19 January 2023

CIS 5200: MACHINE LEARNING

LINEAR AND LOGISTIC REGRESSION

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Content here draws from material by Vatsal Sharan (USC), Christopher De Sa and Kilian Weinberger (Cornell)

Spring 2023

LOGISTICS - UPCOMING

Homework:

- HW0 due on **Friday, Jan 20, 2023** end of day
- For those on waitlist, email your HW0 to Keshav and Wendi (head TAs)
- HW1 will be out on Monday, Jan 23, 2023

Recitation:

- Sign up link will be posted on Ed this Friday
- Math background recitation next week

Instructor OH:

- Eric and I will run joint office hours after class on Tuesdays 3:30-4:30

OUTLINE - TODAY

- Quick Review of Perceptron
- Logistic Regression
  - MLE perspective
- Linear Regression
  - Least squares solution
  - MLE perspective
- Regularization

PERCEPTRON - SUMMARY

Input space: $\mathcal{X} \subseteq \mathbb{R}^d$

Output space: $\mathcal{Y} = \{-1,1\}$

Hypothesis Class: $\mathcal{F} := \{x \mapsto \text{sign}(w^\top x + b) \,|\, w \in \mathbb{R}^d, b \in \mathbb{R}\}$

Loss function: $\ell(f(x), y) = \begin{cases} 0 & \text{if } f(x) = y \\ 1 & \text{otherwise.} \end{cases}$

Assumption: Linearly separable data

Guarantee: Zero-error on training data after $1/\gamma^2$ iterations for margin γ

PERCEPTRON - FAILURES

XOR:

Led to the AI winter till mid 1980s

Minsky and Papert in a 1969 book "Perceptrons" showed that Perceptron fails on XOR problems

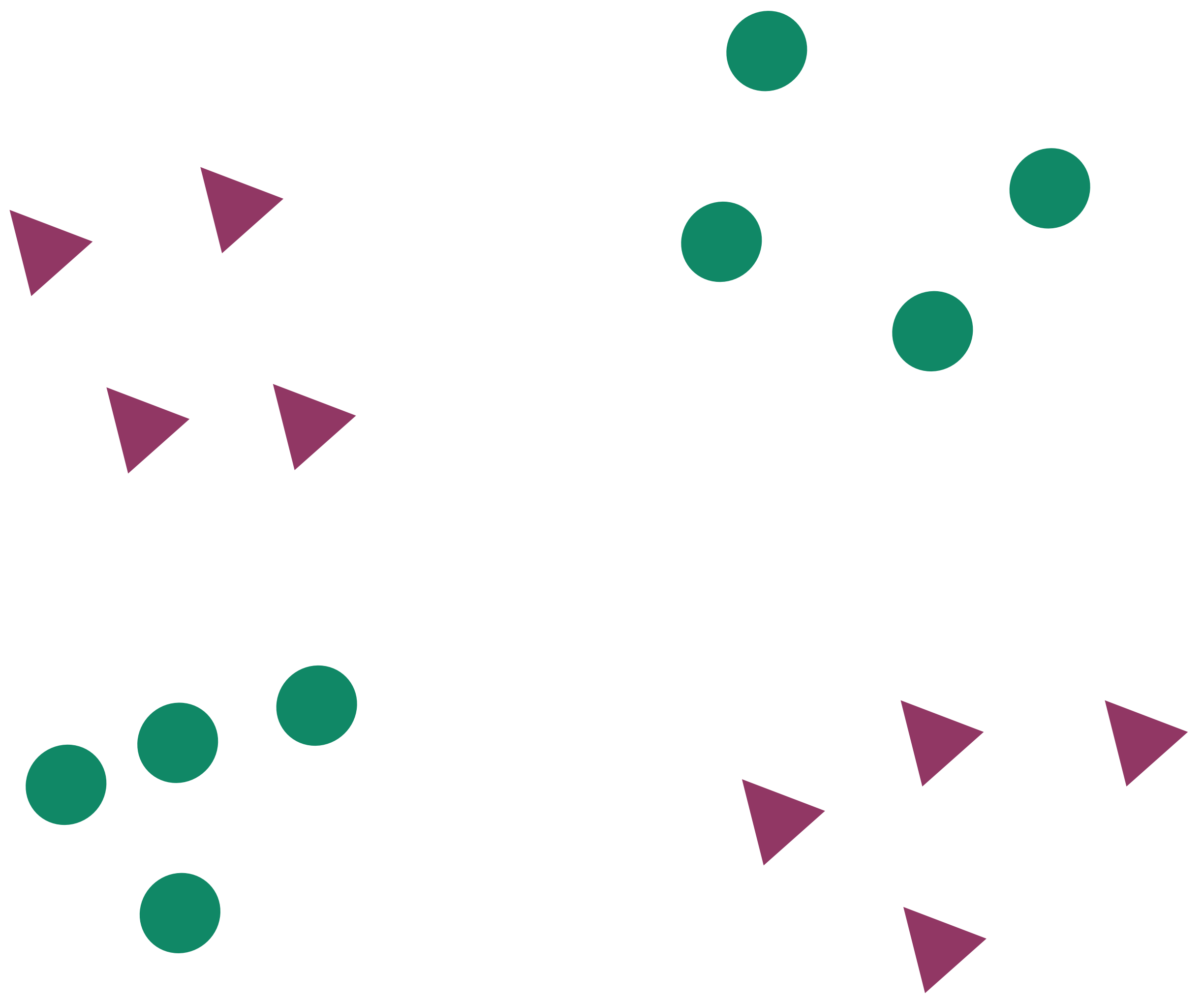
Non-linearly separable data:

Kernels (later in class)

