Linear Classifiers

CS 444: Deep Learning for Computer Vision

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Slides from Lana Lazebnik

Outline

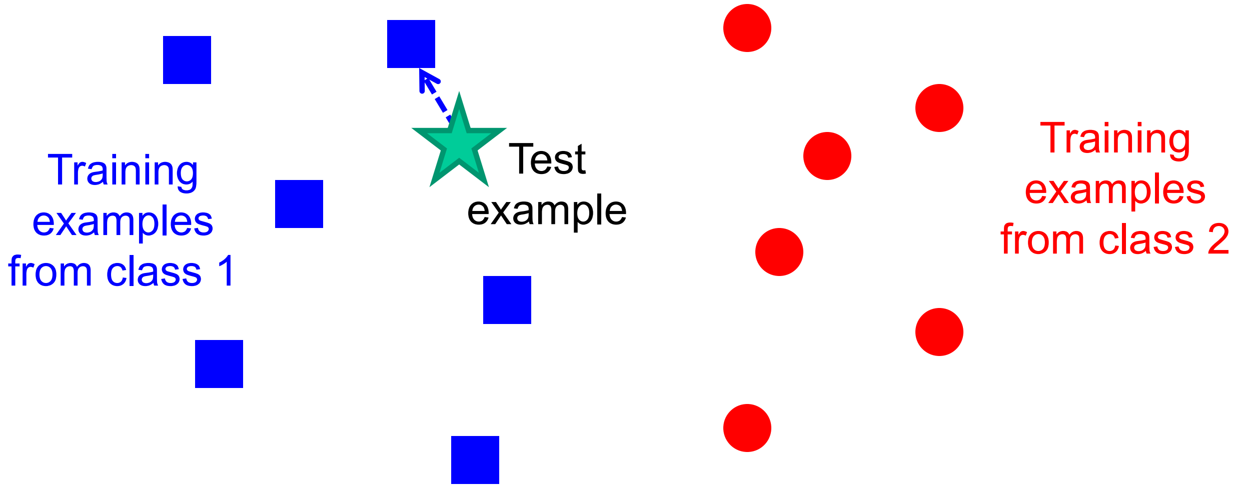
- Examples of classification models: nearest neighbor, linear
- Empirical loss minimization framework
- Linear classification models
    1. Linear regression
    2. Logistic regression
    3. Perceptron training algorithm
    4. Support vector machines

Recall: The basic *supervised learning* framework

$$\underset{\text{output}}{\underset{\uparrow}{y}} = \underset{\substack{\text{prediction}\\ \text{function}}}{\underset{\uparrow}{f}}\left(\underset{\text{input}}{\underset{\nwarrow}{x}}\right)$$

- **Training** (or **learning**): given a *training set* of labeled examples $\{(x_1, y_1), \ldots, (x_N, y_N)\}$, instantiate a predictor f
- **Testing** (or **inference**): apply f to a new *test example* x and output the predicted value $y = f(x)$

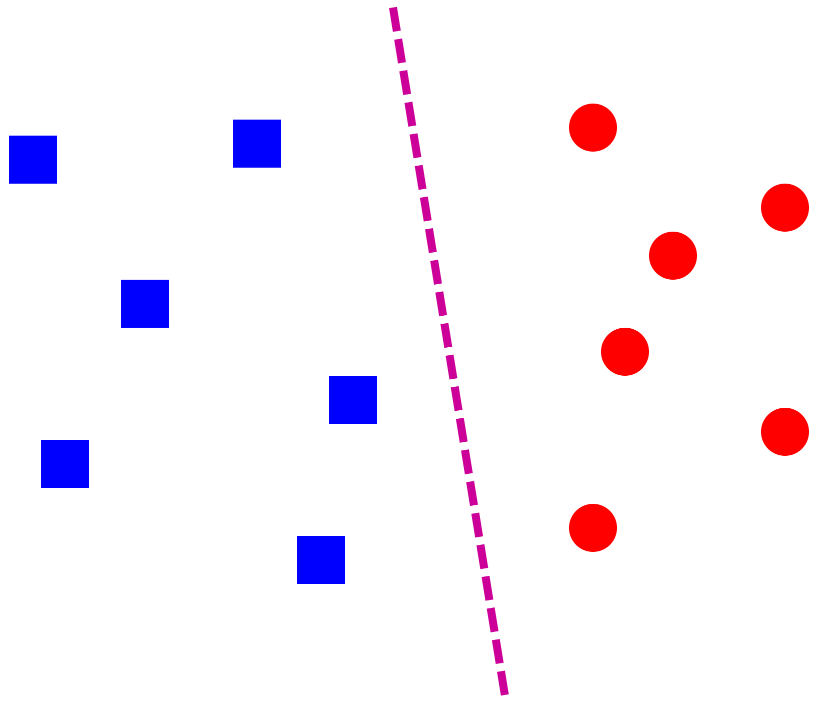
Nearest neighbor classifier


Training examples from class 1
Test example
Training examples from class 2

$f(x)$ = label of the training example nearest to x

- All we need is a distance function for our inputs
- No training required!

Linear classifier

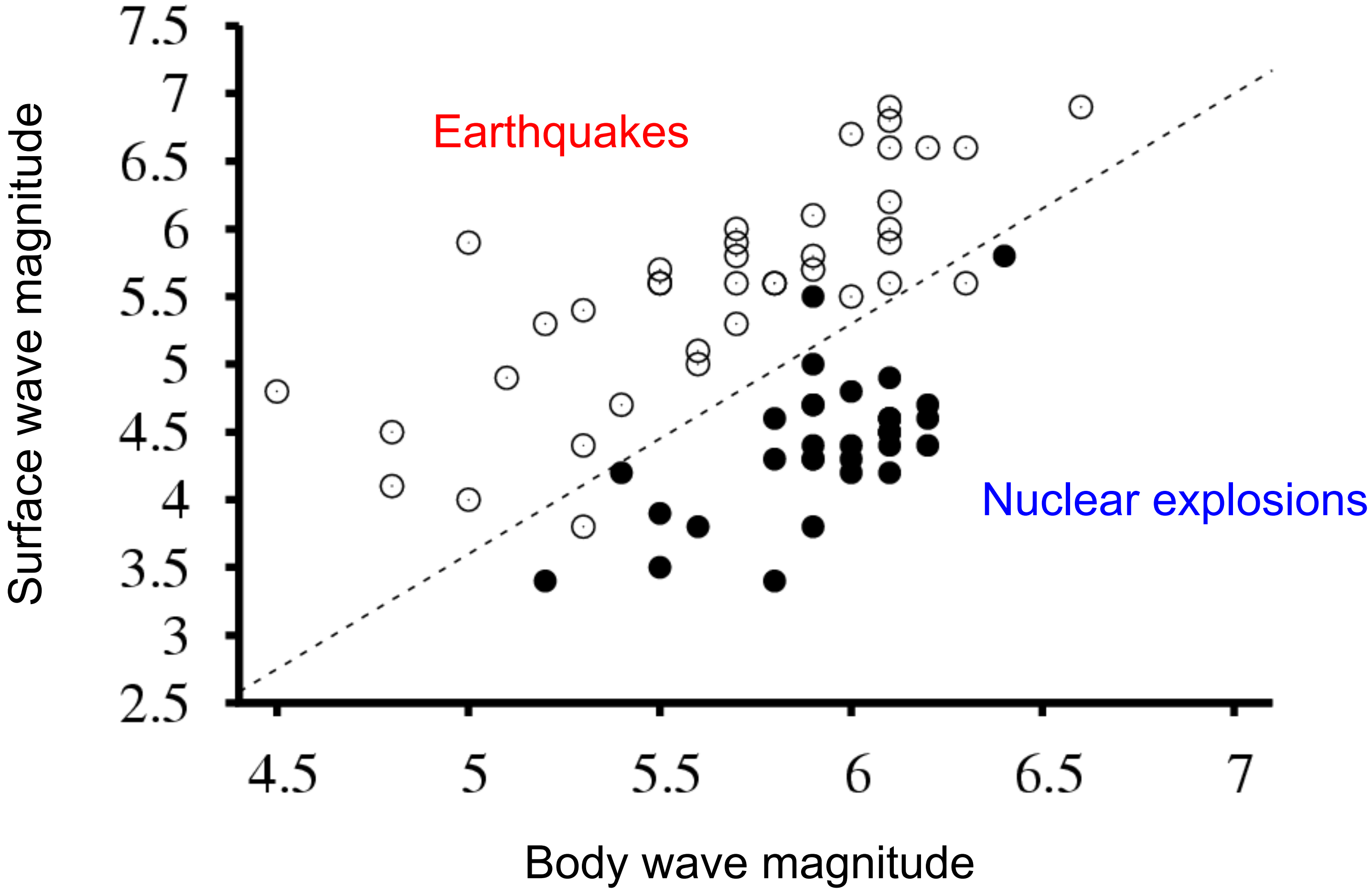


- Find a *linear function* to separate the classes:

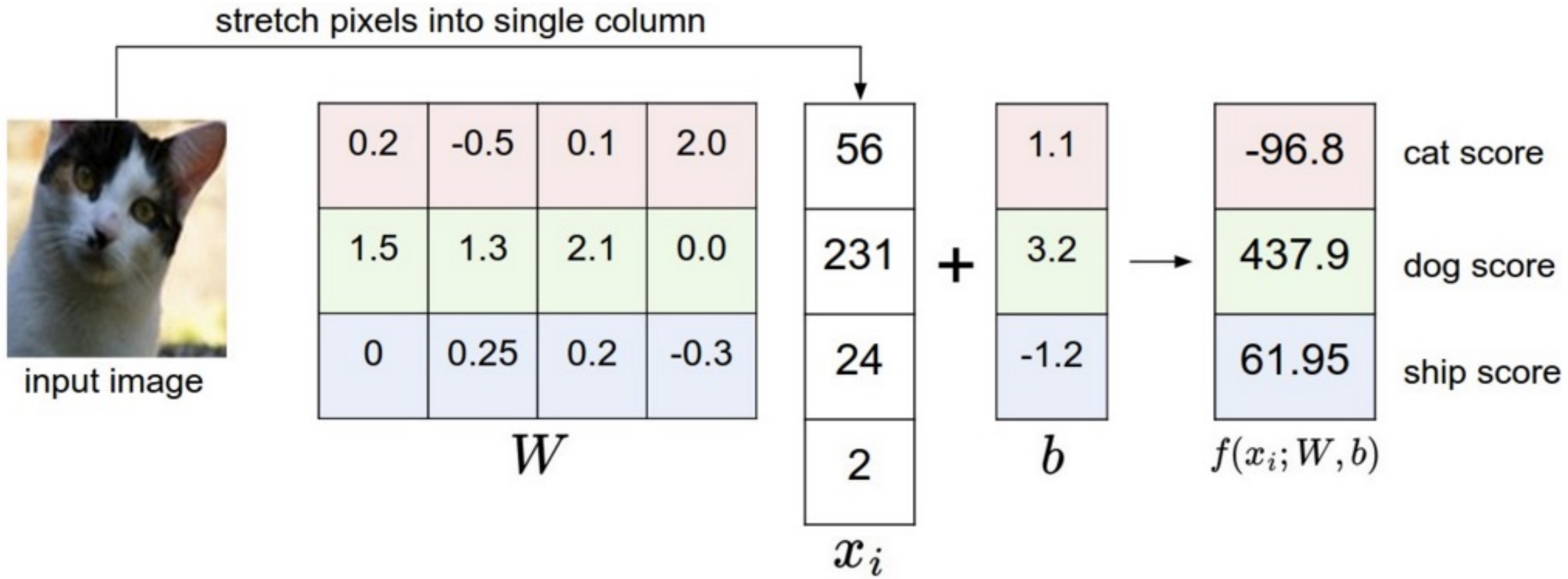
$$f(x) = \mathrm{sgn}\left(w^{(1)}x^{(1)} + w^{(2)}x^{(2)} + \cdots + w^{(D)}x^{(D)} + b\right) = \mathrm{sgn}(w \cdot x + b)$$

Visualizing linear classifiers

Seismic data classification



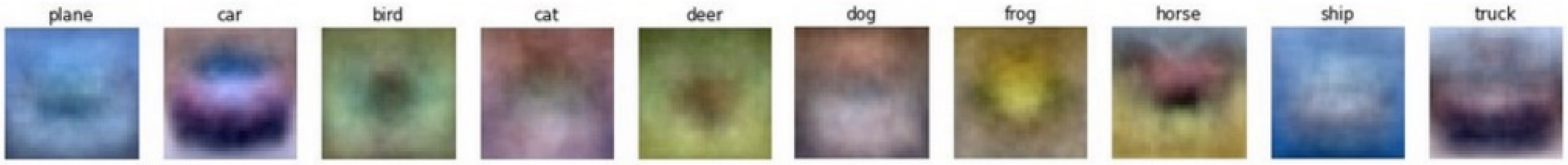
Visualizing linear classifiers



stretch pixels into single column

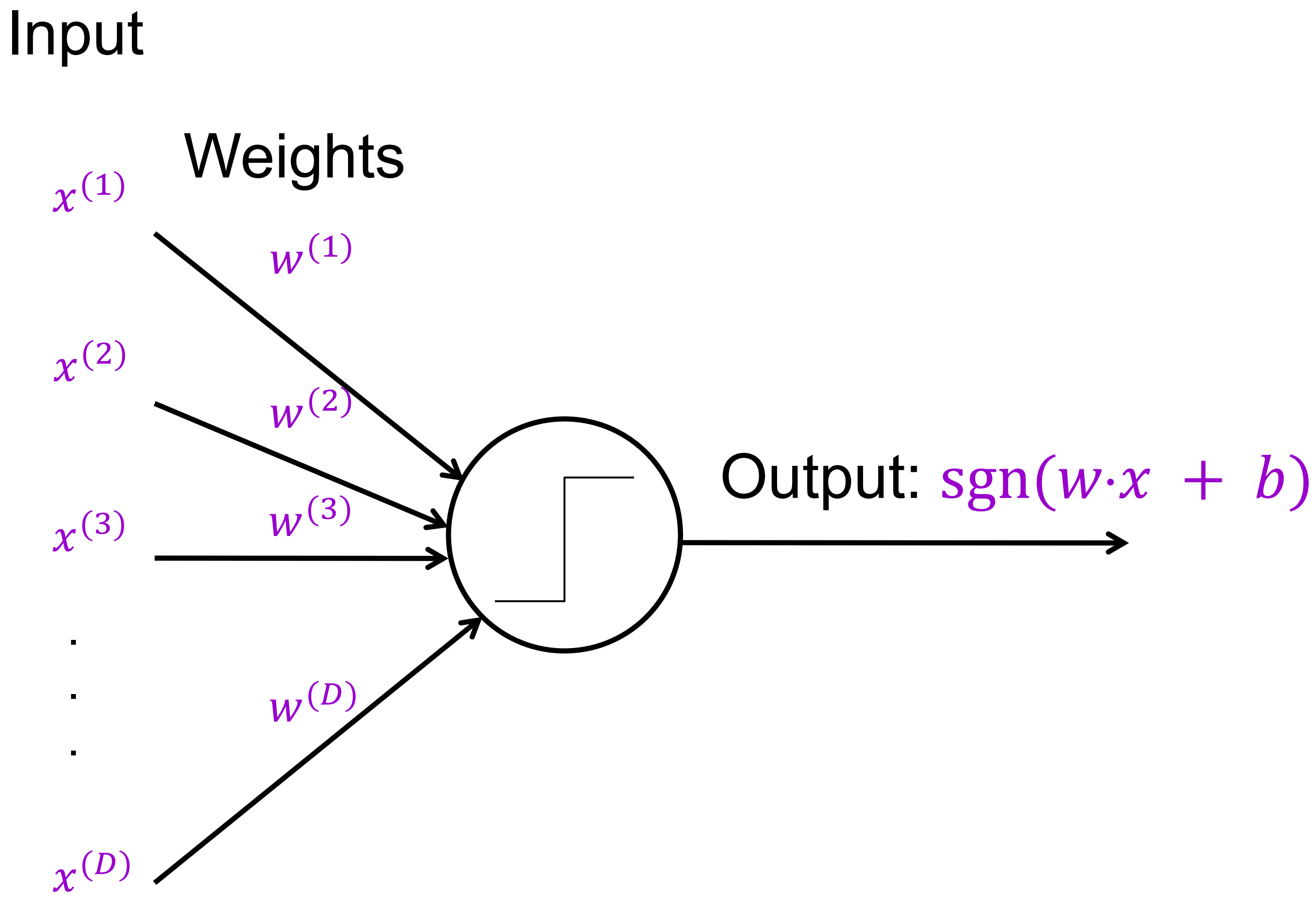
input image

$$\underbrace{\begin{bmatrix}0.2 & -0.5 & 0.1 & 2.0\\ 1.5 & 1.3 & 2.1 & 0.0\\ 0 & 0.25 & 0.2 & -0.3\end{bmatrix}}_{W}\underbrace{\begin{bmatrix}56\\ 231\\ 24\\ 2\end{bmatrix}}_{x_i} + \underbrace{\begin{bmatrix}1.1\\ 3.2\\ -1.2\end{bmatrix}}_{b} \rightarrow \underbrace{\begin{bmatrix}-96.8\\ 437.9\\ 61.95\end{bmatrix}}_{f(x_i;W,b)}\begin{array}{l}\text{cat score}\\ \text{dog score}\\ \text{ship score}\end{array}$$

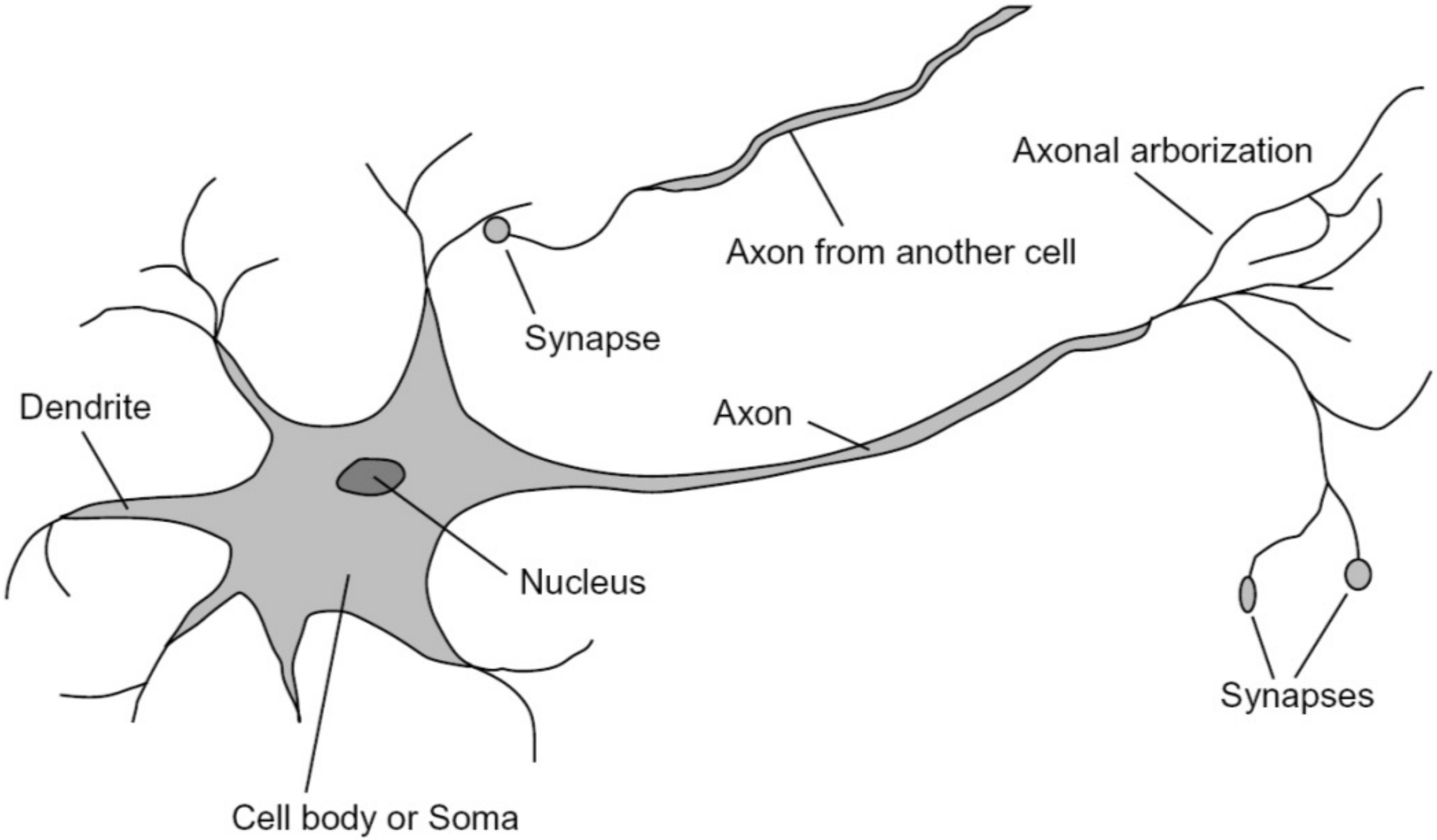


Source: http://cs231n.github.io/linear-classify/

Linear classifier: Perceptron view



Loose inspiration: Biological neurons



NN vs. linear classifiers: Pros and cons

- NN pros:
  - + Simple to implement
  - + Decision boundaries not necessarily linear
  - + Works for any number of classes
  - + *Nonparametric* method
- NN cons:
  - - Need good distance function
  - - Slow at test time
- Linear pros:
  - + Low-dimensional *parametric* representation
  - + Very fast at test time
- Linear cons:
  - - Works for two classes
  - - How to train the linear function?
  - - What if data is not linearly separable?

