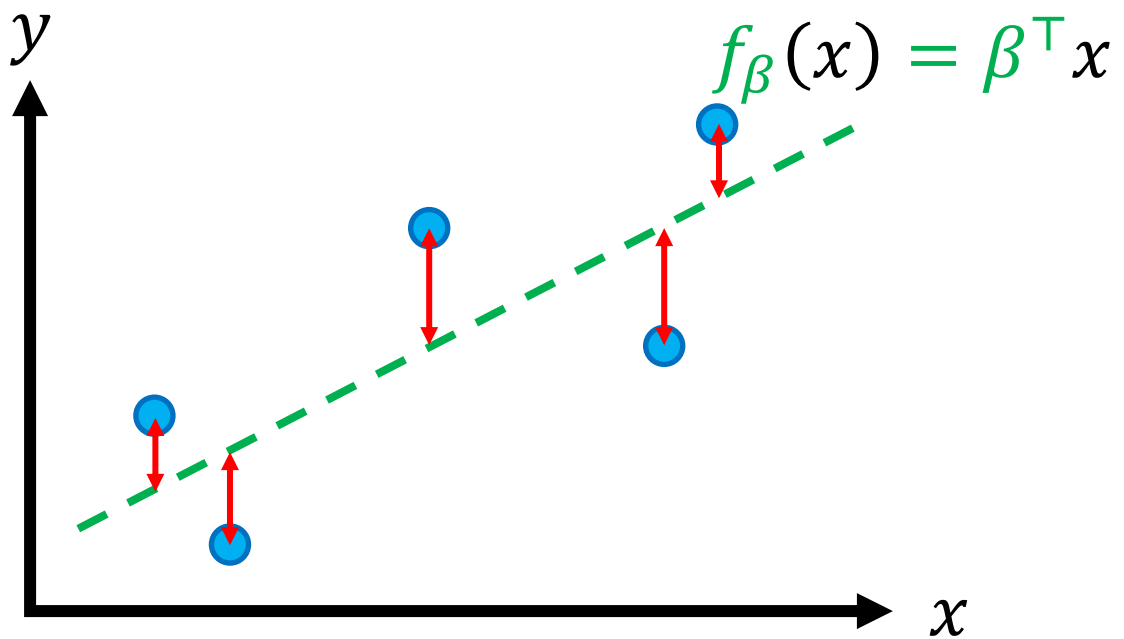
Image: https://www.flickr.com/photos/gsfc/5937599688/
Data from https://nsidc.org/arcticseaicenews/sea-ice-tools/

Choice of Loss Function

- $y_i \approx \beta^\top x_i$ if $(y_i - \beta^\top x_i)^2$ small
- **Mean squared error (MSE):**

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

- Computationally convenient and works well in practice



$$L(\beta; Z) = \frac{\updownarrow^2 + \updownarrow^2 + \updownarrow^2 + \updownarrow^2 + \updownarrow^2}{n}$$

Linear Regression Problem

- **Input:** Data $Z = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$
- **Output:** A linear function $f_\beta(x) = \beta^\top x$ that minimizes the MSE:

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

Linear Regression Algorithm

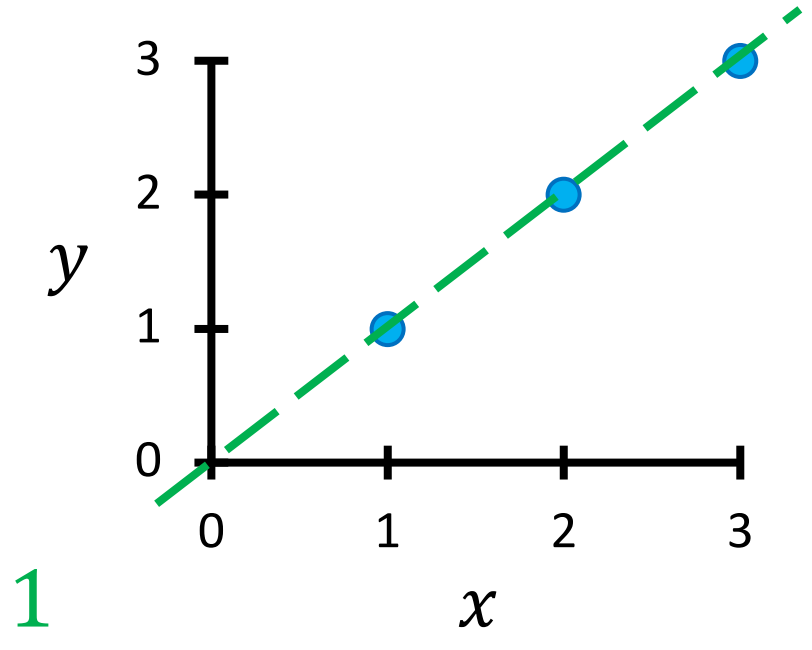
- **Input:** Dataset $Z = \{(x_1, y_1), \ldots, (x_n, y_n)\}$
- Compute

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

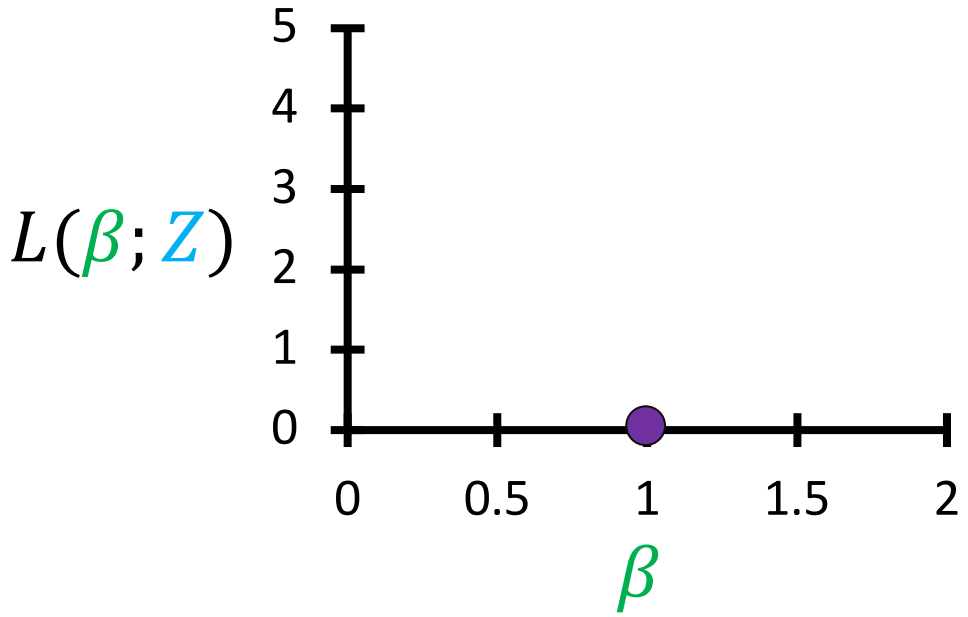
- **Output:** $f_{\hat{\beta}(Z)}(x) = \hat{\beta}(Z)^\top x$
- Discuss algorithm for computing the minimal β later

Intuition on Minimizing MSE Loss

- Consider $x \in \mathbb{R}$ and $\beta \in \mathbb{R}$

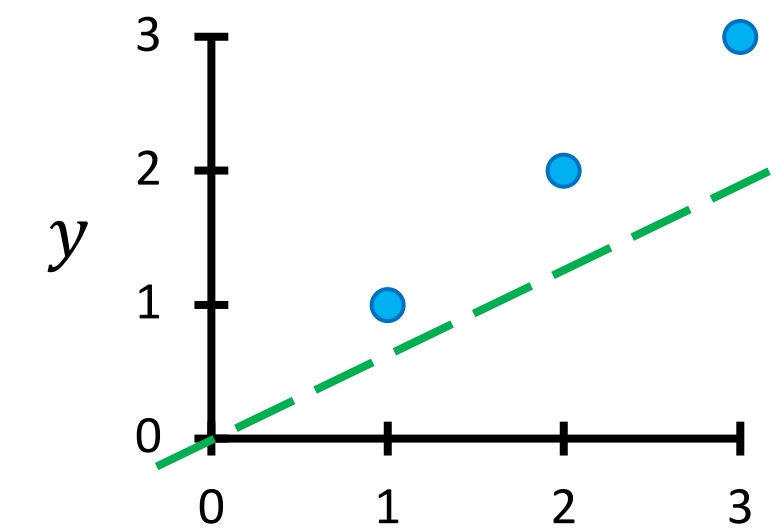


$\beta = 1$

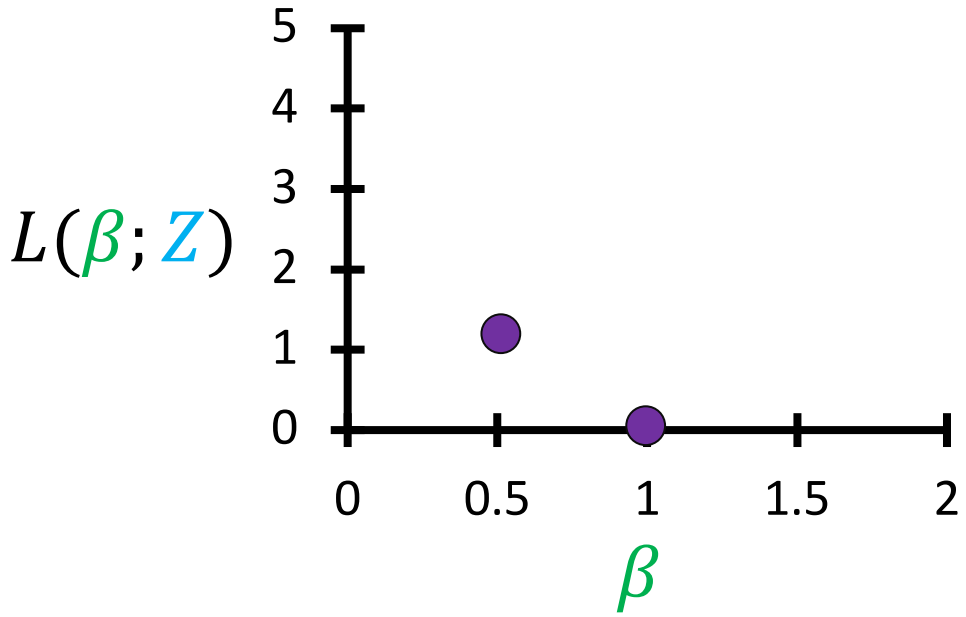


Intuition on Minimizing MSE Loss

- Consider $x \in \mathbb{R}$ and $\beta \in \mathbb{R}$

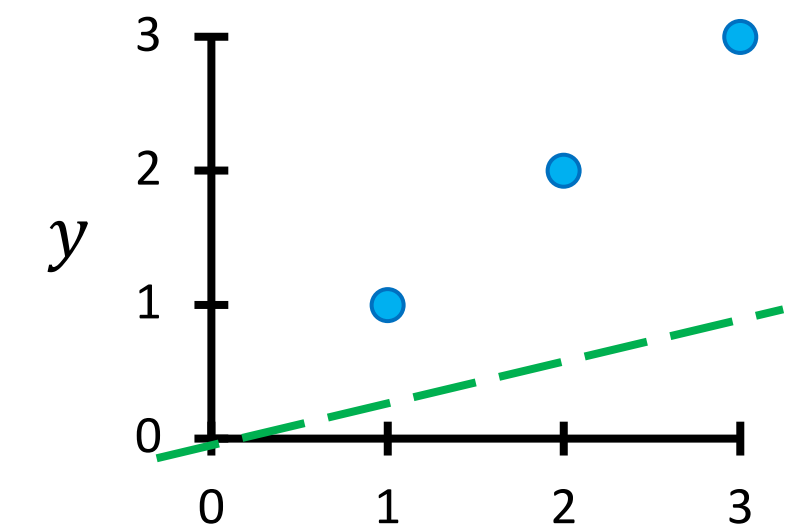


$\beta = 0.5$

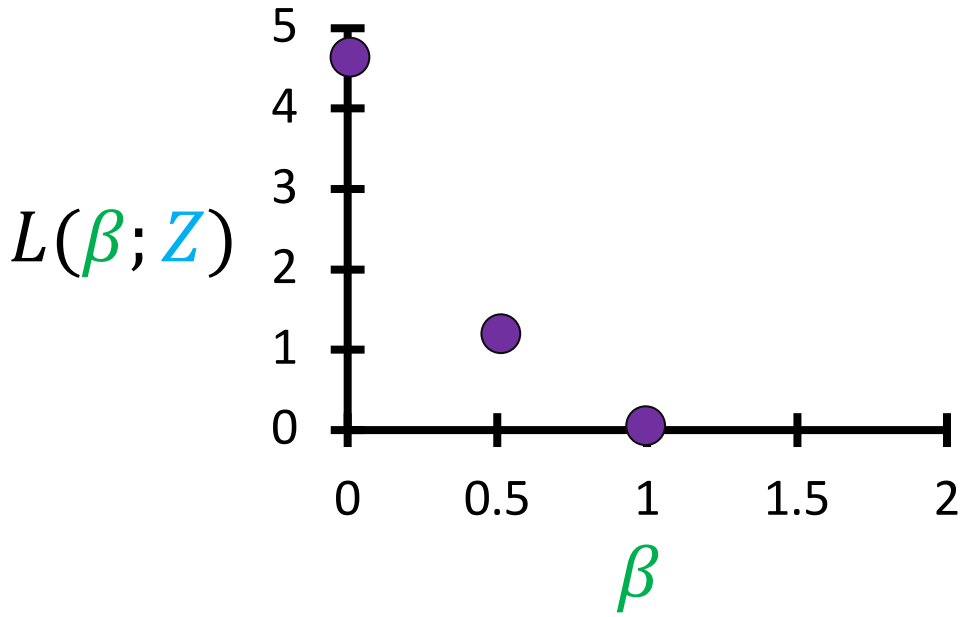


Intuition on Minimizing MSE Loss

- Consider $x \in \mathbb{R}$ and $\beta \in \mathbb{R}$

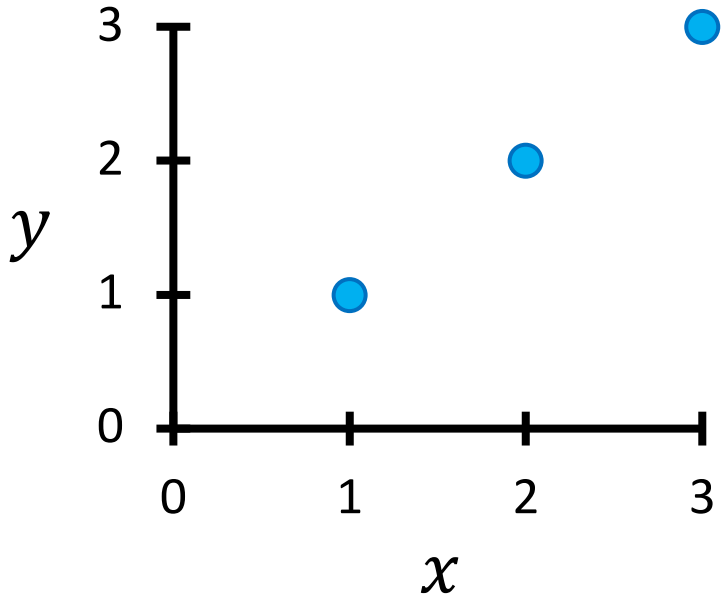


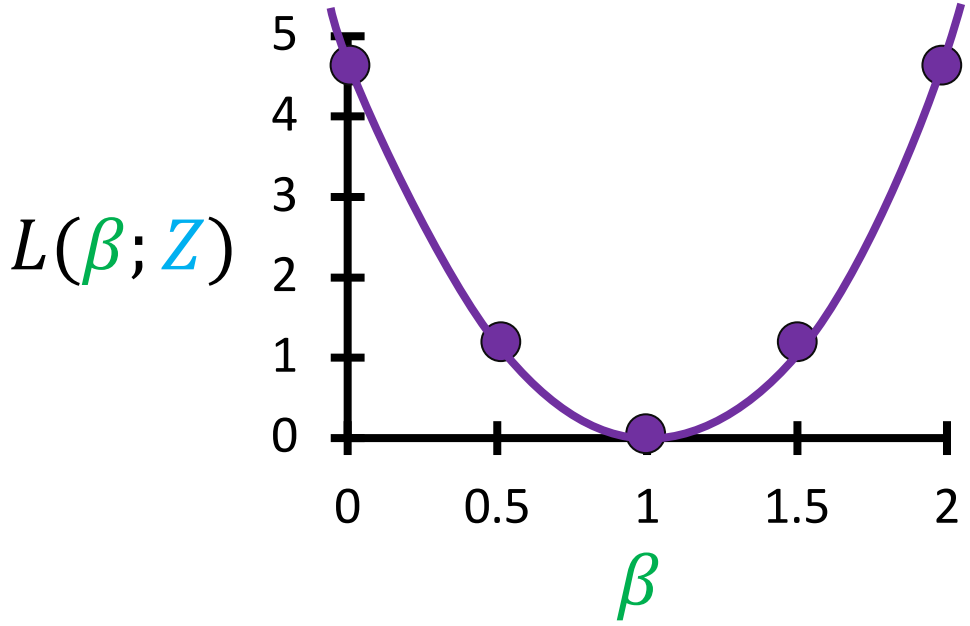
$\beta = 0.25$



Intuition on Minimizing MSE Loss

- Consider $x \in \mathbb{R}$ and $\beta \in \mathbb{R}$

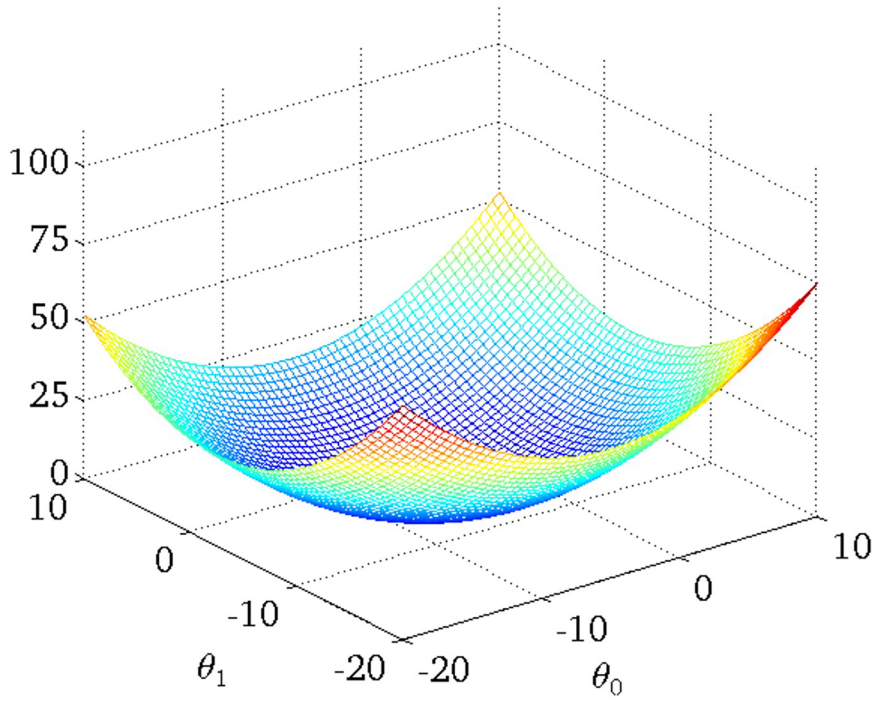


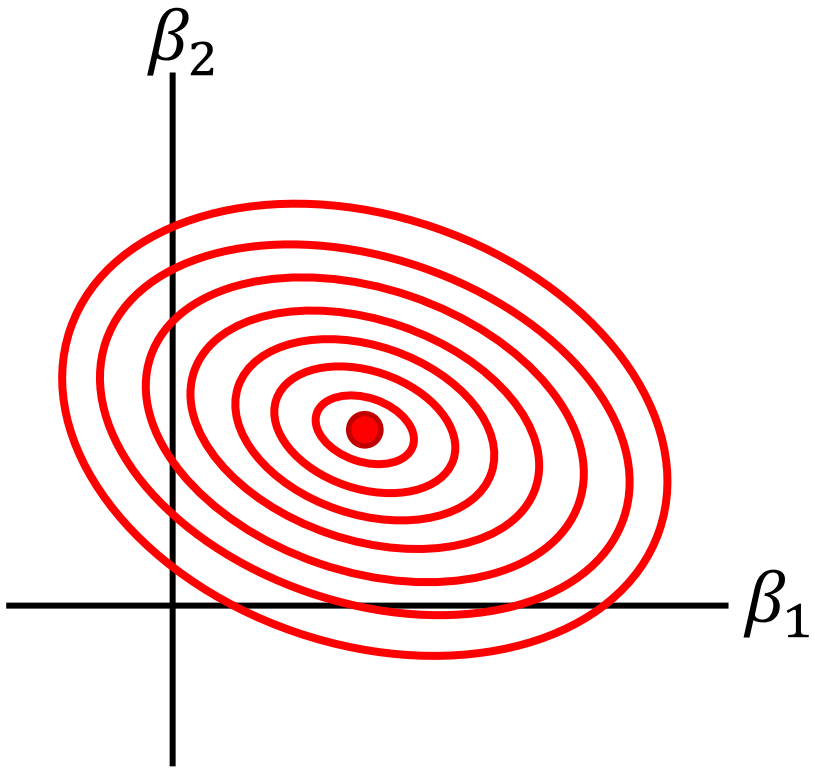


Intuition on Minimizing MSE Loss

- **Convex** (“bowl shaped”) in general

$L(\beta; Z)$





Slide by Andrew Ng

Alternative Loss Functions

- **Mean absolute error:** $\frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i|$
- **Mean relative error:** $\frac{1}{n}\sum_{i=1}^{n}\frac{|\widehat{y_i}-y_i|}{|y_i|}$
- $\boldsymbol{R^2}$ **score:** $1 - \frac{\text{MSE}}{\text{Variance}}$
  - "Coefficient of determination"
  - Higher is better, $R^2 = 1$ is perfect