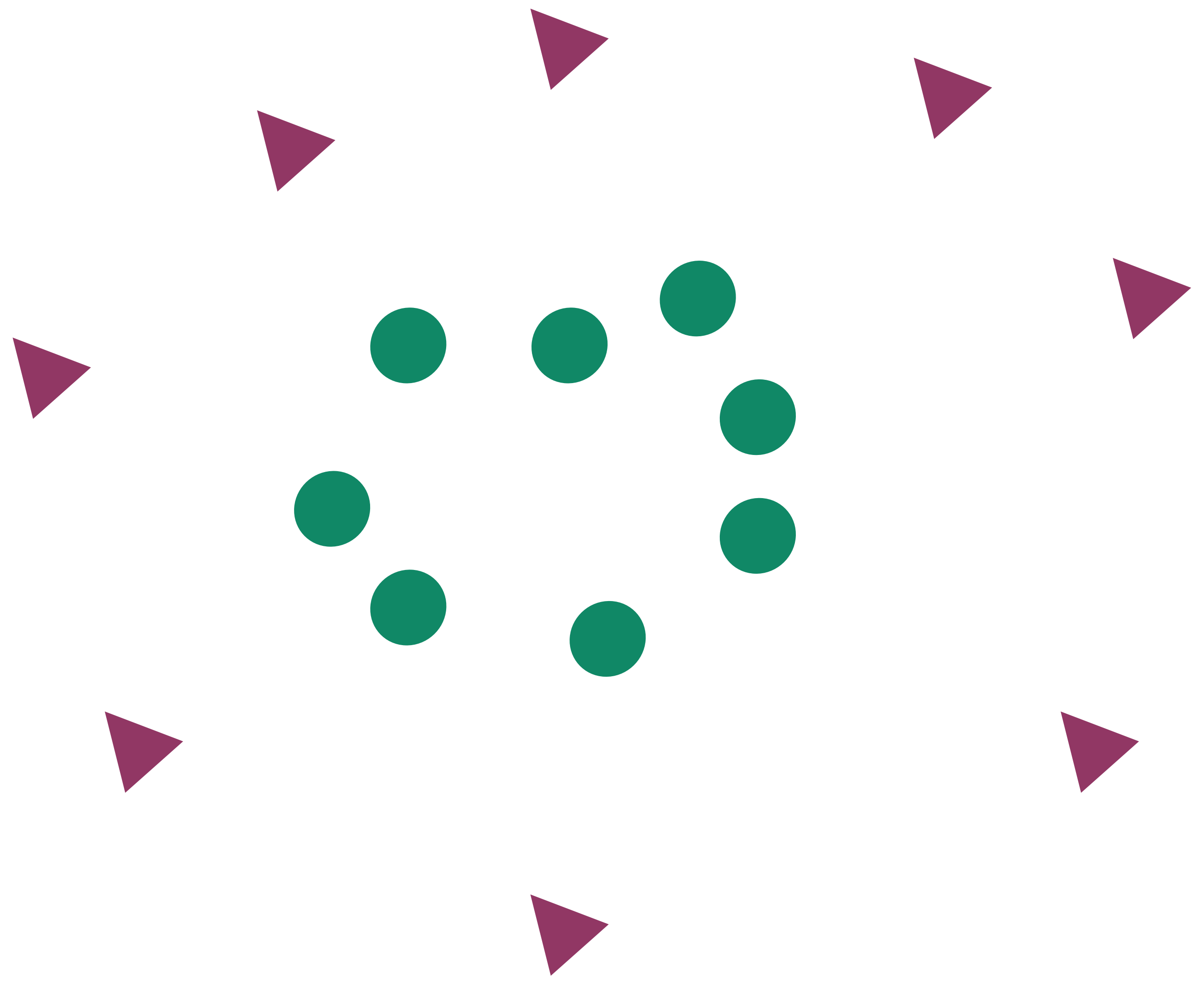
Separable in a lifted space

Noise:

Hard classifier, cannot model inherent noise



XOR

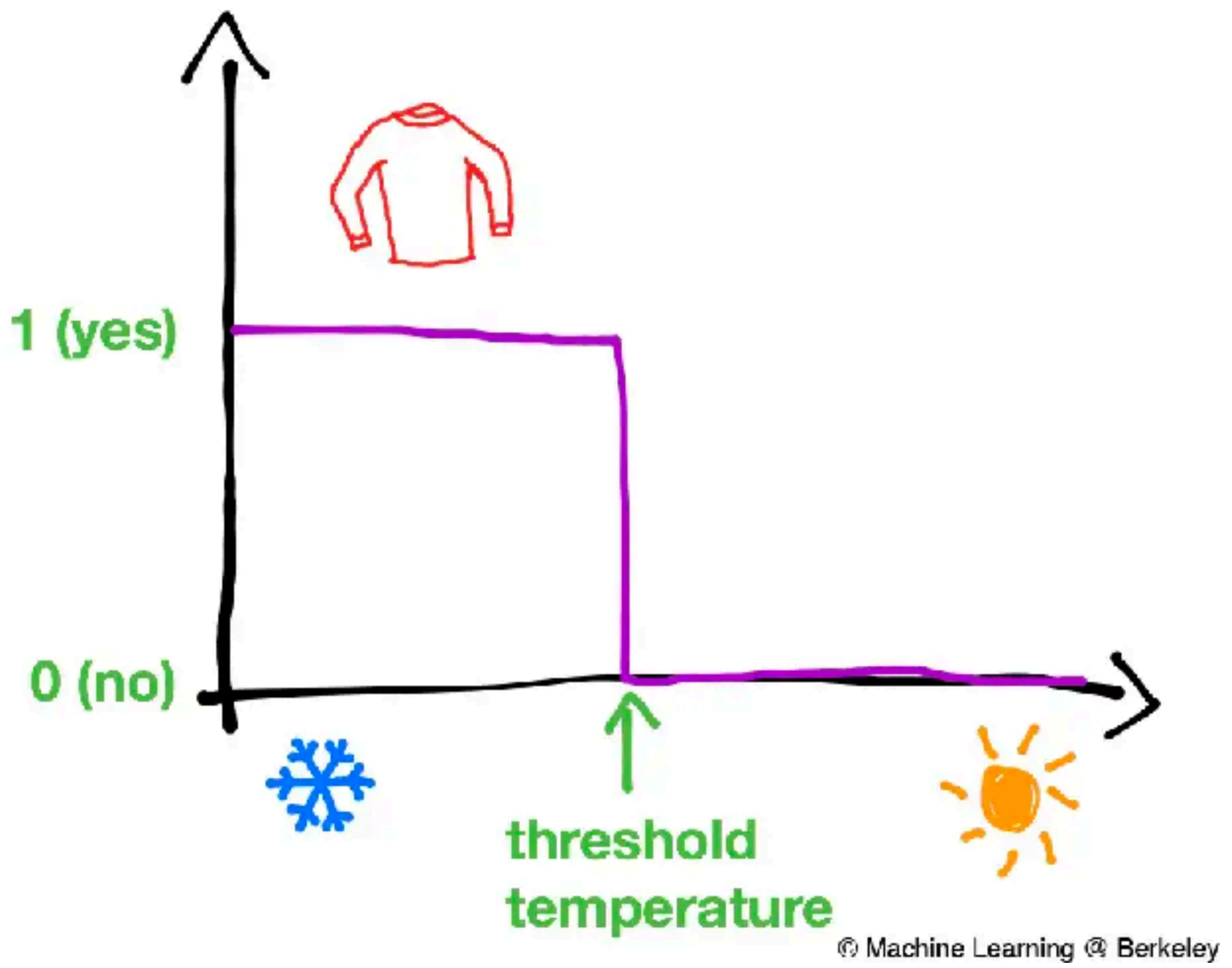


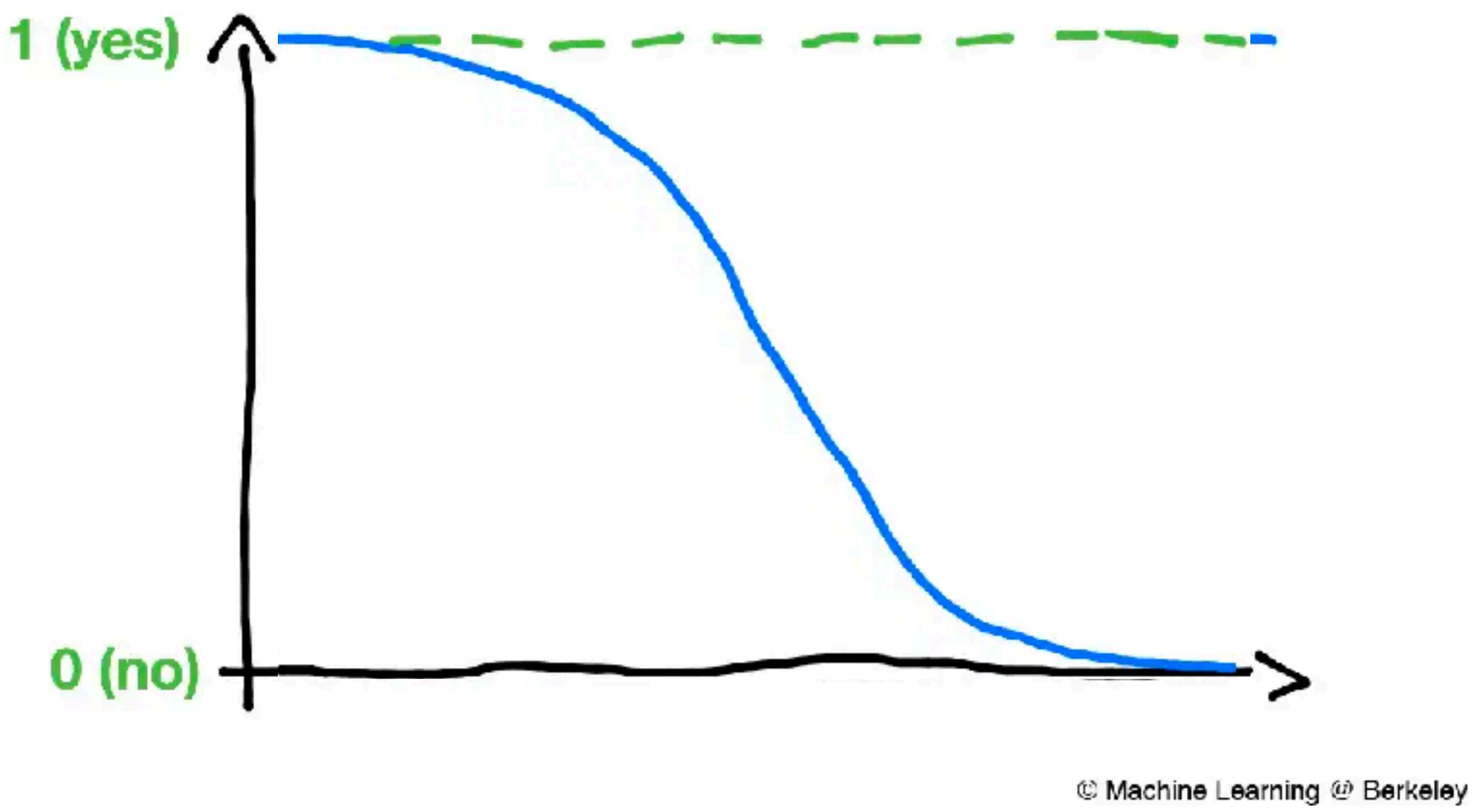
Non-separable Data

NON-DETERMINISTIC INPUTS

Perceptron assumed deterministic labels

But there may be inherent uncertainty in the label





We can model this uncertainty using some function $\eta(x) = P(y = 1 \mid x)$

LOGISTIC FUNCTION

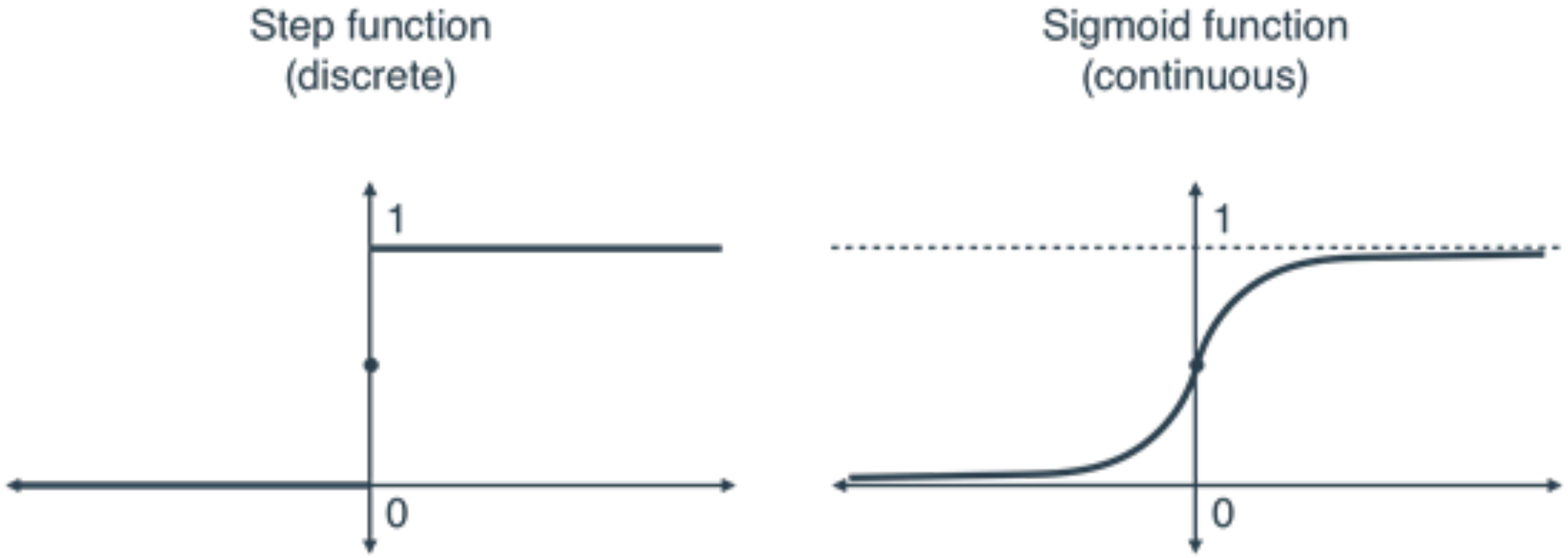
We can model $\eta(x) = P(y = 1 \,|\, x)$ using different functions

$$\text{sign}_{0/1}(a) = \begin{cases} 1 & \text{if } a \geq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Step function

$$\text{sigmoid}(a) = \frac{1}{1 + \exp(-a)}$$

Sigmoid function



$$P(y = 1 \,|\, x) = \eta(x) = \text{sigmoid}(w^\top x) = \frac{1}{1 + \exp(-w^\top x)}$$

More unsure near the decision boundary

$$P(y = -1 \,|\, x) = 1 - \eta(x) = 1 - \text{sigmoid}(w^\top x) = \frac{1}{1 + \exp(w^\top x)}$$