Outline

- Examples of classification models: nearest neighbor, linear
- Empirical loss minimization framework

Empirical loss minimization

- Let’s formalize the setting for learning of a *parametric model* in a supervised scenario

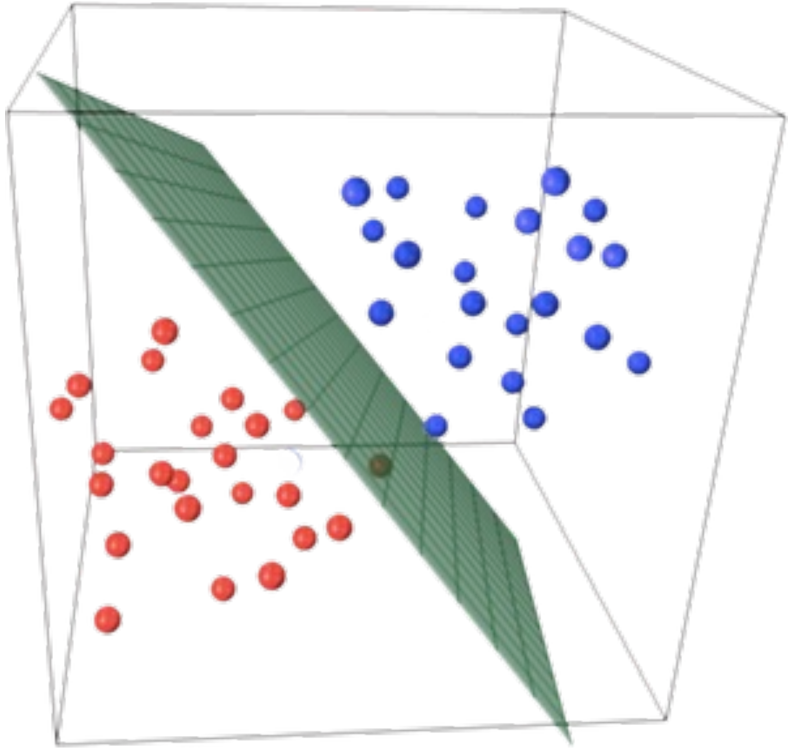


Image source

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \dots, n\}$
- Find: predictor f
- Goal: make good predictions $\hat{y} = f(x)$ on *test* data

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \ldots, n\}$
- Find: predictor f
- Goal: make good predictions $\hat{y} = f(x)$ on *test* data

What kinds of functions?

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \ldots, n\}$
- Find: predictor $f \in \mathcal{H}$
- Goal: make good predictions $\hat{y} = f(x)$ on *test* data

Hypothesis class

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \dots, n\}$
- Find: predictor $f \in \mathcal{H}$
- Goal: make good predictions $\hat{y} = f(x)$ on *test* data

Connection between training and test data?

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \ldots, n\}$ i.i.d. from distribution D
- Find: predictor $f \in \mathcal{H}$
- Goal: make good predictions $\hat{y} = f(x)$ on *test* data i.i.d. from distribution D

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \dots, n\}$ i.i.d. from distribution D
- Find: predictor $f \in \mathcal{H}$
- Goal: make good predictions $\hat{y} = f(x)$ on *test* data i.i.d. from distribution D

What kind of performance measure?

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \ldots, n\}$ i.i.d. from distribution D
- Find: predictor $f \in \mathcal{H}$
- S.t. the *expected loss* is small:

$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

Various loss functions

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \ldots, n\}$ i.i.d. from distribution D
- Find: predictor $f \in \mathcal{H}$
- S.t. the *expected loss* is small:

$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

- Example losses:

$0 - 1$ loss: $l(f, x, y) = \mathbb{I}[f(x) \neq y]$ and $L(f) = \Pr[f(x) \neq y]$

l_2 loss: $l(f, x, y) = [f(x) - y]^2$ and $L(f) = \mathbb{E}[\,[f(x) - y]^2]$

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \dots, n\}$ i.i.d. from distribution D
- Find: predictor $f \in \mathcal{H}$
- S.t. the *expected loss* is small:

$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

Can't optimize this directly

Source: Y. Liang

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \dots, n\}$ i.i.d. from distribution D
- Find: predictor $f \in \mathcal{H}$ that minimizes

$$\hat{L}(f) = \frac{1}{n}\sum_{i=1}^{n} l(f, x_i, y_i)$$

Empirical loss

Source: Y. Liang

Supervised learning in a nutshell

1. **Collect *training data* and labels**
2. **Specify model:** select *hypothesis class* and *loss function*
3. **Train model:** find the function in the hypothesis class that minimizes the *empirical loss* on the training data

Outline

- Example classification models: nearest neighbor, linear
- Empirical loss minimization
- Linear classification models
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  2. Logistic regression
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Training linear classifiers

- Given: i.i.d. training data $\{(x_i, y_i), i = 1, \ldots, n\}$,
  $y_i \in \{-1,1\}$
- Hypothesis class: $f_w(x) = \mathrm{sgn}(w^T x)$
- Classification with *bias*, i.e. $f_w(x) = \mathrm{sgn}(w^T x + b)$, can be reduced to the case w/o bias by letting $\tilde{w} = [w; b]$ and $\tilde{x} = [x; 1]$

Source: Y. Liang

Training linear classifiers

- Given: i.i.d. training data $\{(x_i, y_i), i = 1, \dots, n\}$,
  $y_i \in \{-1,1\}$
- Hypothesis class: $f_w(x) = \text{sgn}(w^T x)$
- Loss: how about minimizing the number of mistakes on the training data?

$$\hat{L}(f_w) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}[\text{sgn}(w^T x_i) \neq y_i]$$

- Difficult to optimize directly (NP-hard), so people resort to *surrogate loss functions*

Source: Y. Liang

Linear regression ("straw man" model)

- Find $f_w(x) = w^T x$ that minimizes l_2 *loss* or *mean squared error*

$$\hat{L}(f_w) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2$$

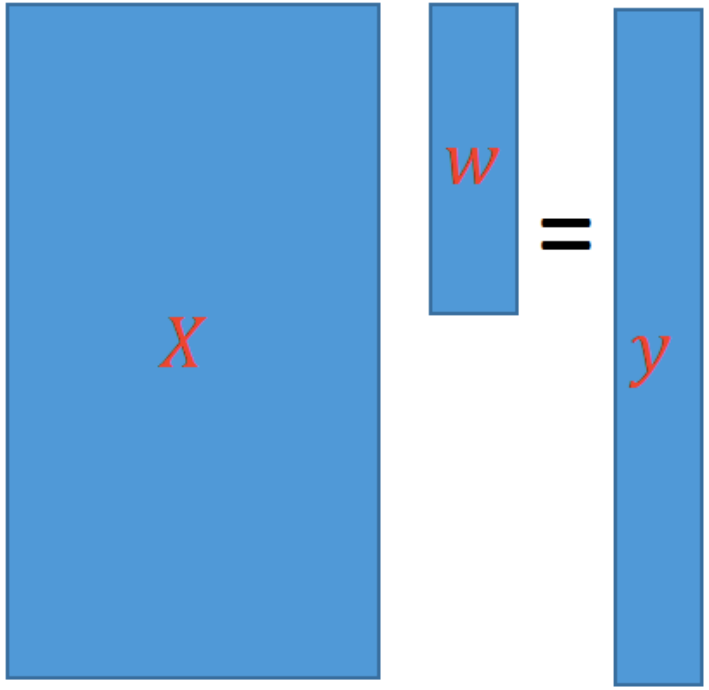
- Ignores the fact that $y \in \{-1,1\}$ but is easy to optimize

Source: Y. Liang

Linear regression: Optimization

- Let X be a matrix whose ith row is x_i^T, Y be the vector $(y_1, \ldots, y_n)^T$

$$\hat{L}(f_w) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2 = \frac{1}{n}\|Xw - Y\|_2^2$$



Source: Y. Liang

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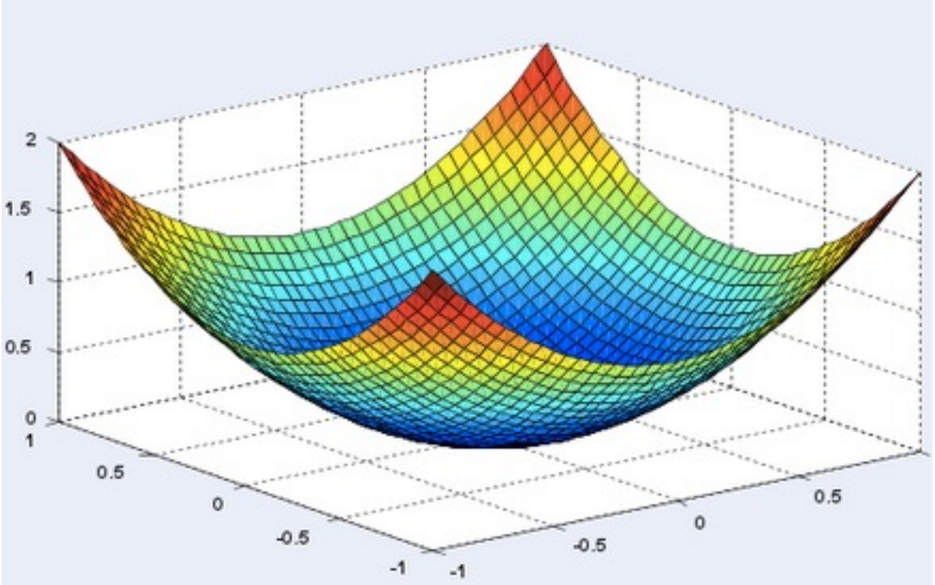
$$\hat{L}(f_w) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2 = \frac{1}{n}\|Xw - Y\|_2^2$$

- This is a *convex* function of the weights



Source: Y. Liang

Linear regression: Optimization

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- Find the *gradient* w.r.t. w:

  $\nabla_w \|Xw - Y\|_2^2$

Source: Y. Liang

Linear regression: Optimization

- Let X be a matrix whose ith row is x_i^T, Y be the vector $(y_1, \dots, y_n)^T$

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- Find the *gradient* w.r.t. w:

$$\begin{aligned} \nabla_w \|Xw - Y\|_2^2 &= \nabla_w[(Xw - Y)^T(Xw - Y)] \\ &= \nabla_w[w^T X^T X w - 2w^T X^T Y + Y^T Y] \\ &= 2X^T X w - 2X^T Y \end{aligned}$$

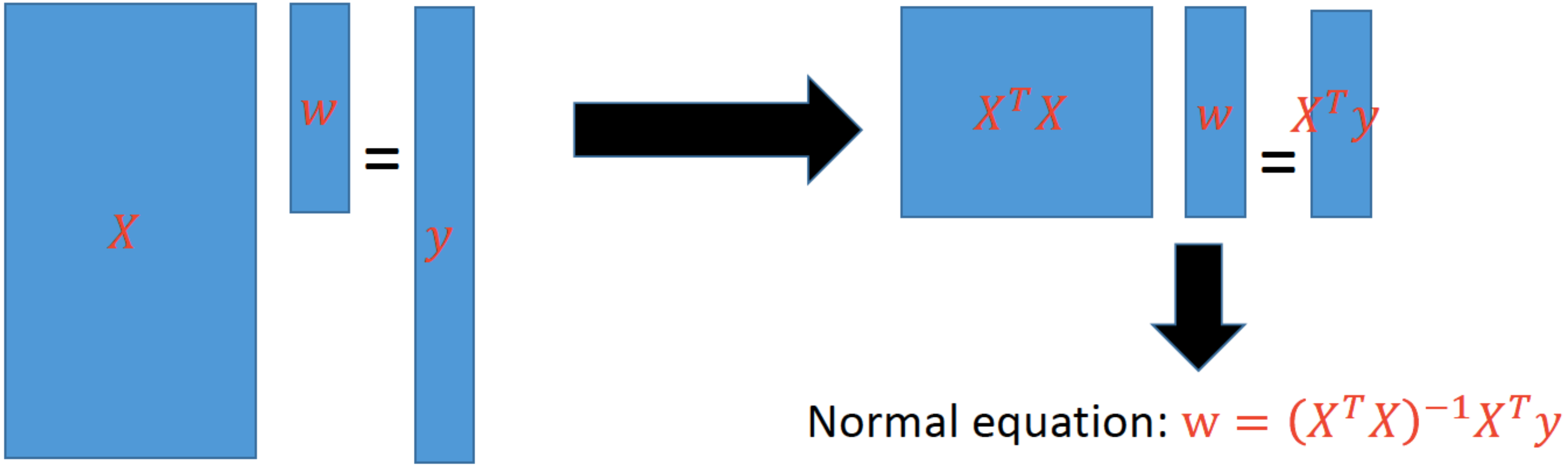
- Set gradient to zero to get the minimizer:

$$X^T X w = X^T Y$$
$$w = (X^T X)^{-1} X^T Y$$

Source: Y. Liang

Linear regression: Optimization

- Linear algebra view
  - If X is invertible, simply solve $Xw = Y$ and get $w = X^{-1}Y$
  - But typically X is a "tall" matrix so you need to find the *least squares solution* to an over-constrained system

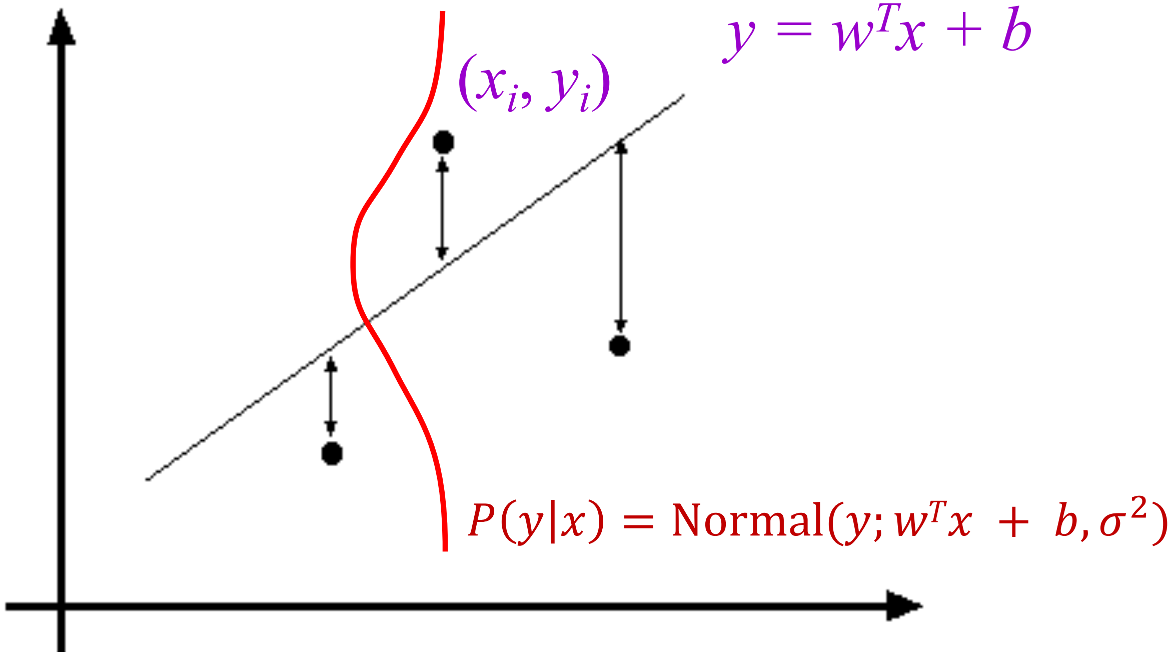


Normal equation: $\mathrm{w} = (X^TX)^{-1}X^Ty$

Source: Y. Liang

Linear regression as maximum likelihood estimation

- Interpretation of l_2 loss: *negative log likelihood* assuming y is normally distributed with mean $f_w(x) = w^T x + b$



Maximum likelihood estimation

- Given: i.i.d. training data $\{(x_i, y_i), i = 1, \ldots, n\}$
- Let $\{P_\theta(y|x), \theta \in \Theta\}$ be a family of distributions parameterized by θ
- Maximum (conditional) likelihood estimate:

$$\theta_{ML} = \mathrm{argmax}_\theta \prod_i P_\theta(y_i|x_i)$$

$$= \mathrm{argmin}_\theta - \sum_i \log P_\theta(y_i|x_i)$$

Maximum likelihood estimation

$$\theta_{ML} = \text{argmin}_\theta - \textstyle\sum_i \log P_\theta(y_i|x_i)$$

- Assume $P_\theta(y|x) = \text{Normal}(y; f_\theta(x), \sigma^2)$

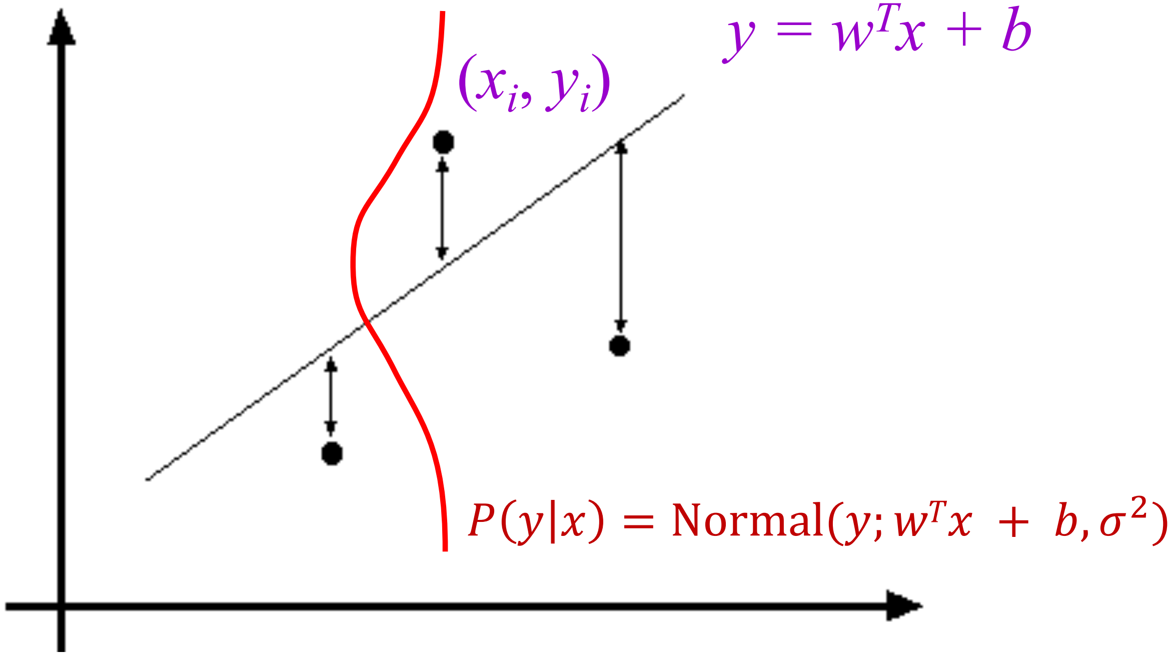
$$\log P_\theta(y|x) = \log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{\left(y - f_\theta(x)\right)^2}{2\sigma^2}\right]\right]$$

$$= -\frac{1}{2\sigma^2}\left(y - f_\theta(x)\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)$$

$$\theta_{ML} = \text{argmin}_\theta \sum_i \left(y_i - f_\theta(x_i)\right)^2$$

Linear regression as maximum likelihood estimation

- Interpretation of l_2 loss: *negative log likelihood* assuming y is normally distributed with mean $f_w(x) = w^T x + b$



- Does this make sense for binary classification?

