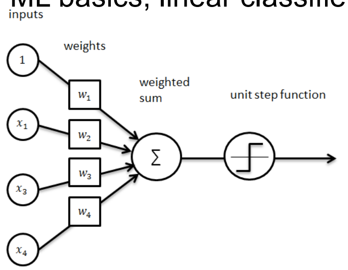
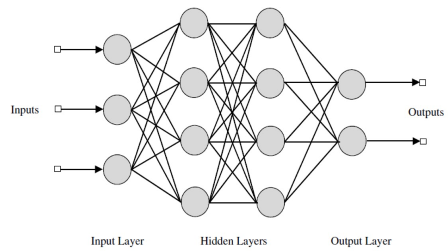
Topics to be covered in class

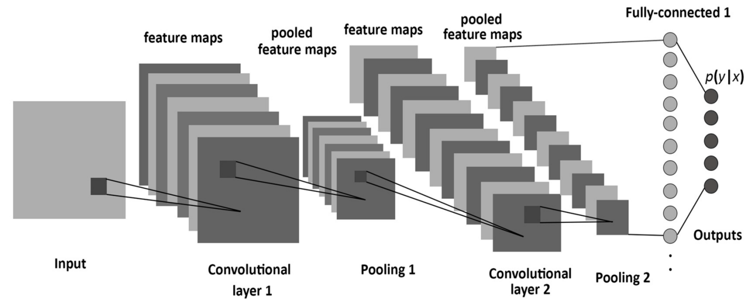
ML basics, linear classifiers



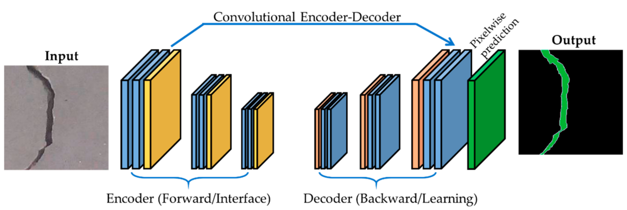
Multilayer neural networks, backpropagation



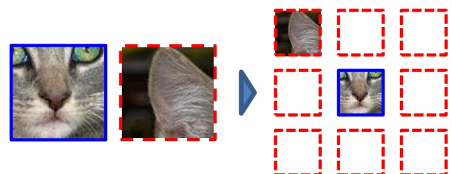
Convolutional networks for classification



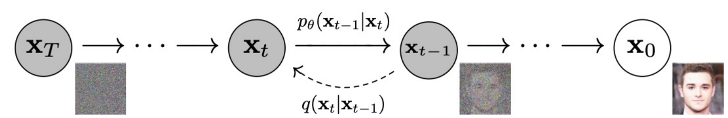
Networks for detection, dense prediction



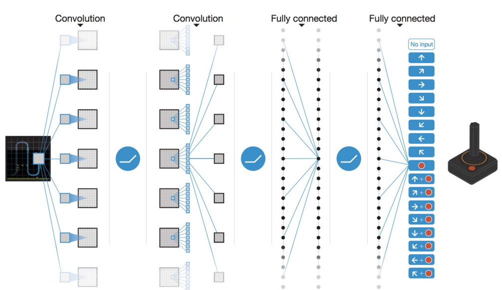
Self-supervised learning



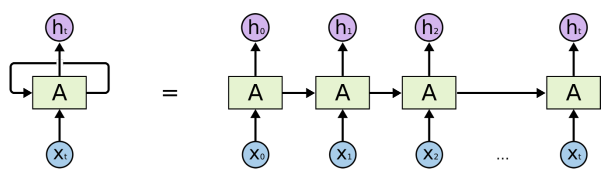
Generative models: GANs, image-to-image translation, diffusion models