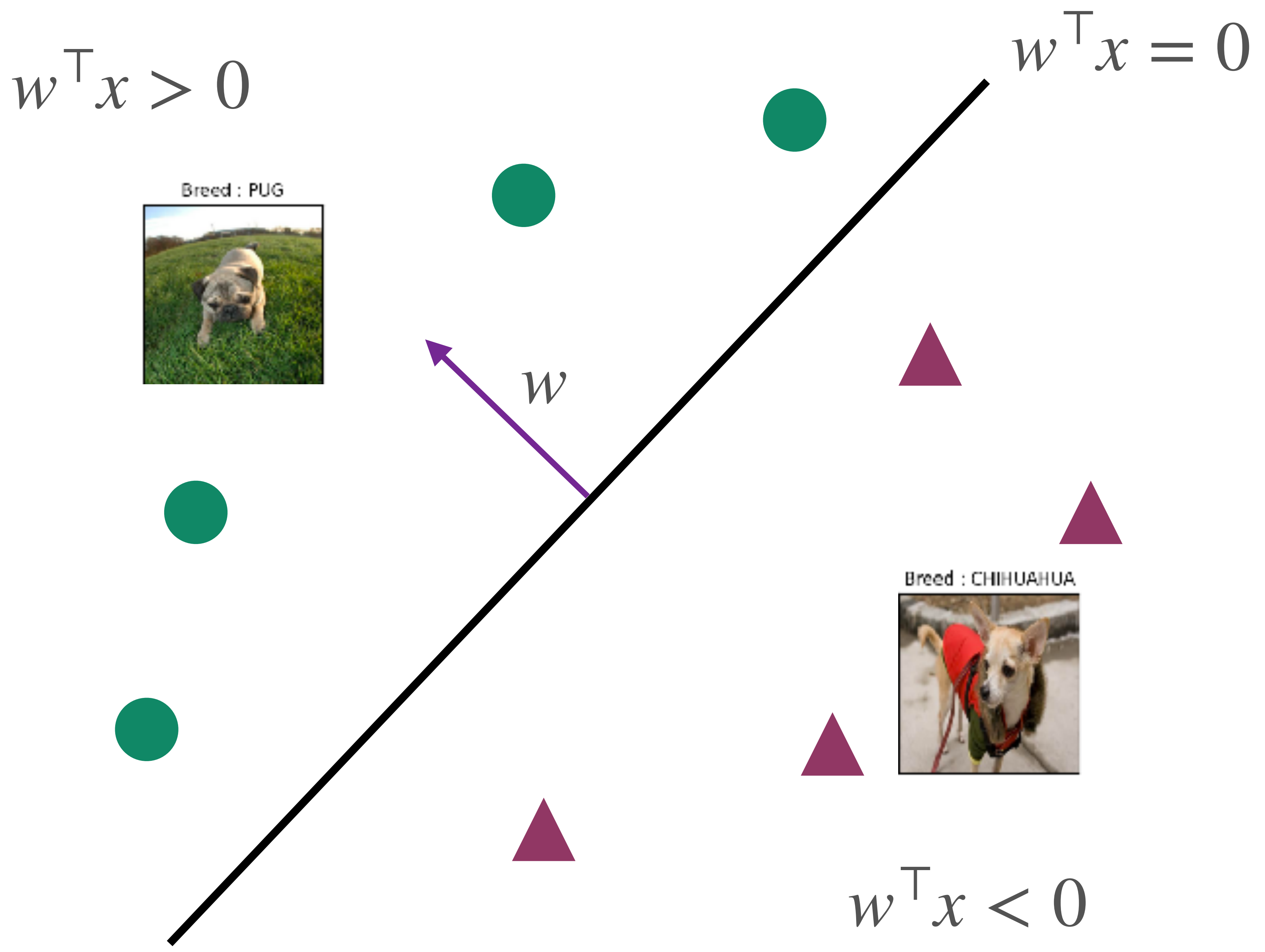
Like perceptron away from the decision boundary

DECISION BOUNDARY

How do we decide the label given the logistic model?

$$\frac{P(y=+1\,|\,x)}{P(y=-1\,|\,x)} = \frac{1+\exp(w^\top x)}{1+\exp(-w^\top x)} = \exp(w^\top x)$$

$= 1$ *when* $w^\top x = 0$



Linear decision boundary

LOSS FUNCTION

Logistic Loss

$$\ell(f(x), y) = \begin{cases} -\log(f(x)) & \text{if } y = 1 \\ -\log(1 - f(x)) & \text{otherwise} \end{cases}$$

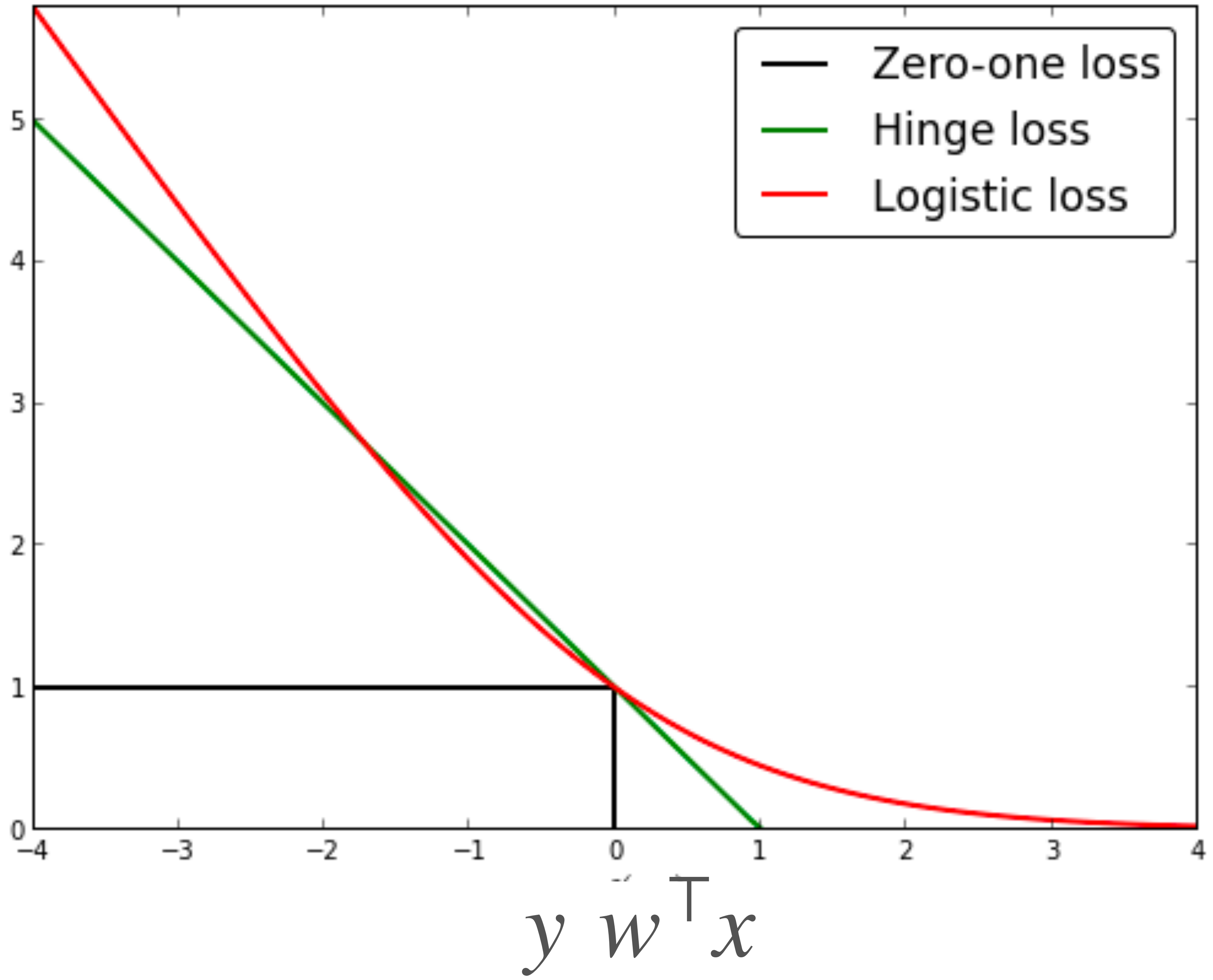
For our setting logistic loss is $\log\left(1 + \exp(-y\, w^\top x)\right)$

0/1 Loss

$$\ell_{0/1}(f(x), y) = 1[f(x) \neq y]$$

For linear classifier this is $1[\mathrm{sgn}(w^\top x) \neq y] = 1[y\, w^\top x < 0]$

Why this loss?