Problem with linear regression

- In practice, very sensitive to outliers

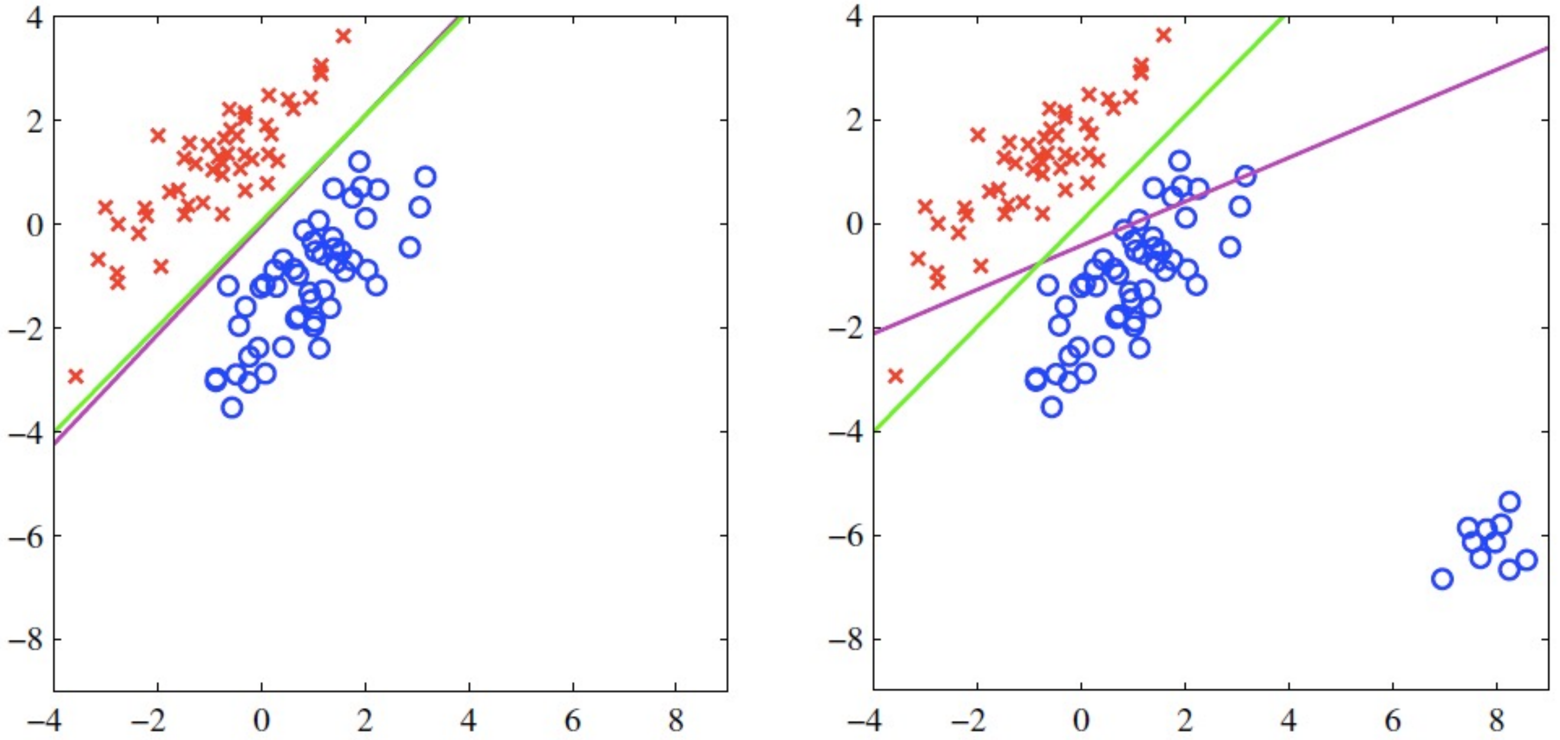
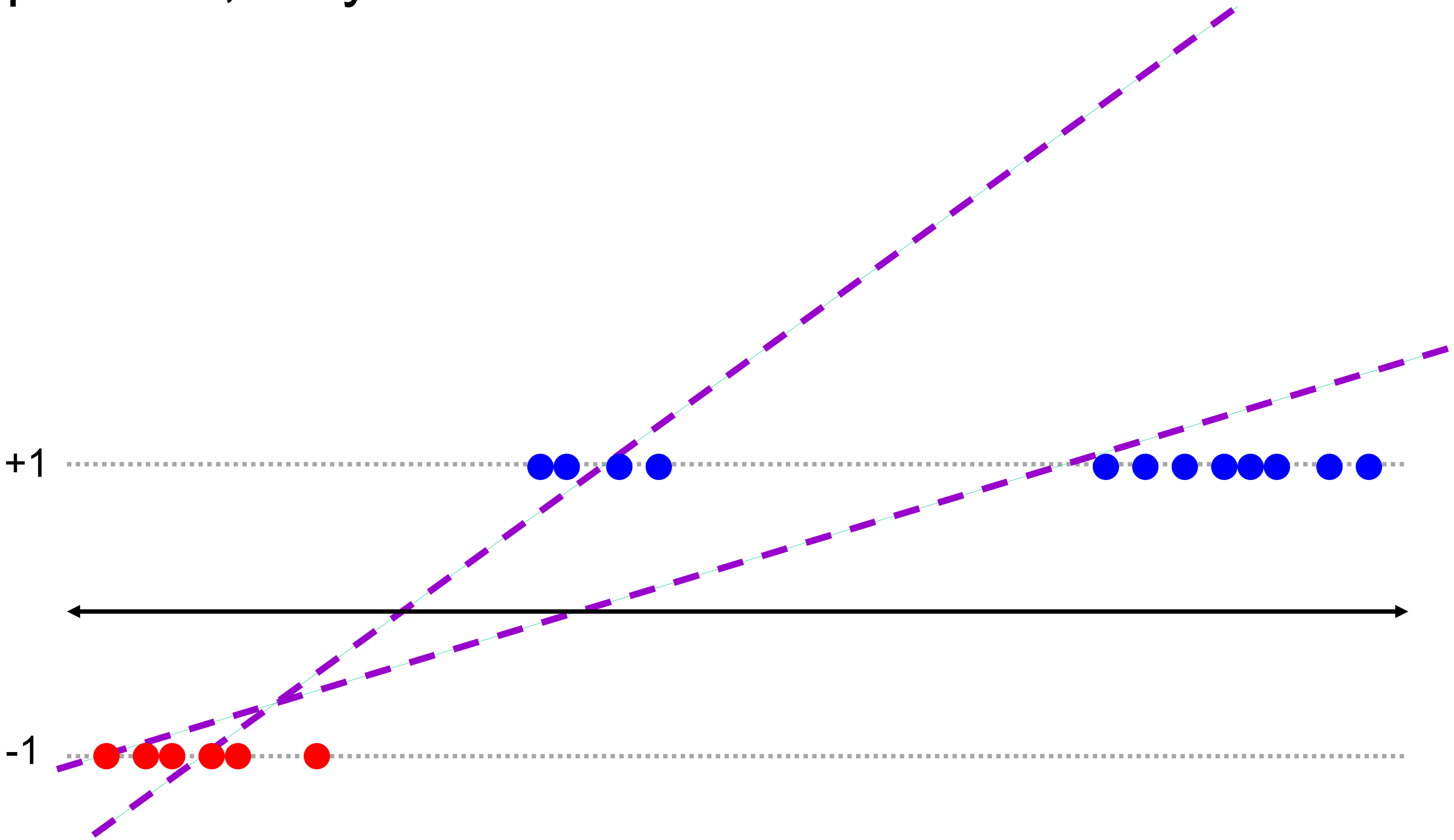


Figure 4.4 The left plot shows data from two classes, denoted by red crosses and blue circles, together with the decision boundary found by least squares (magenta curve) and also by the logistic regression model (green curve), which is discussed later in Section 4.3.2. The right-hand plot shows the corresponding results obtained when extra data points are added at the bottom left of the diagram, showing that least squares is highly sensitive to outliers, unlike logistic regression.

Figure from *Pattern Recognition and Machine Learning*, Bishop

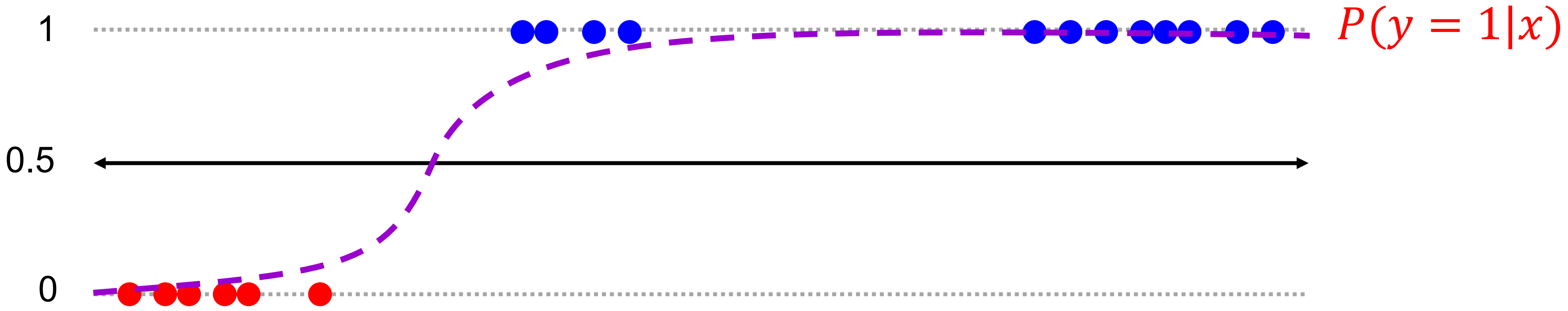
Problem with linear regression

- In practice, very sensitive to outliers



Next idea

- Instead of a linear function, how about we fit a function representing the *confidence* of the classifier?



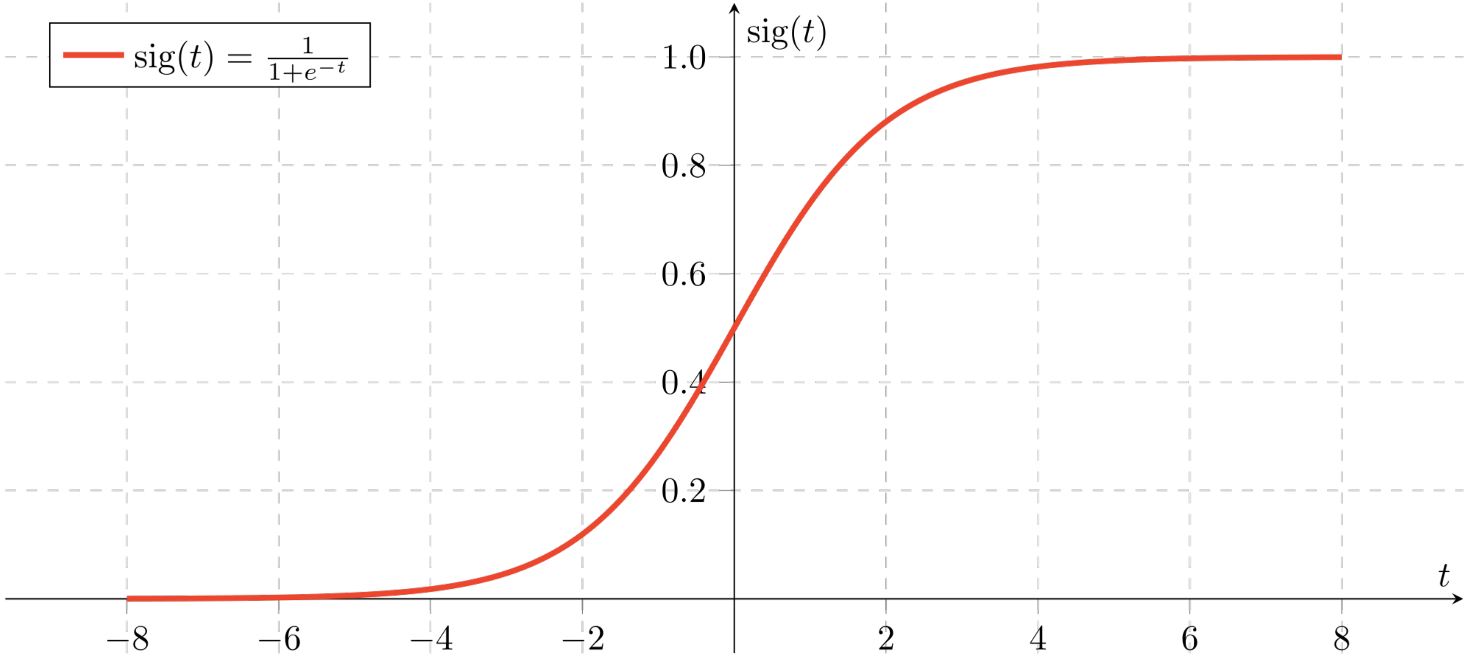
Linear classifiers: Outline

- Example classification models: nearest neighbor, linear
- Empirical loss minimization
- Linear classification models
    1. Linear regression (least squares)
    2. Logistic regression

Logistic regression

- Let's learn a probabilistic classifier estimating the probability of the input x having a positive label, given by putting a *sigmoid function* around the linear response $w^T x$:

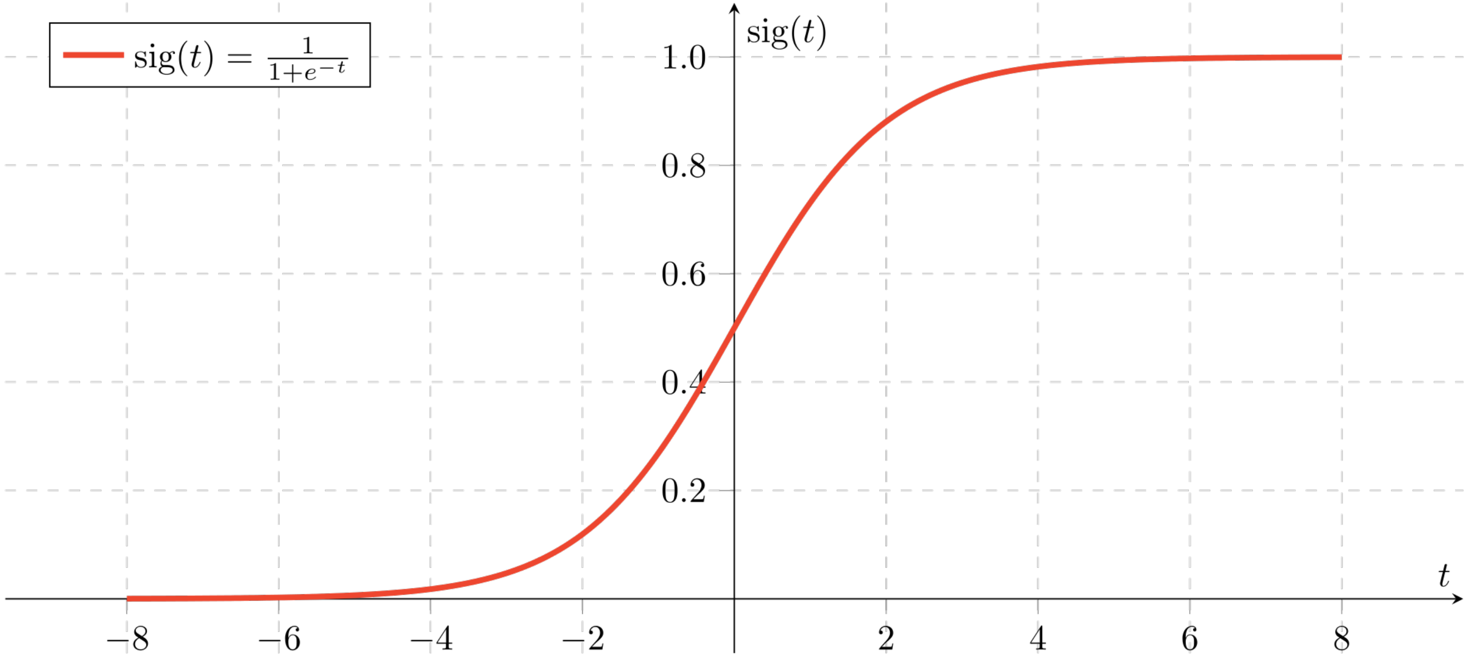
$$P_w(y = 1|x) = \sigma(w^T x) = \frac{1}{1+\exp(-w^T x)}$$



Sigmoid: Properties

$$P_w(y = 1|x) = \sigma(w^T x) = \frac{1}{1 + \exp(-w^T x)}$$

- What is the range?
- What is $\sigma(0)$?
- What is $P_w(y = -1|x)$?



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- What is $P_w(y = -1|x)$?

$$P_w(y = -1|x) = 1 - P_w(y = 1|x) = 1 - \sigma(w^T x)$$

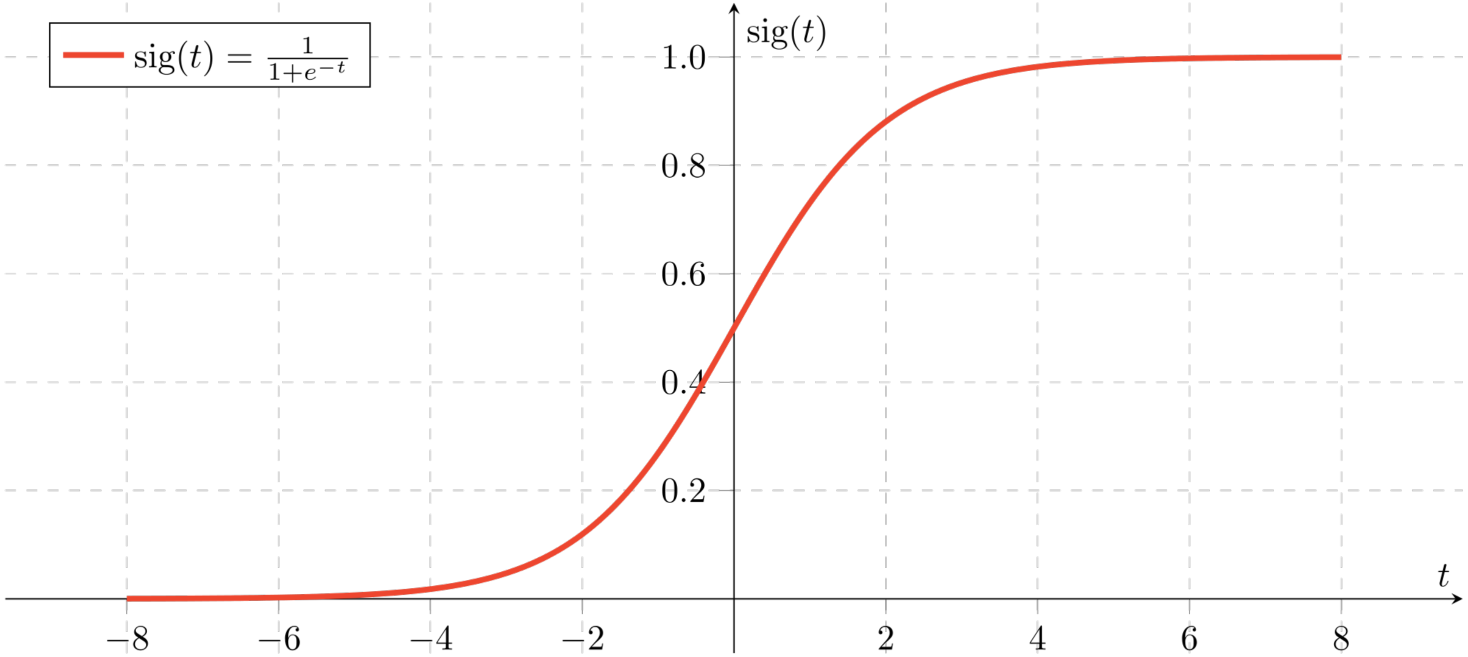
$$= \frac{1+\exp(-w^T x)-1}{1+\exp(-w^T x)} = \frac{\exp(-w^T x)}{1+\exp(-w^T x)} = \frac{1}{\exp(w^T x)+1}$$

$$= \sigma(-w^T x)$$

Sigmoid: Properties

$$P_w(y = 1|x) = \sigma(w^T x) = \frac{1}{1 + \exp(-w^T x)}$$

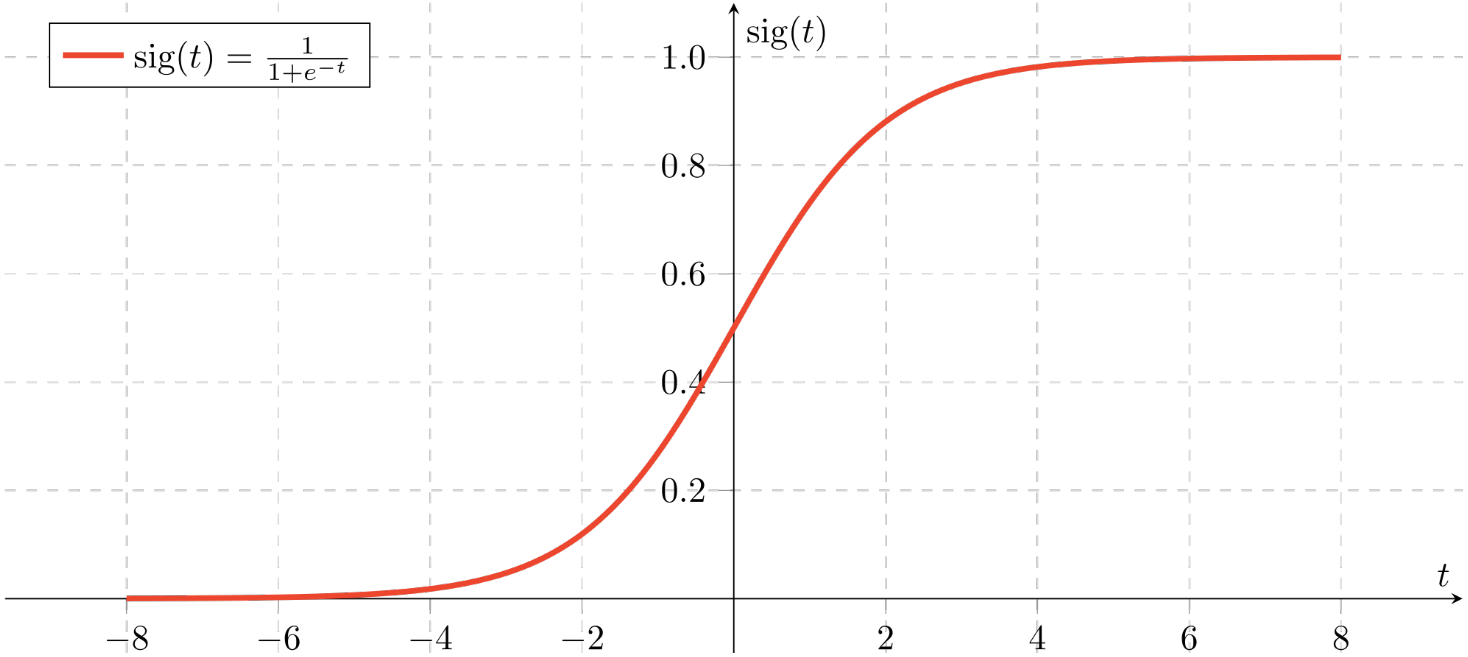
- Sigmoid is *symmetric* in the following sense: $1 - \sigma(t) = \sigma(-t)$



Sigmoid: Properties

$$P_w(y = 1|x) = \sigma(w^T x) = \frac{1}{1 + \exp(-w^T x)}$$

- What happens if we scale w by a constant?