Linear Regression

General strategy

- Model family $F = \{f_\beta\}_\beta$
- Loss function $L(\beta; Z)$

Linear regression strategy

- Linear functions $F = \{f_\beta(x) = \beta^\top x\}$
- MSE $L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$

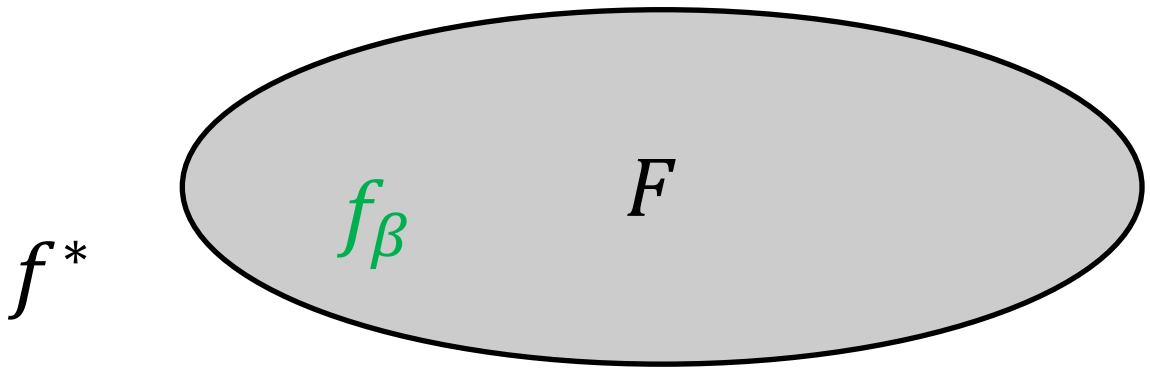
Linear regression algorithm

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

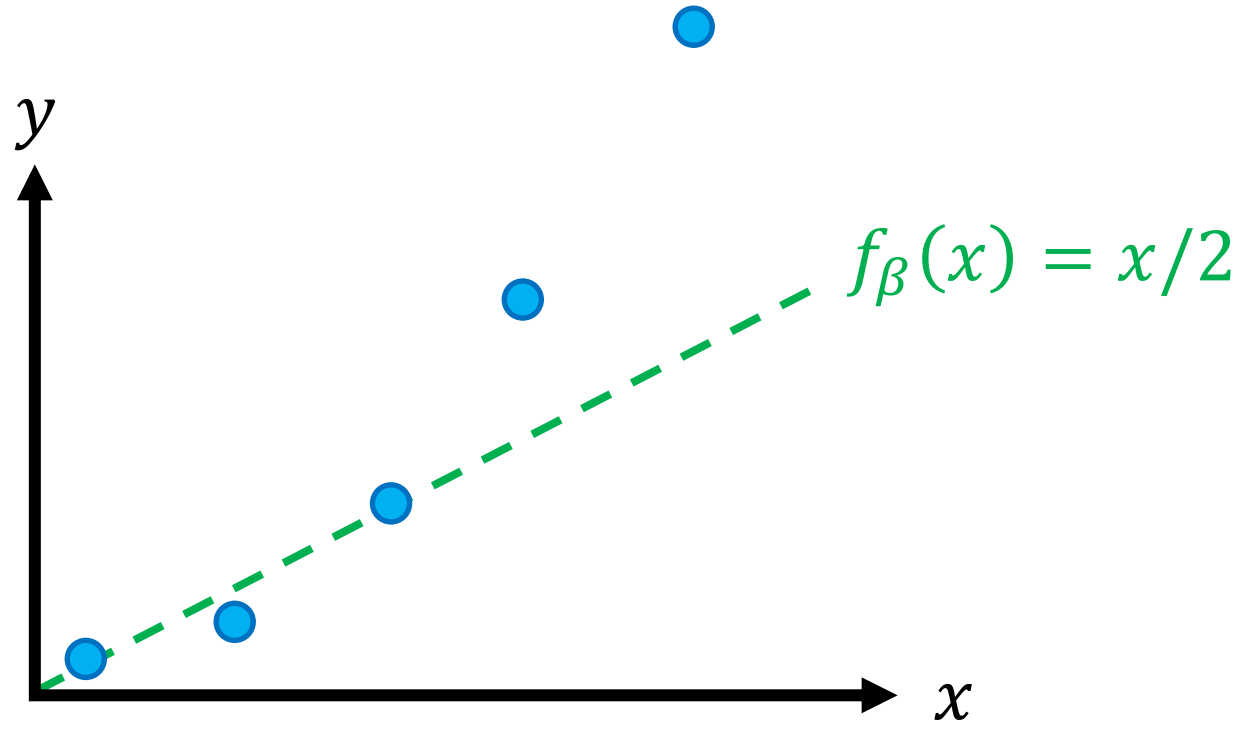
Aside: "True Function"

- **Input:** Dataset Z
  - Presume there is an unknown function f^* that **generates** Z

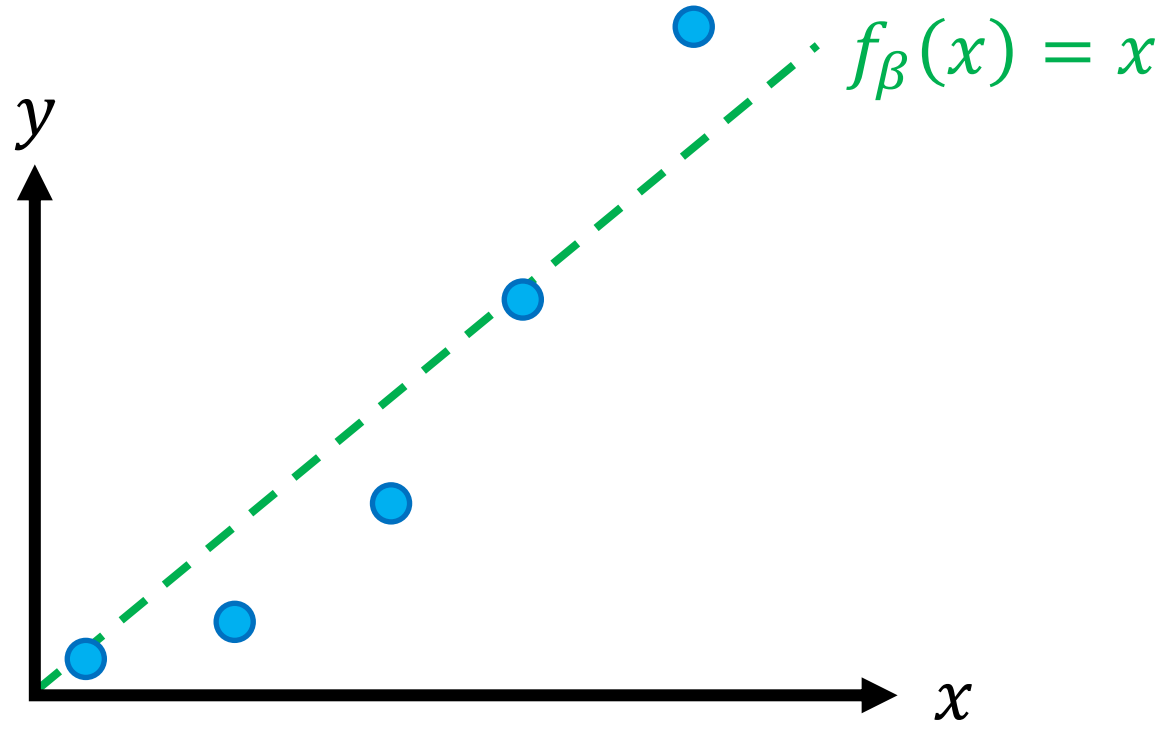
- **Goal:** Find an approximation $f_\beta \approx f^*$ in our model family $f_\beta \in F$
  - Typically, f^* not in our model family F



Example: Quadratic Function



Example: Quadratic Function



Can we get a better fit?

Feature Maps

General strategy

- Model family $F = \{f_\beta\}_\beta$
- Loss function $L(\beta; Z)$

Linear regression with feature map

- Linear functions over a given **feature map** $\phi: X \to \mathbb{R}^d$

$$F = \{f_\beta(x) = \beta^\top \phi(x)\}$$

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

Quadratic Feature Map

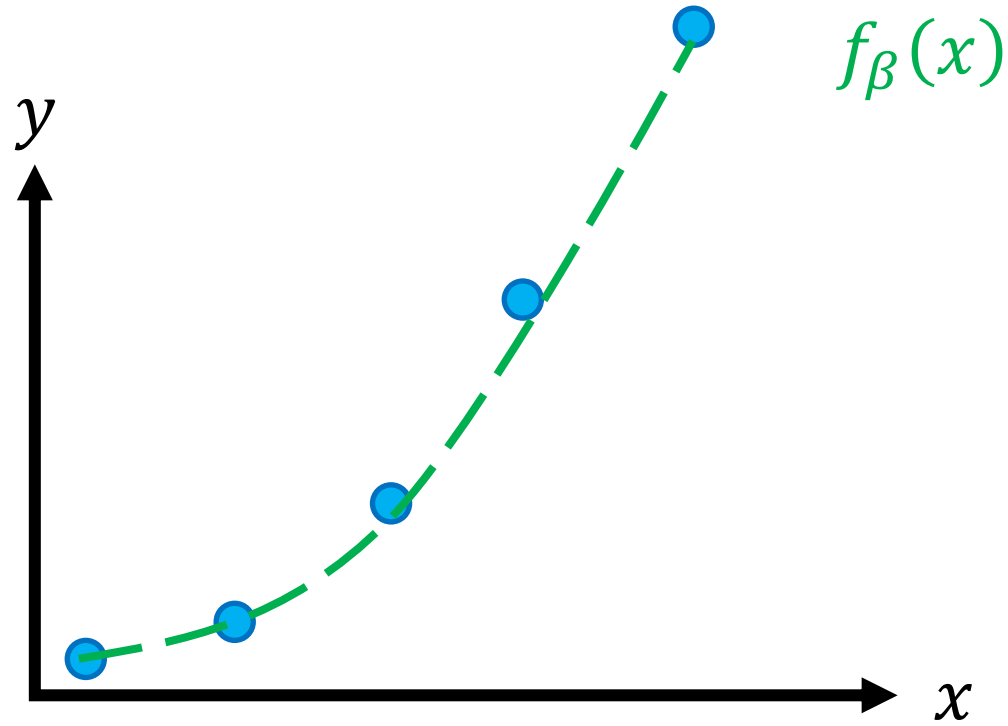
- Consider the feature map $\phi: \mathbb{R} \to \mathbb{R}^2$ given by

$$\phi(x) = \begin{bmatrix} x \\ x^2 \end{bmatrix}$$

- Then, the model family is

$$f_\beta(x) = \beta_1 x + \beta_2 x^2$$

Quadratic Feature Map



In our family for $\beta = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$!

Feature Maps

- Powerful strategy for encoding prior knowledge

- **Terminology**
  - x is the **input** and $\phi(x)$ are the **features**
  - Often used interchangeably

Examples of Feature Maps

- **Polynomial features**
  - $\phi(x) = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_1^2 + \beta_5 x_1 x_2 + \beta_6 x_2^2 + \cdots$
  - Quadratic features are very common; capture "feature interactions"
  - Can use other nonlinearities (exponential, logarithm, square root, etc.)

- **Intercept term**
  - $\phi(x) = [1 \quad x_1 \quad \dots \quad x_d]^\top$
  - Almost always used; captures constant effect

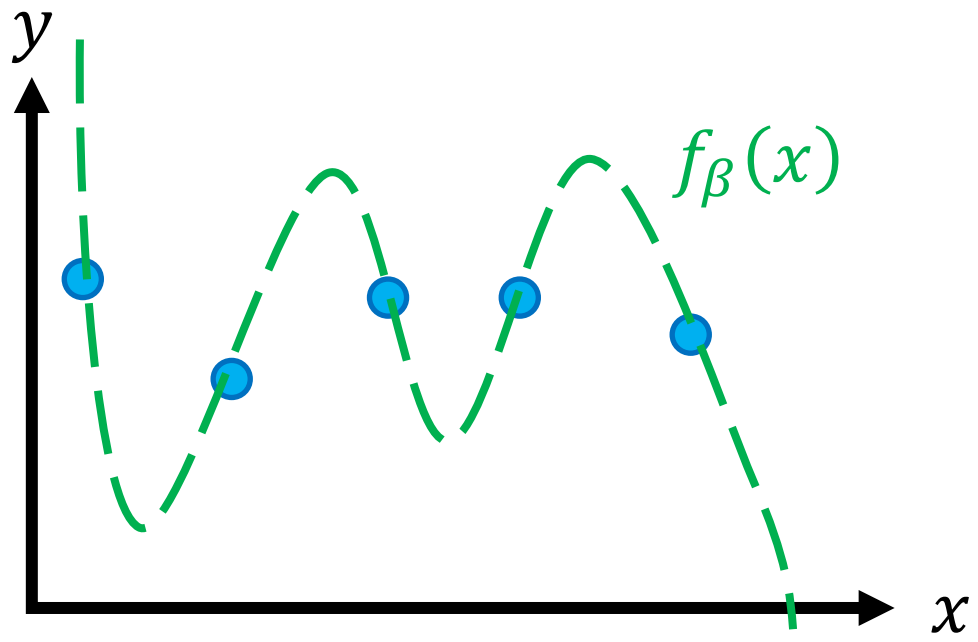
- **Encoding non-real inputs**
  - E.g., $x =$ "the food was good" and $y = 4$ stars
  - $\phi(x) = [1(\text{“good”} \in x) \quad 1(\text{“bad”} \in x) \quad \dots]^\top$

Algorithm

- Reduces to linear regression
- **Step 1:** Compute $\phi_i = \phi(x_i)$ for each x_i in Z
- **Step 2:** Run linear regression with $Z' = \{(\phi_1, y_1), \ldots, (\phi_n, y_n)\}$

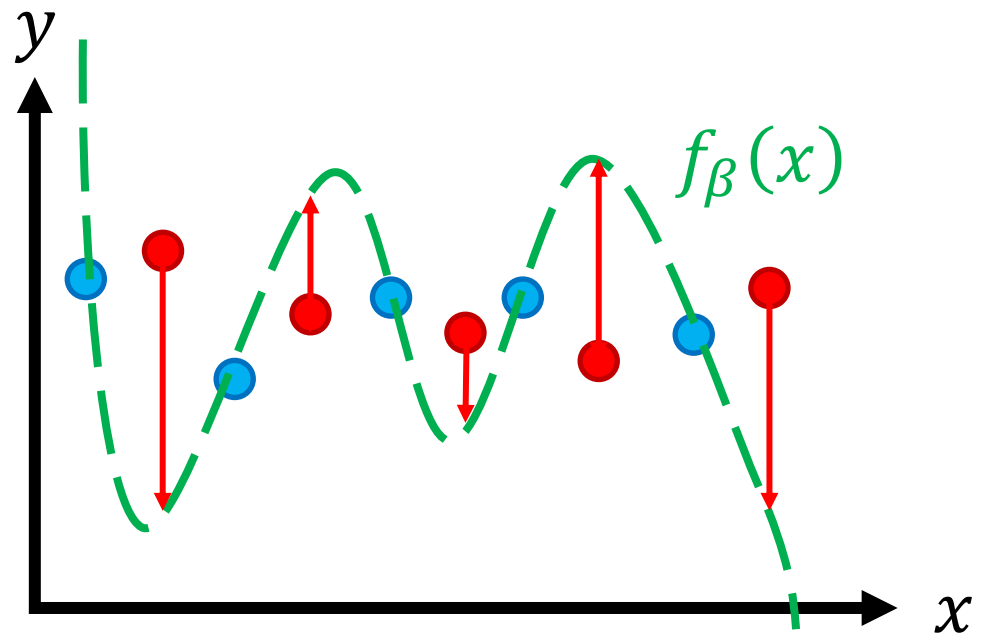
Question

- **Why not throw in lots of features?**
  - $\phi(x) = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_1^2 + \beta_5 x_1 x_2 + \beta_6 x_2^2 + \cdots$
  - Can fit any n points using a polynomial of degree n



Prediction

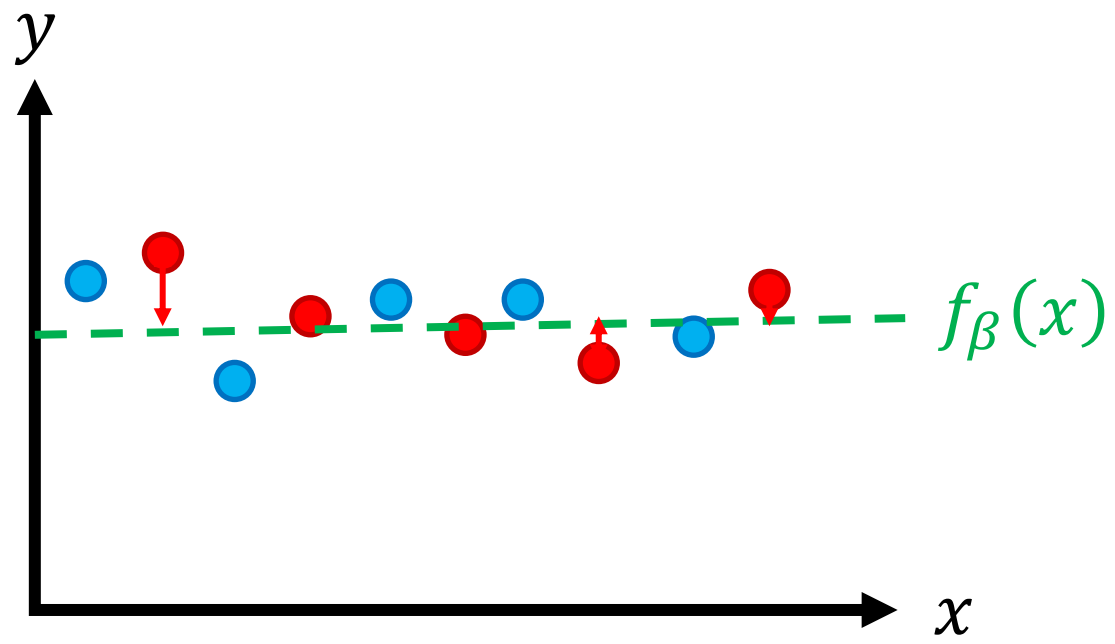
- **Issue:** The goal in machine learning is **prediction**
  - Given a **new** input x, predict the label $\hat{y} = f_\beta(x)$



The errors on new inputs is very large!