Logistic loss is an upper bound of 0/1 loss

PROBABILISTIC VIEW - MAXIMUM LIKELIHOOD ESTIMATOR

Another way to view the supervised learning task is to maximize the likelihood of seeing the training data

- Make an explicit modeling condition on the data distribution
- Find parameters that maximize the probability of seeing the data

Suppose the parameters of the model are denoted by θ

$$\hat{\mathscr{L}}(\theta) = P(S \mid \theta)$$

S is the training data

$$= \prod_{i=1}^{m} P(x_i, y_i \mid \theta)$$

Training data is i.i.d.

MAXIMUM (CONDITIONAL) LOG LIKELIHOOD

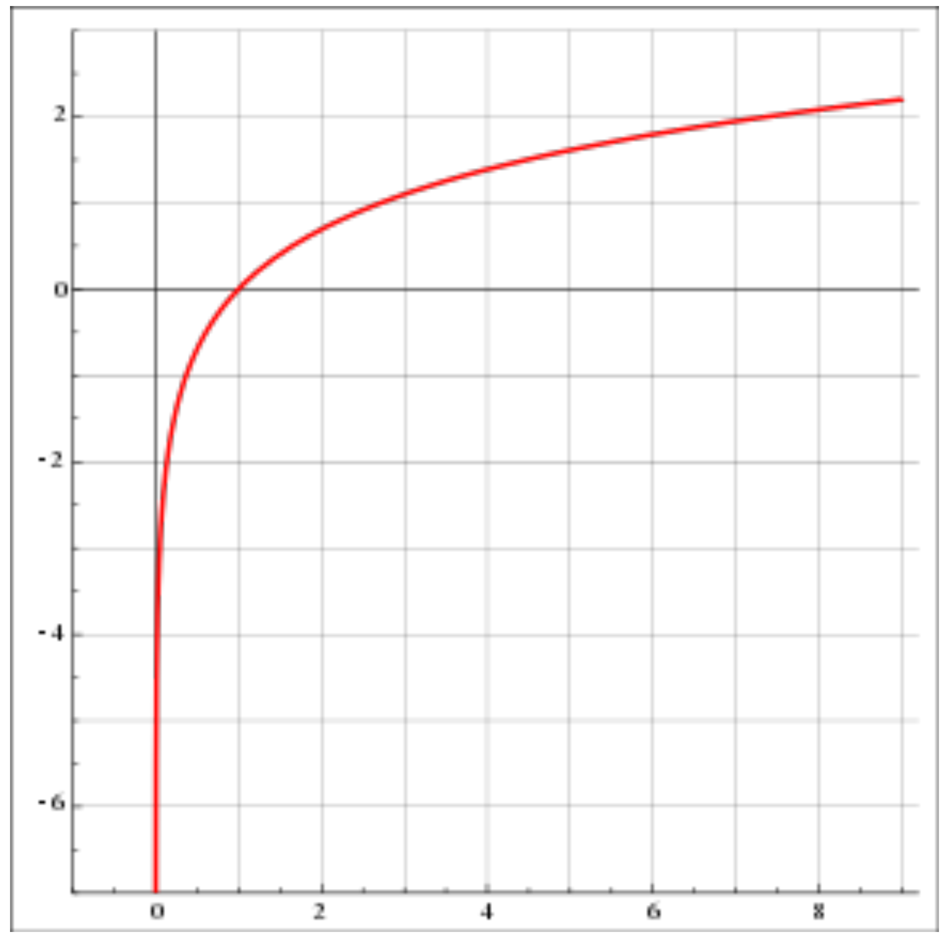
Suppose we don't have any assumption on the generation process of $\boldsymbol{x}$, then we can maximize a conditional likelihood

$$\hat{\mathscr{L}}(\theta) = \prod_{i=1}^{m} P(y_i \mid x_i, \theta)$$

The log-likelihood is then equivalent to:

$$\log \hat{\mathscr{L}}(\theta) = \log\left(\prod_{i=1}^{m} P(y_i \mid x_i, \theta)\right)$$

$$= \sum_{i=1}^{m} \log\left(P(y_i \mid x_i, \theta)\right)$$



$\log$ is an increasing function
Maximizers of both are identical

M(C)LE - LOGISTIC REGRESSION

We have the model for $P(y \mid x, w)$, substituting it gives us

$$\begin{aligned}\log \hat{\mathscr{L}}(w) &= \sum_{i=1}^{m} \log\left(P(y_i \mid x_i, w)\right) \\ &= \sum_{i=1}^{m} \log\left(\frac{1}{1+\exp(-y_i w^\top x_i)}\right) \\ &= -\sum_{i=1}^{m} \log\left(1+\exp(-y_i w^\top x_i)\right)\end{aligned}$$

This is the negative of the logistic loss!

$$\max_w \log \hat{\mathscr{L}}(w) = \min_w \hat{R}(w)$$

LOGISTIC REGRESSION - TRAINING

Training Dataset: $\mathcal{S} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)\}$,
$x_i \in \mathbb{R}^d, y_i \in \{-1,1\}$

Empirical Risk Minimization: Find $\hat{w}$ that minimizes

$$\widehat{R}(w) = \frac{1}{m} \sum_{i=1}^{m} \log\left(1 + \exp(-y_i\, w^\top x_i)\right)$$

How do we solve this minimization problem?