Sigmoid: Properties

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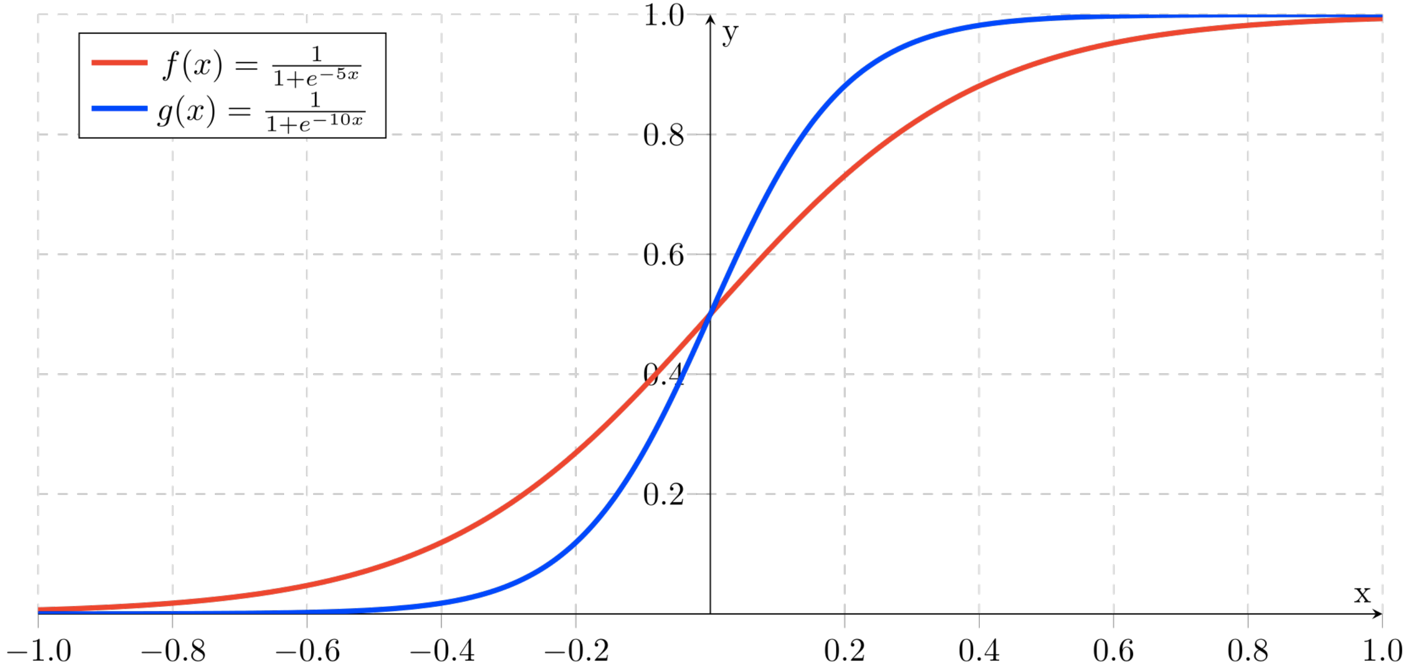


Image source

Logistic loss

- Given: $\{(x_i, y_i), i = 1, \dots, n\}$, $y_i \in \{-1,1\}$
- Maximum (conditional) likelihood estimate: find w that minimizes

$$\hat{L}(w) = -\frac{1}{n}\sum_{i=1}^{n} \log P_w(y_i|x_i)$$

$$l(w, x_i, y_i) = -\log P_w(y_i|x_i)$$

- If $y_i = 1$:

$$P_w(y_i|x_i) = \sigma(w^T x_i)$$

- If $y_i = -1$:

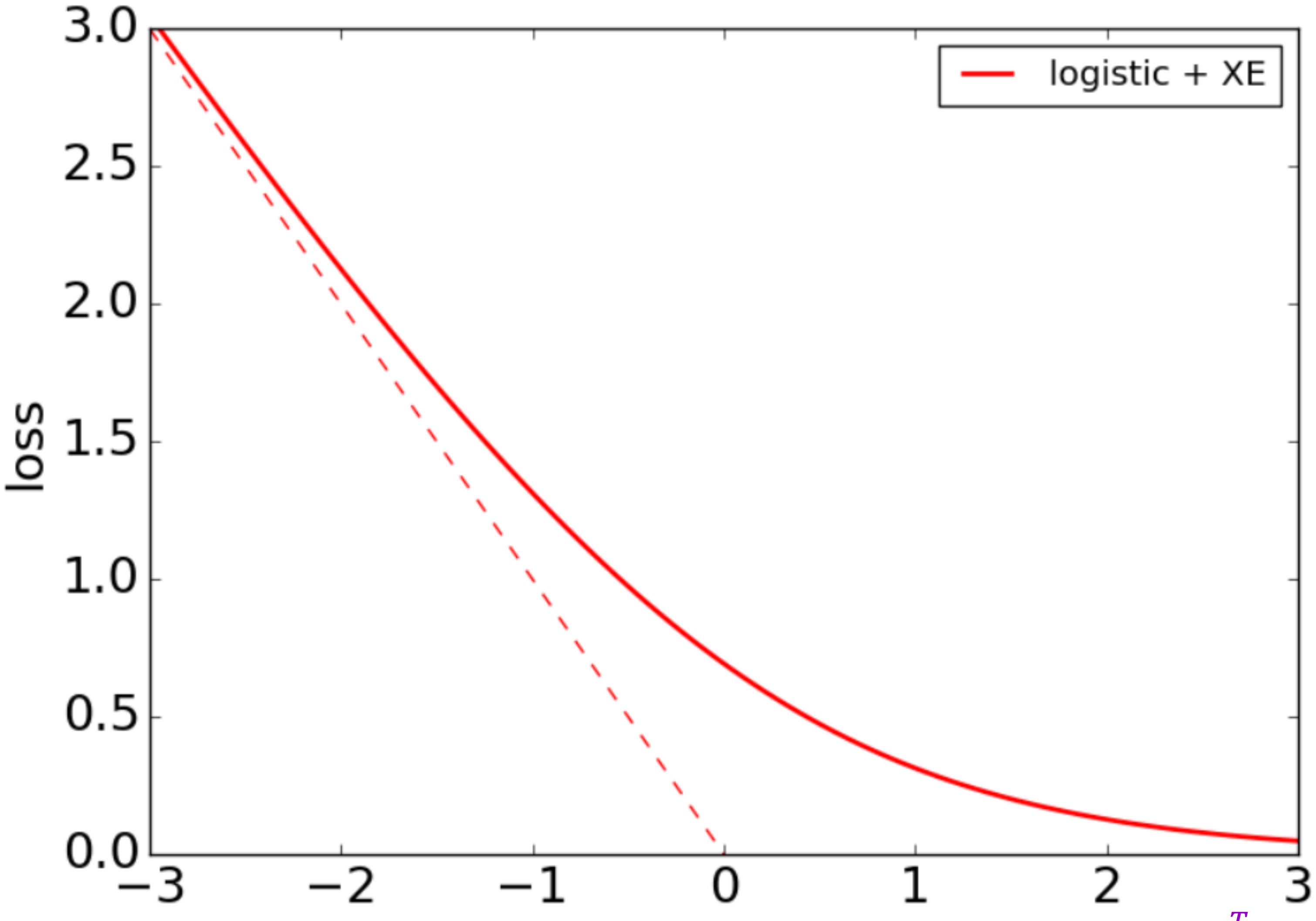
$$P_w(y_i|x_i) = 1 - \sigma(w^T x_i) = \sigma(-w^T x_i)$$

- Thus,

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

Logistic loss

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$



$y_i w^T x_i$

Figure source

Logistic loss: Optimization

- Given: $\{(x_i, y_i), i = 1, \ldots, n\}$, $y_i \in \{-1,1\}$
- Find w that minimizes

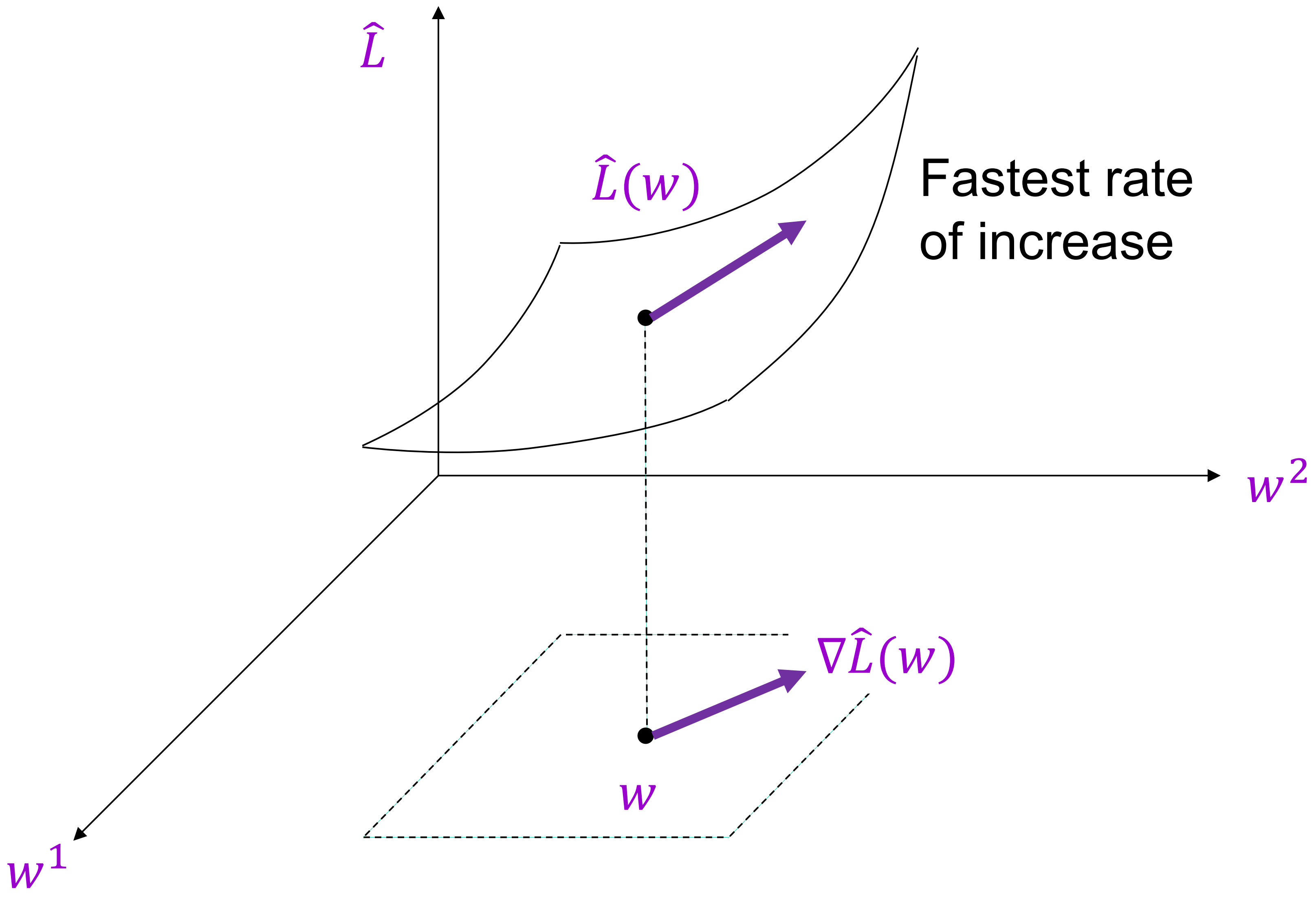
$$\hat{L}(w) = -\frac{1}{n}\sum_{i=1}^{n} \log P_w(y_i|x_i)$$

- There is no closed-form expression for the minimum and we need to use *gradient descent* to find it

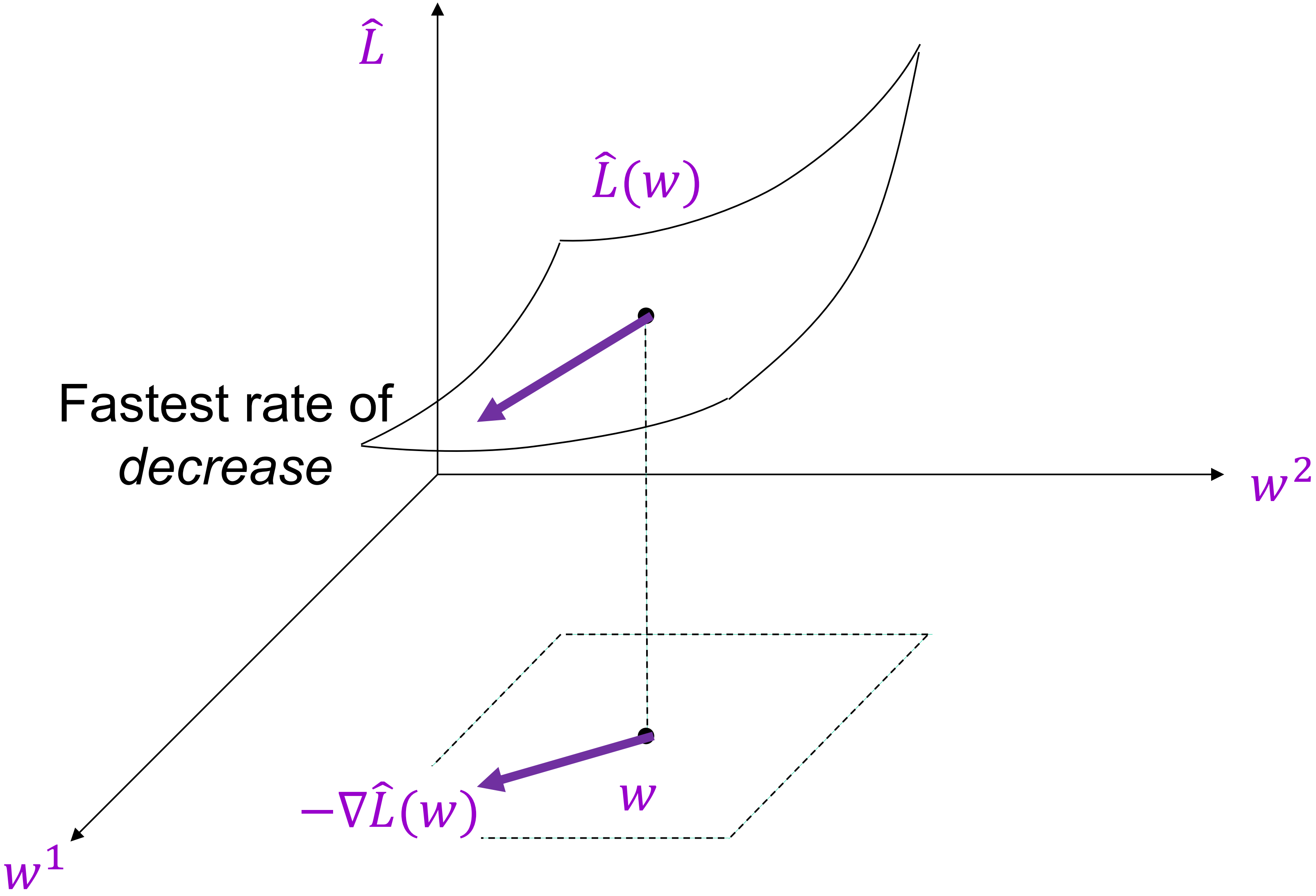
Gradient descent

- Goal: find w to minimize loss $\hat{L}(w)$
- Start with some initial estimate of w
- Repeat until convergence:
  - Find $\nabla\hat{L}(w)$, the *gradient* of the loss w.r.t. w
  - Take a small step in the *opposite* direction: $w \leftarrow w - \eta \, \nabla\hat{L}(w)$

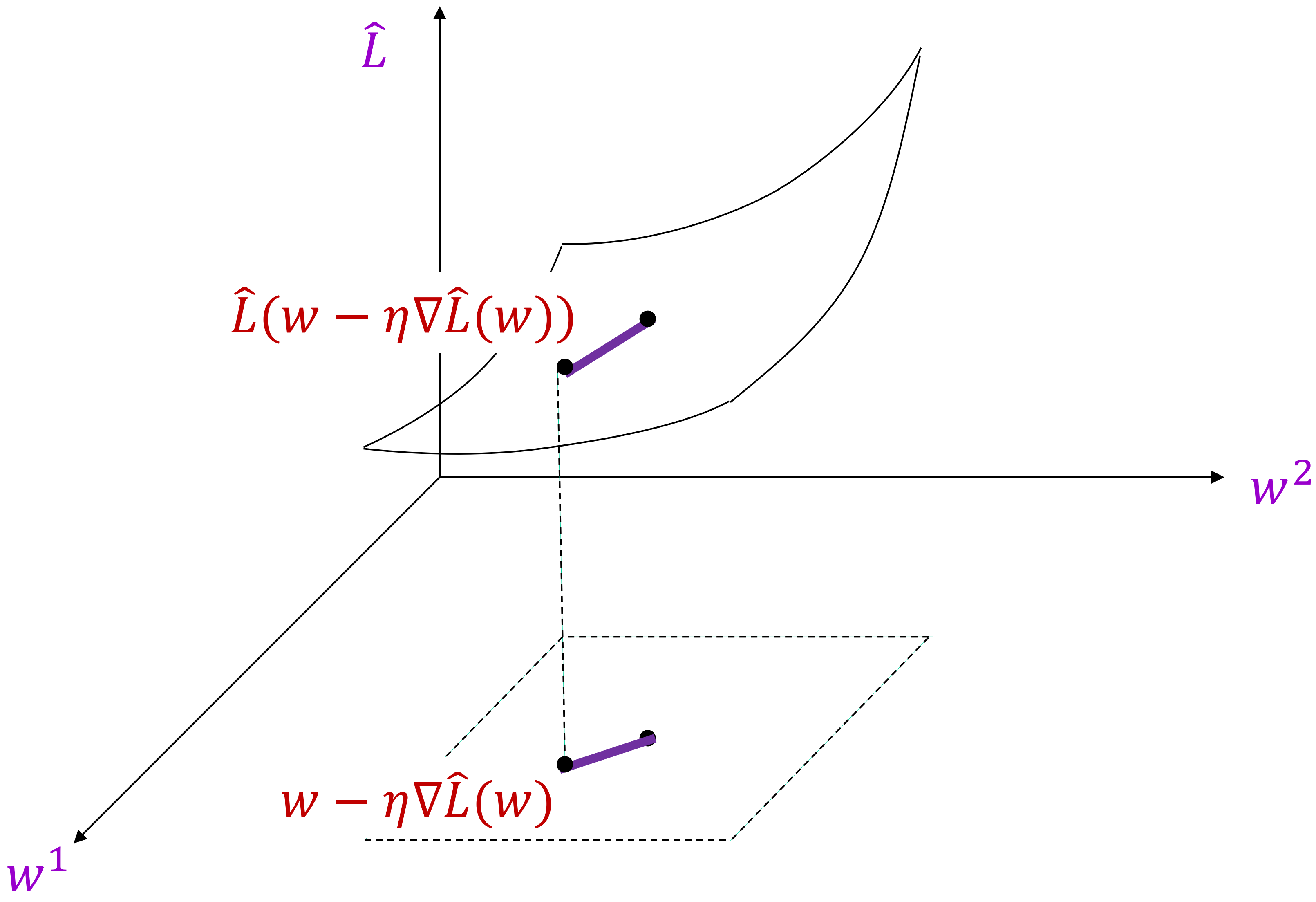
The gradient vector



The gradient vector



Gradient descent


$\hat{L}$
$\hat{L}(w - \eta\nabla\hat{L}(w))$
w^2
$w - \eta\nabla\hat{L}(w)$
w^1

Gradient descent

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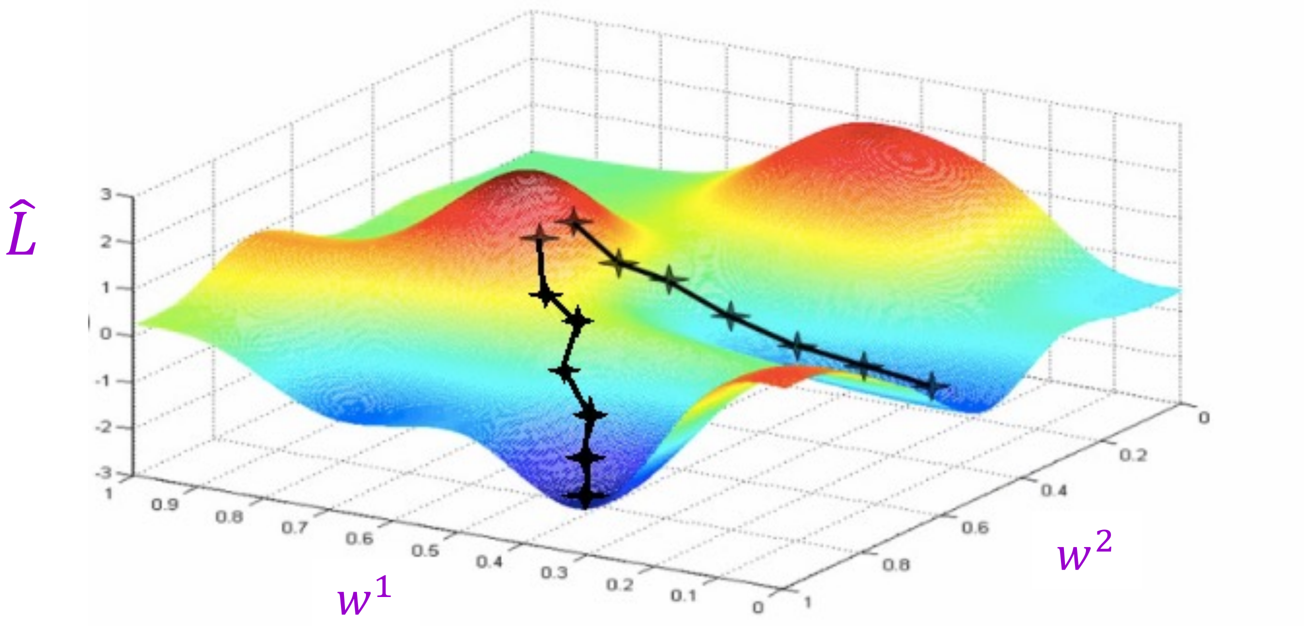

Gradient descent

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- Start with some initial estimate of w
- Repeat until convergence:
  - Find $\nabla\hat{L}(w)$, the *gradient* of the loss w.r.t. w
  - Take a small step in the *opposite* direction: $w \leftarrow w - \eta\,\nabla\hat{L}(w)$
  - η is the step size or *learning rate*

Full batch gradient descent

- Since $\hat{L}(w) = \frac{1}{n}\sum_{i=1}^{n} l(w, x_i, y_i)$, we have

$$\nabla \hat{L}(w) = \frac{1}{n}\sum_{i=1}^{n} \nabla l(w, x_i, y_i)$$

- For a single parameter update, need to cycle through the entire training set!