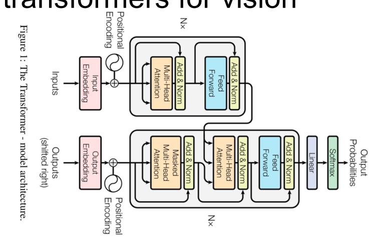
Deep reinforcement learning



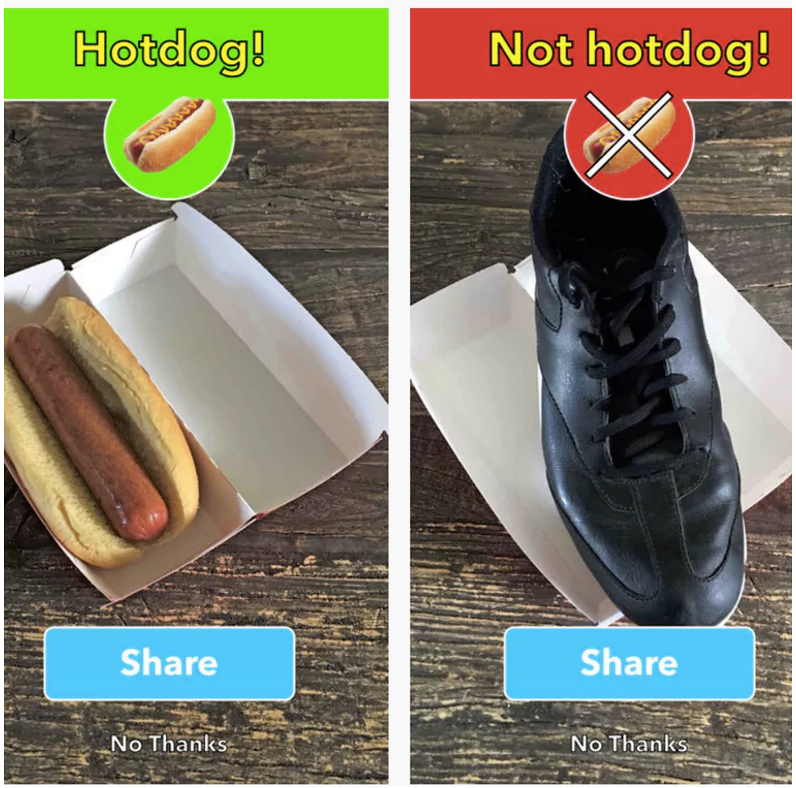
Models for sequence data



Transformers, large language models, transformers for vision



Everything you've ever wanted to know about linear classifiers (Part 1)



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

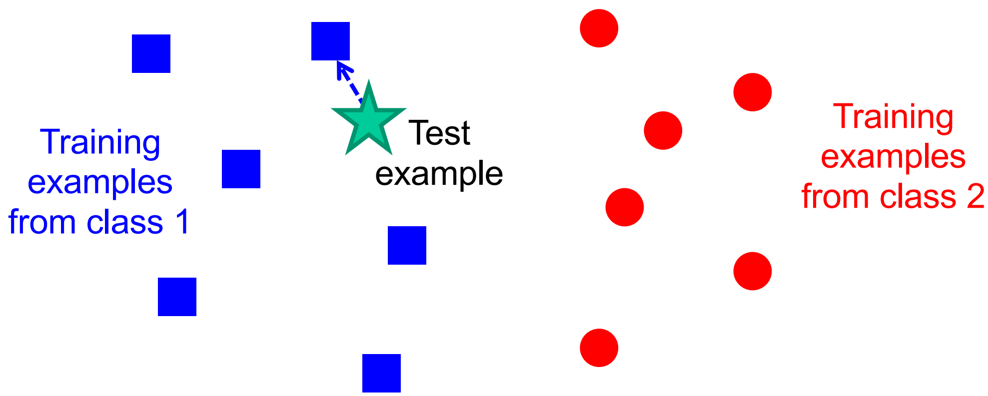
The basic *supervised learning* framework