The problem is convex so we can use convex optimization (will discuss in later lectures)

LOGISTIC REGRESSION - SUMMARY

Input space: $\mathscr{X} \subseteq \mathbb{R}^d$ Perceptron

Output space: $\mathscr{Y} = [0,1]$ $\mathscr{Y} = \{-1,1\}$

Hypothesis Class: $\mathscr{F} := \{x \mapsto \text{sigmoid}(w^\top x + b) \mid w \in \mathbb{R}^d, b \in \mathbb{R}\}$

$$\mathscr{F} := \{x \mapsto \text{sign}(w^\top x + b) \mid w \in \mathbb{R}^d, b \in \mathbb{R}\}$$

Loss function: $\ell(f(x), y) = \begin{cases} -\log(f(x)) & \text{if } y = 1 \\ -\log(1 - f(x)) & \text{otherwise} \end{cases}$

$$\ell(f(x), y) = \begin{cases} 0 & \text{if } f(x) = y \\ 1 & \text{otherwise.} \end{cases}$$

SUPERVISED LEARNING

Predict future outcomes based on past outcomes

Inputs $x \in \mathcal{X}$

Labels $y \in \mathcal{Y}$

($\mathcal{Y}$ = Breeds)
"Pug"
"Chihuahua"

Classification

Discrete labels

($\mathcal{Y}$ = Stock prices)
"$130.02"

Regression

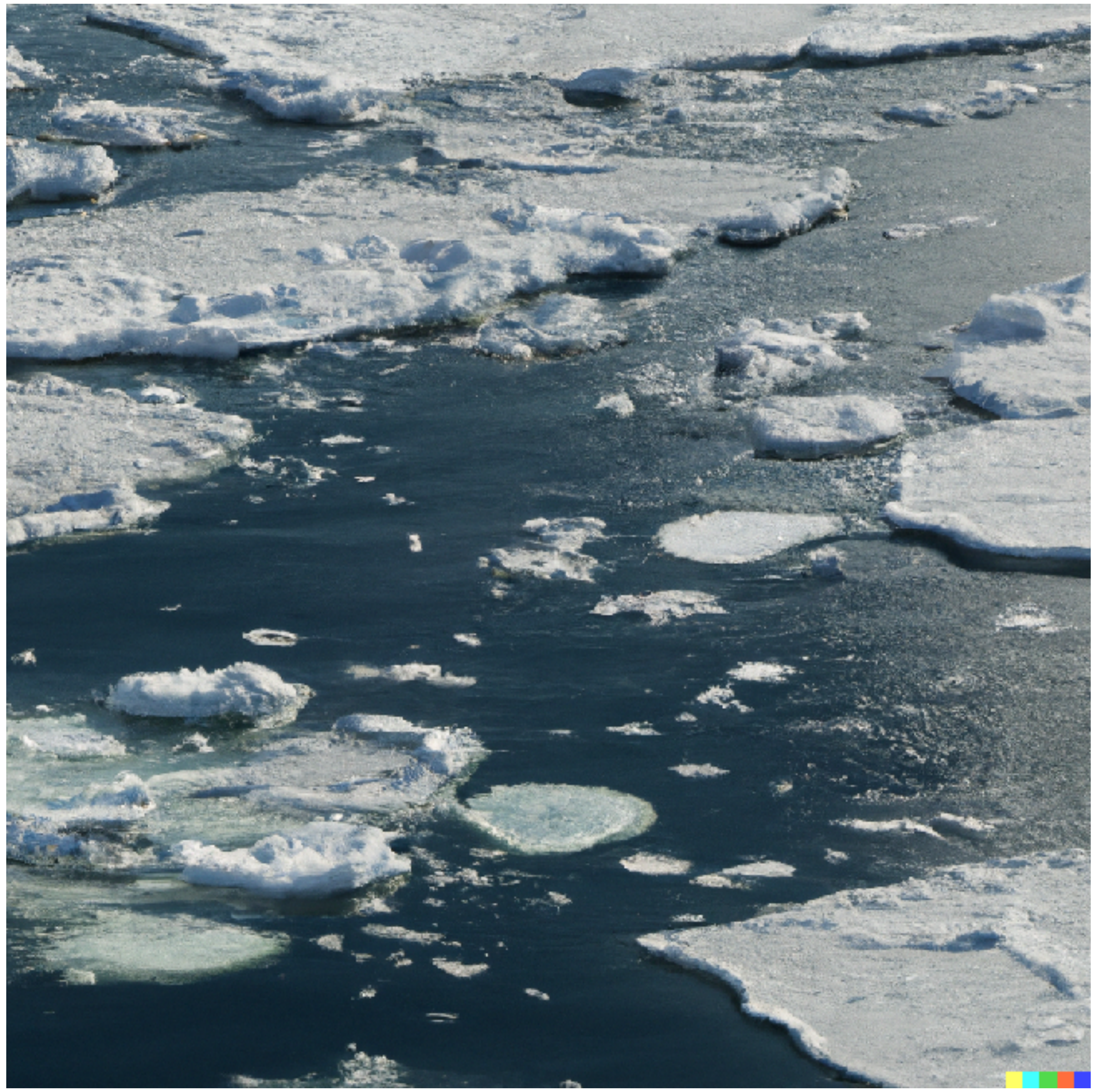
Continuous labels

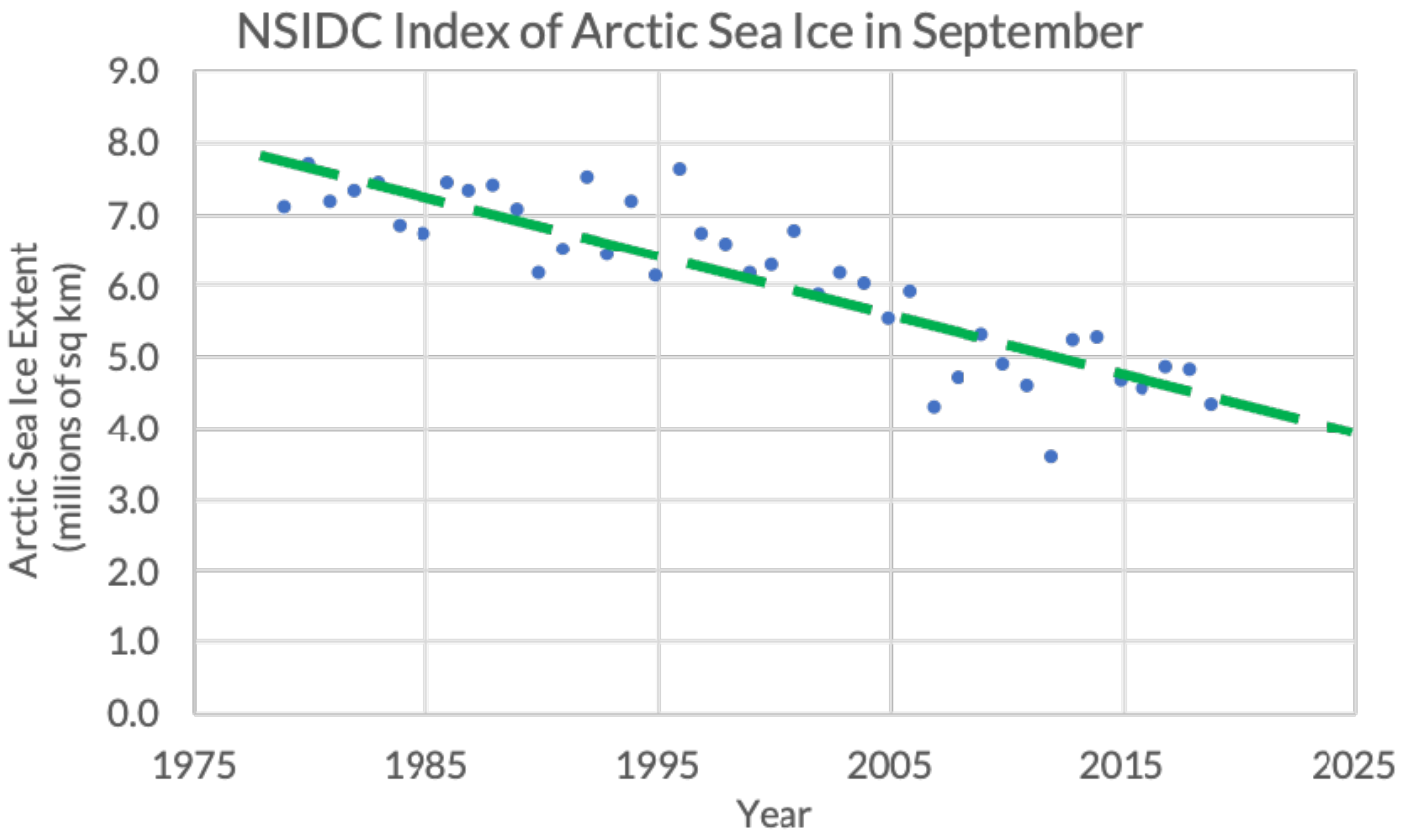
Task: Learn predictor $f : \mathcal{X} \rightarrow \mathcal{Y}$