Stochastic gradient descent (SGD)

- At each iteration, take a *single data point* (x_i, y_i) and perform a parameter update using $\nabla l(w, x_i, y_i)$, the gradient of the loss for that point:

$$w \leftarrow w - \eta \, \nabla l(w, x_i, y_i)$$

- This is called an *online* or *stochastic* update
- In practice, *mini-batch SGD* is typically used:
  - Group data into mini-batches of size b
    - Compute gradient of the loss for the mini-batch $(x_1, y_1), \dots, (x_b, y_b)$:

$$\nabla \hat{L} = \frac{1}{b} \sum_{i=1}^{b} \nabla l(w, x_i, y_i)$$

    - Update parameters: $w \leftarrow w - \eta \nabla \hat{L}$

SGD for logistic regression

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

- Let's find the gradient:

$$\nabla l(w, x_i, y_i) = -\nabla_w \log \sigma(y_i w^T x_i)$$
$$= -\frac{\nabla_w \sigma(y_i w^T x_i)}{\sigma(y_i w^T x_i)}$$

- Derivative of log:

$$\left[\log(g(a))\right]' = \frac{g'(a)}{g(a)}$$

SGD for logistic regression

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$$= -\frac{\nabla_w \sigma(y_i w^T x_i)}{\sigma(y_i w^T x_i)}$$

$$= -\frac{\sigma(y_i w^T x_i)\sigma(-y_i w^T x_i) y_i x_i}{\sigma(y_i w^T x_i)}$$

Derivative of sigmoid:

$$\sigma'(a) = \sigma(a)(1 - \sigma(a)) = \sigma(a)\sigma(-a)$$

SGD for logistic regression

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

- Let's find the gradient:

$$\nabla l(w, x_i, y_i) = -\nabla_w \log \sigma(y_i w^T x_i)$$

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$$= -\frac{\sigma(y_i w^T x_i)\sigma(-y_i w^T x_i) y_i x_i}{\sigma(y_i w^T x_i)}$$

- We also used the *chain rule*: $\left[g_2(g_1(a))\right]' = g_2{}'(g_1(a))g_1{}'(a)$

SGD for logistic regression

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$

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$$= -\frac{\sigma(y_i w^T x_i)\sigma(-y_i w^T x_i) y_i x_i}{\sigma(y_i w^T x_i)}$$
$$= -\sigma(-y_i w^T x_i) y_i x_i$$

- SGD update:

$$w \leftarrow w + \eta\, \sigma(-y_i w^T x_i) y_i x_i$$

SGD for logistic regression

- Let’s take a close look at the SGD update:

$$w \leftarrow w + \eta\, \sigma(-y_i w^T x_i) y_i x_i$$

- What happens if x_i is *incorrectly,* but confidently, classified?
  - The update rule approaches $w \leftarrow w + \eta\, y_i x_i$
- What happens if x_i is *correctly,* and confidently, classified?
  - The update approaches zero (but never actually reaches zero)

SGD for logistic regression

- Logistic regression *does not converge* for linearly separable data!
  - Scaling w by ever larger constants makes the classifier more confident and keeps increasing the likelihood of the data

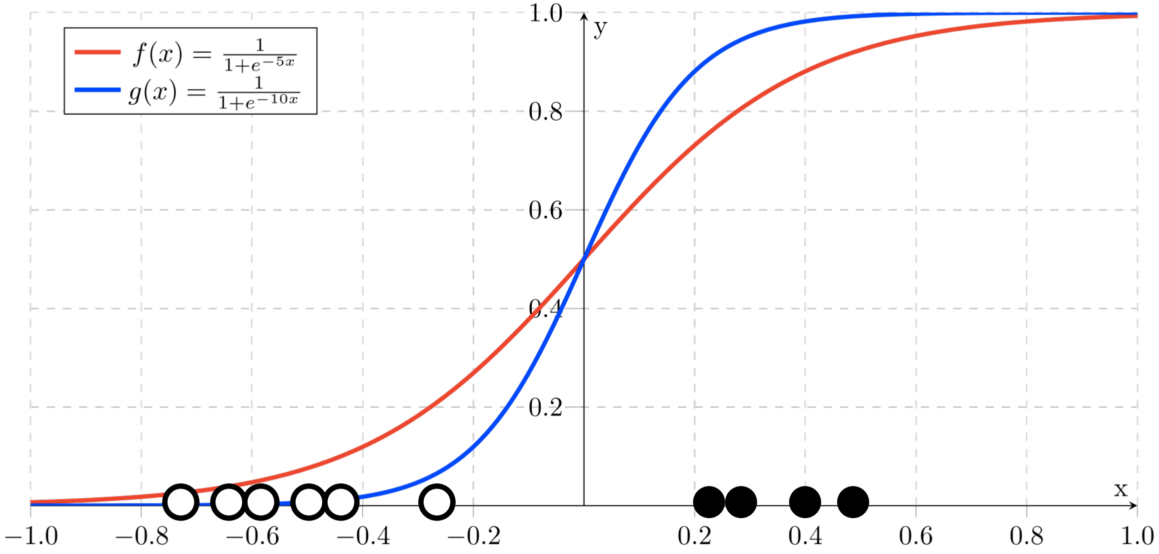

Image source

SGD for logistic regression

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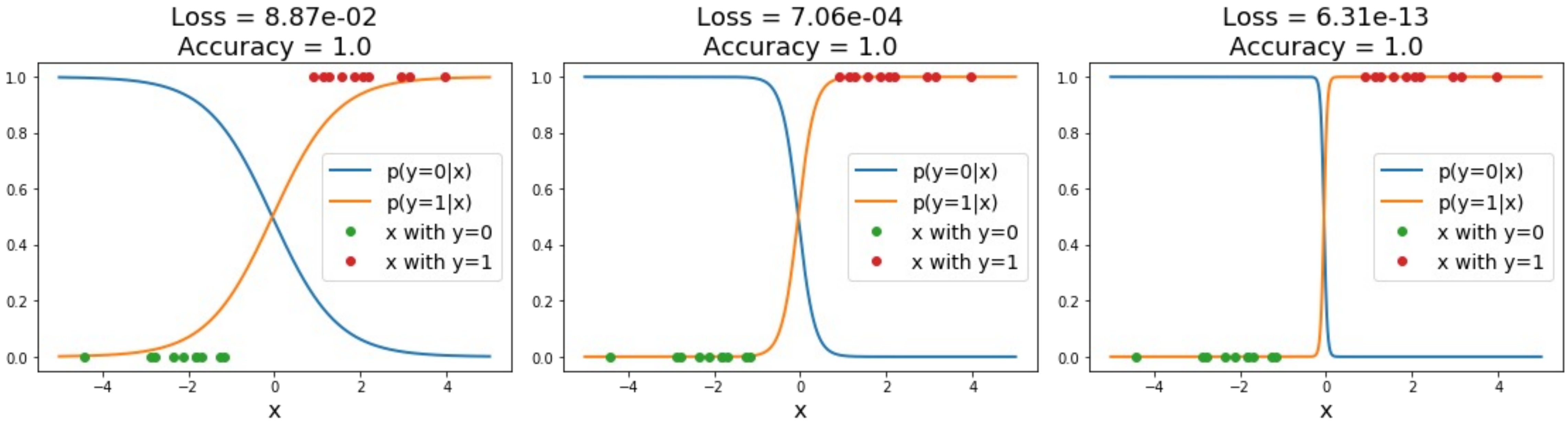


Source: J. Johnson

Sigmoid: Interpretation

- We can write out the connection between the *posteriors* $P(y|x)$ and the *class-conditional densities* $P(x|y)$:

$$P(y=1|x) = \frac{P(x|y=1)P(y=1)}{P(x)}$$

$$= \frac{P(x|y=1)P(y=1)}{P(x|y=1)P(y=1) + P(x|y=-1)P(y=-1)}$$

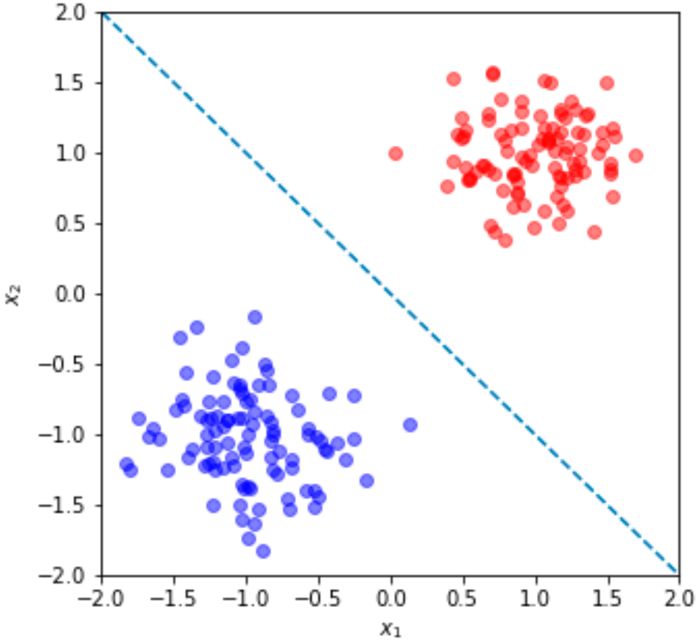
$$= \frac{1}{1+\exp(-a)} = \sigma(a), \qquad a = \log\frac{P(y=1|x)}{P(y=-1|x)}$$

Sigmoid: Interpretation

- Adopting a linear + sigmoid model is equivalent to assuming *linear log odds*:

$$\log \frac{P(y=1|x)}{P(y=-1|x)} = w^T x + b$$

- This happens when $P(x|y=1)$ and $P(x|y=-1)$ are Gaussians with different means and the same covariance matrices (w is related to the difference between the means)

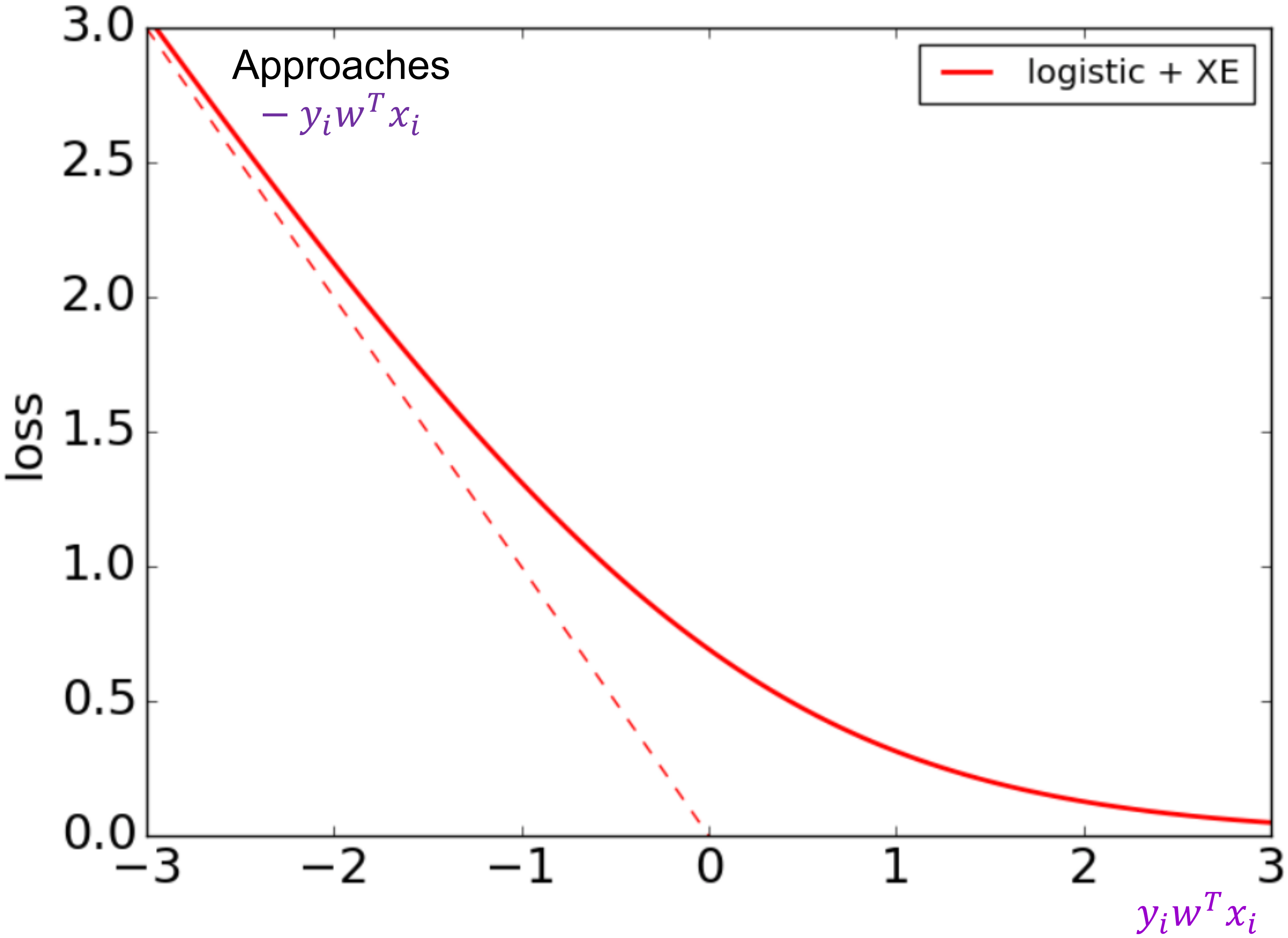


Linear classifiers: Outline

- Example classification models: nearest neighbor, linear
- Empirical loss minimization
- Linear classification models
  1. Linear regression (least squares)
  2. Logistic regression
  3. Perceptron loss

Recall: The shape of logistic loss

$$l(w, x_i, y_i) = -\log \sigma(y_i w^T x_i)$$



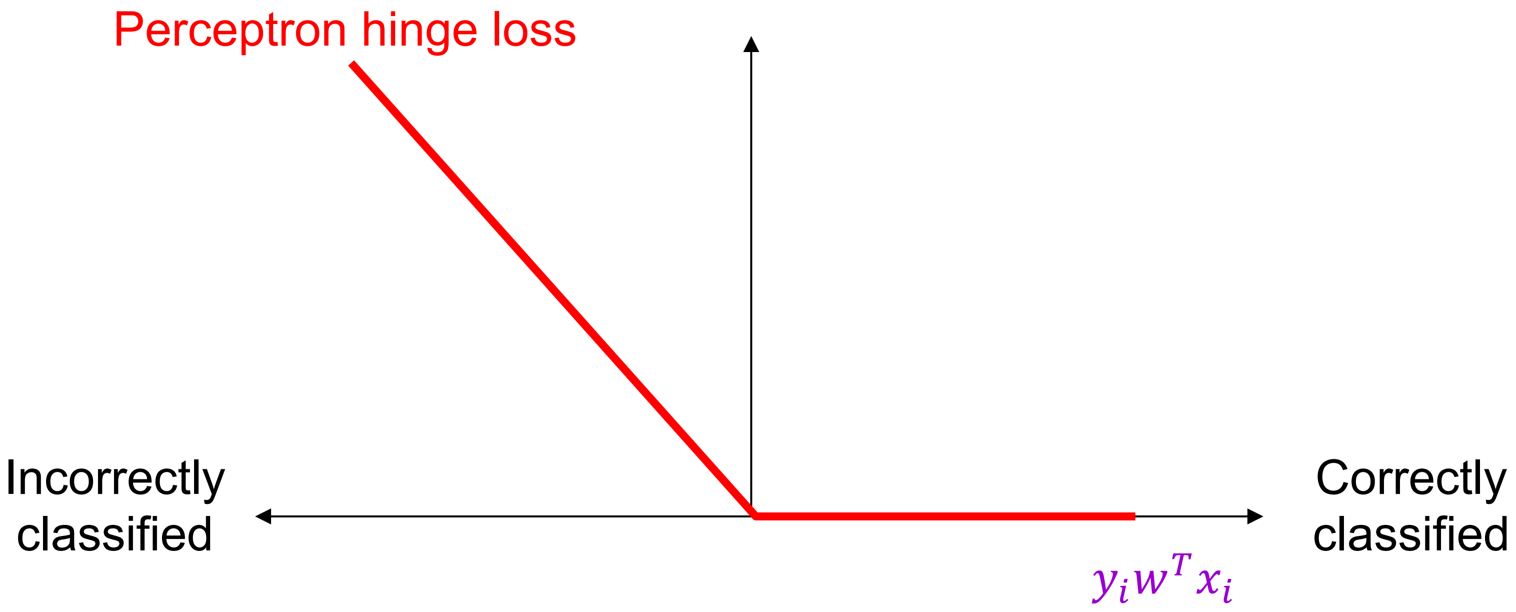
Approaches 0

Figure source

Perceptron

- Let's define the *perceptron hinge loss*:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$



Perceptron

- Let's define the *perceptron hinge loss*:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$

- Training: find w that minimizes

$$\hat{L}(w) = \frac{1}{n}\sum_{i=1}^{n} l(w, x_i, y_i) = \frac{1}{n}\sum_{i=1}^{n} \max(0, -y_i w^T x_i)$$

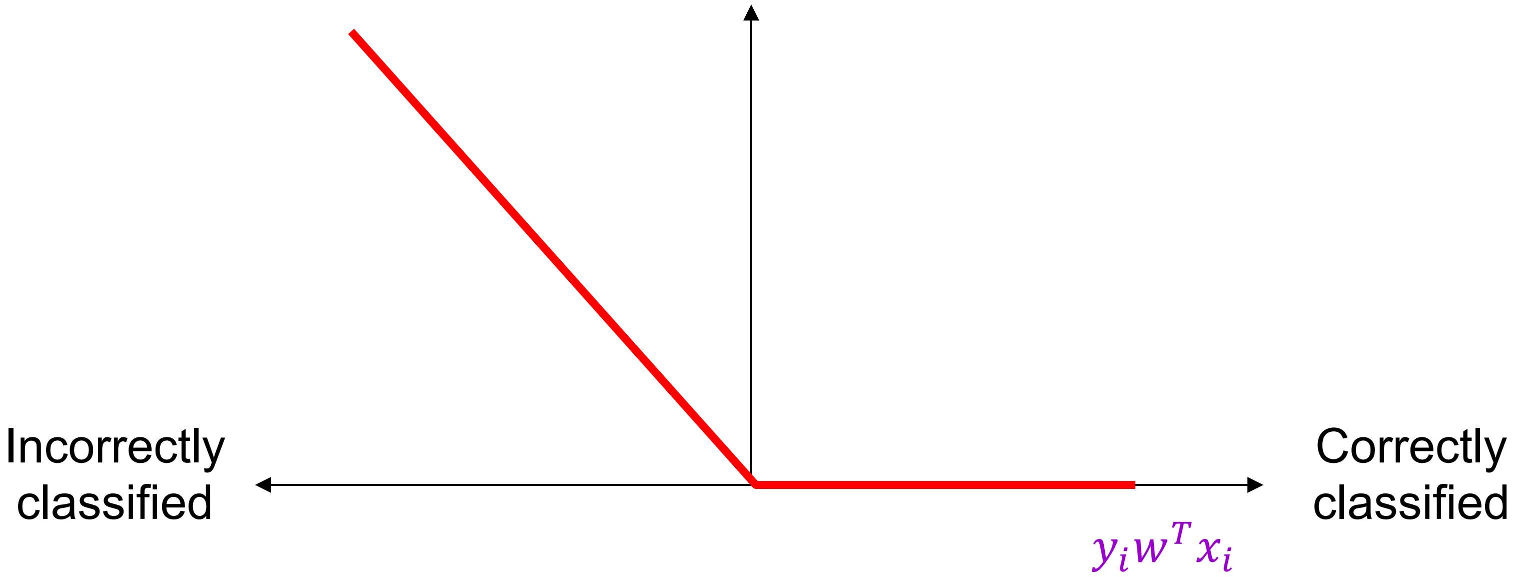
- Once again, there is no closed-form solution, so let's go straight to SGD

Deriving the perceptron update

- Let's differentiate the perceptron hinge loss:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$

(Strictly speaking, this loss is not differentiable, so we need to find a *sub-gradient*: A vector $g \in R^n$ is a sub-gradient of $f: R^n \to R$ at x if for all z, $f(z) \geq f(x) + g^T(z - x)$.)