$$y = f(x)$$

output   prediction function   input

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

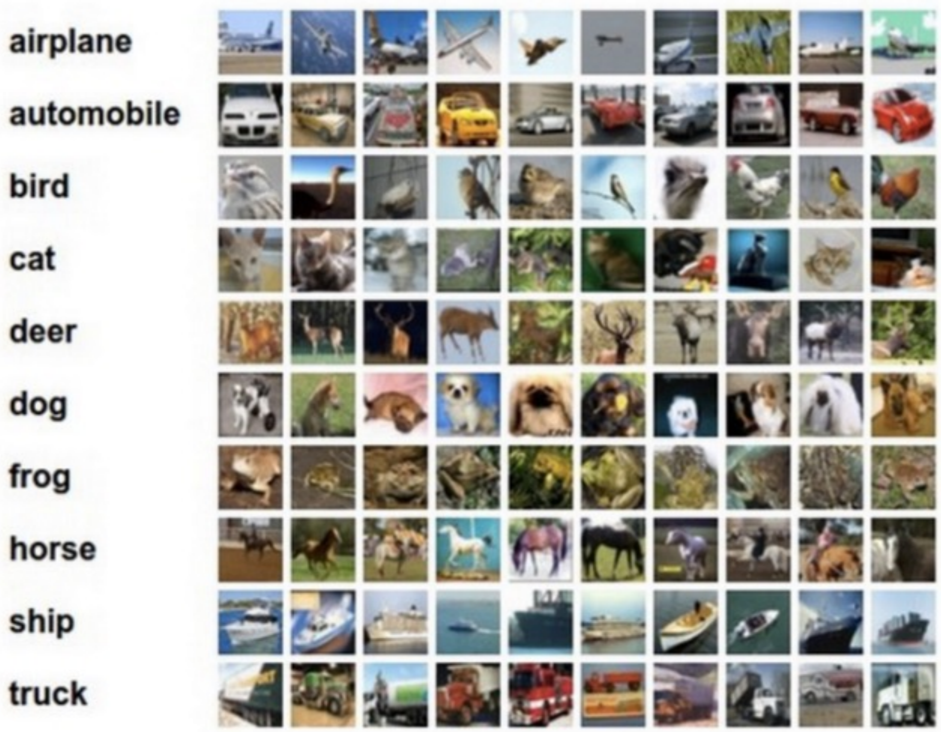
Nearest neighbor classifier



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

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

Nearest neighbors of images based on raw pixel values

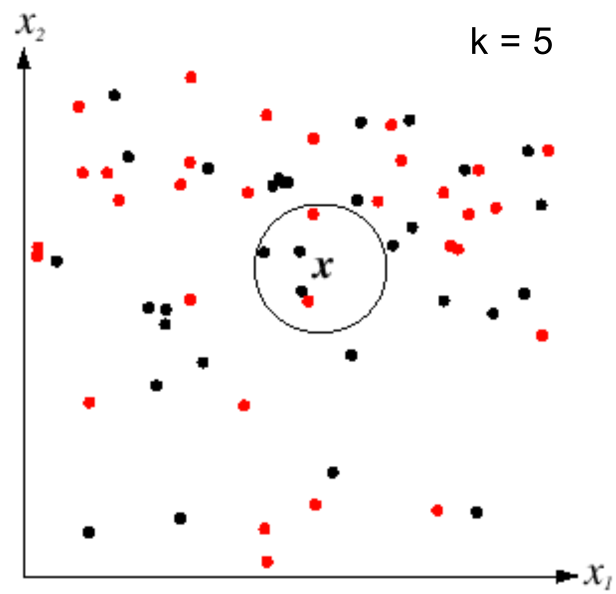


Left: Example images from the CIFAR-10 dataset. Right: first column shows a few test images and next to each we show the top 10 nearest neighbors in the training set according to pixel-wise difference.

Source: http://cs231n.github.io/classification/

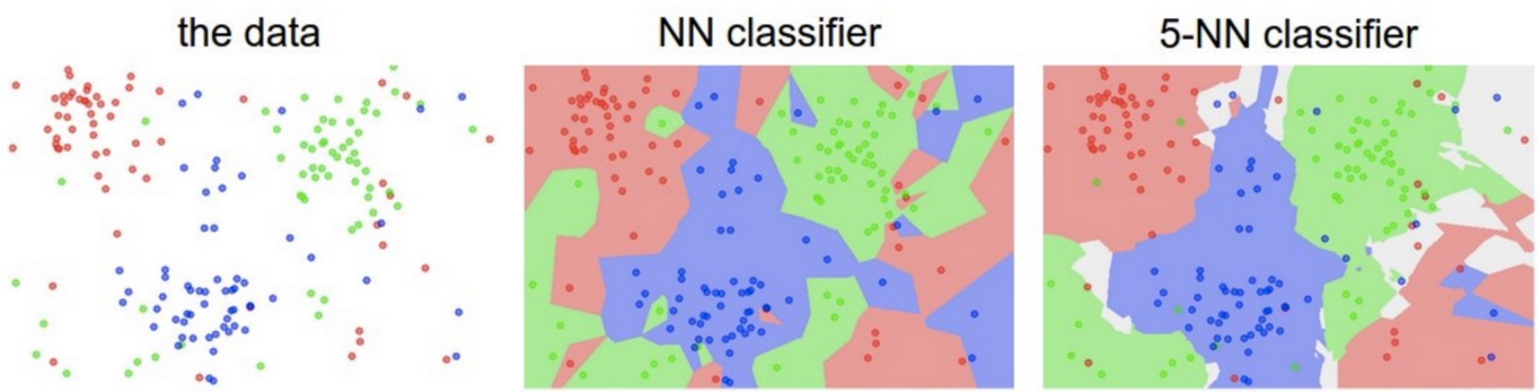
K-nearest neighbor classifier

- For a new point, find the k closest points from training data
- Vote for class label with labels of the k points



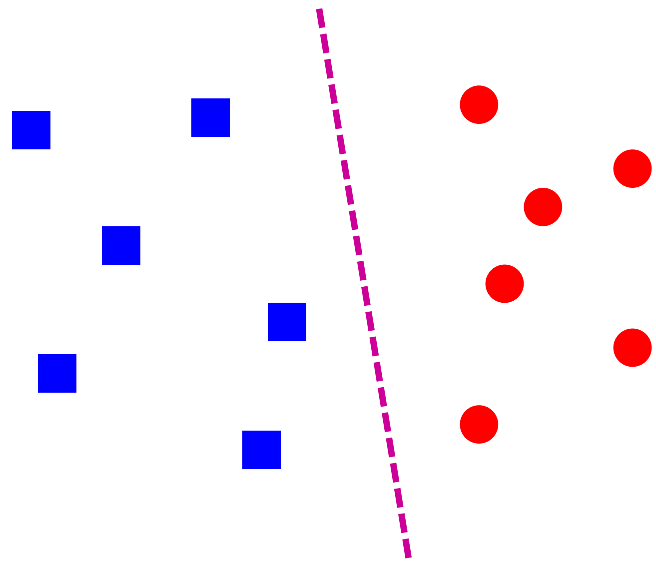
K-nearest neighbor classifier

- For a new point, find the k closest points from training data
- Vote for class label with labels of the k points
- 1-NN vs. k-NN