HYPOTHESIS CLASS - LINEAR REGRESSORS

Similar to perceptron, can ignore bias

Linear regressors $\mathcal{F} := \{x \mapsto w^\top x + b \,|\, w \in \mathbb{R}^d, b \in \mathbb{R}\}$





NSIDC Index of Arctic Sea Ice in September
Arctic Sea Ice Extent (millions of sq km)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1975
1985
1995
2005
2015
2025
Year

Data from https://nsidc.org/arcticseaicenews/sea-ice-tools/

LOSS FUNCTION

Square Loss

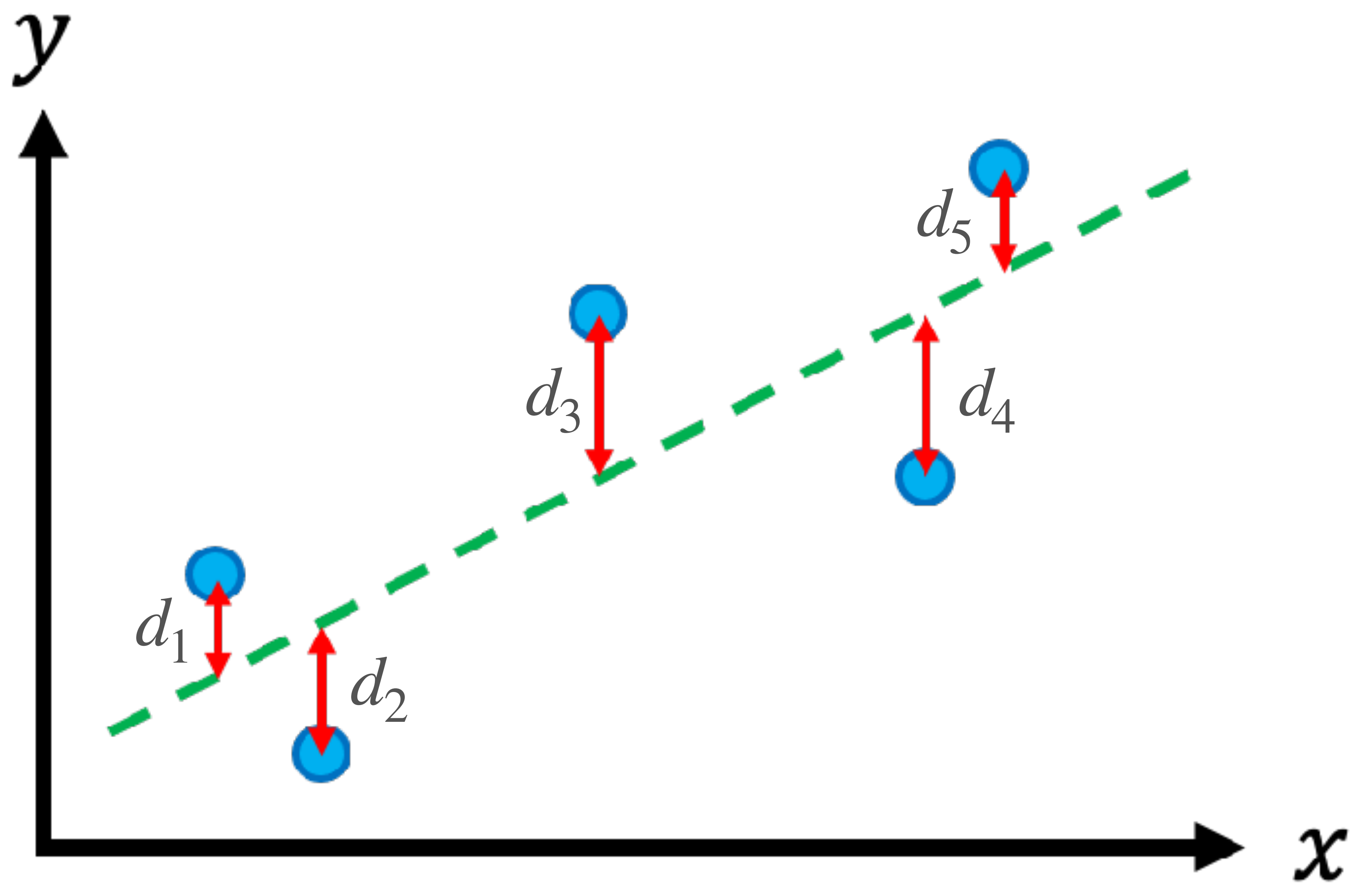
$$\ell(f(x), y) = (f(x) - y)^2$$

$$\text{Square-loss} = \frac{d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2}{5}$$

Absolute Loss

$$\ell(f(x), y) = |f(x) - y|$$

$$\text{Absolute-loss} = \frac{|d_1| + |d_2| + |d_3| + |d_4| + |d_5|}{5}$$



How does square loss behave on outliers?

LINEAR REGRESSION - TRAINING

Training Dataset: $\mathcal{S} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)\}, x_i \in \mathbb{R}^d, y_i \in \mathbb{R}$

Empirical Risk Minimization: Find $\hat{w}$ that minimizes

$$\widehat{R}(w) = \frac{1}{m} \sum_{i=1}^{m} (y_i - w^\top x_i)^2$$

How do we solve this minimization problem?