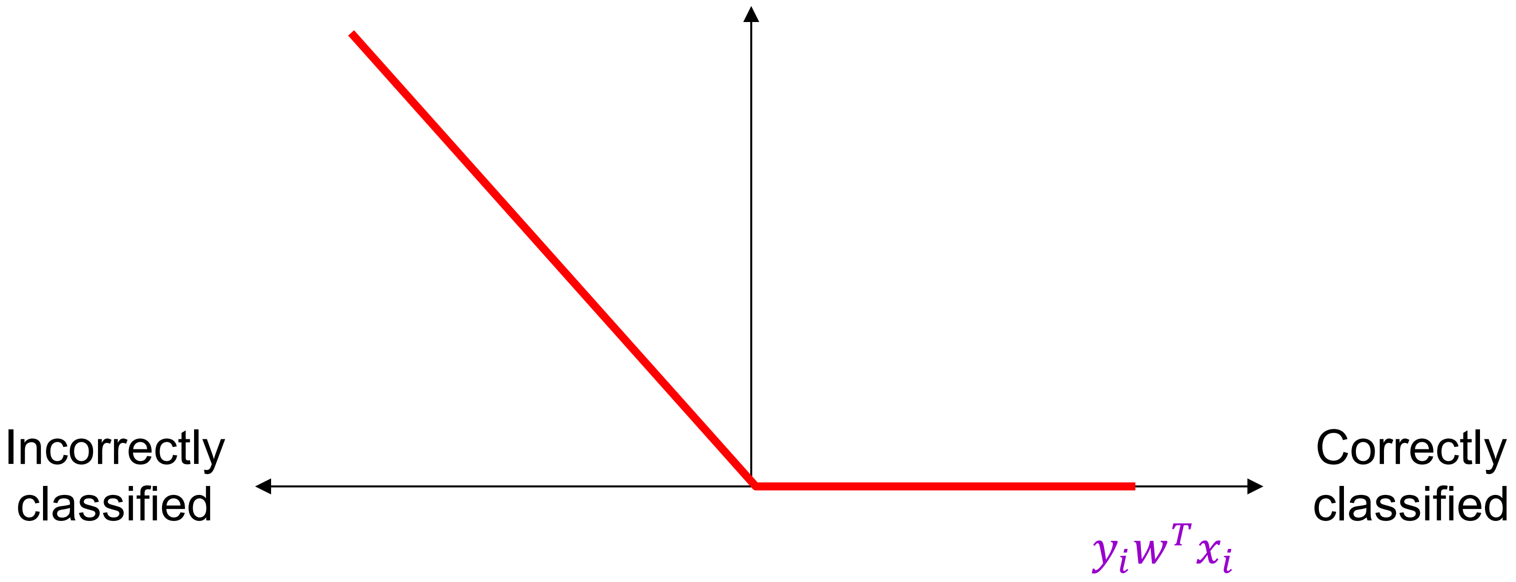
Deriving the perceptron update

- Let's differentiate the perceptron hinge loss:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$

$$\nabla l(w, x_i, y_i) = -\mathbb{I}[y_i w^T x_i < 0] y_i x_i$$

$$\frac{d}{da}\max(0, a) =$$



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- We also used the chain rule: $\left[g_2\left(g_1(a)\right)\right]' = g_2'\left(g_1(a)\right) g_1'(a)$

Deriving the perceptron update

- Let’s differentiate the perceptron hinge loss:

$$l(w, x_i, y_i) = \max(0, -y_i w^T x_i)$$

$$\nabla l(w, x_i, y_i) = -\mathbb{I}[y_i w^T x_i < 0] y_i x_i$$

- Corresponding SGD update ($w \leftarrow w - \eta \, \nabla l(w, x_i, y_i)$):

$$w \leftarrow w + \eta \, \mathbb{I}[y_i w^T x_i < 0] y_i x_i$$

  - If x_i is correctly classified: do nothing
  - If x_i is incorrectly classified: $w \leftarrow w + \eta \, y_i x_i$

Understanding the perceptron update rule

- **Perceptron update rule:** If $y_i \neq \text{sgn}(w^T x_i)$ then update weights:

$$w \leftarrow w + \eta \, y_i x_i$$

- The raw response of the classifier changes to

$$w^T x_i + \eta \, y_i \|x_i\|^2$$

- How does the response change if $y_i = 1$?
  - The response $w^T x_i$ is initially *negative* and will be *increased*

- How does the response change if $y_i = -1$?
  - The response $w^T x_i$ is initially *positive* and will be *decreased*

Linear classifiers: Outline

- Example classification models: nearest neighbor, linear
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  2. Logistic regression
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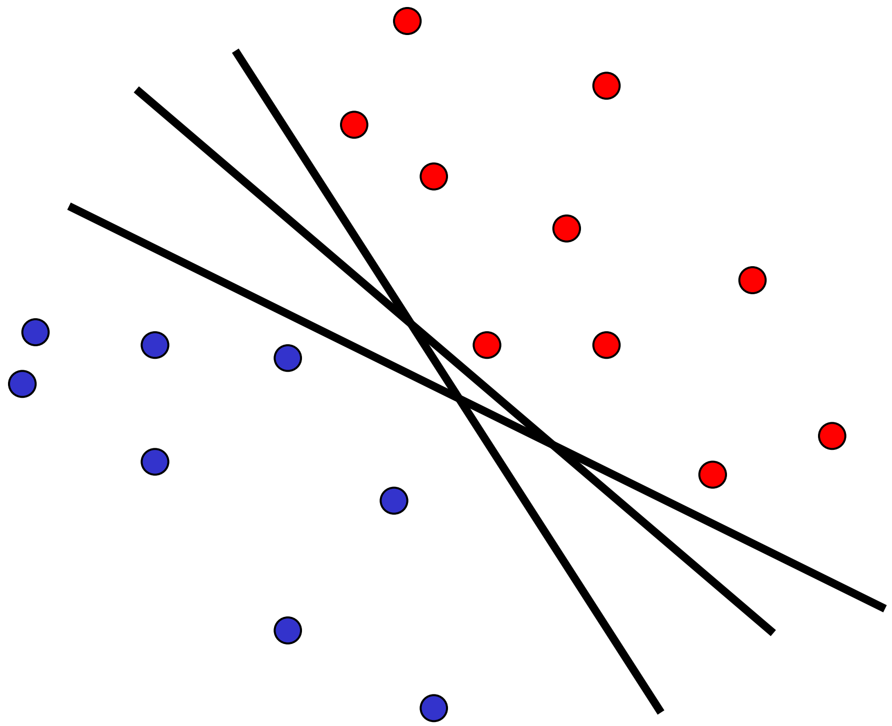
  4. Support vector machine (SVM) loss

Support vector machines

- When the data is linearly separable, which of the many possible solutions should we prefer?

  - **Perceptron training algorithm:** no special criterion, solution depends on initialization

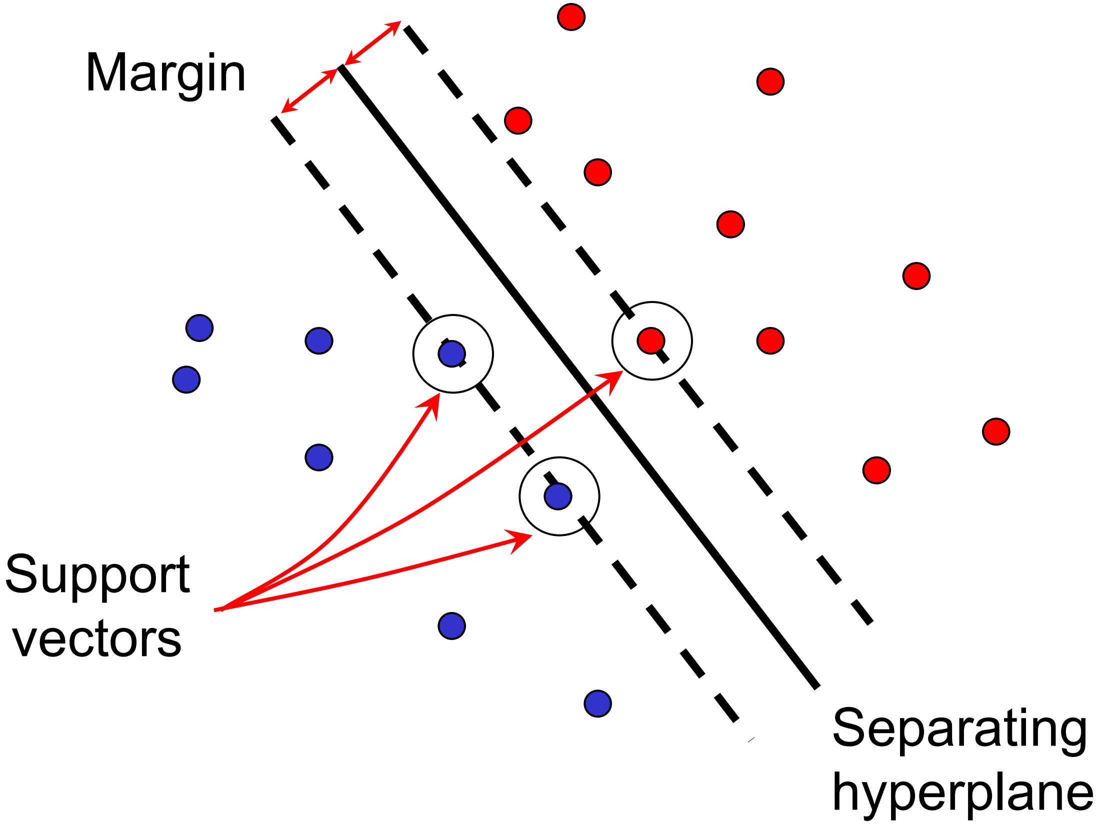


Support vector machines

- When the data is linearly separable, which of the many possible solutions should we prefer?

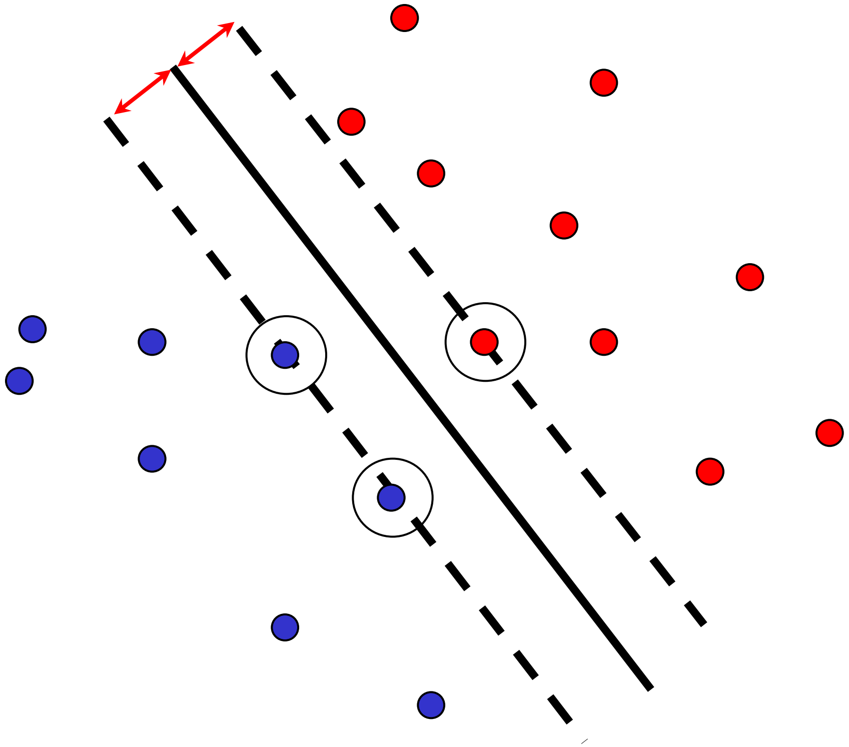
  - **Perceptron training algorithm:** no special criterion, solution depends on initialization

  - **SVM criterion:** maximize the *margin*, or distance between the hyperplane and the closest training example



Finding the maximum margin hyperplane

- We want to maximize the margin, or distance between the hyperplane $w^T x = 0$ and the closest training example x_0
- This distance is given by $\frac{|w^T x_0|}{\|w\|}$ (for derivation see, e.g., here)
- Assuming the data is linearly separable, we can fix the scale of w so that $y_i w^T x_i = 1$ for support vectors and $y_i w^T x_i \geq 1$ for all other points
- Then the margin is given by $\frac{1}{\|w\|}$



Finding the maximum margin hyperplane

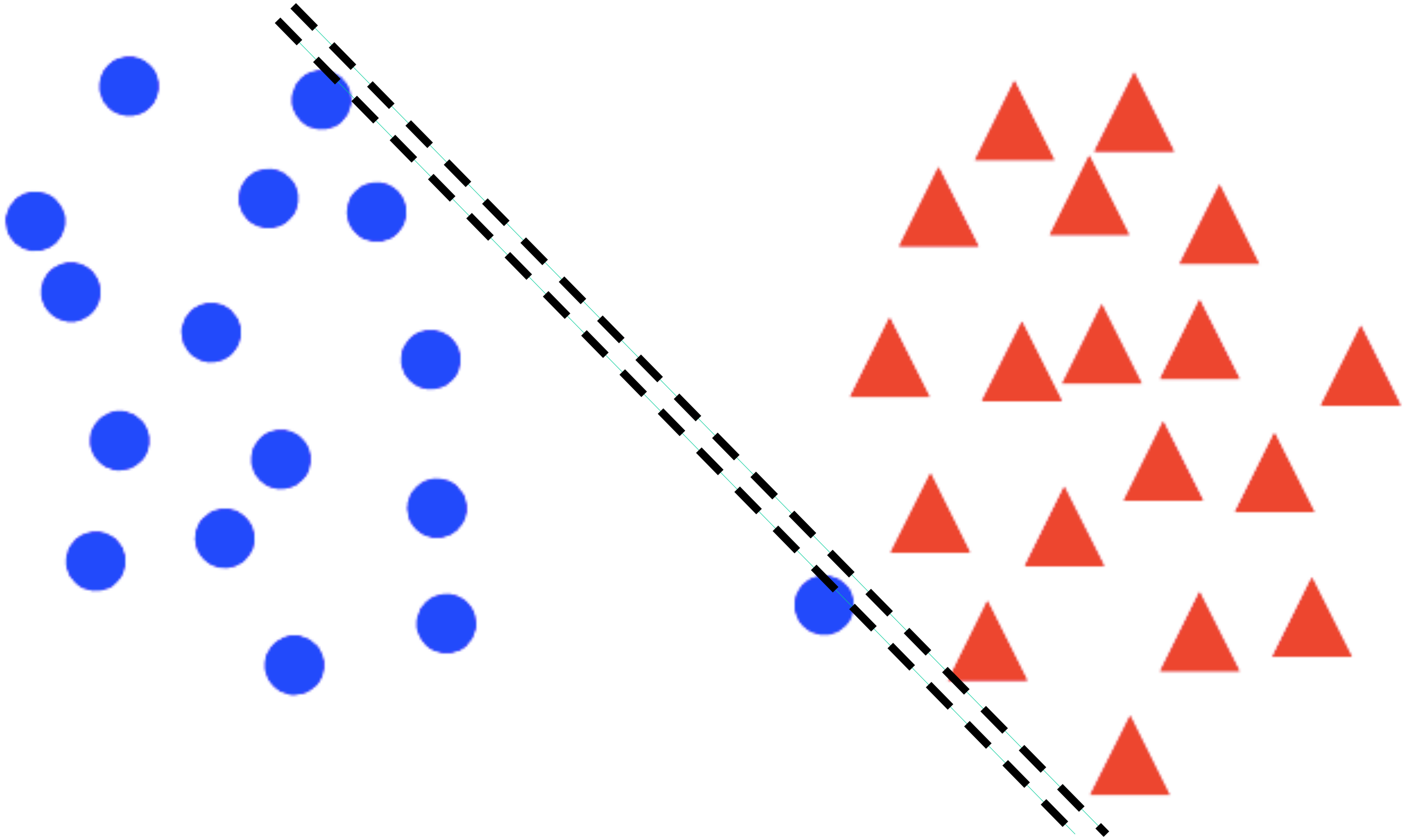
- We want to maximize margin $\frac{1}{\|w\|}$ while correctly classifying all training data: $y_i w^T x_i \geq 1$
- Equivalent problem:

$$\min_w \frac{1}{2}\|w\|^2 \quad \text{s.t.} \quad y_i w^T x_i \geq 1 \;\; \forall i$$

- This is a quadratic objective with linear constraints: convex optimization problem, global optimum can be found using well-studied methods

“Soft margin” formulation

- What about non-separable data?
- And even for separable data, we may prefer a larger margin with a few constraints violated



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“Soft margin” formulation

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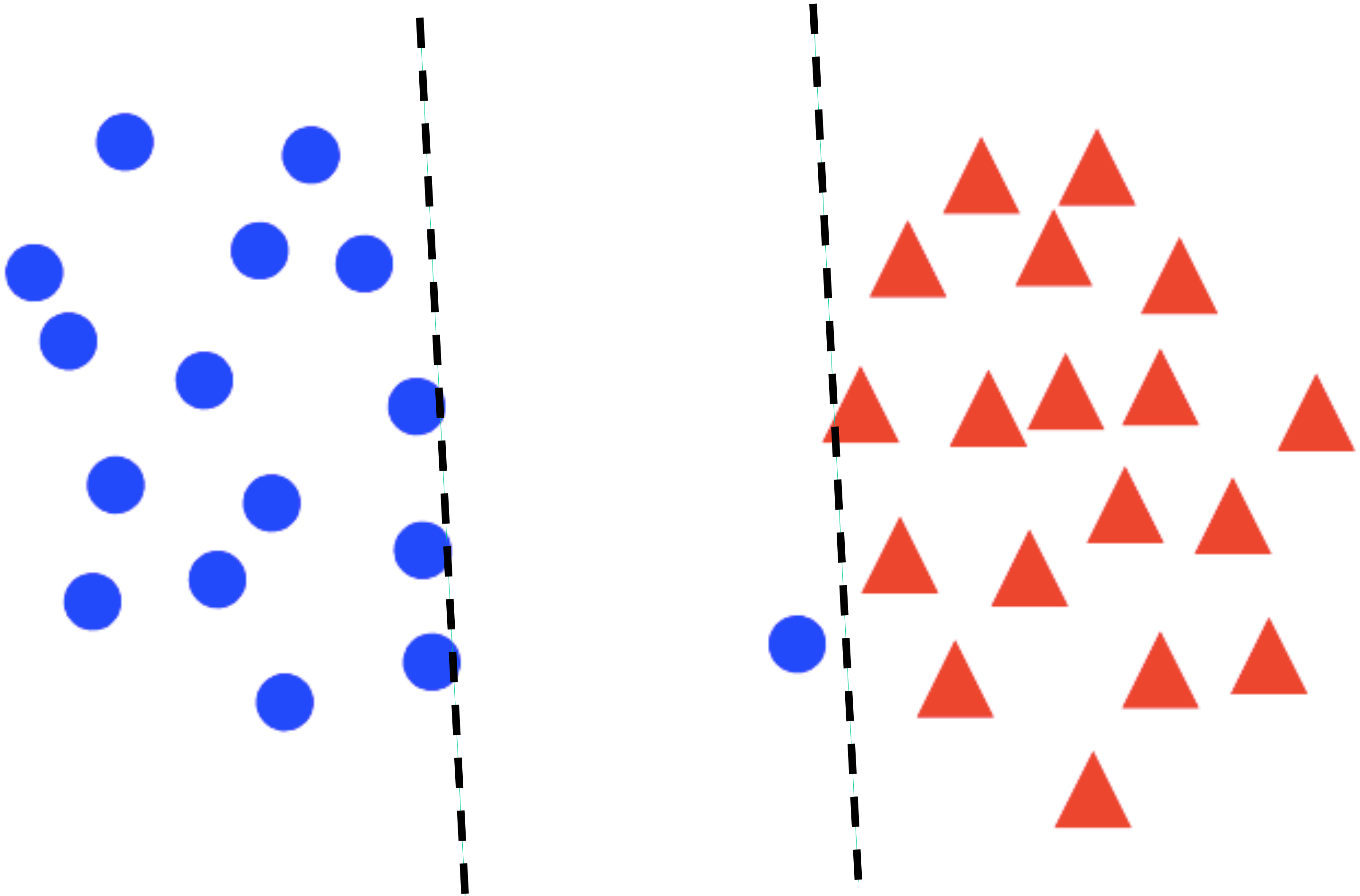

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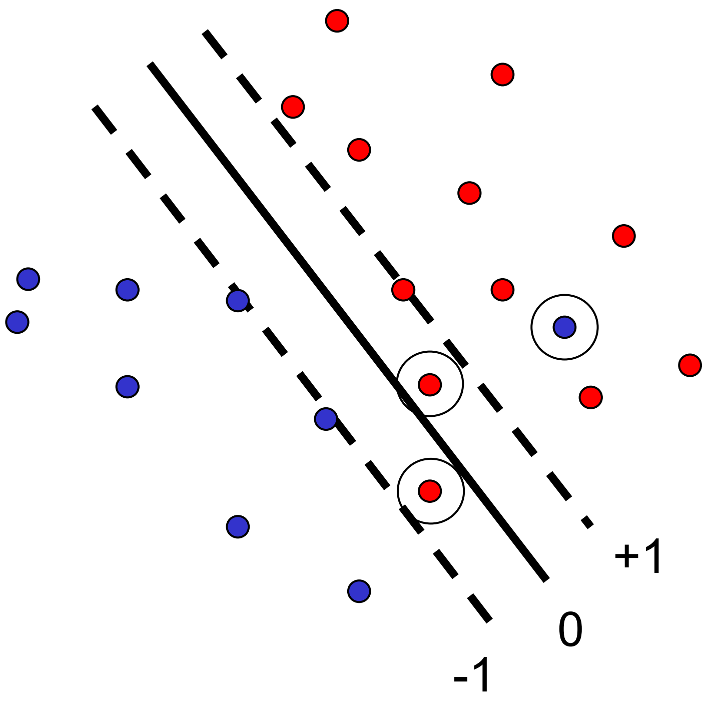
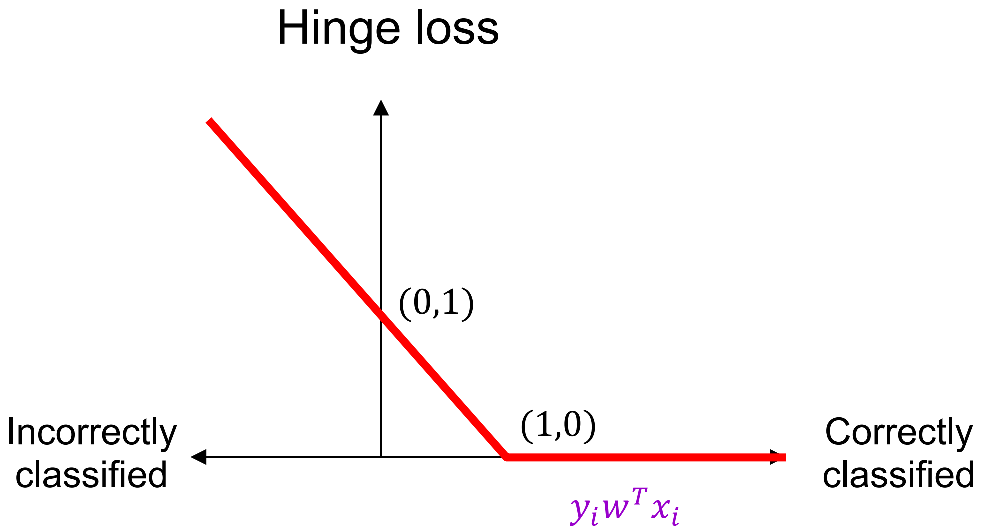
“Soft margin” formulation