Source: http://cs231n.github.io/classification/

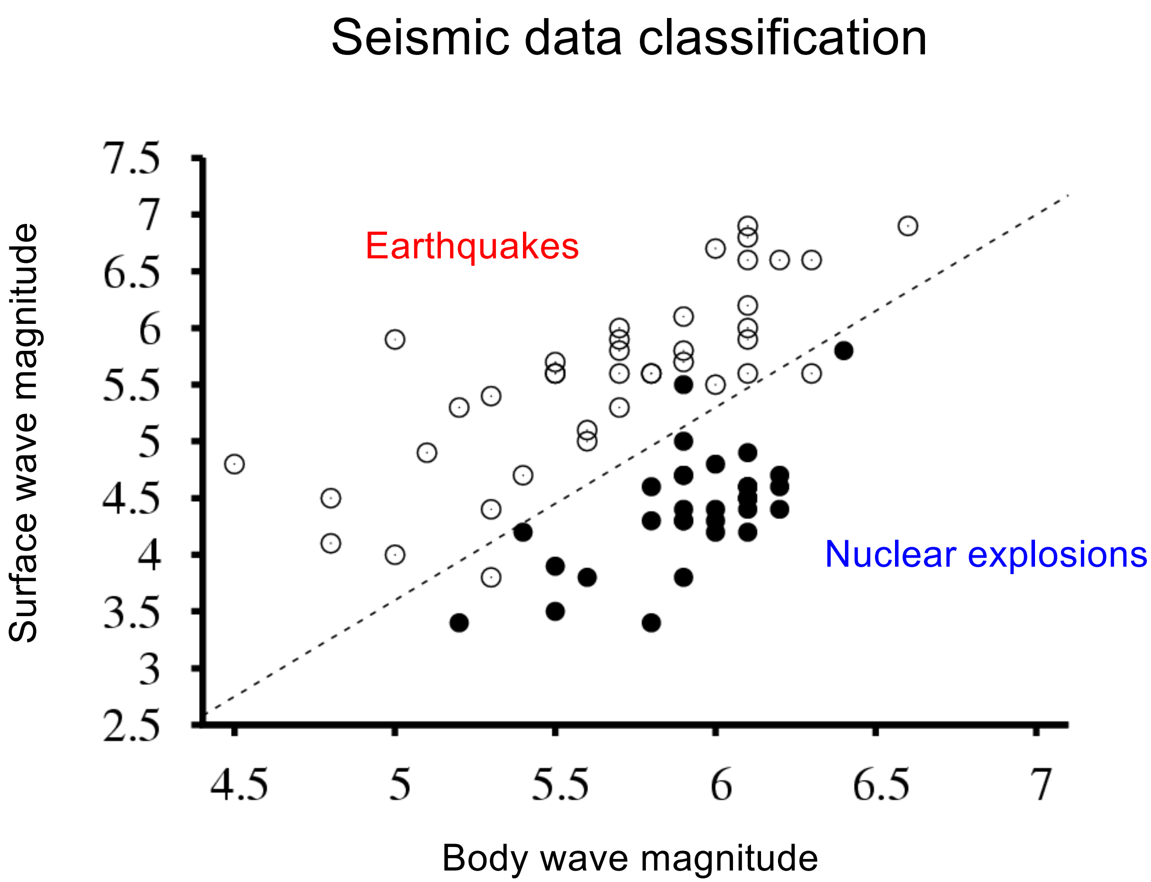
Linear classifier



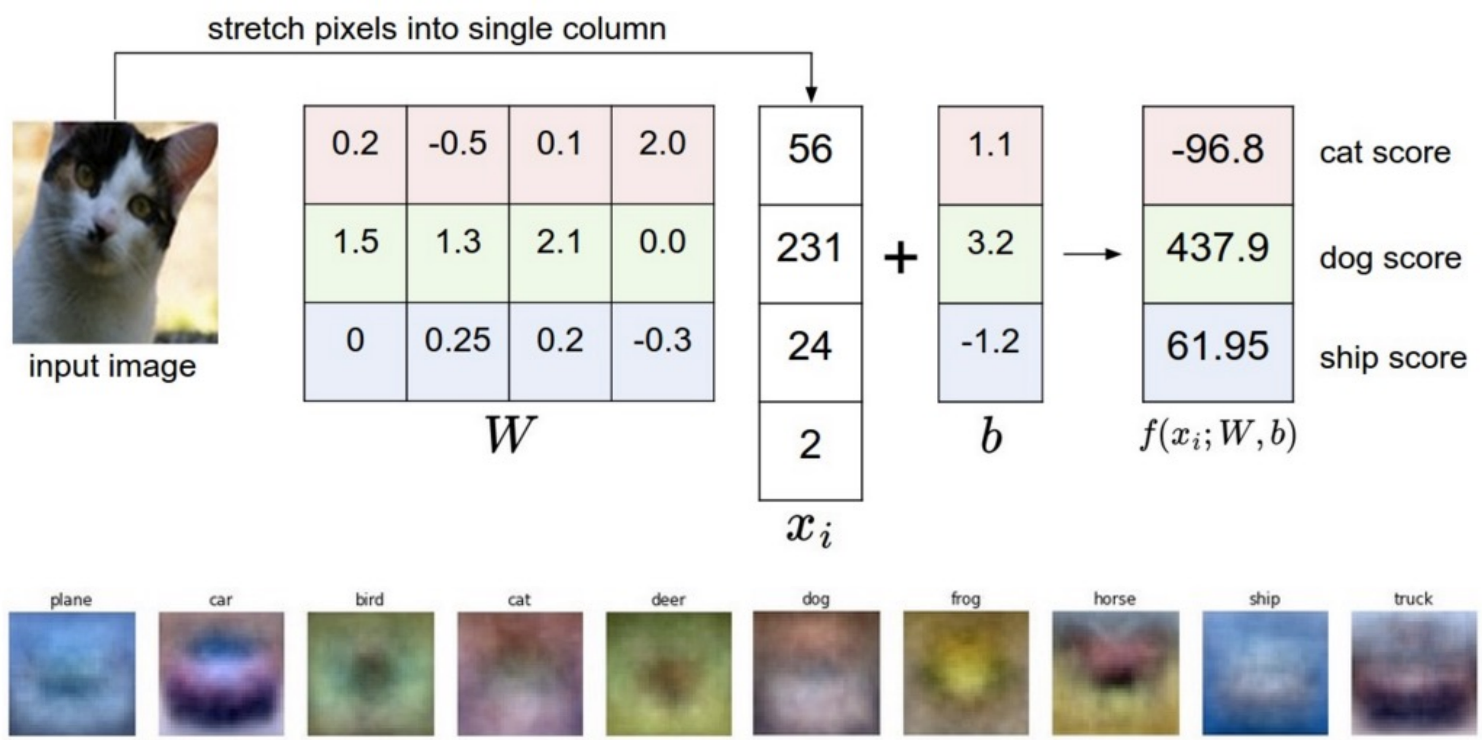
- Find a *linear function* to separate the classes:

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

Visualizing linear classifiers

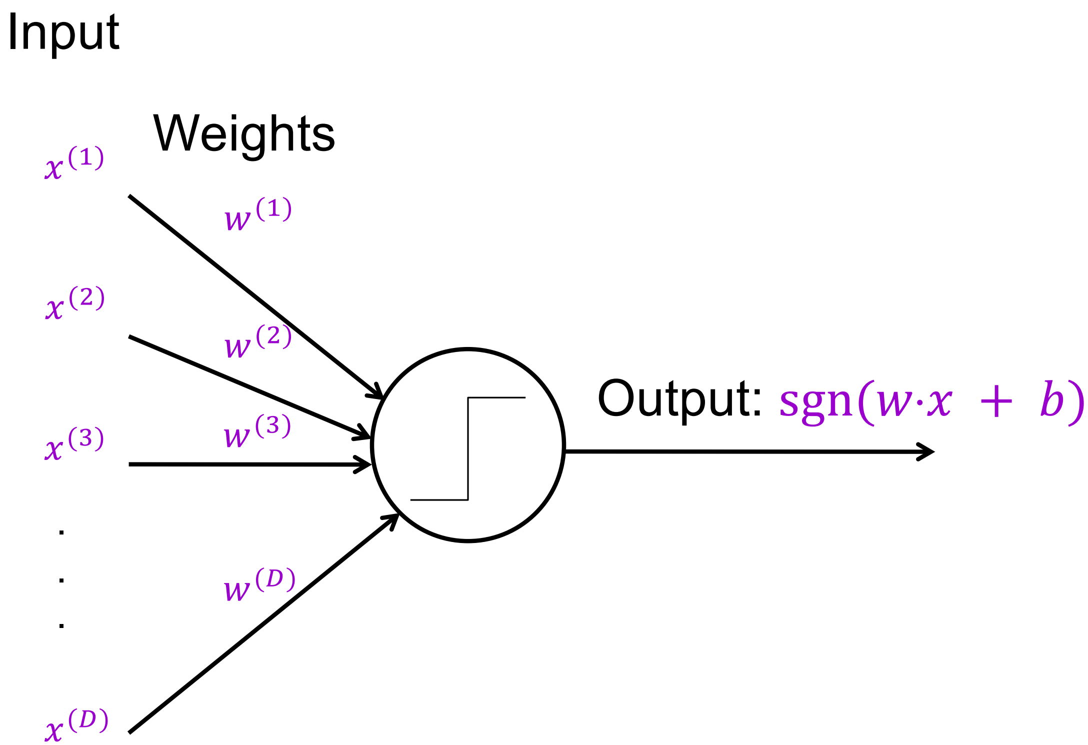


Visualizing linear classifiers

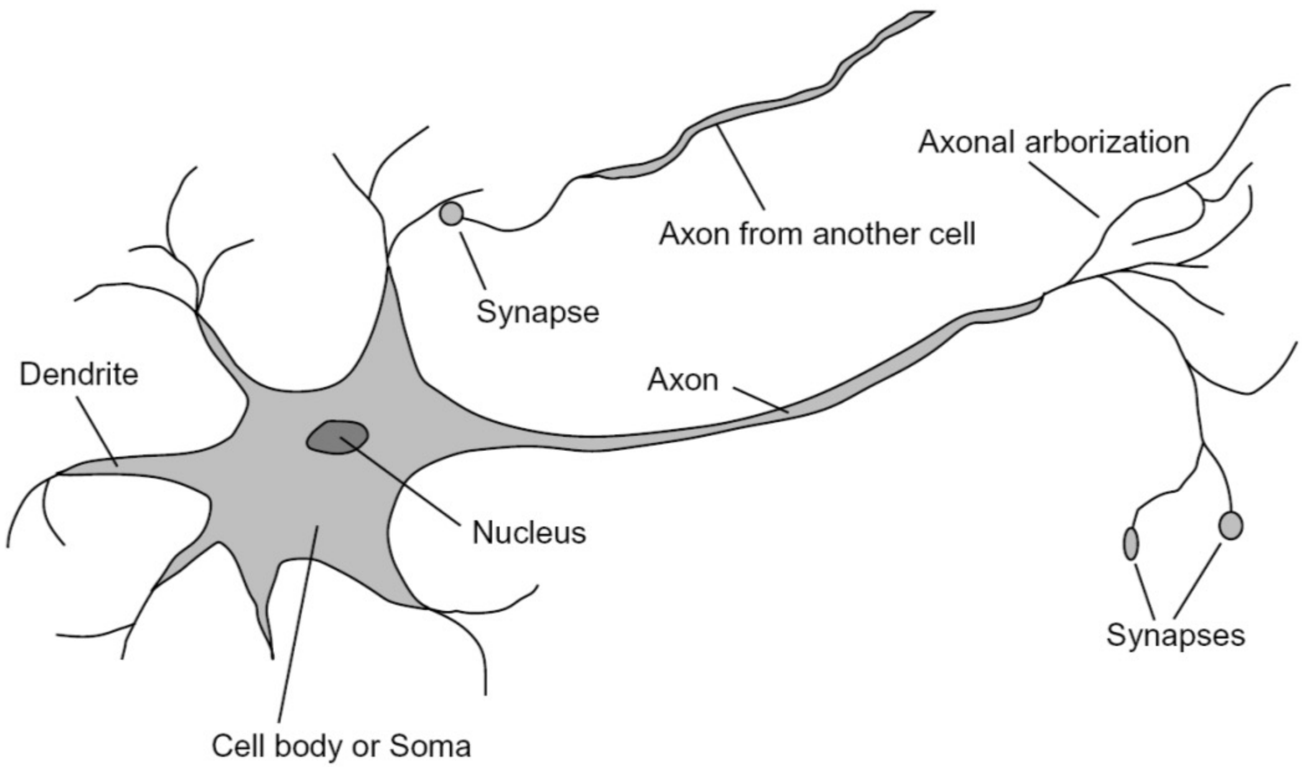


Source: http://cs231n.github.io/linear-classify/

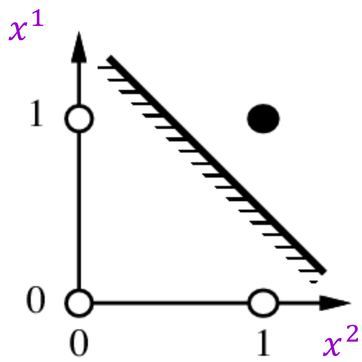
Linear classifier: Perceptron view