Prediction

- **Issue:** The goal in machine learning is **prediction**
  - Given a **new** input x, predict the label $\hat{y} = f_\beta(x)$



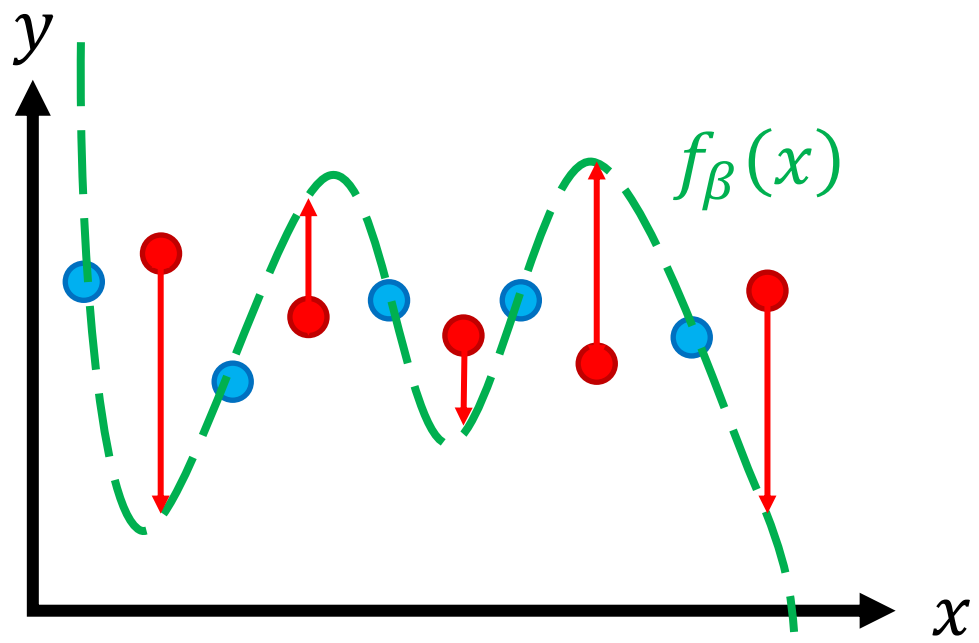
Vanilla linear regression actually works better!

Training vs. Test Data

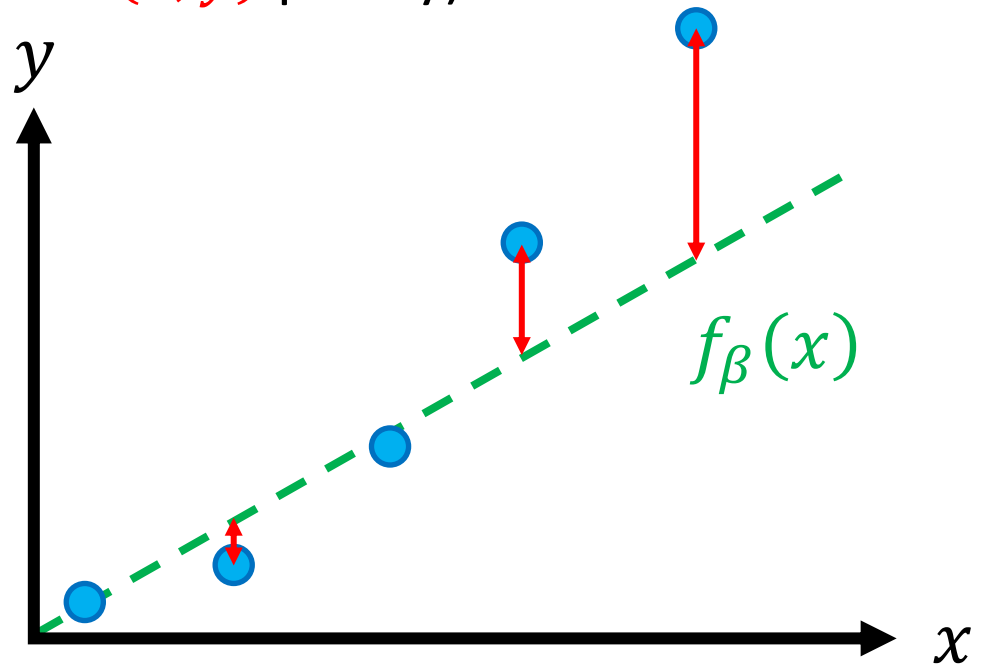
- **Training data:** Examples $Z = \{(x, y)\}$ used to fit our model
- **Test data:** New inputs x whose labels y we want to predict

Overfitting vs. Underfitting

- **Overfitting**
  - Fit the **training data** Z well
  - Fit new **test data** (x, y) poorly



- **Underfitting**
  - Fit the **training data** Z poorly
  - (Necessarily fit new **test data** (x, y) poorly)



Aside: Why Does Overfitting Happen?

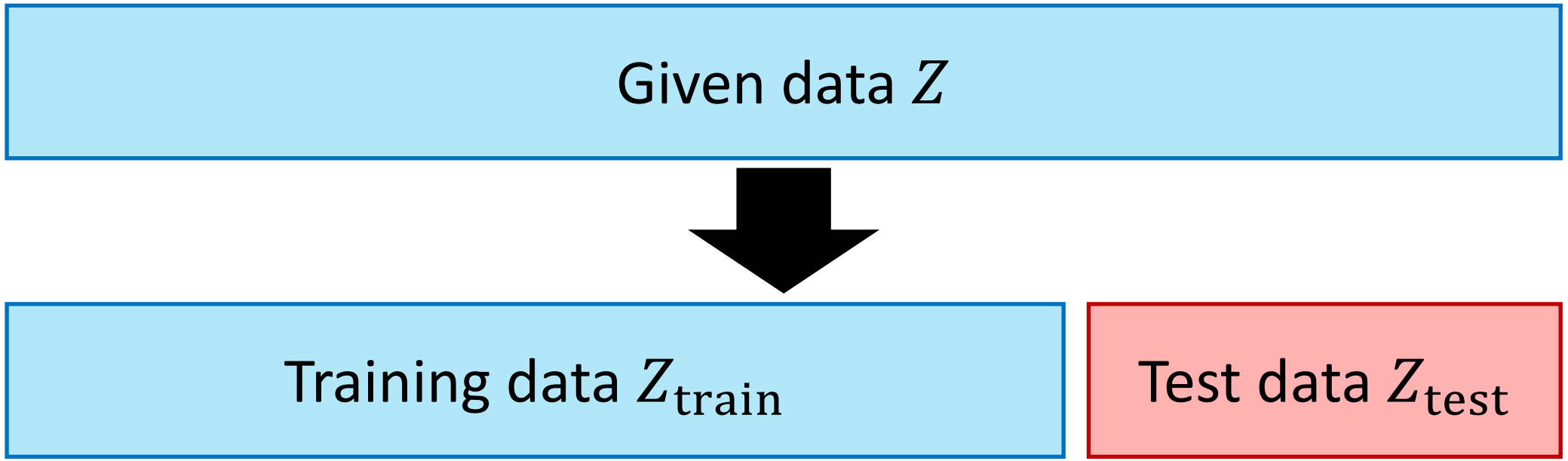
- Overfitting typically due to fitting noise in the data

- **Noise in labels $\boldsymbol{y}_i$**
  - True data generating process is more complex than we can capture
  - May depend on unobserved features

- **Noise in features $\boldsymbol{x}_i$**
  - Measurement error in the feature values
  - Errors due to preprocessing
  - Some features might be irrelevant to the decision function

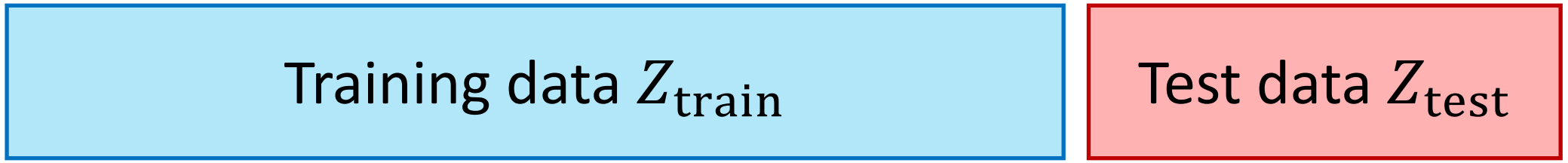
Training/Test Split

- **Issue:** How to detect overfitting vs. underfitting?
- **Solution:** Use **held-out test data** to estimate loss on new data
  - Typically, randomly shuffle data first



Training/Test Split Algorithm

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

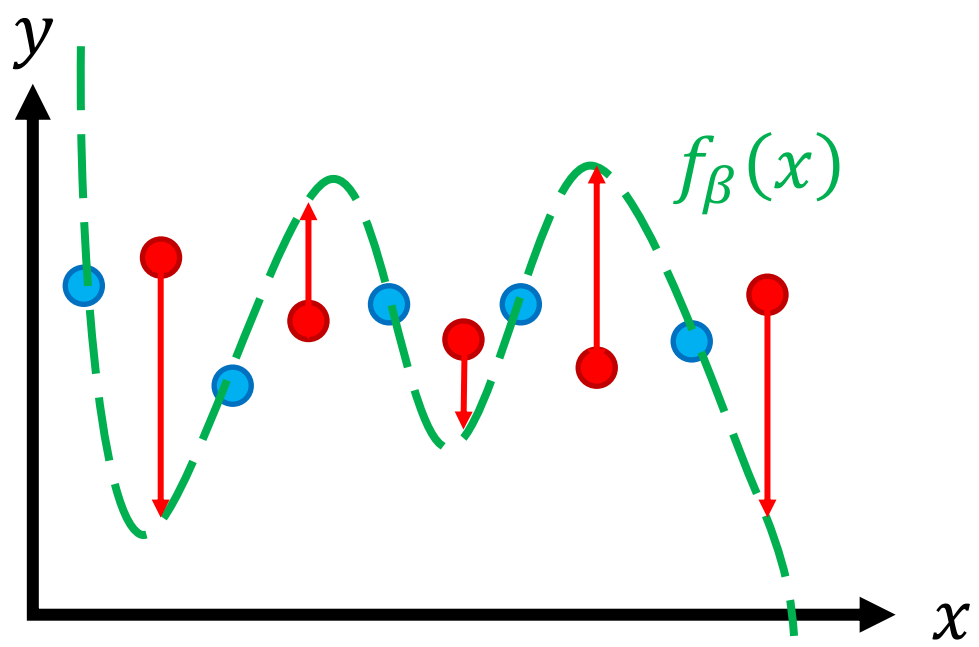


- **Step 2:** Run linear regression with Z_{train} to obtain $\hat{\beta}(Z_{\text{train}})$

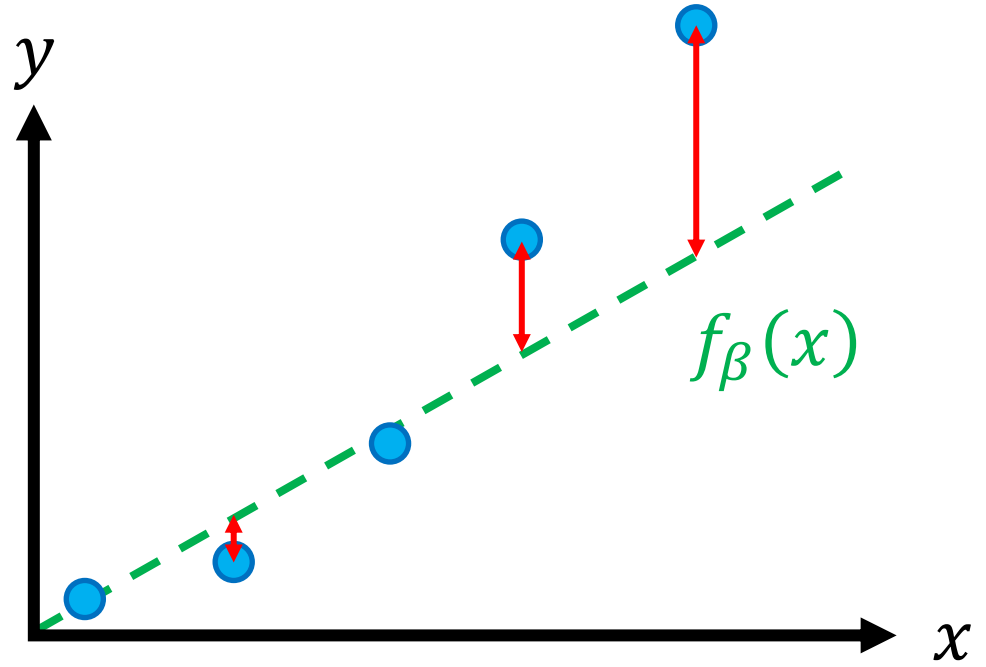
- **Step 3:** Evaluate
  - **Training loss:** $L_{\text{train}} = L\left(\hat{\beta}(Z_{\text{train}}); Z_{\text{train}}\right)$
  - **Test (or generalization) loss:** $L_{\text{test}} = L\left(\hat{\beta}(Z_{\text{train}}); Z_{\text{test}}\right)$

Training/Test Split Algorithm

- **Overfitting**
  - L_{train} is small
  - L_{test} is large



- **Underfitting**
  - L_{train} is large
  - L_{test} is large



How to Fix Underfitting/Overfitting?

- Choose the right model family!

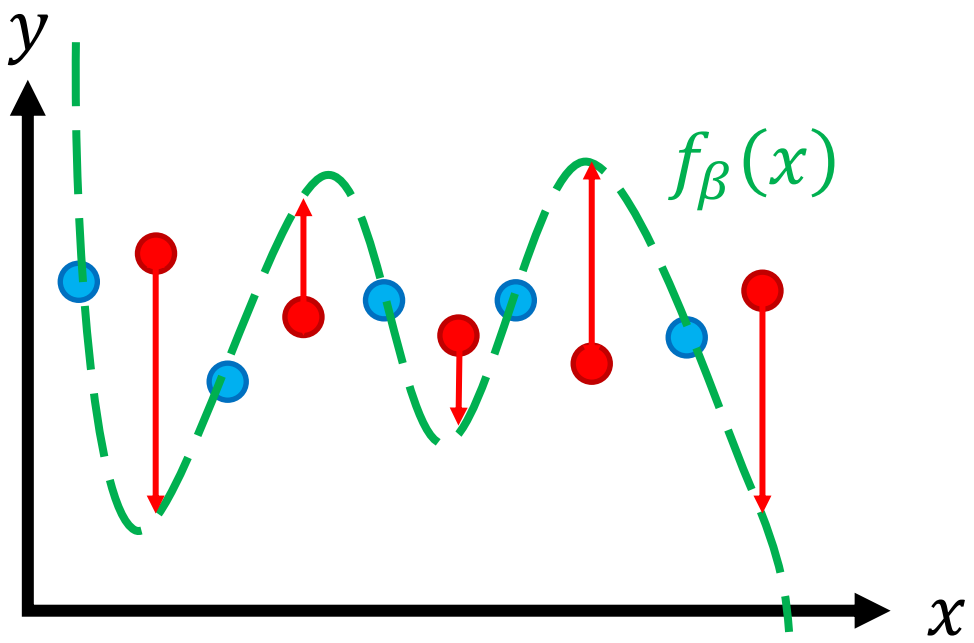
Role of Capacity

- **Capacity** of a model family captures "complexity" of data it can fit
  - Higher capacity → more likely to overfit (model family has high **variance**)
  - Lower capacity → more likely to underfit (model family has high **bias**)

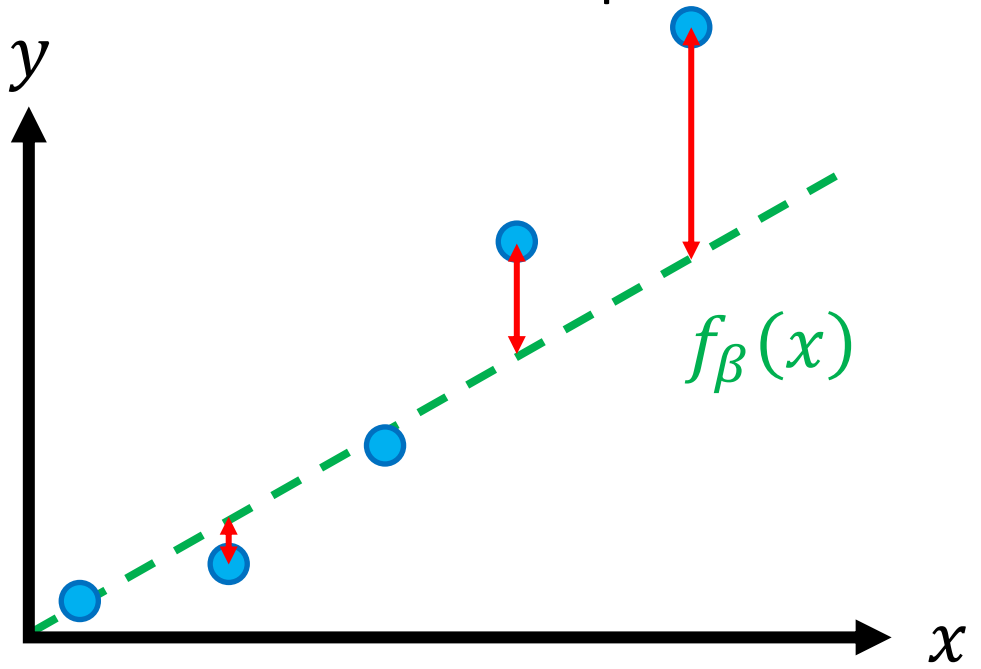
- For linear regression, capacity corresponds to feature dimension d
  - I.e., number of features in $\phi(x)$

Bias-Variance Tradeoff

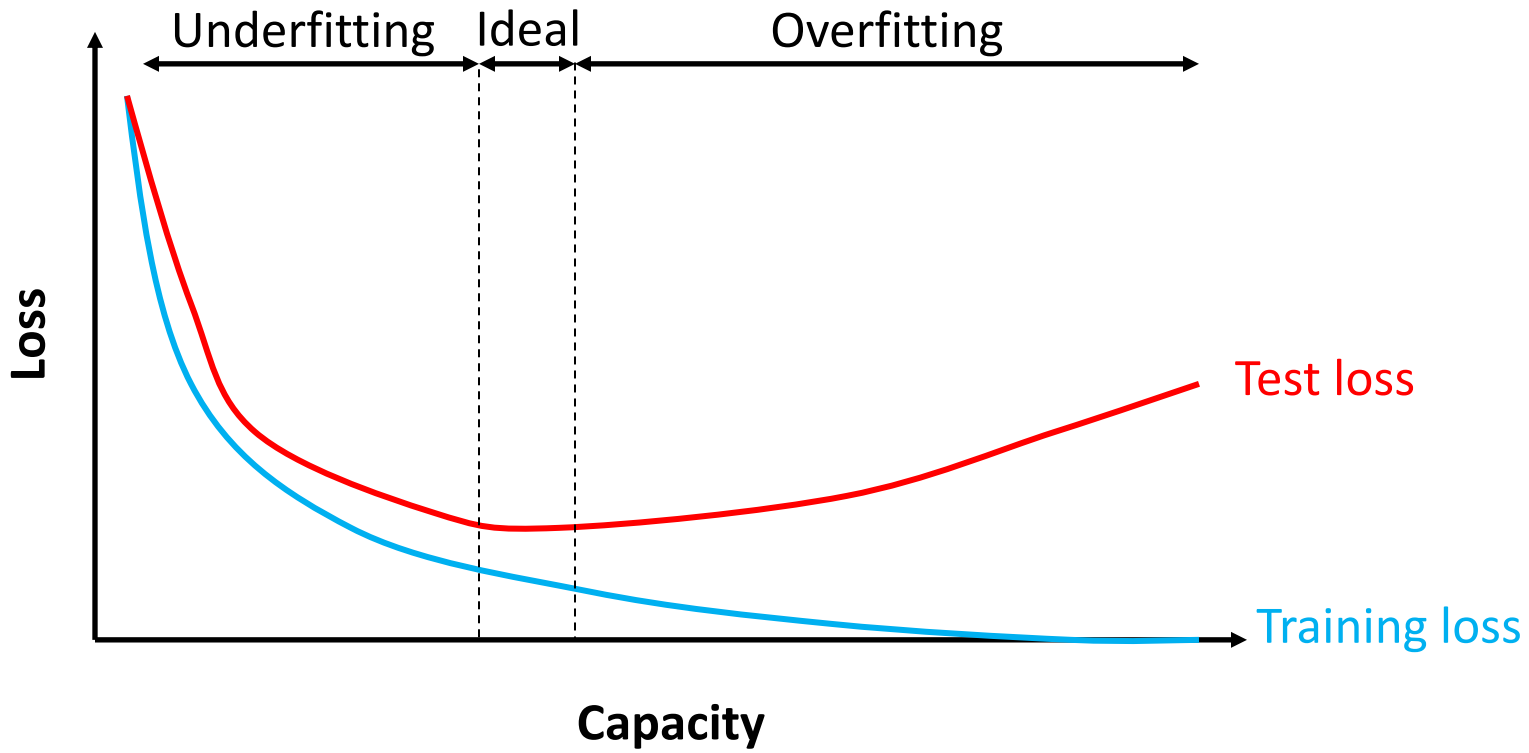
- **Overfitting (high variance)**
  - High capacity model capable of fitting complex data
  - Insufficient data to constrain it