- Penalize margin violations using SVM hinge loss:

$$\min_w \frac{\lambda}{2}\|w\|^2 \quad + \quad \sum_{i=1}^{n} \max[0, 1 - y_i w^T x_i]$$





“Soft margin” formulation

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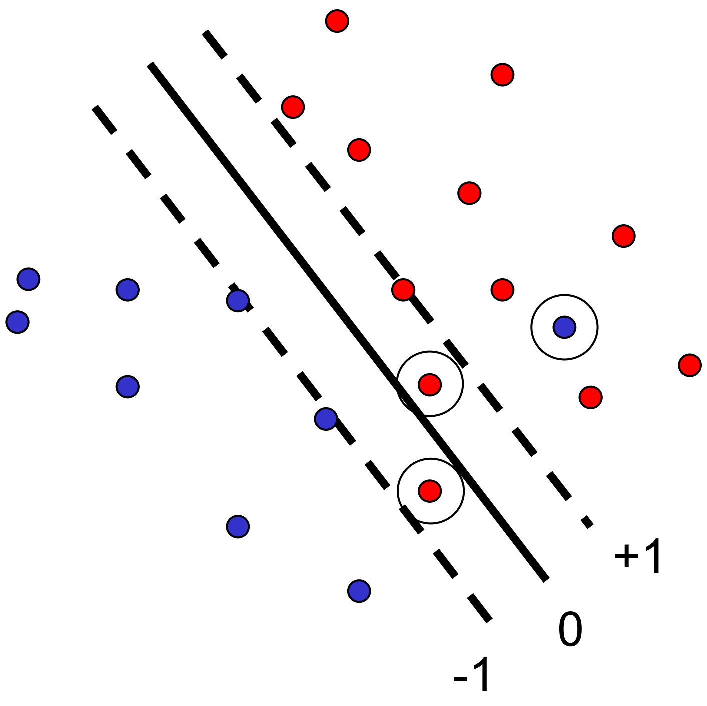
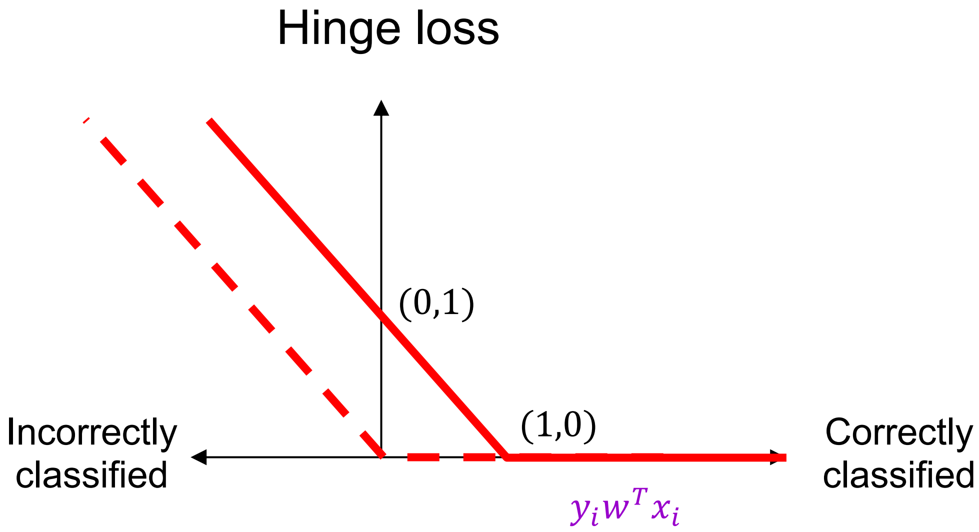




Recall hinge loss used by the perceptron update algorithm!

“Soft margin” formulation

- Penalize margin violations using SVM hinge loss:

$$\min_w \underbrace{\frac{\lambda}{2}\|w\|^2}_{\text{Maximize margin – a.k.a. }\textit{regularization}} \quad + \quad \underbrace{\sum_{i=1}^{n} \max[0, 1 - y_i w^T x_i]}_{\text{Minimize misclassification loss}}$$

SGD update for SVM

$$l(w, x_i, y_i) = \frac{\lambda}{2n}\|w\|^2 + \max[0, 1 - y_i w^T x_i]$$

$$\nabla l(w, x_i, y_i) = \frac{\lambda}{n} w - \mathbb{I}[y_i w^T x_i < 1] y_i x_i$$

Recall: $\frac{d}{da}\max(0, a) = \mathbb{I}[a > 0]$

SGD update for SVM

$$l(w, x_i, y_i) = \frac{\lambda}{2n}\|w\|^2 + \max[0, 1 - y_i w^T x_i]$$

$$\nabla l(w, x_i, y_i) = \frac{\lambda}{n} w - \mathbb{I}[y_i w^T x_i < 1] y_i x_i$$

- SGD update:
  - If $y_i w^T x_i \geq 1$: $w \leftarrow w - \eta \frac{\lambda}{n} w$
  - If $y_i w^T x_i < 1$: $w \leftarrow w + \eta \left(y_i x_i - \frac{\lambda}{n} w \right)$

S. Shalev-Schwartz et al., Pegasos: Primal Estimated sub-GrAdient SOlver for SVM, *Mathematical Programming*, 2011

Linear classifiers: Outline

- Examples of classification models: nearest neighbor, linear
- Empirical loss minimization framework
- Linear classification models
  1. Linear regression
  2. Logistic regression
  3. Perceptron training algorithm
  4. Support vector machines
- General recipe: data loss, regularization

General recipe

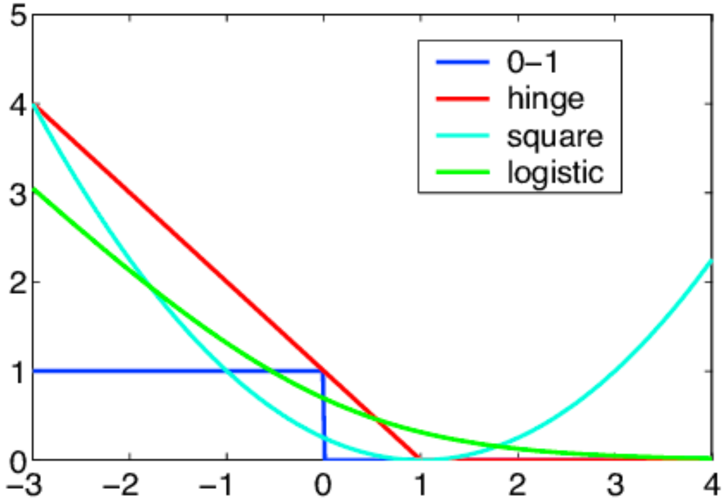
- Find parameters w that minimize the sum of a *regularization loss* and a *data loss*:

$$\hat{L}(w) = \lambda R(w) + \frac{1}{n}\sum_{i=1}^{n} l(w, x_i, y_i)$$

empirical loss regularization data loss

L2 regularization:

$$R(w) = \frac{1}{2}\|w\|_2^2$$



Closer look at L2 regularization

- Regularized objective: $\hat{L}(w) = \frac{\lambda}{2}\|w\|_2^2 + \sum_{i=1}^{n} l(w, x_i, y_i)$
- Gradient of objective:

$$\nabla\hat{L}(w) = \lambda w + \sum_{i=1}^{n} \nabla l(w, x_i, y_i)$$

- SGD update:

$$w \leftarrow w - \eta\left(\frac{\lambda}{n} w + \nabla l(w, x_i, y_i)\right)$$

$$w \leftarrow \left(1 - \frac{\eta\lambda}{n}\right) w - \eta\nabla l(w, x_i, y_i)$$

- Interpretation: weight decay

General recipe

- Find parameters w that minimize the sum of a *regularization loss* and a *data loss*:

$$\hat{L}(w) = \lambda R(w) + \frac{1}{n}\sum_{i=1}^{n} l(w, x_i, y_i)$$

empirical loss

regularization

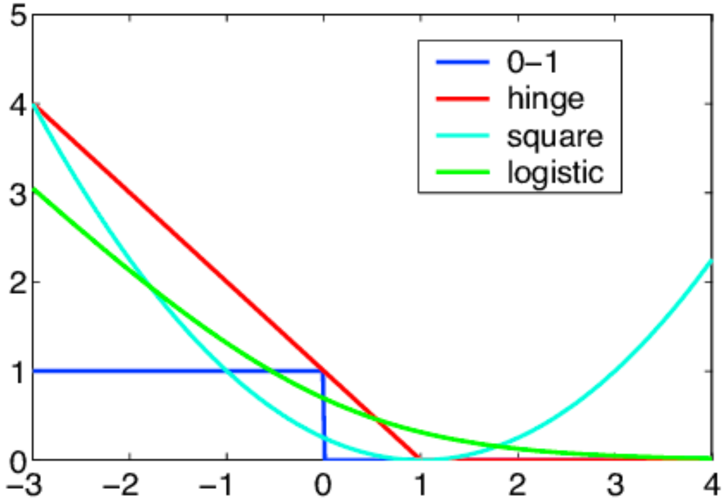
data loss

L2 regularization:

$$R(w) = \frac{1}{2}\|w\|_2^2$$

L1 regularization:

$$R(w) = \|w\|_1$$



Closer look at L1 regularization

- Regularized objective:

$$\hat{L}(w) = \lambda \|w\|_1 + \sum_{i=1}^{n} l(w, x_i, y_i)$$

$$= \lambda \sum_{d} \left| w^{(d)} \right| + \sum_{i=1}^{n} l(w, x_i, y_i)$$

- Gradient: $\nabla \hat{L}(w) = \lambda \operatorname{sgn}(w) + \sum_{i=1}^{n} \nabla l(w, x_i, y_i)$

  (here sgn is an elementwise function)

- SGD update:

$$w \leftarrow w - \frac{\eta\lambda}{n} \operatorname{sgn}(w) - \eta \nabla l(w, x_i, y_i)$$

- Interpretation: encouraging sparsity

Linear classifiers: Outline

- Examples of classification models: nearest neighbor, linear
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- General recipe: data loss, regularization
- Multi-class classification with a Softmax Function

One-vs-all Classification with a Softmax

- Let $y \in \{1, \ldots, C\}$
- Learn C scoring functions $f_1, f_2, \ldots, f_C$
- We can squash the vector of responses $(f_1, \ldots, f_c)$ into a vector of "probabilities":

$$\text{softmax}(f_1, \ldots, f_c) = \left(\frac{\exp(f_1)}{\sum_j \exp(f_j)}, \ldots, \frac{\exp(f_C)}{\sum_j \exp(f_j)} \right)$$

- The outputs are between 0 and 1 and sum to 1
- If one of the inputs (*logits*) is much larger than the others, then the corresponding softmax value will be close to 1 and others will be close to 0

Softmax and sigmoid

- For two classes:

$$\mathrm{softmax}(0, f) = \left(\frac{\exp(0)}{\exp(0) + \exp(f)}, \frac{\exp(f)}{\exp(0) + \exp(f)}\right)$$

$$= \left(\frac{1}{1+\exp(f)}, \frac{\exp(f)}{1+ \exp(f)}\right)$$

$$= (1 - \sigma(f), \sigma(f))$$

- Thus, softmax is the generalization of sigmoid for more than two classes

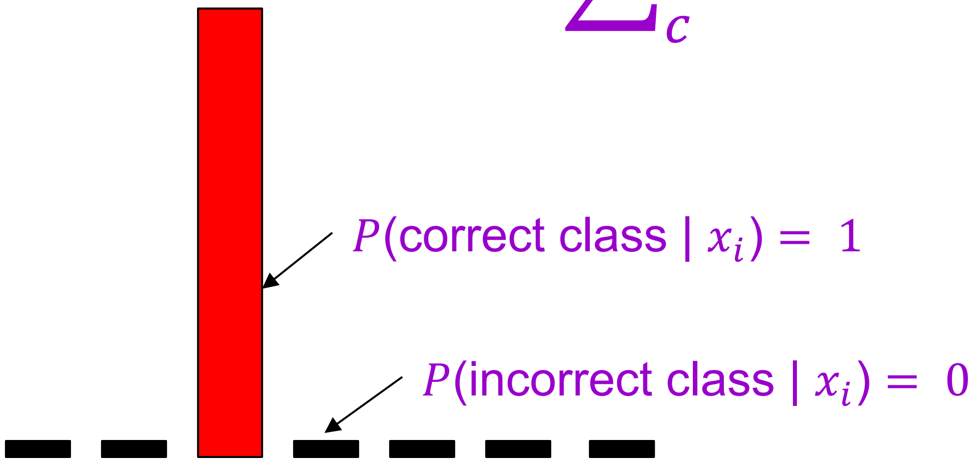
Cross-entropy loss

- It is natural to use negative log likelihood loss with softmax:

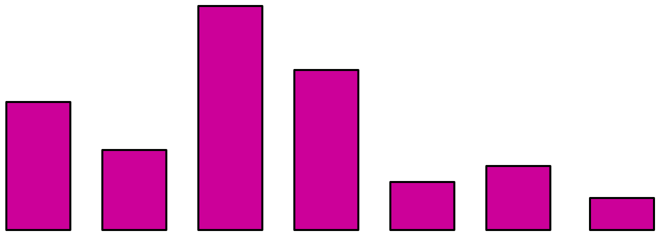
$$l(W, x_i, y_i) = -\log P_W(y_i|x_i) = -\log\left(\frac{\exp(w_{y_i}^T x_i)}{\sum_j \exp(w_j^T x_i)}\right)$$

- This is also the *cross-entropy* between the “empirical” distribution $\hat{P}(c|x_i) = \mathbb{I}[c = y_i]$ and “estimated” distribution $P_W(c|x_i)$:

$$-\sum_c \hat{P}(c|x_i) \log P_W(c|x_i)$$



Empirical distribution $\hat{P}(c|x_i)$



Estimated distribution $P_W(c|x_i)$

SGD with cross-entropy loss

$$l(W, x_i, y_i) = -\log P_W(y_i|x_i) = -\log\left(\frac{\exp(w_{y_i}^T x_i)}{\sum_j \exp(w_j^T x_i)}\right)$$

$$= -w_{y_i}^T x_i + \log\left(\sum_j \exp(w_j^T x_i)\right)$$

- Gradient w.r.t. w_{y_i}:

$$-x_i + \frac{\exp(w_{y_i}^T x_i)x_i}{\sum_j \exp(w_j^T x_i)} = (P_W(y_i|x_i) - 1)x_i$$

- Gradient w.r.t. w_c, $c \neq y_i$:

$$\frac{\exp(w_c^T x_i)x_i}{\sum_j \exp(w_j^T x_i)} = P_W(c|x_i)x_i$$

SGD with cross-entropy loss

- Gradient w.r.t. w_{y_i}: $(P_W(y_i|x_i) - 1)x_i$
- Gradient w.r.t. w_c, $c \neq y_i$: $P_W(c|x_i)x_i$
- Update rule:
  - For y_i:

    $$w_{y_i} \leftarrow w_{y_i} + \eta\big(1 - P_W(y_i|x_i)\big)x_i$$
  - For $c \neq y_i$:

    $$w_c \leftarrow w_c - \eta P_W(c|x_i)x_i$$

Softmax trick: Avoiding overflow

- Exponentiated values $\exp(f_c)$ can become very large and cause overflow
- Note that adding the same constant to all softmax inputs (*logits*) does not change the output of the softmax:

$$\frac{\exp(f_c + K)}{\sum_j \exp\left(f_j + K\right)} = \frac{\exp(K)\exp(f_c)}{\sum_j \exp(K)\exp\left(f_j\right)} = \frac{\exp(f_c)}{\sum_j \exp\left(f_j\right)}$$

- Then we can let $\mathrm{K} = -\max_j f_j$ (i.e., make largest input to softmax be 0)

Softmax trick: Temperature scaling

- Suppose we divide every input to the softmax by the same constant T:

$$\text{softmax}(f_1, \dots, f_c; T) = \left(\frac{\exp(f_1/T)}{\sum_j \exp(f_j/T)}, \dots, \frac{\exp(f_c/T)}{\sum_j \exp(f_j/T)} \right)$$

- What does this accomplish?
  - Prior to normalization, each entry $\exp(f_1)$ is raised to the power $1/T$
  - If T is close to 0, the largest entry will dominate and output distribution will tend to *one-hot*
  - If T is high, output distribution will tend to uniform

Softmax trick: Temperature scaling

Low temperature:
More concentrated
distribution

Higher temperature:
More uniform
distribution

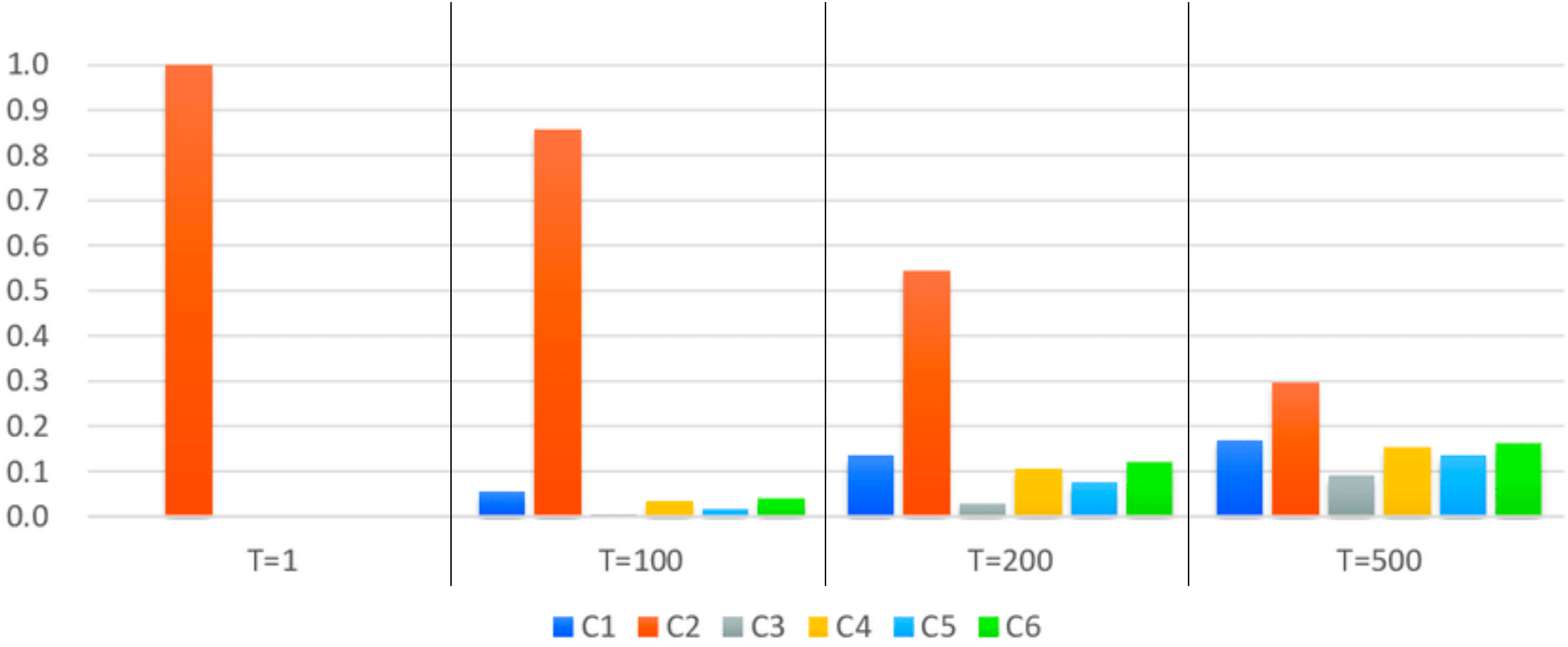


Figure source

Linear classifiers: Outline

- Examples of classification models: nearest neighbor, linear
- Empirical loss minimization framework
- Linear classification models
  1. Linear regression
  2. Logistic regression
  3. Perceptron training algorithm
  4. Support vector machines
- General recipe: data loss, regularization
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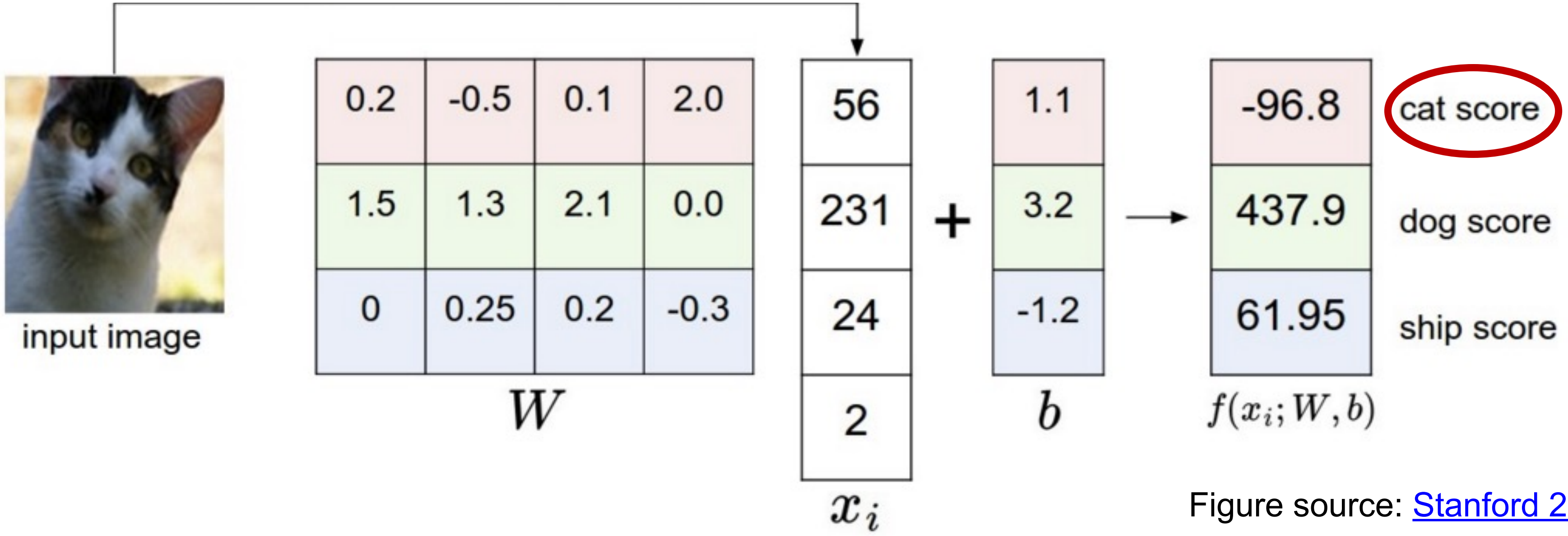
  - Multi-class SVMs and Perceptron (Self-study)