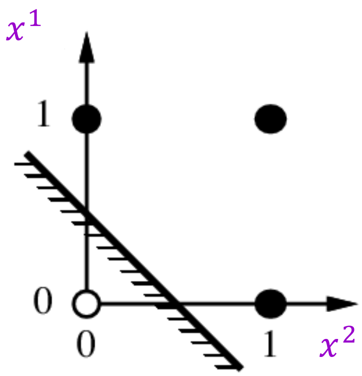
Loose inspiration: Biological neurons



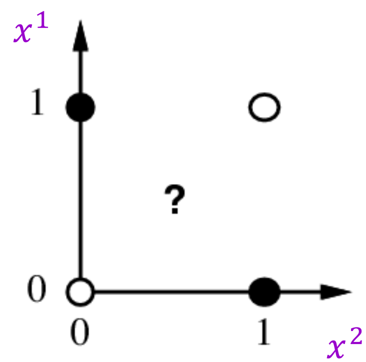
Perceptrons, linear separability, Boolean functions



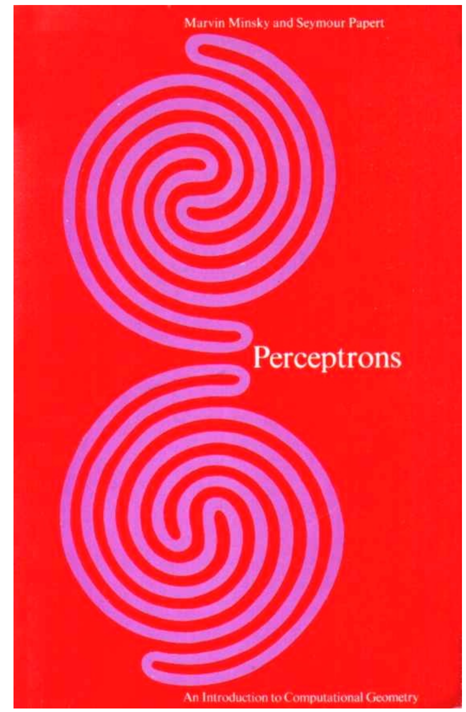
x^1 **and** x^2



x^1 **or** x^2



x^1 **xor** x^2



https://en.wikipedia.org/wiki/Perceptrons_(book)