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



Bias-Variance Tradeoff



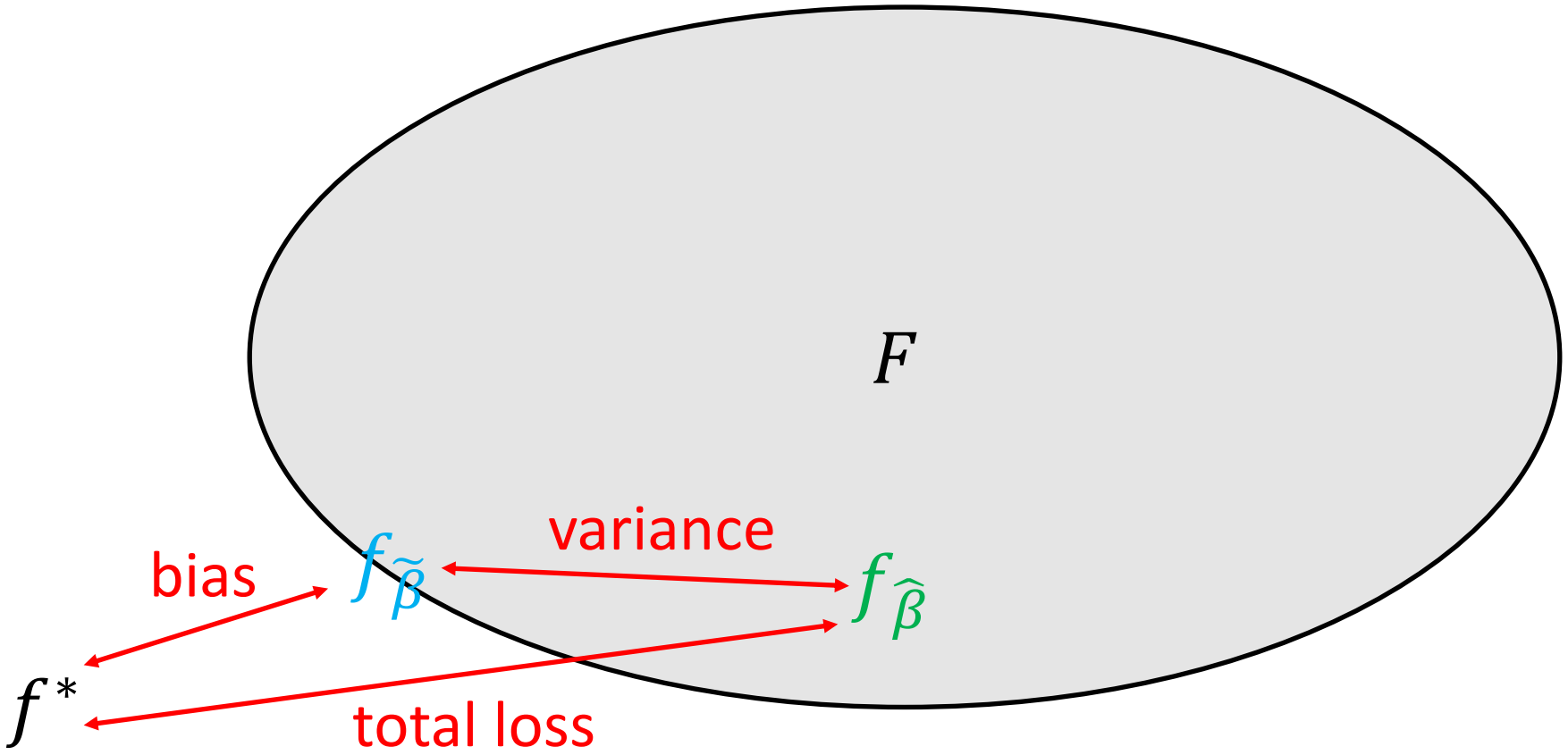
Slide by Padhraic Smyth, UCIrvine

Bias-Variance Tradeoff

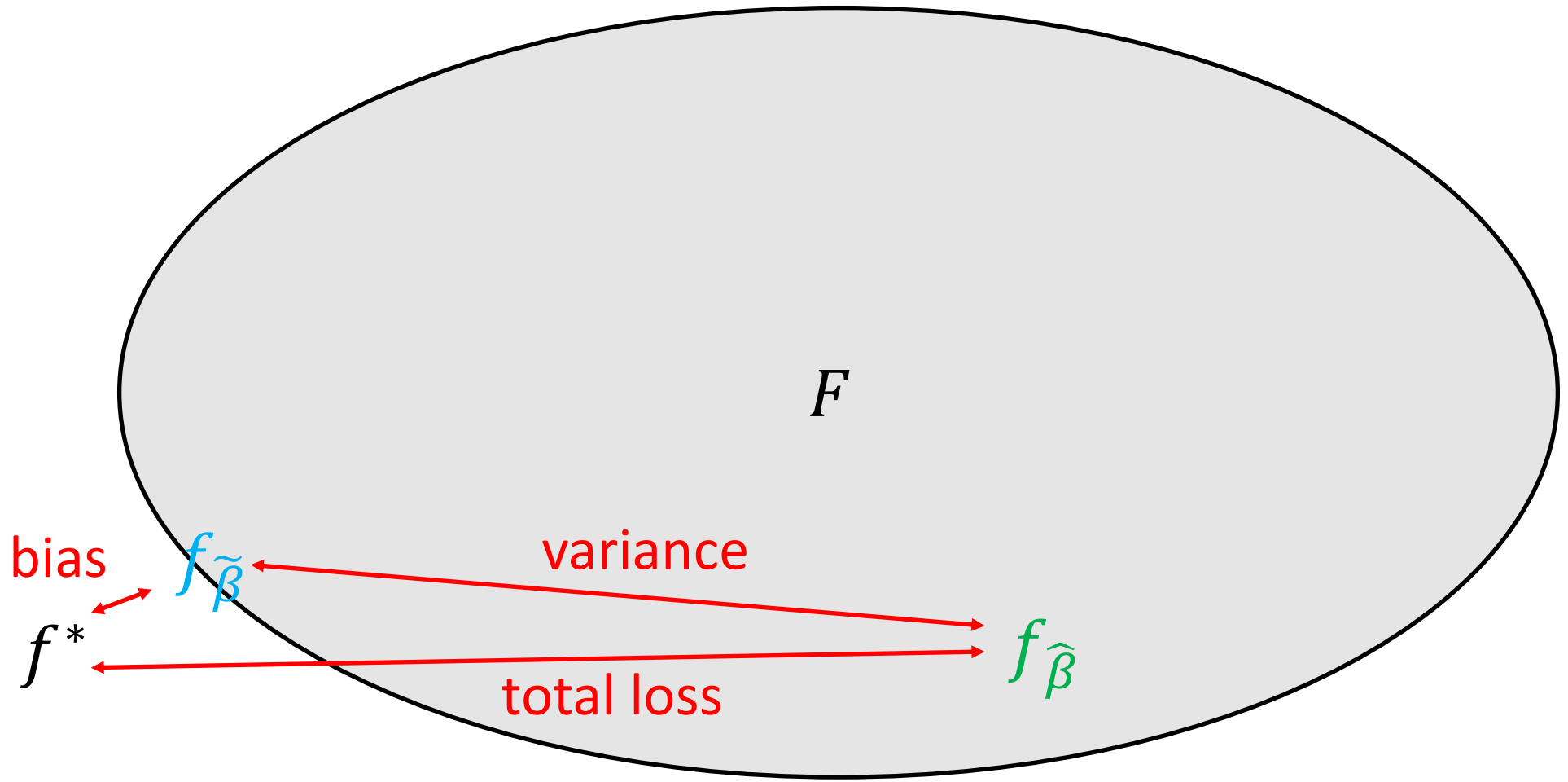
- For linear regression, increasing feature dimension d…
  - Tends to **increase capacity**
  - Tends to **decrease bias** but **increase variance**

- Need to construct ϕ to balance tradeoff between bias and variance
  - **Rule of thumb:** $n \approx d \log d$
  - Large fraction of data science work is data cleaning + feature engineering

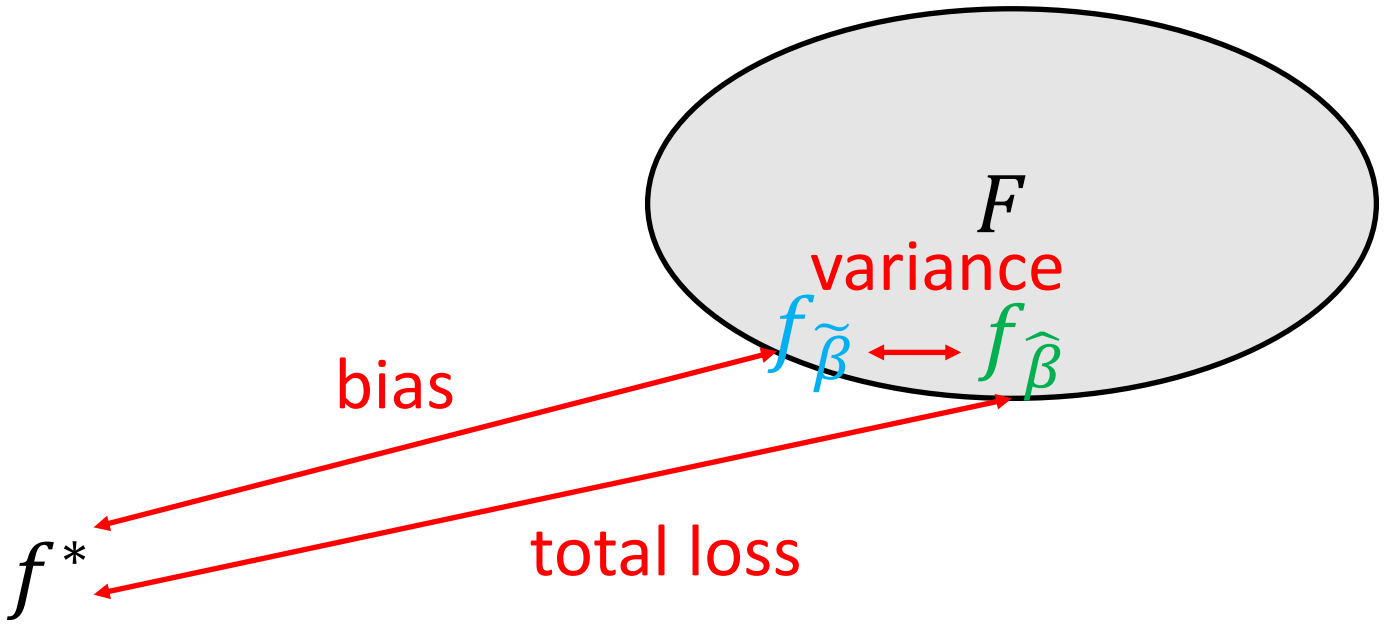
Recap: Bias-Variance Tradeoff



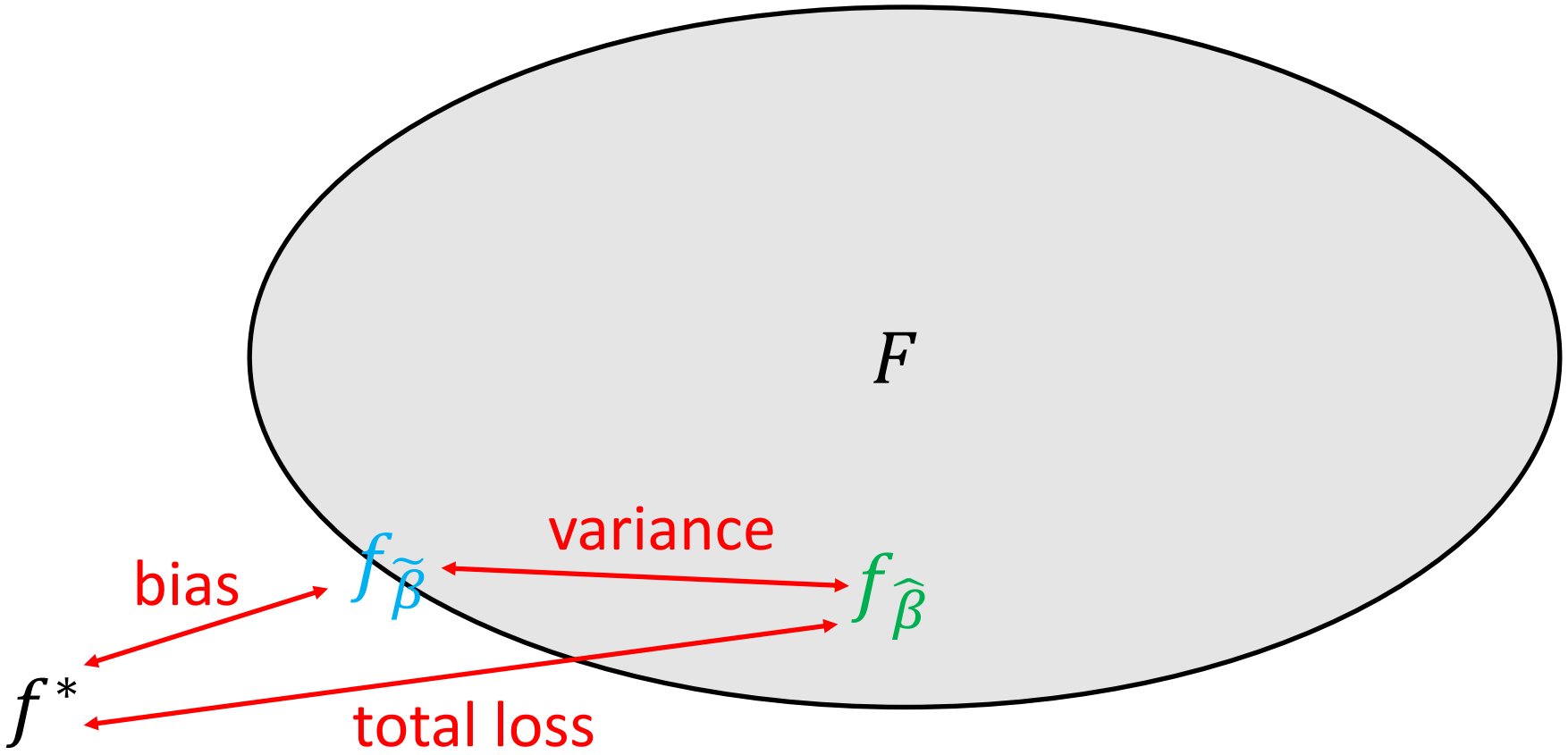
Recap: Bias-Variance Tradeoff (Overfitting)



Recap: Bias-Variance Tradeoff (Underfitting)



Recap: Bias-Variance Tradeoff (Ideal)



Linear Regression with L_2 Regularization

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

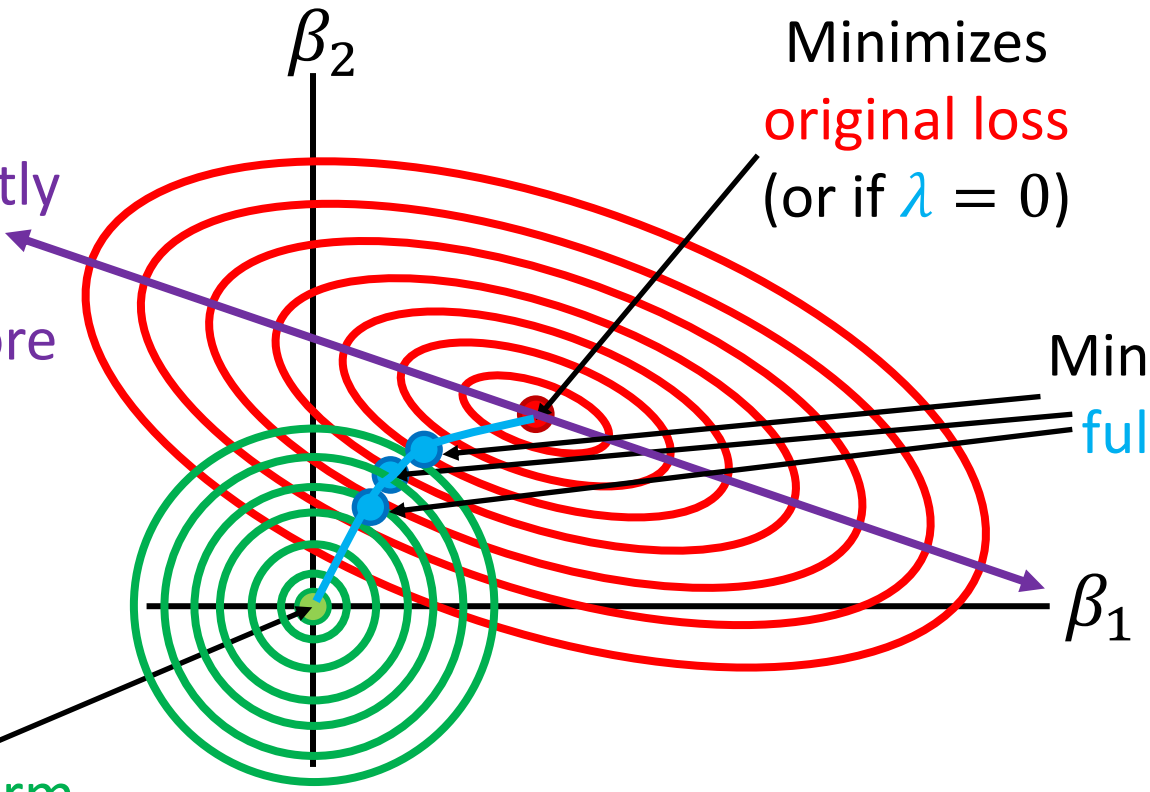
$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \cdot \|\beta\|_2^2$$
$$= \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{j=1}^{d}\beta_j^2$$

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

Intuition on 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

Intuition on L_2 Regularization



Minimizes original loss (or if $\lambda = 0$)

Loss varies greatly in this direction → Penalizes more

Minimizes full loss

Minimizes regularization term (or if $\lambda \to \infty$)

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

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

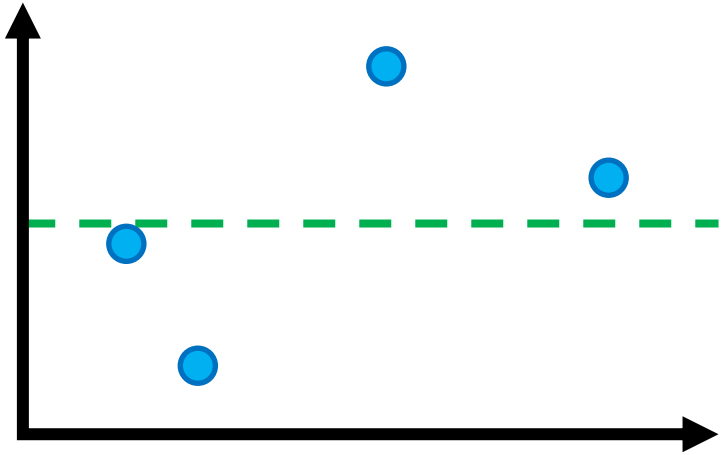
Regularization and Intercept Term

- 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 $\hat{\beta}_1(Z) = \text{mean}(\{y_i\}_{i=1}^n)$)