The problem is convex, in fact we can get a closed form solution

LEAST SQUARES

Loss is convex $\implies$ differentiate to find minimizer

$$\widehat{R}(w) = \frac{1}{m}\sum_{i=1}^{m}(y_i - w^\top x_i)^2 \xrightarrow[]{\text{Take derivative and set to 0}} \frac{2}{m}\sum_{i=1}^{m}(w^\top x_i - y_i)x_i = 0$$

$$\implies \left(\sum_{i=1}^{m} x_i x_i^\top\right) w = \sum_{i=1}^{m} y_i x_i$$

Matrix notation

$$X^\top X w = X^\top Y$$

Normal Equations for Least Squares Regression

Let $X = \begin{bmatrix} - & x_1^\top & - \\ - & x_2^\top & - \\ & \vdots & \\ - & x_m^\top & - \end{bmatrix} \in \mathbb{R}^{m\times d}, Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^{m\times 1}$

SOLVING THE SYSTEM

$$X = \begin{bmatrix} - & x_1^\top & - \\ - & x_2^\top & - \\ & \vdots & \\ - & x_m^\top & - \end{bmatrix} \in \mathbb{R}^{m\times d}, Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^m$$

Normal Equations for Least Squares Regression

$$X^\top X w = X^\top Y$$

If $X^\top X$ is invertible, then

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

$\hat{Y} = X\hat{w}$ is the projection of Y onto the subspace spanned by $x_1, \ldots, x_m$

Recall that $X(X^\top X)^{-1}X$ is the projection matrix on to this subspace

What is the computational cost of computing this?

LINEAR REGRESSION - REGULARIZATION

What if $X^\top X$ is very close to being singular?

This can lead to large values for $\hat{w}$ which might overfit

$$\widehat{G}(w) = \widehat{R}(w) + \lambda\psi(w) = \frac{1}{m}\sum_{i=1}^{m}(y_i - w^\top x_i)^2 + \lambda\psi(w)$$

$\psi(w)$ is chosen to be some function that penalizes complexity of w

Common examples include: $\psi(w) = \|w\|_2^2$ or $\psi(w) = \|w\|_1$

RIDGE REGRESSION

$$X = \begin{bmatrix} - & x_1^\top & - \\ - & x_2^\top & - \\ & \vdots & \\ - & x_m^\top & - \end{bmatrix} \in \mathbb{R}^{m \times d}, Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^{m \times 1}$$

$$\widehat{G}(w) = \frac{1}{m} \sum_{i=1}^{m} (y_i - w^\top x_i)^2 + \lambda \|w\|_2^2$$

Take derivative and set to 0

$$\frac{2}{m} \sum_{i=1}^{m} (w^\top x_i - y_i) x_i + 2\lambda w = 0$$

$$\Longrightarrow \left(\sum_{i=1}^{m} x_i x_i^\top + \lambda m I \right) w = \sum_{i=1}^{m} y_i x_i$$

Matrix notation

$$(X^\top X + \lambda m I) w = X^\top Y$$

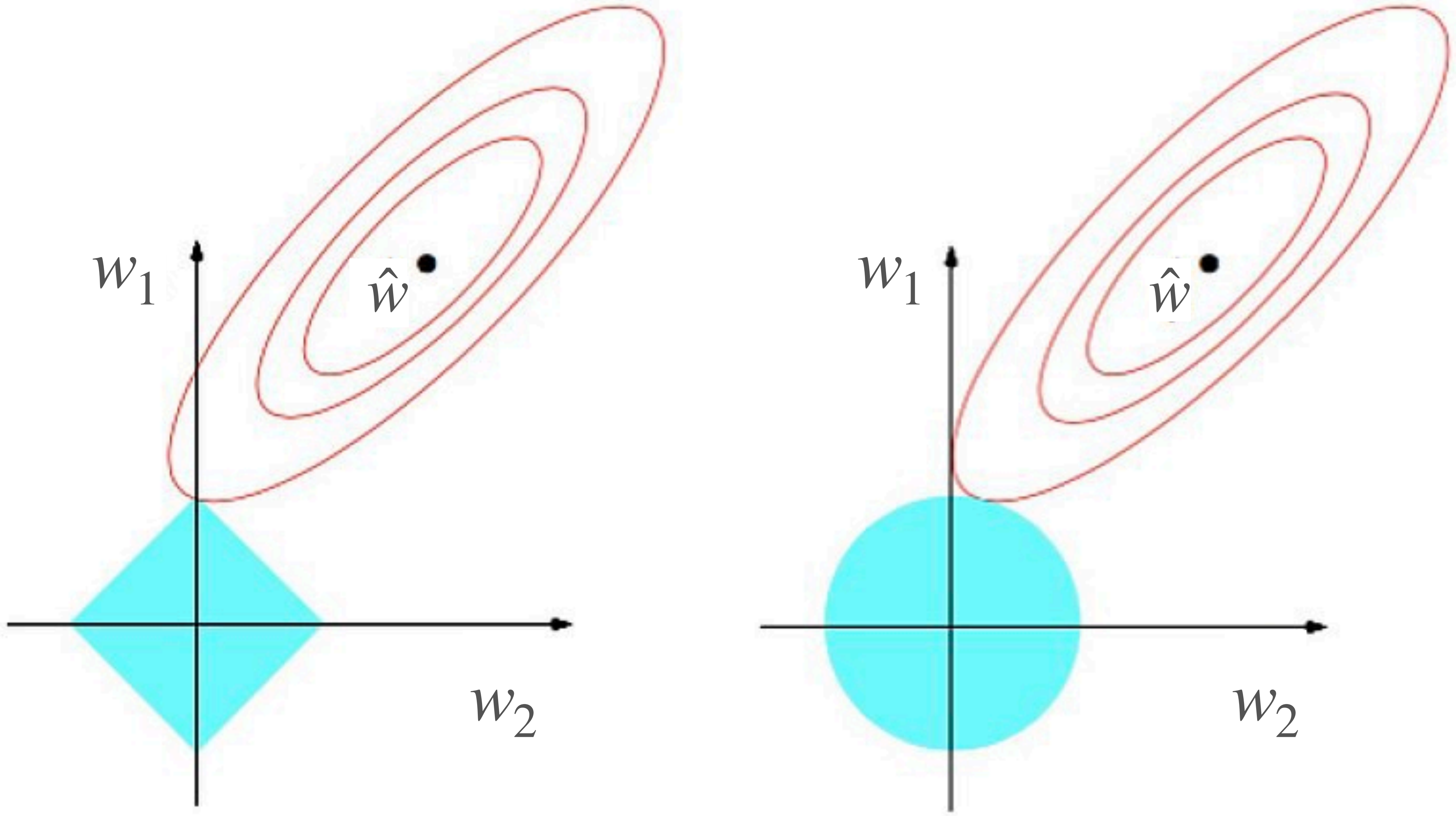
$$\hat{w}_\lambda = (X^\top X + \lambda m I)^{-1} X^\top Y$$

Always invertible,
eigenvalues are $\geq \lambda m$

LASSO REGRESSION

$$\widehat{G}(w) = \frac{1}{m}\sum_{i=1}^{m}(y_i - w^\top x_i)^2 + \lambda\|w\|_1$$

Can model as a quadratic program



Leads to sparsity in the weights!

LINEAR REGRESSION - SUMMARY

Input space: $\mathscr{X} \subseteq \mathbb{R}^d$

Output space: $\mathscr{Y} = \mathbb{R}$

Hypothesis Class: $\mathscr{F} := \{x \mapsto w^\top x + b \,|\, w \in \mathbb{R}^d, b \in \mathbb{R}\}$

Loss function: $\ell(f(x), y) = (f(x) - y)^2$

Least Squares solution: $\hat{w} = (X^\top X)^{-1} X^\top Y$

Next class: Eric will talk about k-nearest neighbors