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

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

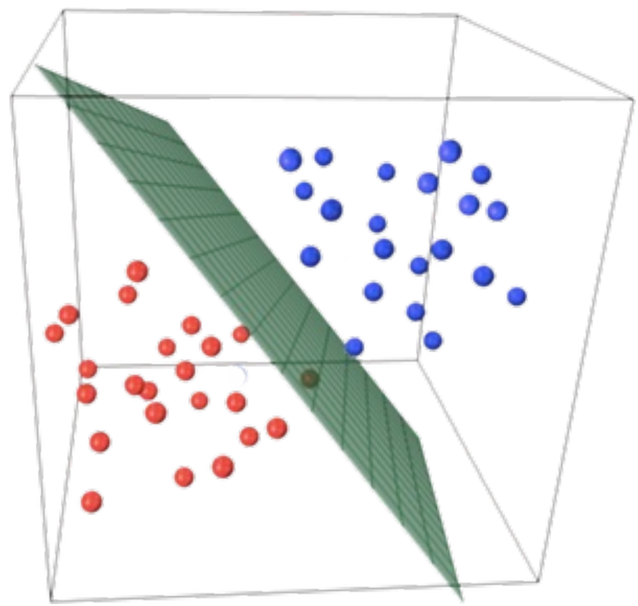


Image source

Empirical loss minimization

- Given: training data $\{(x_i, y_i), i = 1, \ldots, n\}$
- 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 $\{(x_i, y_i), i = 1, \ldots, n\}$
- 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 $\{(x_i, y_i), i = 1, \dots, n\}$ 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

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

What kind of performance measure?

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:

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

Various loss functions

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:

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

- 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 $\{(x_i, y_i), i = 1, \ldots, n\}$ i.i.d. from distribution D
- Find: predictor $f \in \mathcal{H}$
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$$L(f) = \mathbb{E}_{(x,y)\sim D}[l(f, x, y)]$$

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
    1. Linear regression
    2. Logistic regression
    3. Perceptron training algorithm
    4. Support vector machines

Training linear classifiers

- Given: i.i.d. training data $\{(x_i, y_i), i = 1, \dots, n\}$,
  $y_i \in \{-1,1\}$
- Hypothesis class: $f_w(x) = \mathrm{sgn}(w^T x)$
- 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 $\{(x_i, y_i), i = 1, \ldots, n\}$,
  $$y_i \in \{-1,1\}$$
- 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*

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

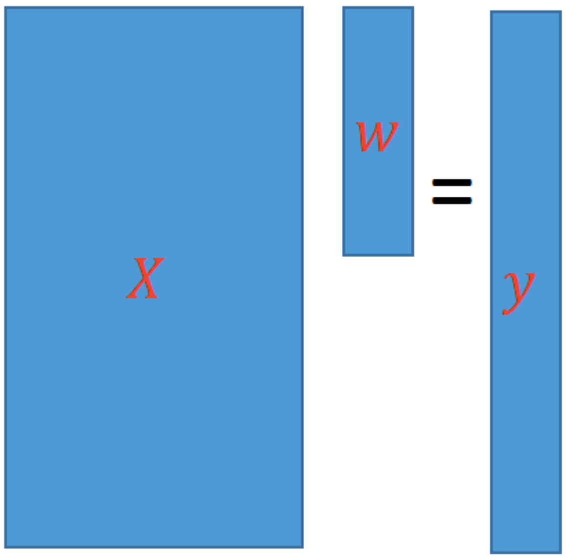
- Ignores the fact that $y \in \{-1,1\}$ but is easy to optimize

Source: Y. Liang

Linear regression: Optimization

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

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



Source: Y. Liang

Linear regression: Optimization

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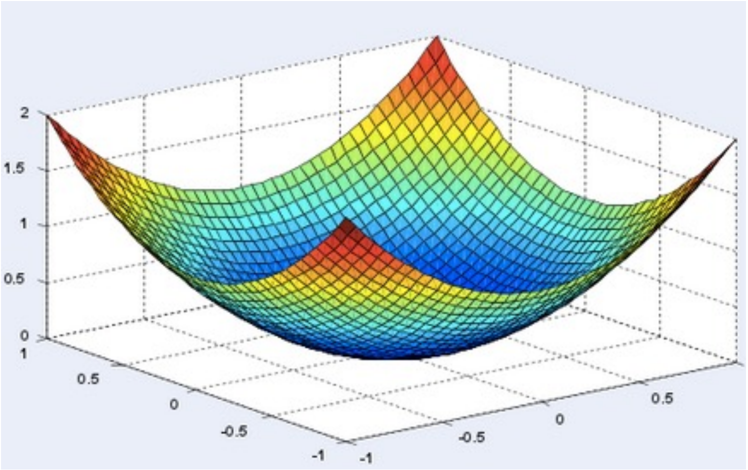
$$\hat{L}(f_w) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2 = \frac{1}{n}\|Xw - Y\|_2^2$$