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 $(\beta_j/2)^2$ 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

- **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:**

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

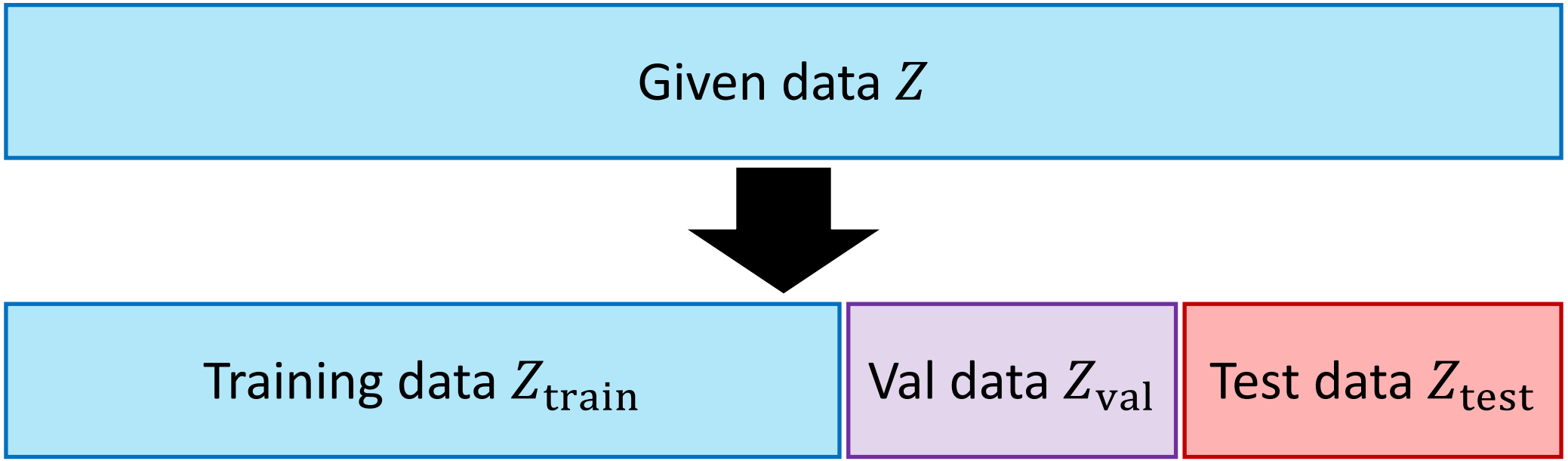
  - Offers a way to express a preference “simpler” functions in family
  - Typically, regularization is independent of data

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



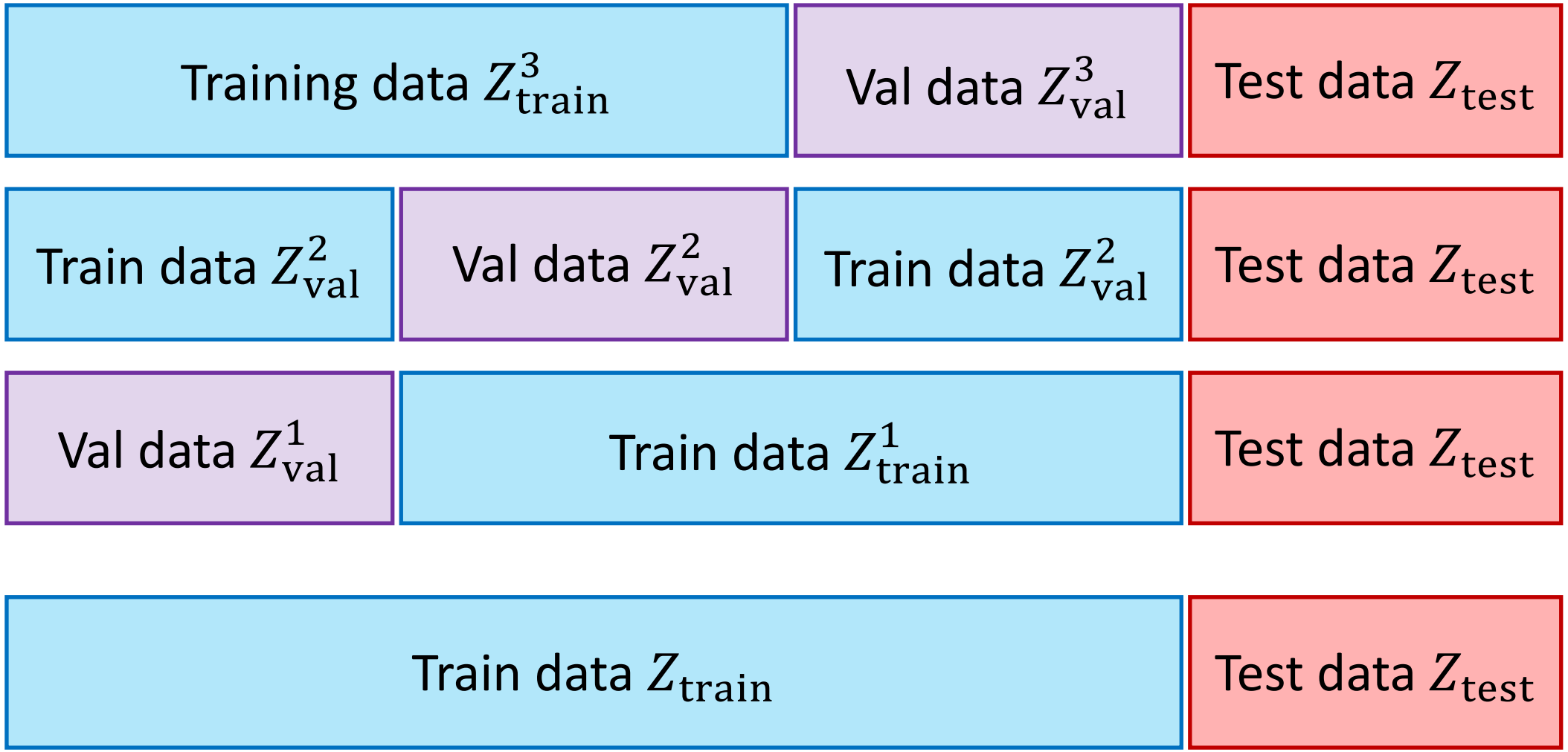
Basic Cross Validation Algorithm

- **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 $\hat{\beta}(Z_{\text{train}}, \lambda_{t'})$

Example: 3-Fold Cross Validation



k-Fold Cross-Validation

- 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 $s \in \{1, \ldots, k\}$ with Z_{train}
  - Chooses better λ' than above strategy

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

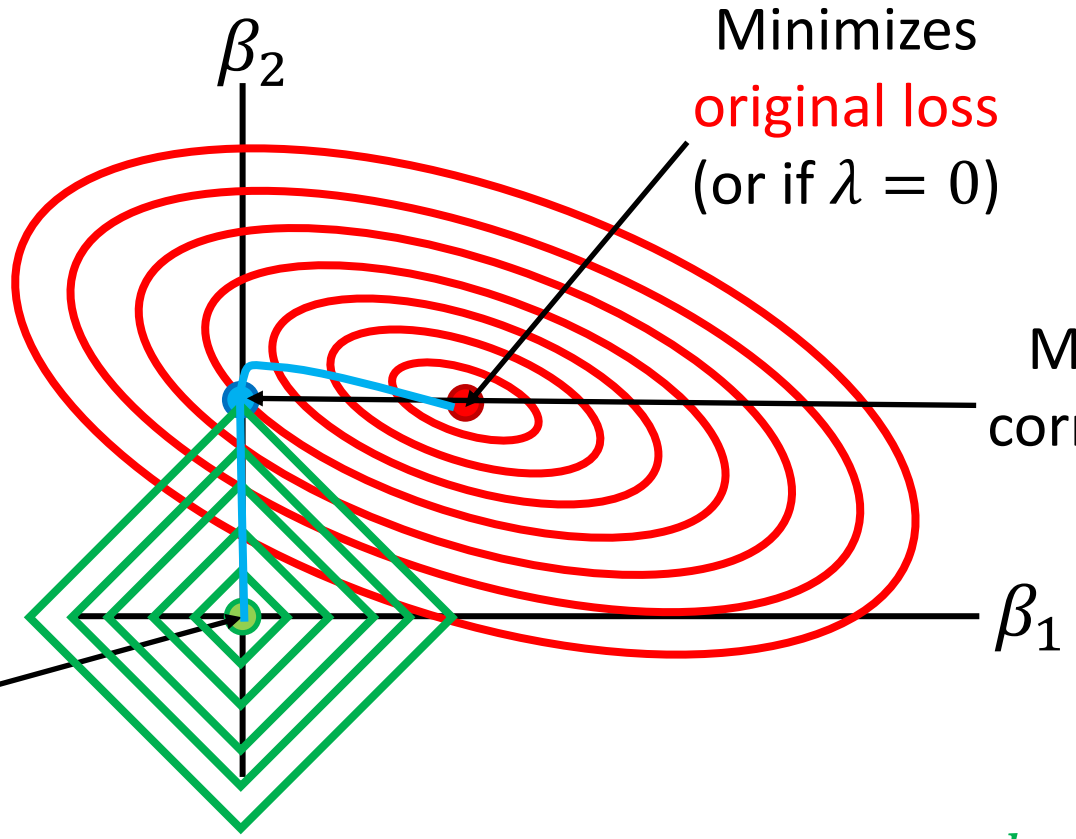
L_1 Regularization

- **Sparsity:** Can we minimize $\|\beta\|_0 = \left|\left\{ j \mid \beta_j \neq 0 \right\}\right|$?
  - 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



Minimizes original loss (or if $\lambda = 0$)

Minimizer of full loss at corner → sparse ($\beta_1 = 0$)!

Minimizes regularization term (or if $\lambda \to \infty$)

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

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)

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

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

$$\approx$$

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

Summary: $Y \approx X\beta$

Vectorizing Mean Squared Error

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

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

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

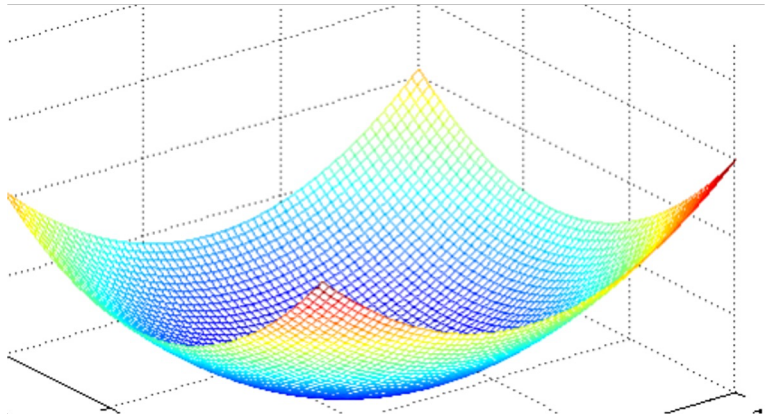
Strategy 1: Closed-Form Solution

- 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:

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



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

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)

Strategy 2: Gradient Descent

- **Gradient descent:** Update β based on **gradient** $\nabla_\beta L(\beta; Z)$ of $L(\beta; Z)$:

$$\beta_{t+1} \leftarrow \beta_t - \alpha \cdot \nabla_\beta L(\beta_t; Z)$$

- **Intuition:** The gradient is the direction along which $L(\beta; Z)$ changes most quickly as a function of β

- $\alpha \in \mathbb{R}$ is a hyperparameter called the **learning rate**
  - More on this later

Strategy 2: Gradient Descent

- Choose initial value for β
- Until we reach a minimum:
  - Choose a new value for β to reduce $L(\beta; Z)$

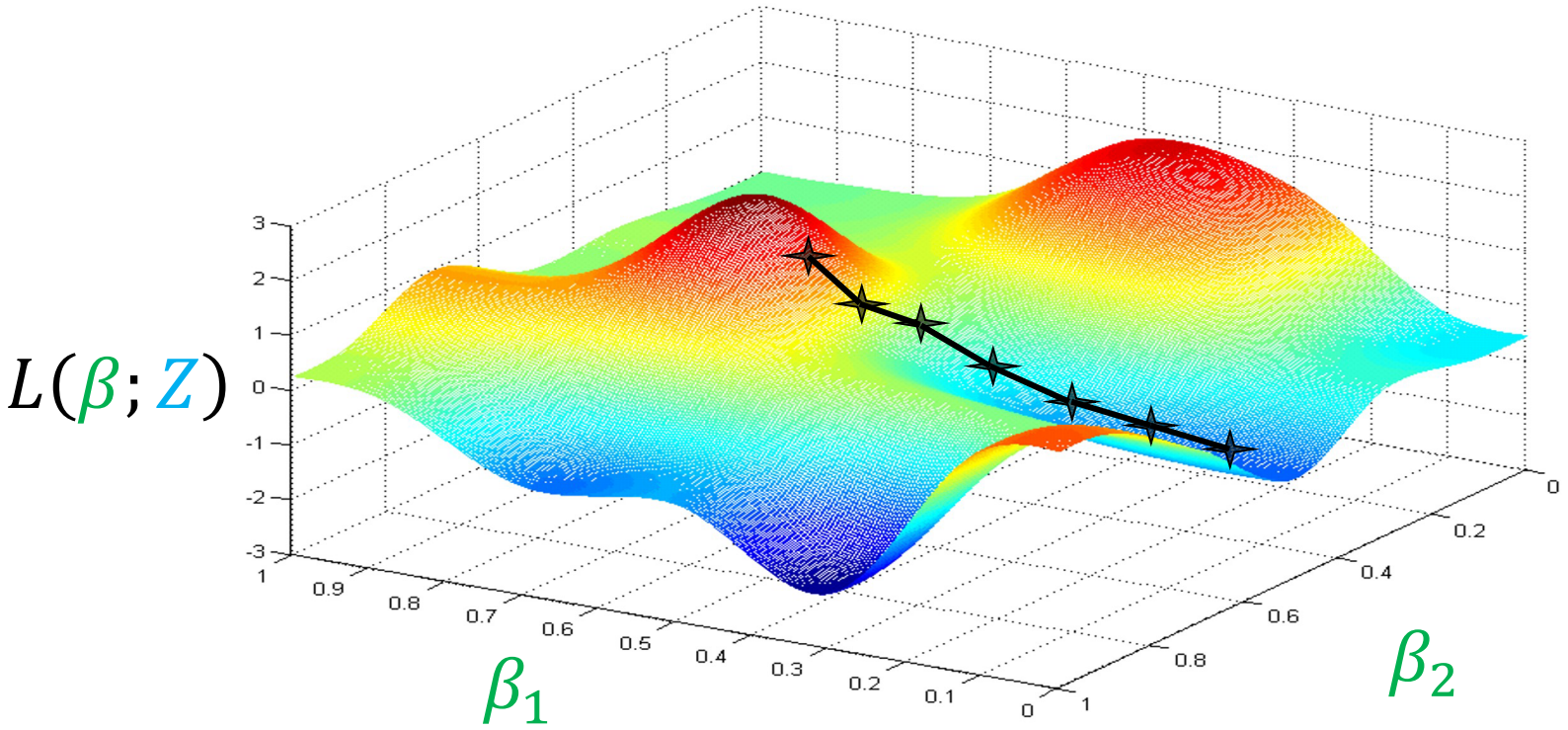


Figure by Andrew Ng

Strategy 2: Gradient Descent

- Choose initial value for β
- Until we reach a minimum:
  - Choose a new value for β to reduce $L(\beta; Z)$

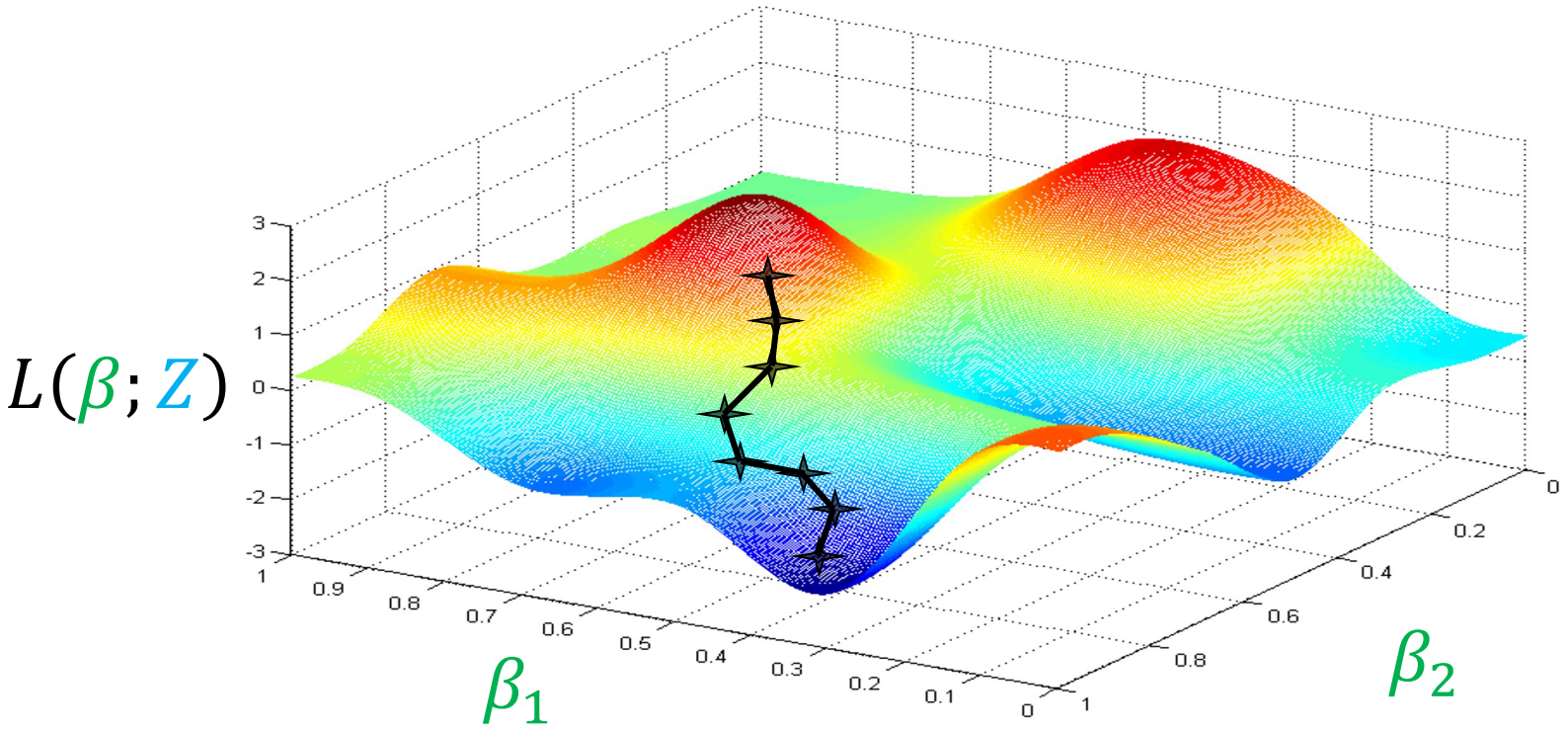
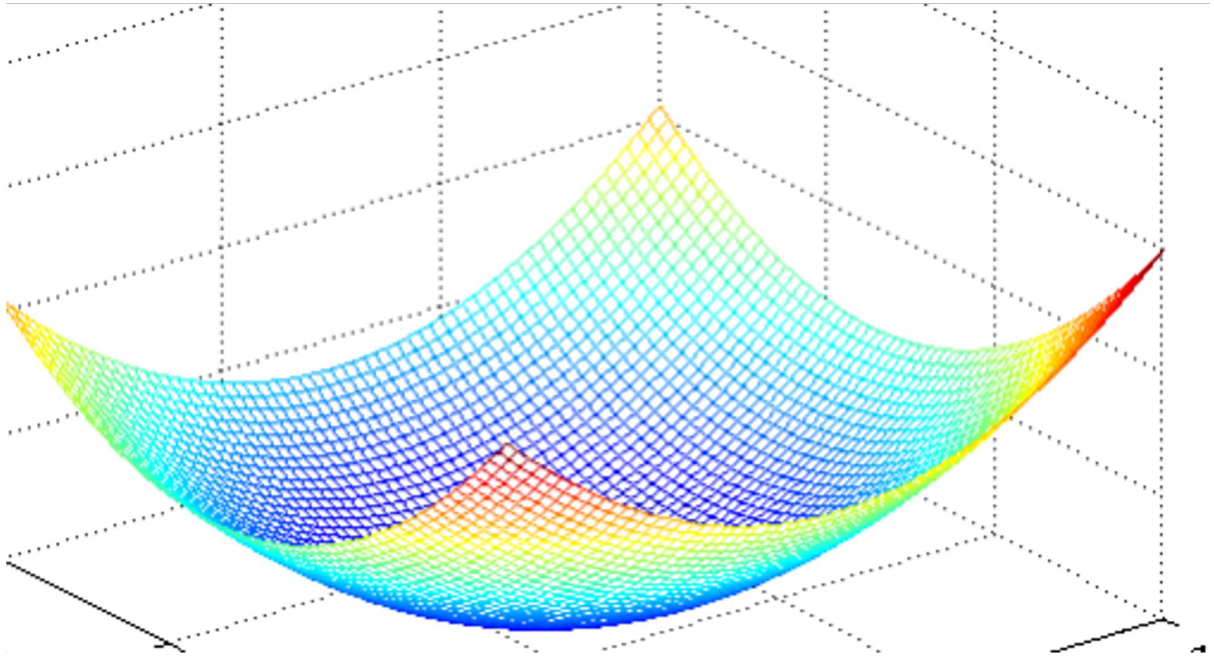