Multi-class perceptrons

- Let $y \in \{1, \dots, C\}$
- Learn C scoring functions $f_1, f_2, \dots, f_C$
- Classify x to class $\hat{y} = \text{argmax}_c\ f_c(x)$
- Multi-class perceptrons: $f_c(x) = w_c^T x$
- Let W be the matrix with rows w_c
- What loss should we use for multi-class classification?



$$\underset{W}{\begin{bmatrix}0.2 & -0.5 & 0.1 & 2.0\\ 1.5 & 1.3 & 2.1 & 0.0\\ 0 & 0.25 & 0.2 & -0.3\end{bmatrix}} \underset{x_i}{\begin{bmatrix}56\\ 231\\ 24\\ 2\end{bmatrix}} + \underset{b}{\begin{bmatrix}1.1\\ 3.2\\ -1.2\end{bmatrix}} \rightarrow \underset{f(x_i; W, b)}{\begin{bmatrix}-96.8\\ 437.9\\ 61.95\end{bmatrix}}$$

Figure source: Stanford 231n

Multi-class perceptrons

- Let $y \in \{1, \dots, C\}$
- Learn C scoring functions $f_1, f_2, \dots, f_C$
- Classify x to class $\hat{y} = \operatorname{argmax}_c f_c(x)$
- Multi-class perceptrons: $f_c(x) = w_c^T x$
- Let W be the matrix with rows w_c
- What loss should we use for multi-class classification?
- For (x_i, y_i), let the loss be the *sum of hinge losses* associated with predictions for all *incorrect* classes:

$$l(W, x_i, y_i) = \sum_{c \neq y_i} \max[0, w_c^T x_i - w_{y_i}^T x_i]$$

Score for correct class (y_i) has to be greater than the score for the incorrect class (c)

Figure source: Stanford 231n

Multi-class perceptrons

$$l(W, x_i, y_i) = \sum_{c \neq y_i} \max[0, w_c^T x_i - w_{y_i}^T x_i]$$

- Gradient w.r.t. w_{y_i}:

$$-\sum_{c \neq y_i} \mathbb{I}\,[w_c^T x_i > w_{y_i}^T x_i] x_i$$

Recall: $\frac{d}{da} \max(0, a) = \mathbb{I}[a > 0]$

Multi-class perceptrons

$$l(W, x_i, y_i) = \sum_{c \neq y_i} \max[0, w_c^T x_i - w_{y_i}^T x_i]$$

- Gradient w.r.t. w_{y_i}:

$$-\sum_{c \neq y_i} \mathbb{I}\,[w_c^T x_i > w_{y_i}^T x_i] x_i$$

- Gradient w.r.t. w_c, $c \neq y_i$:

$$\mathbb{I}[w_c^T x_i > w_{y_i}^T x_i] x_i$$

- Update rule: for each c s.t. $w_c^T x_i > w_{y_i}^T x_i$:

$$w_{y_i} \leftarrow w_{y_i} + \eta x_i$$
$$w_c \leftarrow w_c - \eta x_i$$

Multi-class perceptrons

- Update rule: for each c s.t. $w_c^T x_i > w_{y_i}^T x_i$:

$$w_{y_i} \leftarrow w_{y_i} + \eta x_i$$
$$w_c \leftarrow w_c - \eta x_i$$

- Is this equivalent to training C independent one-vs-all classifiers?

input image

	Independent	Multi-class
Cat score: 65.1	Do nothing	Increase
Dog score: 101.4	Decrease	Decrease
Ship score: 24.9	Decrease	Do nothing

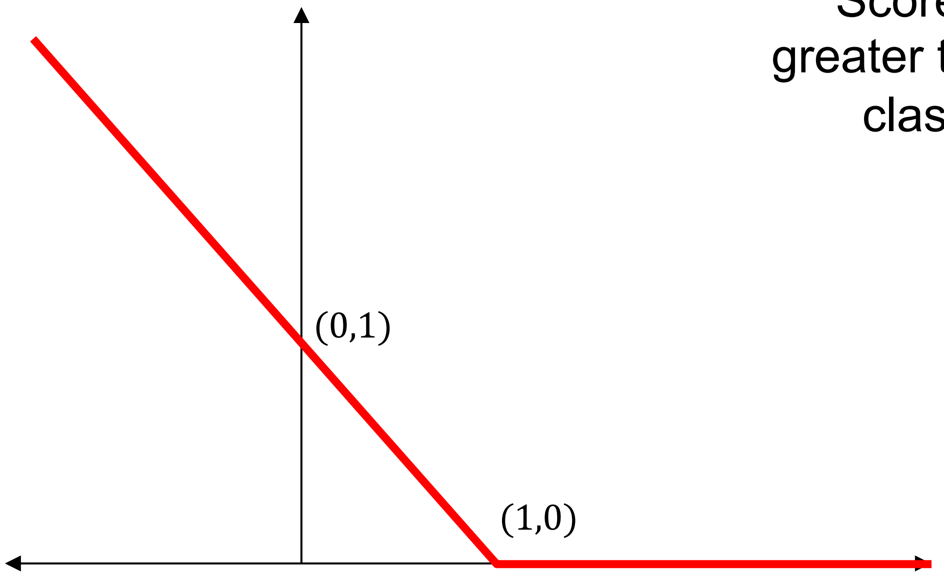
Multi-class SVM

- Recall single-class SVM loss:

$$l(w, x_i, y_i) = \frac{\lambda}{2n}\|w\|^2 + \max[0, 1 - y_i w^T x_i]$$

- Generalization to multi-class:

$$l(W, x_i, y_i) = \frac{\lambda}{2n}\|W\|^2 + \sum_{c \neq y_i} \max[0, 1 - w_{y_i}^T x_i + w_c^T x_i]$$



Score for correct class has to be greater than the score for the incorrect class *by at least a margin of* 1

Score for correct class – score for incorrect class

Source: Stanford 231n

Multi-class SVM

$$l(W, x_i, y_i) = \frac{\lambda}{2n}\|W\|^2 + \sum_{c \neq y_i} \max[0, 1 - w_{y_i}^T x_i + w_c^T x_i]$$

- Gradient w.r.t. w_{y_i}:

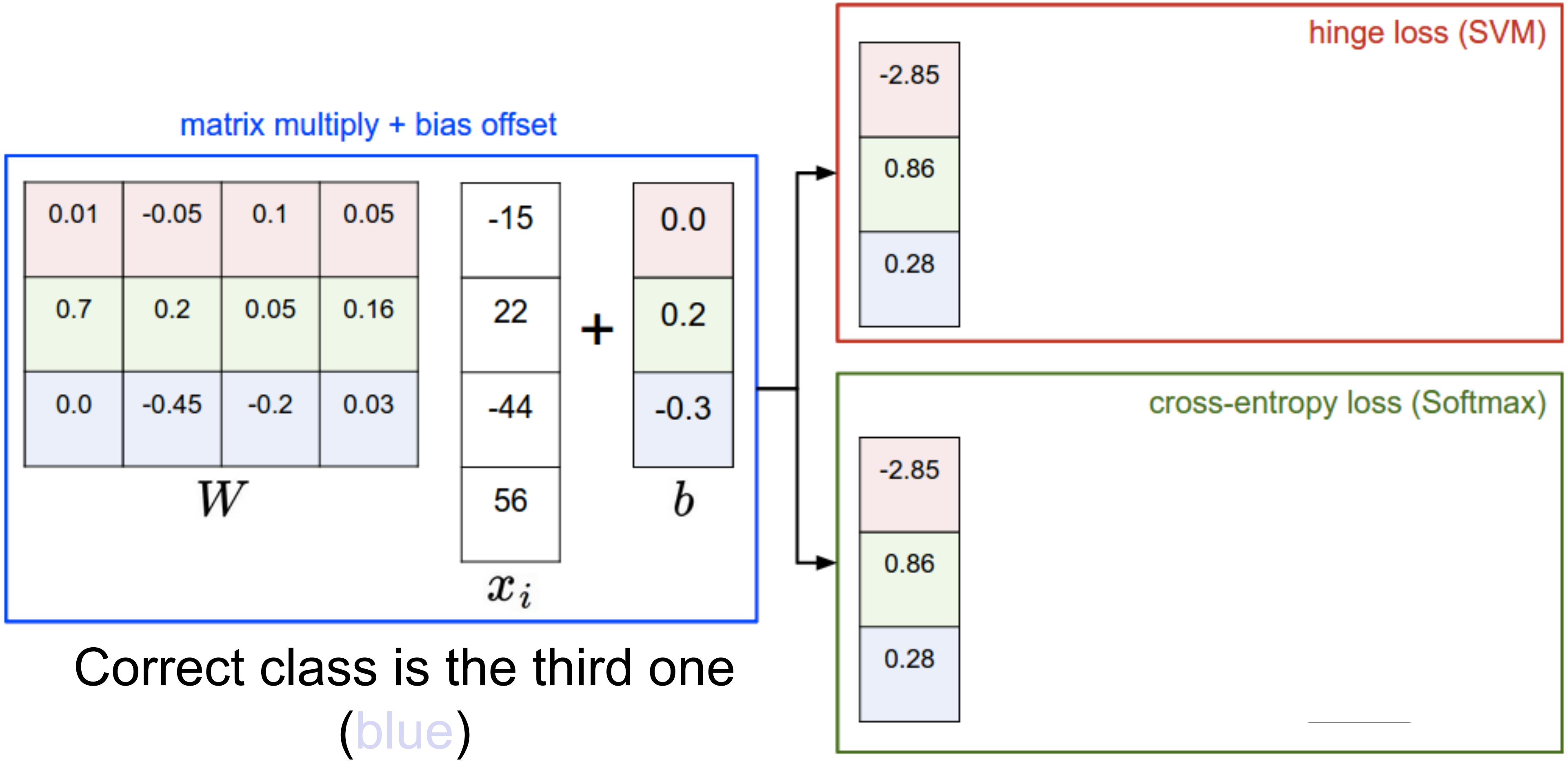
$$\frac{\lambda}{n} w_{y_i} - \sum_{c \neq y_i} \mathbb{I}\left[w_{y_i}^T x_i - w_c^T x_i < 1\right] x_i$$

- Gradient w.r.t. w_c, $c \neq y_i$:

$$\frac{\lambda}{n} w_c + \mathbb{I}[w_{y_i}^T x_i - w_c^T x_i < 1] x_i$$

- Update rule (almost* equivalent to above):
  - For each $c \neq y_i$ s.t. $w_{y_i}^T x_i - w_c^T x_i < 1$: $w_{y_i} \leftarrow w_{y_i} + \eta x_i$, $w_c \leftarrow w_c - \eta x_i$
  - For $c = 1, \ldots, C$: $w_c \leftarrow \left(1 - \eta \frac{\lambda}{n}\right) w_c$

SVM loss vs. cross-entropy loss



0.01	-0.05	0.1	0.05
0.7	0.2	0.05	0.16
0.0	-0.45	-0.2	0.03

x_i: -15, 22, -44, 56

b: 0.0, 0.2, -0.3

hinge loss (SVM): -2.85, 0.86, 0.28

cross-entropy loss (Softmax): -2.85, 0.86, 0.28

Correct class is the third one (blue)

Source: Stanford 231n

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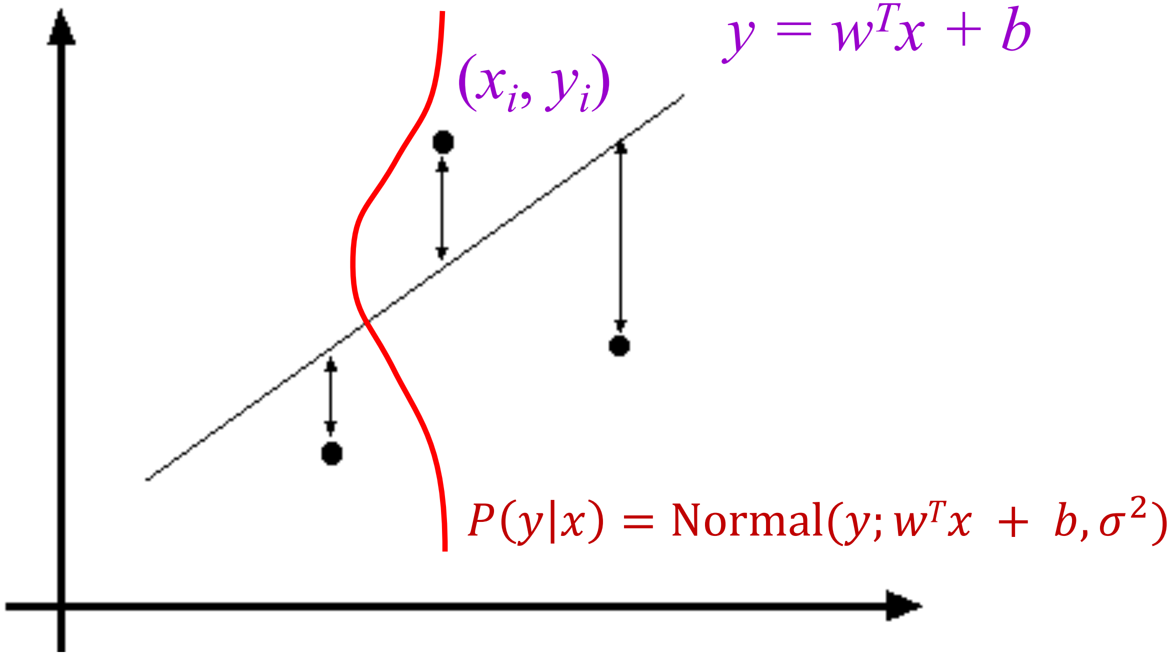
Linear regression as maximum likelihood estimation?

- Interpretation of l_2 loss: *negative log likelihood* assuming y is normally distributed with mean $f_w(x) = w^T x + b$



Maximum likelihood estimation

- Given: i.i.d. training data $\{(x_i, y_i), i = 1, \dots, n\}$
- Let $\{P_\theta(y|x), \theta \in \Theta\}$ be a family of distributions parameterized by θ
- Maximum (conditional) likelihood estimate:

$$\theta_{ML} = \mathrm{argmax}_\theta \prod_i P_\theta(y_i|x_i)$$

$$= \mathrm{argmin}_\theta - \sum_i \log P_\theta(y_i|x_i)$$

Maximum likelihood estimation

$$\theta_{ML} = \operatorname{argmin}_\theta - \textstyle\sum_i \log P_\theta(y_i|x_i)$$

- Assume $P_\theta(y|x) = \mathrm{Normal}(y; f_\theta(x), \sigma^2)$

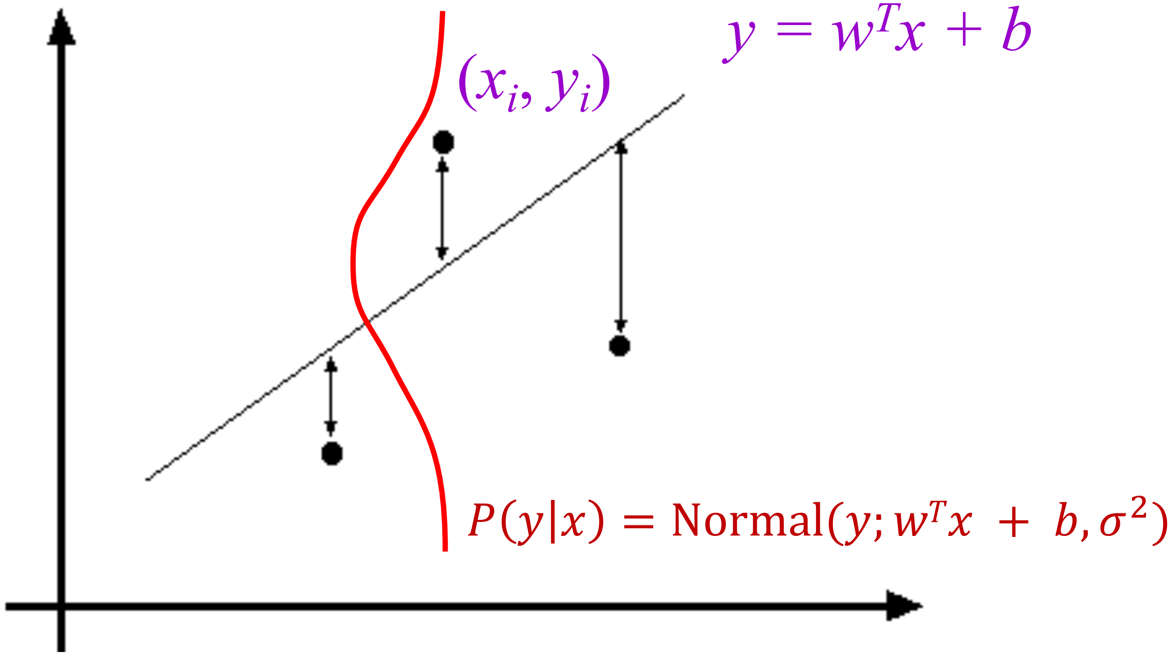
$$\log P_\theta(y|x) = \log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{\left(y - f_\theta(x)\right)^2}{2\sigma^2}\right]\right]$$

$$= -\frac{1}{2\sigma^2}\left(y - f_\theta(x)\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)$$

$$\theta_{ML} = \operatorname{argmin}_\theta \sum_i \left(y_i - f_\theta(x_i)\right)^2$$

Linear regression as maximum likelihood estimation

- Interpretation of l_2 loss: *negative log likelihood* assuming y is normally distributed with mean $f_w(x) = w^T x + b$



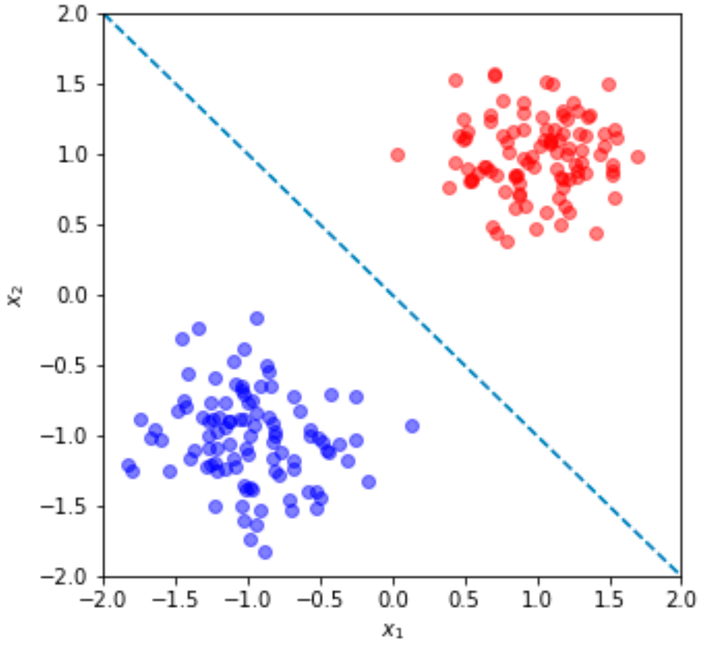
- Does this make sense for binary classification?

Sigmoid: Interpretation

- Adopting a linear + sigmoid model is equivalent to assuming *linear log odds*:

$$\log \frac{P(y=1|x)}{P(y=-1|x)} = w^T x + b$$

- This happens when $P(x|y=1)$ and $P(x|y=-1)$ are Gaussians with different means and the same covariance matrices (w is related to the difference between the means)



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