Figure by Andrew Ng

Strategy 2: Gradient Descent

- Choose initial value for β
- Until we reach a minimum:
  - Choose a new value for β to reduce $L(\beta; Z)$



Linear regression loss is convex, so no local minima

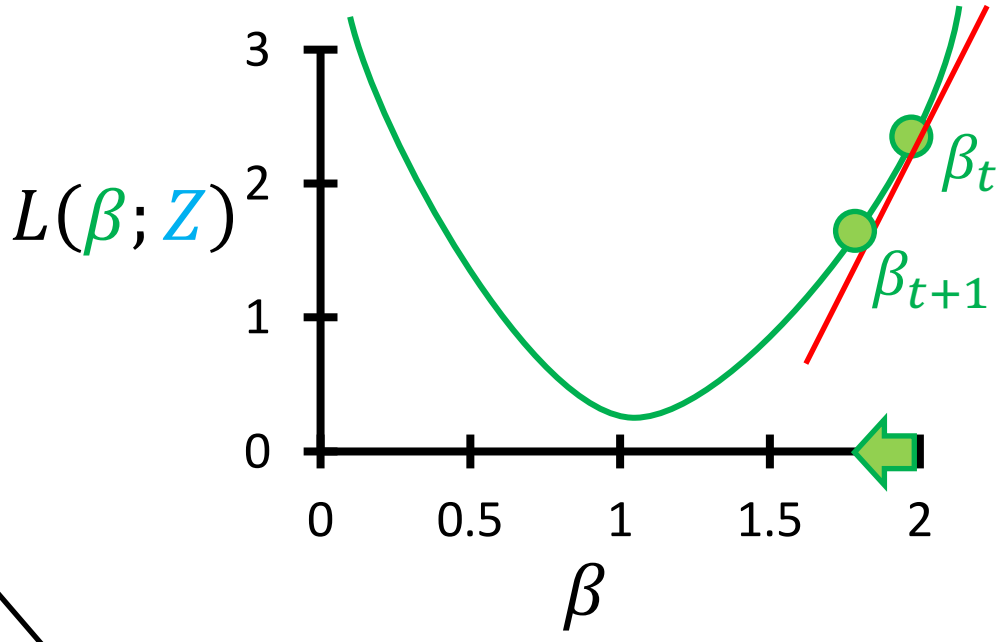
Figure by Andrew Ng

Strategy 2: Gradient Descent

- Initialize $\beta_1 = 0$
- Repeat until convergence:

$$\beta_{t+1} \leftarrow \beta_t - \alpha \cdot \nabla_\beta L(\beta_t; Z)$$

- For linear regression, know the gradient from strategy 1



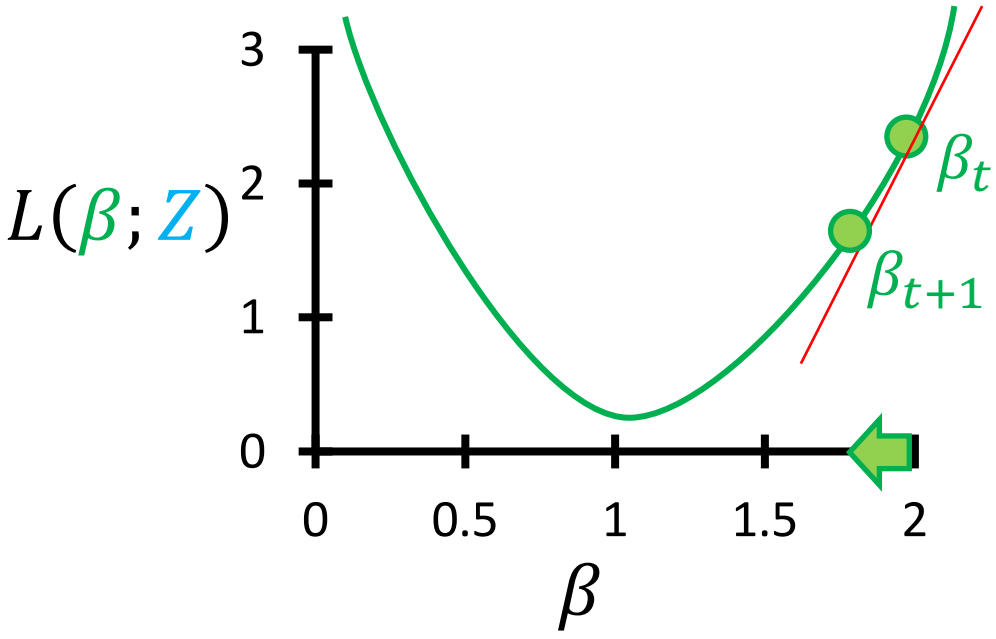
For in-place updates $\beta \leftarrow \beta - \alpha \cdot \nabla_\beta L(\beta; Z)$, compute all components of $\nabla_\beta L(\beta; Z)$ before modifying β

Strategy 2: Gradient Descent

- Initialize $\beta_1 = 0$
- Repeat until convergence:

$$\beta_{t+1} \leftarrow \beta_t - \alpha \cdot \nabla_\beta L(\beta_t; Z)$$

- For linear regression, know the gradient from strategy 1



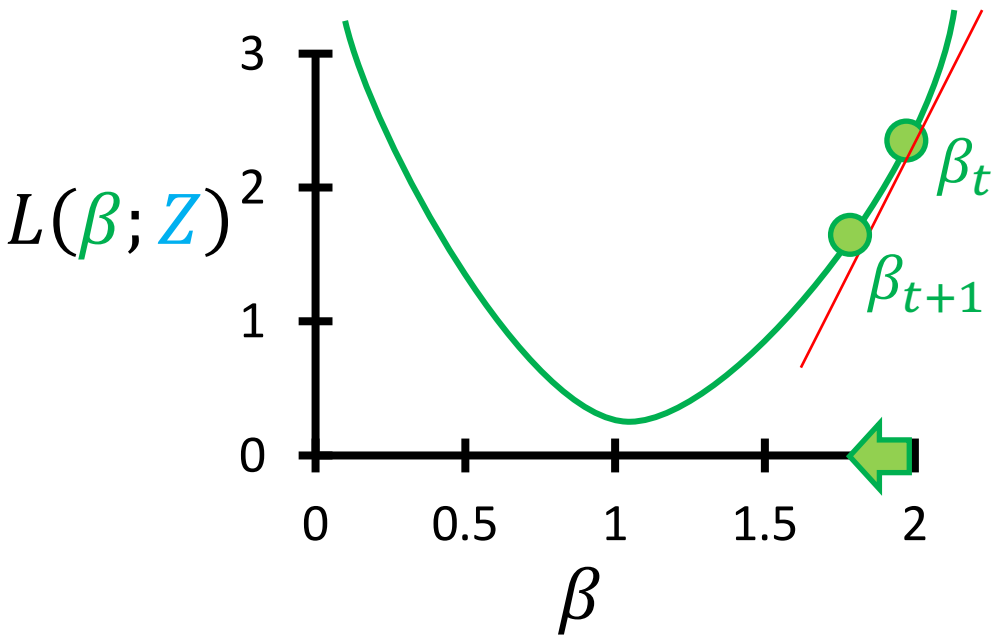
Strategy 2: Gradient Descent

- Initialize $\beta_1 = \vec{0}$
- Repeat until $\|\beta_t - \beta_{t+1}\|_2 \leq \epsilon$:

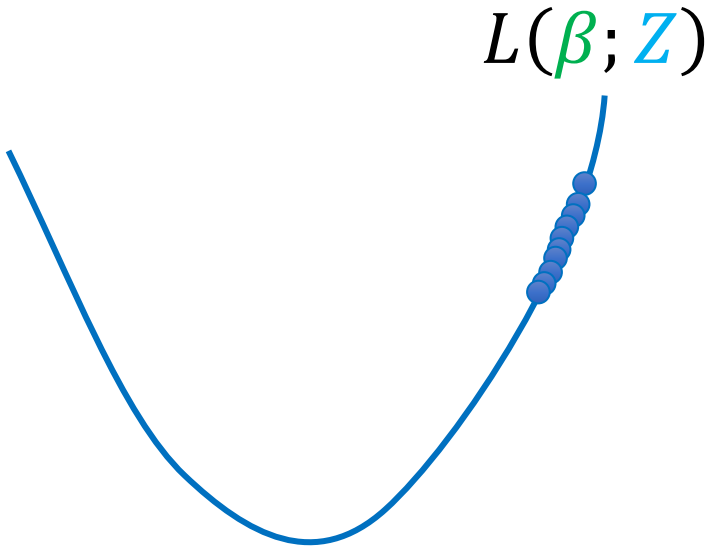
$$\beta_{t+1} \leftarrow \beta_t - \alpha \cdot \nabla_\beta L(\beta_t; Z)$$

- For linear regression, know the gradient from strategy 1

Hyperparameter defining convergence

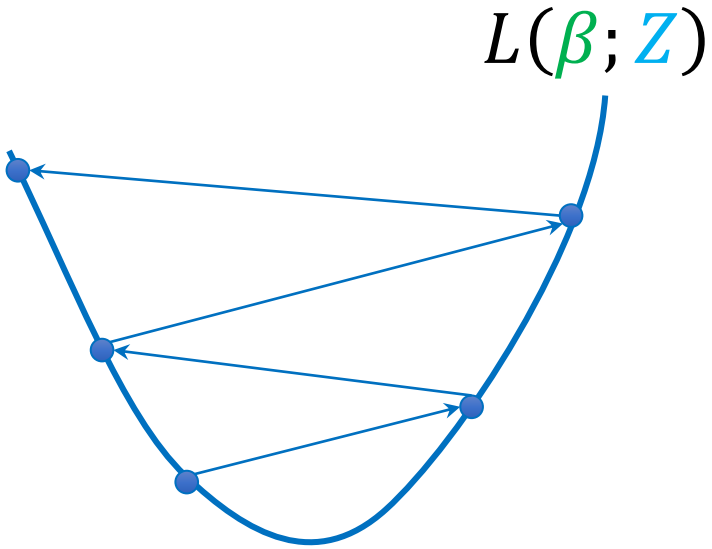


Choice of Learning Rate $\boldsymbol{\alpha}$



Problem: α too small

- $L(\beta; Z)$ decreases slowly



Problem: α too large

- $L(\beta; Z)$ increases!

Plot $L(\beta_t; Z_{\text{train}})$ vs. t to diagnose these problems

Choice of Learning Rate α

- α is a hyperparameter for gradient descent that we need to choose
  - Can set just based on training data

- **Rule of thumb**
  - α **too small:** Loss decreases slowly
  - α **too large:** Loss increases!

- Try rates $\alpha \in \{1.0, 0.1, 0.01, \ldots\}$ (can tune further once one works)

Comparison of Strategies

- **Closed-form solution**
  - No hyperparameters
  - Slow if n or d are large
- **Gradient descent**
  - Need to tune α
  - Scales to large n and d
- For linear regression, there are better optimization algorithms, but gradient descent is very general
  - Accelerated gradient descent is an important tweak that improves performance in practice (and in theory)

L_2 Regularized Linear Regression

- Recall that linear regression with L_2 regularization minimizes the loss

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

L_2 Regularized Linear Regression

- Recall that linear regression with L_2 regularization minimizes the loss

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

- Gradient is

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

Strategy 1: Closed-Form Solution

- Gradient is

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

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

- Always invertible if $\lambda > 0$, so we have

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

Strategy 2: Gradient Descent

- Gradient is

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

- Same algorithm as vanilla linear regression (a.k.a. OLS)
- **Intuition:** The extra term $\lambda\beta$ in the gradient is **weight decay** that encourages β to be small

Supervised Learning

Data $Z = \{(x_i, y_i)\}_{i=1}^{n}$

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

L encodes $y_i \approx f_{\beta}(x_i)$

Model $f_{\hat{\beta}(Z)}$

Regression

Data $Z = \{(x_i, y_i)\}_{i=1}^{n}$

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

L encodes $y_i \approx f_{\beta}(x_i)$

Model $f_{\hat{\beta}(Z)}$

Label is a **real value** $y_i \in \mathbb{R}$

Classification

Data $Z = \{(x_i, y_i)\}_{i=1}^{n}$

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

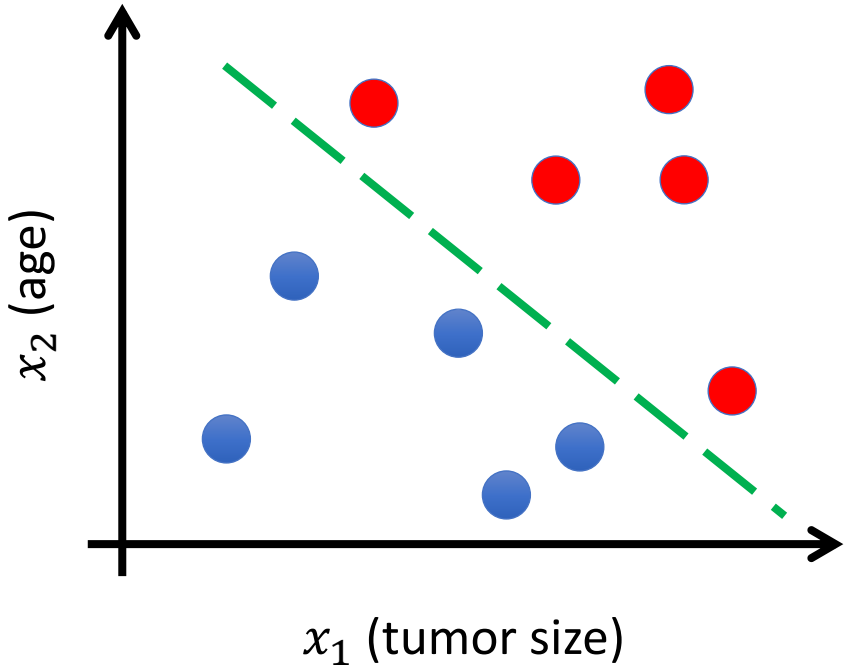
L encodes $y_i \approx f_{\beta}(x_i)$

Model $f_{\hat{\beta}(Z)}$

Label is a **discrete value** $y_i \in \mathcal{Y} = \{1, \ldots, k\}$

(Binary) Classification

- **Input:** Dataset $Z = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
- **Output:** Model $y_i \approx f_\beta(x_i)$



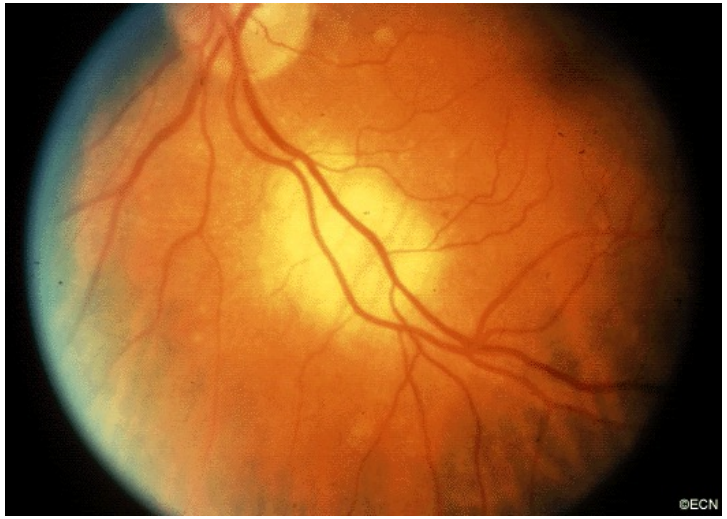


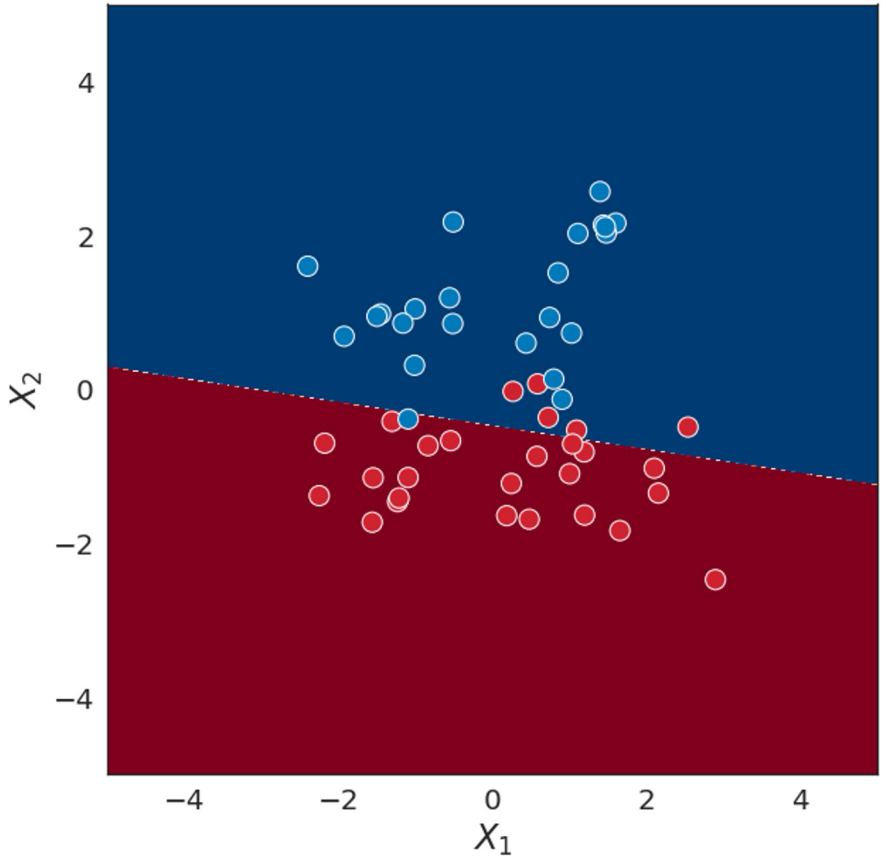
Image: https://eyecancer.com/uncategorized/choroidal-metastasis-test/

Example: Malignant vs. Benign Ocular Tumor

Linear Functions for (Binary) Classification

- **Input:** Dataset $Z = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$

- **Classification:**
  - Labels $y_i \in \{0, 1\}$
  - Predict $y_i \approx 1(\beta^\top x_i \geq 0)$
  - $1(C)$ equals 1 if C is true and 0 if C is false
  - How to learn β? **Need a loss function!**

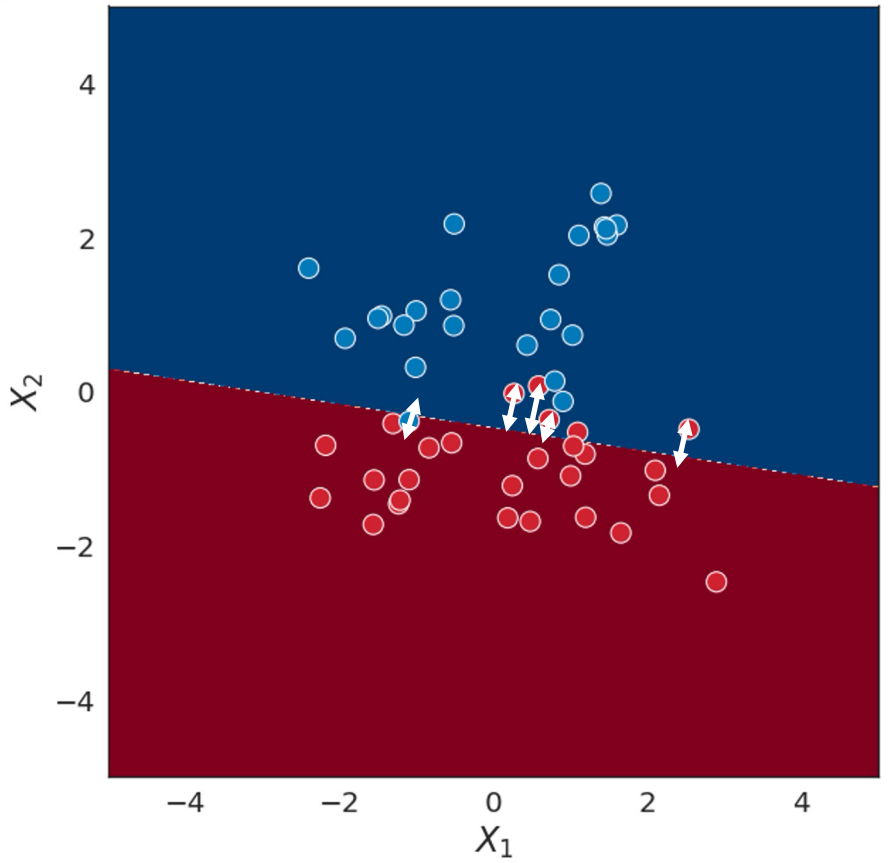


Loss Functions for Linear Classifiers

- **Distance:**

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n} \text{dist}(x_i, f_\beta) \cdot 1\left(f_\beta(x_i) \neq y_i\right)$$

- If $L(\beta; Z) = 0$, then 100% accuracy
- Variant of this loss results in SVM
- But, we will consider a more general strategy



$$L(\beta; Z) = 1.2$$

Maximum Likelihood Estimation

- Our first **probabilistic** viewpoint on learning (from statistics)

- Given x_i, **suppose** y_i is drawn i.i.d. from distribution $p_{Y|X}(Y = y \mid x; \beta)$ with parameters β (or density, if y_i is continuous):

$$y_i \sim p_{Y|X}(\cdot \mid x_i; \beta)$$

Y is random variable, not vector

- Typically write $p_\beta(Y = y \mid x)$ or just $p_\beta(y \mid x)$
  - Called a **model** (and $\{p_\beta\}_\beta$ is the **model family**)
  - Will show up convert p_β to f_β later

Maximum Likelihood Estimation

- **Compare to loss function minimization:**
  - **Before:** $y_i \approx f_\beta(x_i)$
  - **Now:** $y_i \sim p_\beta(\cdot | x_i; \beta)$

- **Intuition the difference:**
  - $f_\beta(x_i)$ just provides a point that y_i should be close to
  - $p_\beta(\cdot | x_i; \beta)$ provides a score for each possible y_i

- Maximum likelihood estimation combines the **loss function** and **model family** design decisions

Maximum Likelihood Estimation

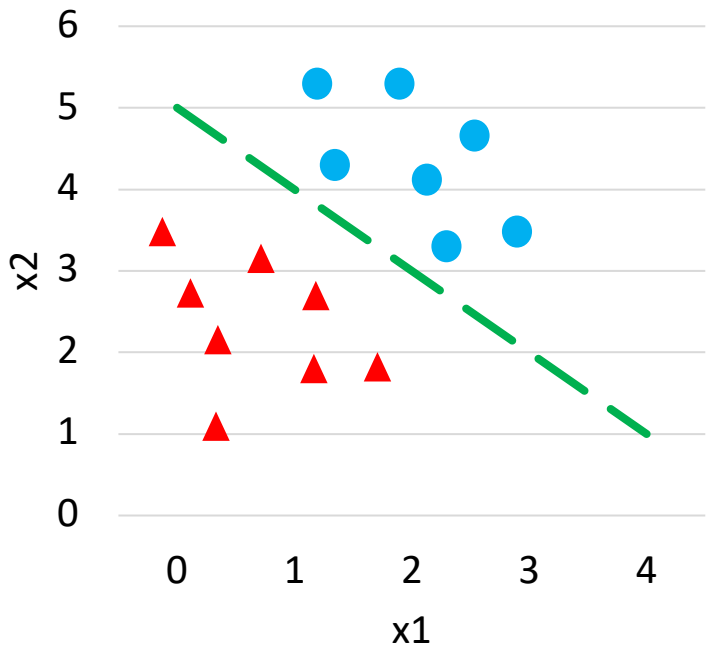
- **Likelihood:** Given model p_β, the probability of dataset Z (replaces loss function in loss minimization view):

$$L(\beta; Z) = p_\beta(Y \mid X) = \prod_{i=1}^{n} p_\beta(y_i \mid x_i)$$

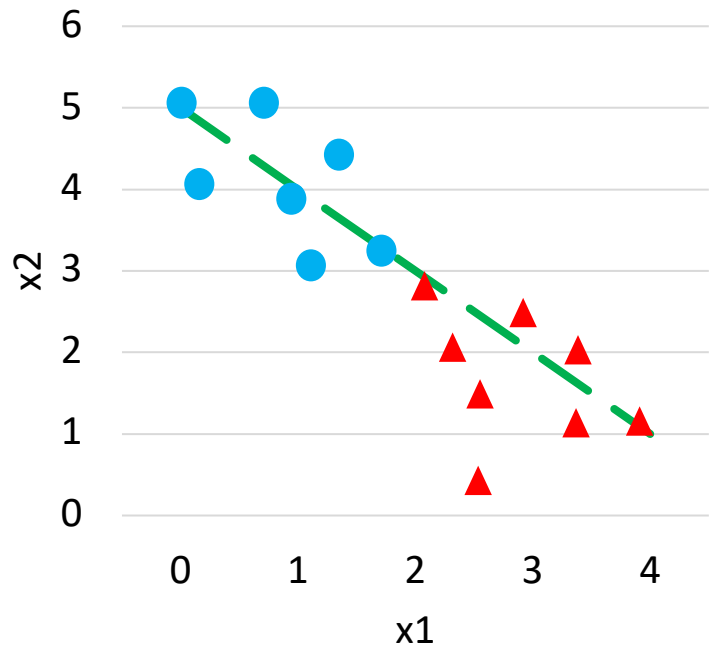
- **Negative Log-likelihood (NLL):** Computationally better behaved form:

$$\ell(\beta; Z) = -\log L(\beta; Z) = -\sum_{i=1}^{n} \log p_\beta(y_i \mid x_i)$$

Intuition on the Likelihood



High likelihood
(Low NLL)



Low likelihood
(High NLL)

Example: Linear Regression

- Assume that the conditional density is

$$p_\beta(y_i \mid x_i) = N(y_i; \beta^\top x_i, 1) = \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{(\beta^\top x_i - y_i)^2}{2}}$$

- $N(y; \mu, \sigma^2)$ is the density of the normal (a.k.a. Gaussian) distribution with mean μ and variance σ^2

Example: Linear Regression

- Then, the likelihood is

$$L(\beta; Z) = \prod_{i=1}^{n} p_\beta(y_i \mid x_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{(\beta^\top x_i - y_i)^2}{2}}$$

- The NLL is

$$\ell(\beta; Z) = -\sum_{i=1}^{n} \log p_\beta(y_i \mid x_i) = \underbrace{\frac{n \log(2\pi)}{2}}_{\text{constant}} + \underbrace{\sum_{i=1}^{n} (\beta^\top x_i - y_i)^2}_{\text{MSE!}}$$

Example: Linear Regression

- Loss minimization for maximum likelihood estimation:

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

- **Note:** Called maximum likelihood estimation since maximizing the likelihood equivalent to minimizing the NLL

Example: Linear Regression

- What about the model family?

$$f_\beta(x) = \arg\max_y p_\beta(y \mid x)$$

$$= \arg\max_y \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{\|\beta^\top x - y\|_2^2}{2}}$$

$$= \beta^\top x$$

- **Recovers linear functions!**

Maximum Likelihood View of ML

- **Two design decisions**
  - **Likelihood:** Probability $p_\beta(\, y \mid x \,)$ of data (x, y) given parameters β
  - **Optimizer:** How do we optimize the NLL? (E.g., gradient descent)

- **Corresponding Loss Minimization View:**
  - **Model family:** Most likely label $f_\beta(x) = \arg\max_y p_\beta(\, y \mid x \,)$
  - **Loss function:** Negative log likelihood (NLL) $\ell(\beta; Z) = -\sum_{i=1}^{n} \log p_\beta(\, y_i \mid x_i \,)$

- Very powerful framework for designing cutting edge ML algorithms
  - Write down the “right” likelihood, form tractable approximation if needed
  - Especially useful for thinking about non-i.i.d. data

What about classification?

Compare to linear regression:

$$p_\beta(y \mid x_i) \propto e^{-\frac{(\beta^\top x_i - y)^2}{2}}$$

- Consider the following choice:

$$p_\beta(Y = 0 \mid x_i) \propto e^{-\frac{\beta^\top x_i}{2}} \text{ and } p_\beta(Y = 1 \mid x_i) \propto e^{\frac{\beta^\top x_i}{2}}$$

- Then, we have

Sigmoid function

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$p_\beta(Y = 1 \mid x_i) = \frac{e^{\frac{\beta^\top x_i}{2}}}{e^{\frac{\beta^\top x_i}{2}} + e^{-\frac{\beta^\top x_i}{2}}} = \frac{1}{1 + e^{-\beta^\top x_i}}$$

What about classification?

Compare to linear regression:

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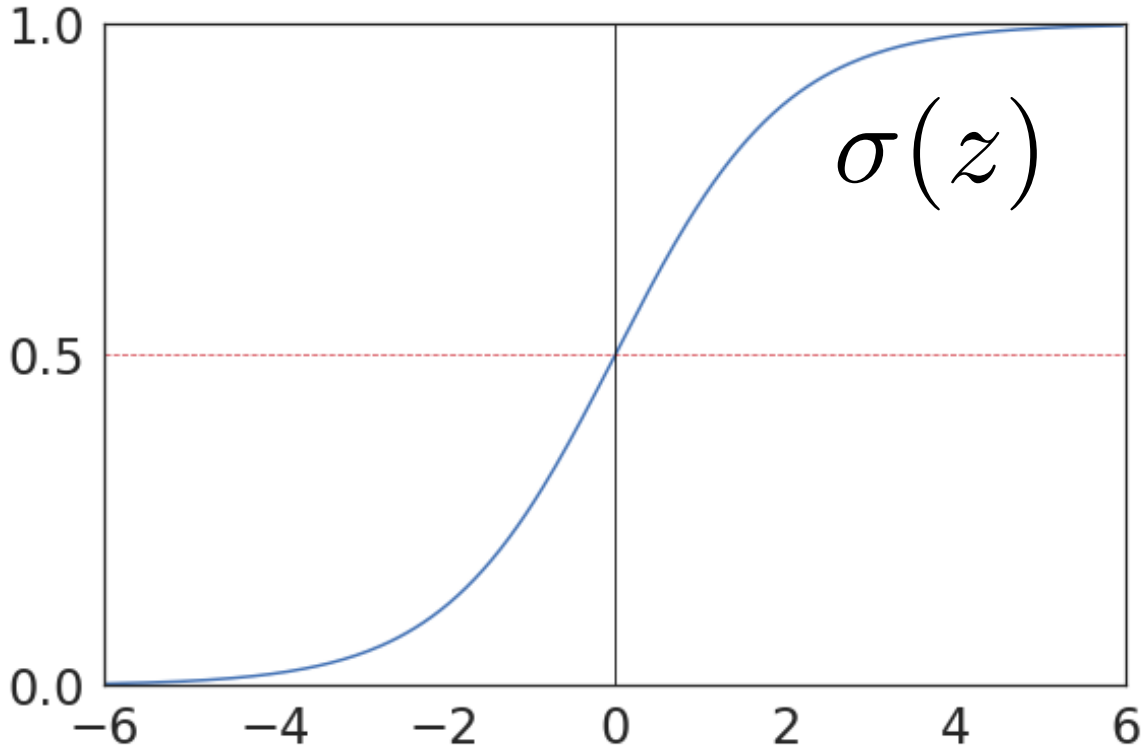
$$p_\beta(Y = 1 \mid x_i) = \frac{e^{\frac{\beta^\top x_i}{2}}}{e^{\frac{\beta^\top x_i}{2}} + e^{-\frac{\beta^\top x_i}{2}}} = \sigma(\beta^\top x_i)$$

- Furthermore, $p_\beta(Y = 0 \mid x_i) = 1 - \sigma(\beta^\top x_i)$

Logistic/Sigmoid Function



$$p_\beta(Y = 1 \mid x_i) = \sigma(\beta^\top x_i)$$

Logistic Regression Model Family

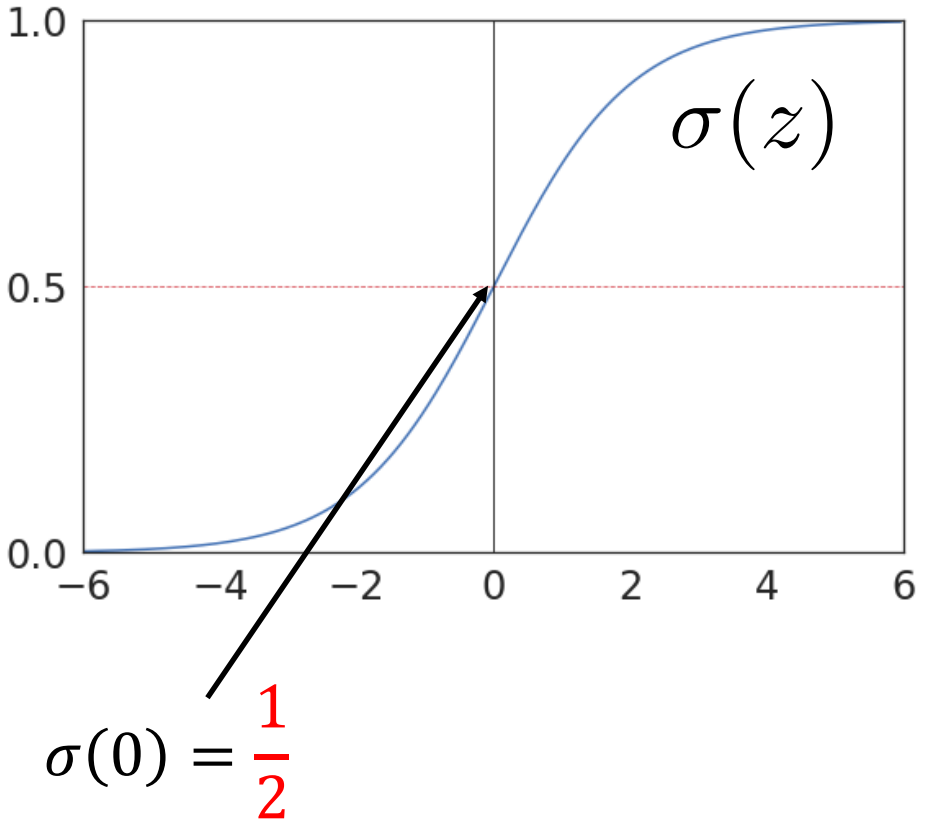
$$f_\beta(x) = \arg\max_y p_\beta(y \mid x)$$

$$= \arg\max_y \begin{cases} \sigma(\beta^\top x) & \text{if } y = 1 \\ 1 - \sigma(\beta^\top x) & \text{if } y = 0 \end{cases}$$

$$= \begin{cases} 1 & \text{if } \sigma(\beta^\top x) \geq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

$$= \begin{cases} 1 & \text{if } \beta^\top x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

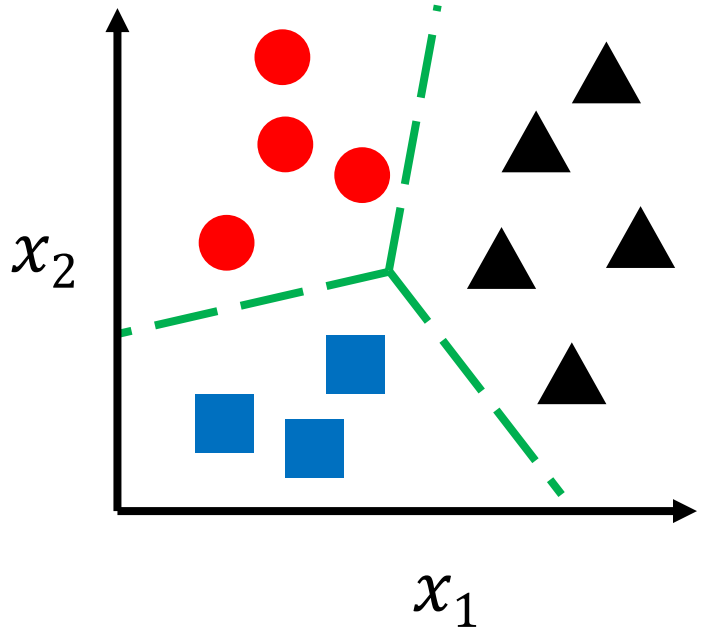
$$= 1(\beta^\top x \geq 0)$$



- **Recovers linear classifiers!**

Multi-Class Classification

- What about more than two classes?
  - **Disease diagnosis:** healthy, cold, flu, pneumonia
  - **Object classification:** desk, chair, monitor, bookcase
  - In general, consider a finite space of labels $\mathcal{Y}$



Multi-Class Logistic Regression

- **Strategy:** Include separate β_y for each label $y \in \mathcal{Y} = \{1, \ldots, k\}$
- Let $p_\beta(\, y \mid x \,) \propto e^{\beta_y^\top x}$, i.e.

$$p_\beta(\, y \mid x \,) = \frac{e^{\beta_y^\top x}}{\sum_{y' \in \mathcal{Y}} e^{\beta_{y'}^\top x}}$$

- We define $\text{softmax}(z_1, \ldots, z_k) = \left[\frac{e^{z_1}}{\sum_{i=1}^k e^{z_i}} \quad \cdots \quad \frac{e^{z_k}}{\sum_{i=1}^k e^{z_i}} \right]$
- Then, $p_\beta(\, y \mid x \,) = \text{softmax}\left(\beta_1^\top x, \ldots, \beta_k^\top x\right)_y$
  - Thus, sometimes called **softmax regression**

Multi-Class Logistic Regression

- **Model family**
  - $f_\beta(x) = \arg\max_y p_\beta(y \mid x) = \arg\max_y \frac{e^{\beta_y^\top x}}{\sum_{y' \in y} e^{\beta_{y'}^\top x}} = \arg\max_y \beta_y^\top x$

- **Optimization**
  - Gradient descent on NLL
  - Simultaneously update all parameters $\{\beta_y\}_{y \in y}$

Classification Metrics

- While we minimize the NLL, we often evaluate using **accuracy**

- However, even accuracy isn't necessarily the "right" metric
  - If 99% of labels are negative (i.e., $y_i = 0$), accuracy of $f_\beta(x) = 0$ is 99%!
  - For instance, very few patients test positive for most diseases
  - "Imbalanced data"

- What are alternative metrics for these settings?

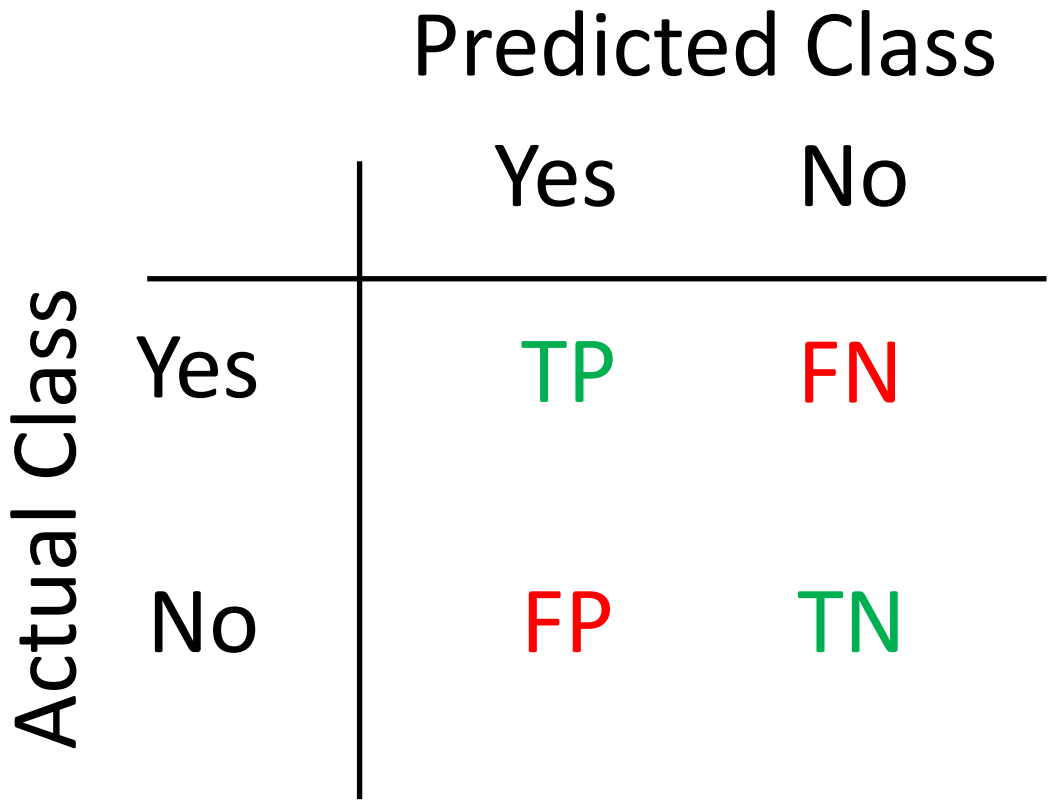
Classification Metrics

- **Classify test examples as follows:**
  - **True positive (TP):** Actually positive, predictive positive
  - **False negative (FN):** Actually positive, predicted negative
  - **True negative (TN):** Actually negative, predicted negative
  - **False positive (FP):** Actually negative, predicted positive

- Many metrics expressed in terms of these; for example:

$$\text{accuracy} = \frac{TP + TN}{n} \qquad \text{error} = 1 - \text{accuracy} = \frac{FP + FN}{n}$$

Confusion Matrix



Confusion Matrix

		Predicted Class: Yes	Predicted Class: No
Actual Class	Yes	3 TP	4 FN
	No	6 FP	37 TN

Accuracy = 0.8

Classification Metrics

- For imbalanced metrics, we roughly want to disentangle:
  - Accuracy on “positive examples”
  - Accuracy on “negative examples”

- Different definitions are possible (and lead to different meanings)!

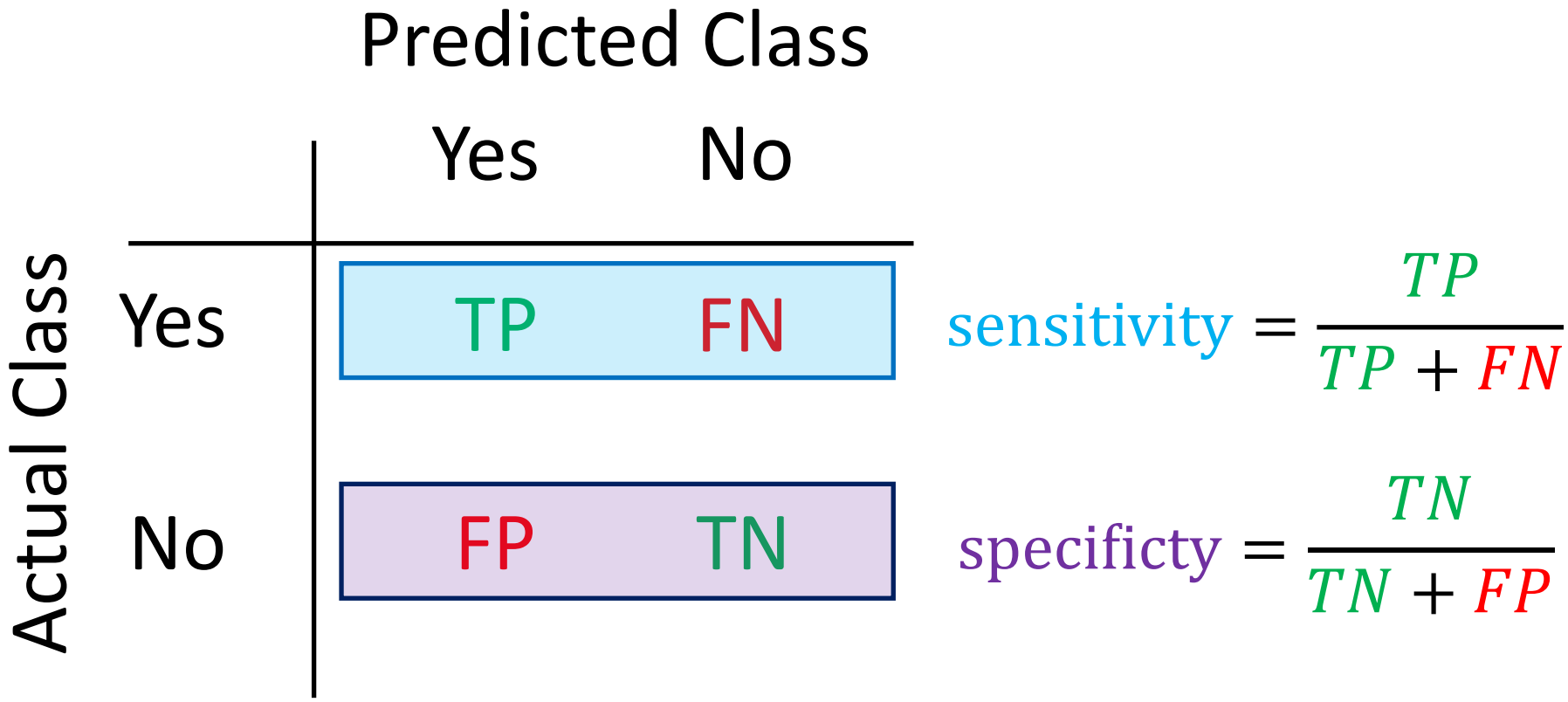
Sensitivity & Specificity

- **Sensitivity:** What fraction of **actual positives** are **predicted positive**?
  - **Good sensitivity:** If you have the disease, the test correctly detects it
  - Also called **true positive rate**

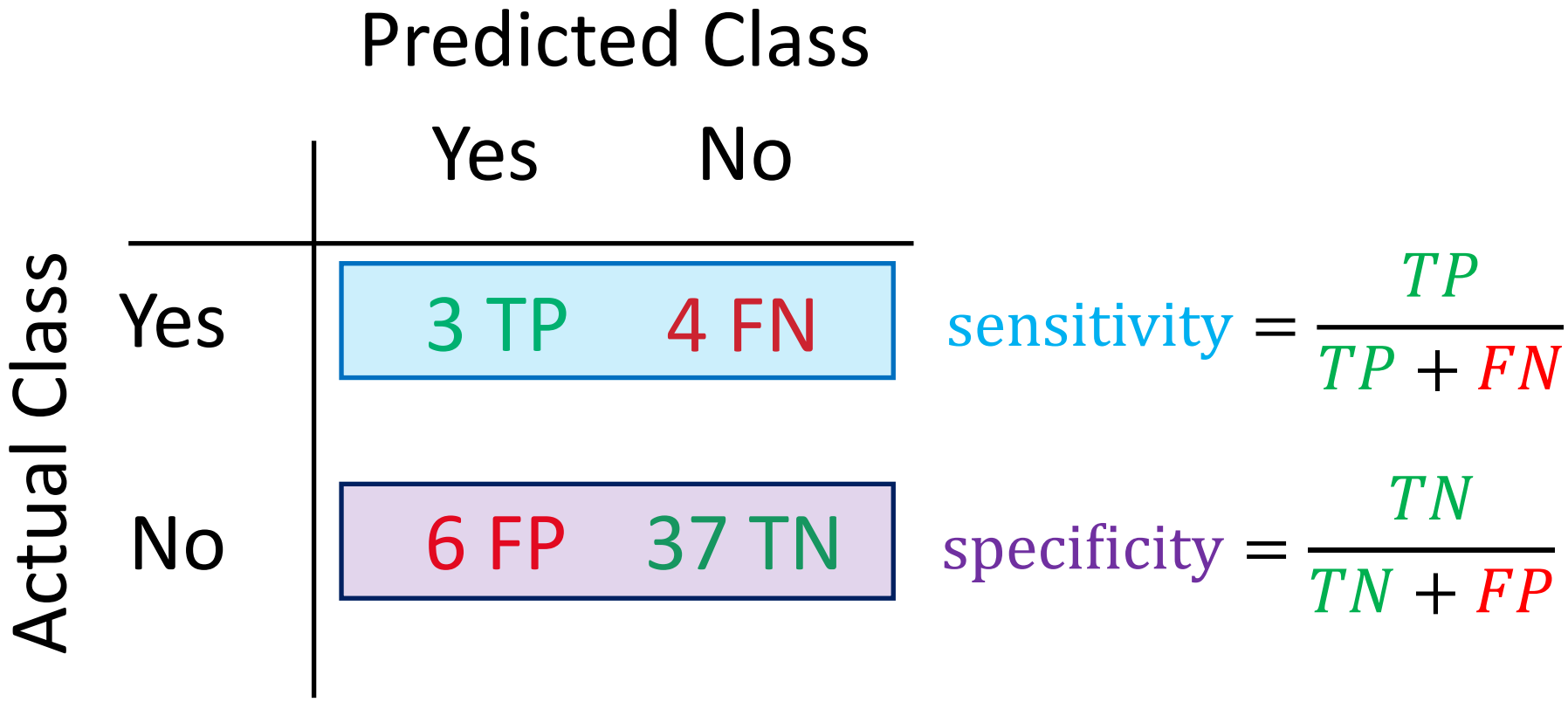
- **Specificity:** What fraction of **actual negatives** are **predicted negative**?
  - **Good specificity:** If you do not have the disease, the test says so
  - Also called **true negative rate**

- Commonly used in medicine

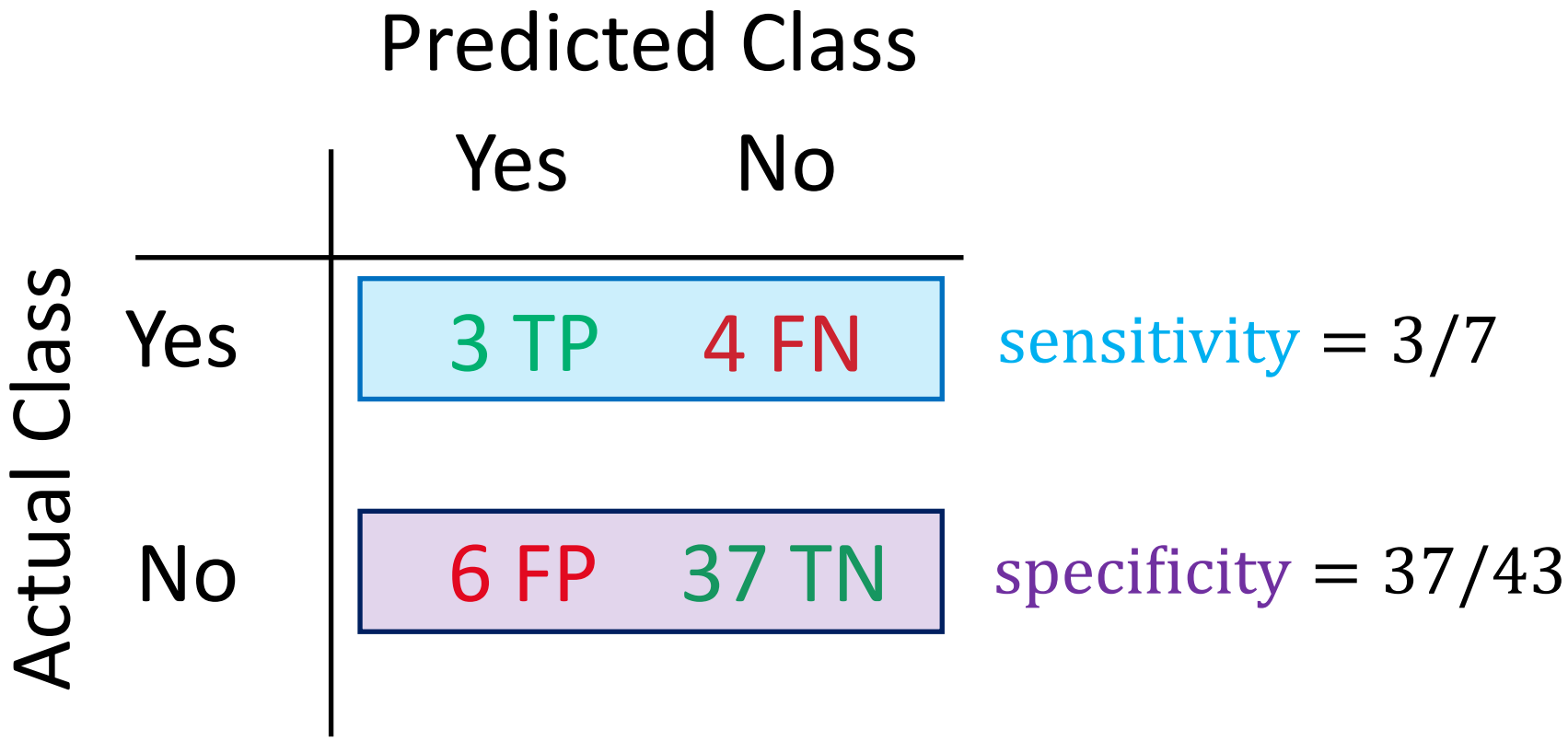
Sensitivity & Specificity



Sensitivity & Specificity



Sensitivity & Specificity



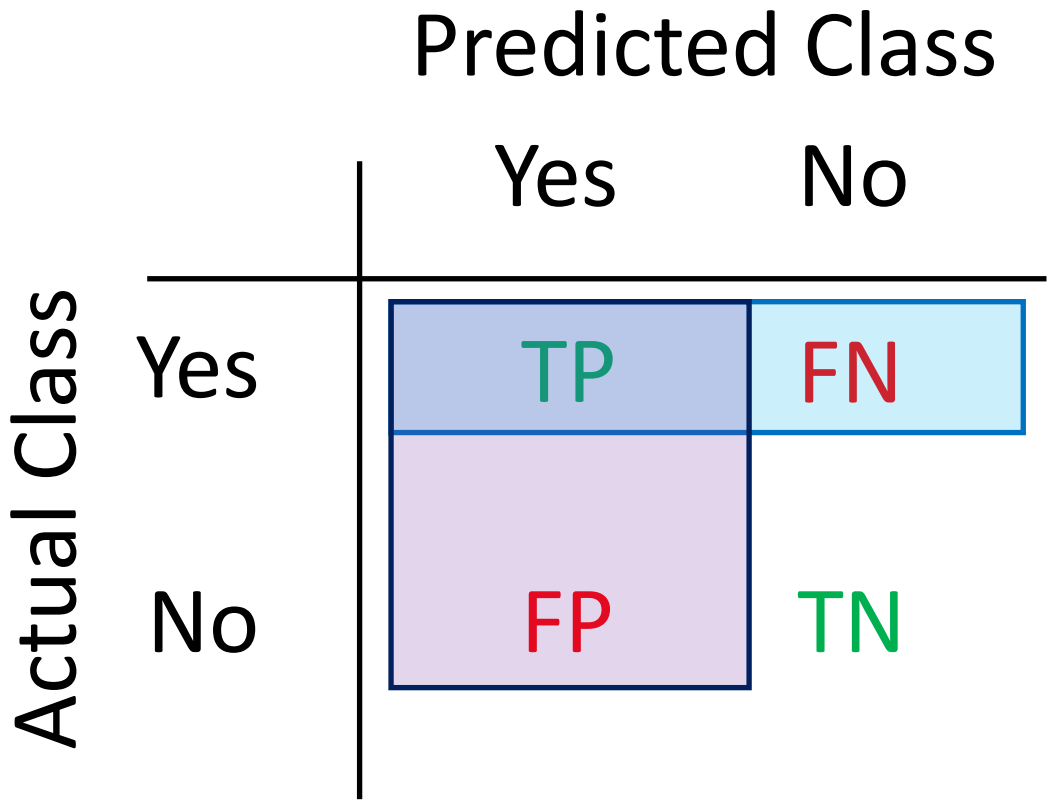
Precision & Recall

- **Recall:** What fraction of **actual positives** are **predicted positive**?
  - **Good recall:** If you have the disease, the test correctly detects it
  - Also called the **true positive rate** (and sensitivity)

- **Precision:** What fraction of **predicted positives** are **actual positives**?
  - **Good precision:** If the test says you have the disease, then you have it
  - Also called **positive predictive value**

- Used in information retrieval, NLP

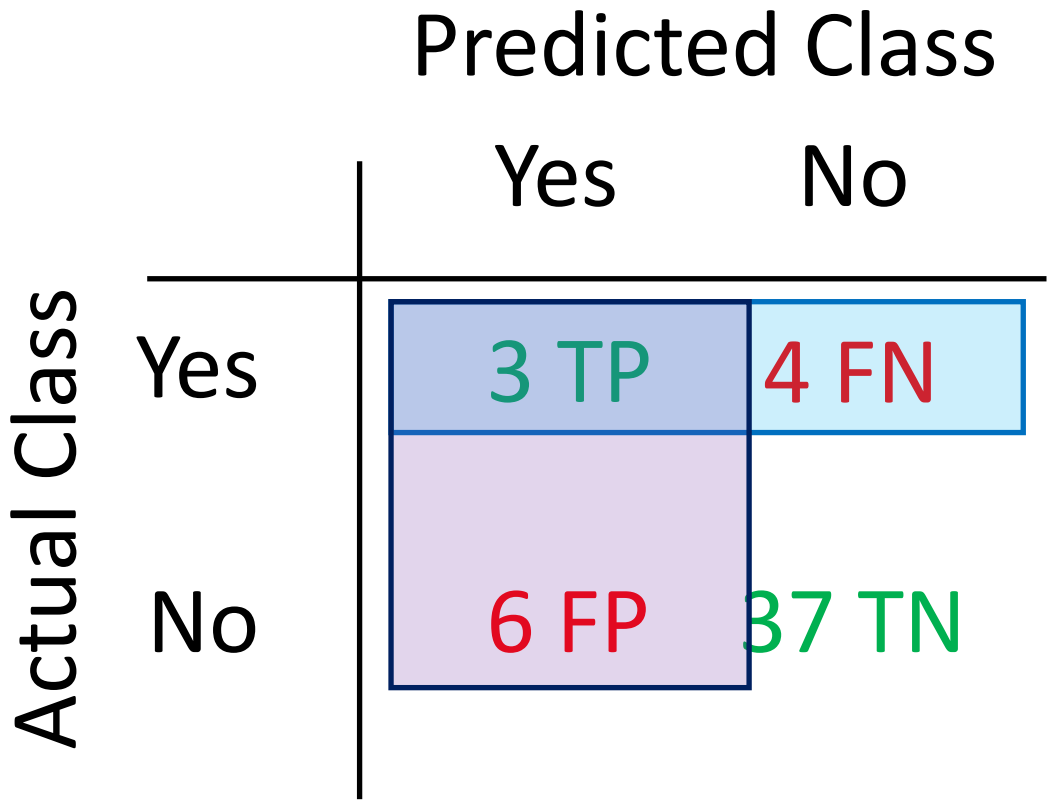
Precision & Recall



$$\text{recall} = \frac{TP}{TP + FN}$$

$$\text{precision} = \frac{TP}{TP + FP}$$

Precision & Recall



$$\text{recall} = \frac{TP}{TP + FN}$$

$$\text{precision} = \frac{TP}{TP + FP}$$

Precision & Recall