- This is a *convex* function of the weights



Source: [Y. Liang]

Linear regression: Optimization

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

- 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 $(y_1, \dots, y_n)^T$

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

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

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

- Set gradient to zero to get the minimizer:

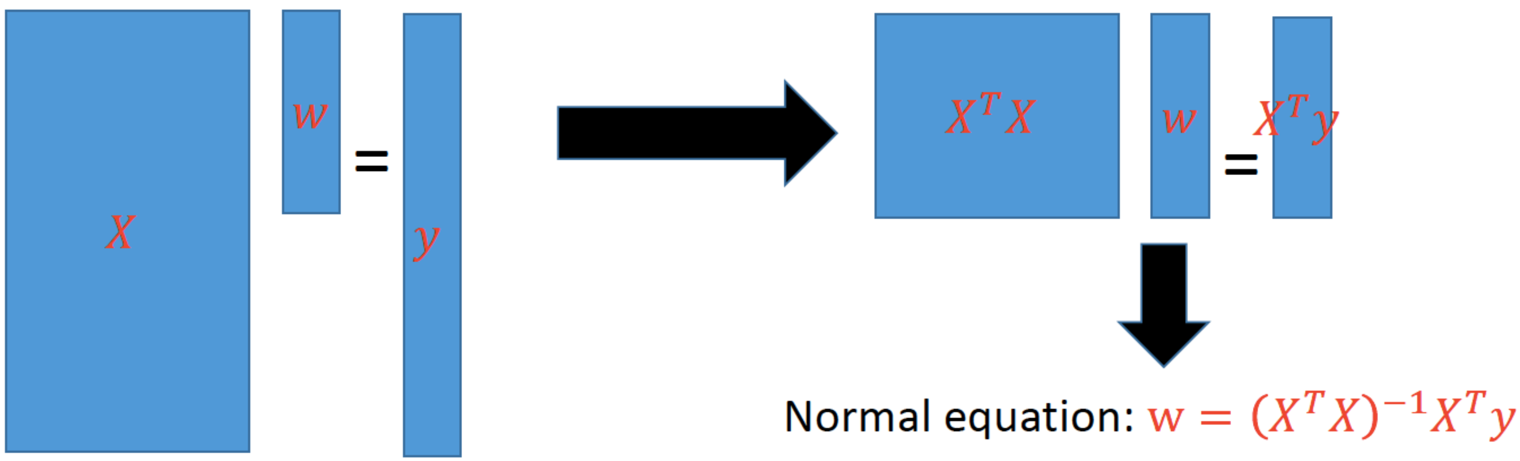
$$X^T Xw = X^T Y$$

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

Source: Y. Liang

Linear regression: Optimization

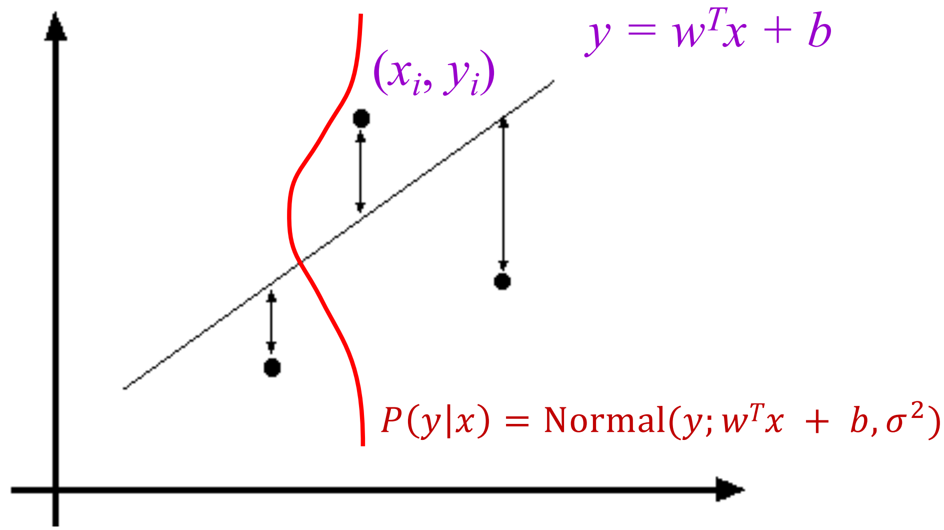
- Linear algebra view
  - If X is invertible, simply solve $Xw = Y$ and get $w = X^{-1}Y$
  - But typically X is a “tall” matrix so you need to find the *least squares solution* to an over-constrained system



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 $P_w(y|x)$ be a density function parameterized by w
- Maximum (conditional) likelihood estimate:

$$w_{ML} = \operatorname{argmax}_w \prod_i P_w(y_i|x_i)$$
$$= \operatorname{argmin}_w - \sum_i \log P_w(y_i|x_i)$$

Maximum likelihood estimation

$$w_{ML} = \text{argmin}_w - \sum_i \log P_w(y_i|x_i)$$

- Assume $P_w(y|x) = \text{Normal}(y; f_w(x), \sigma^2)$

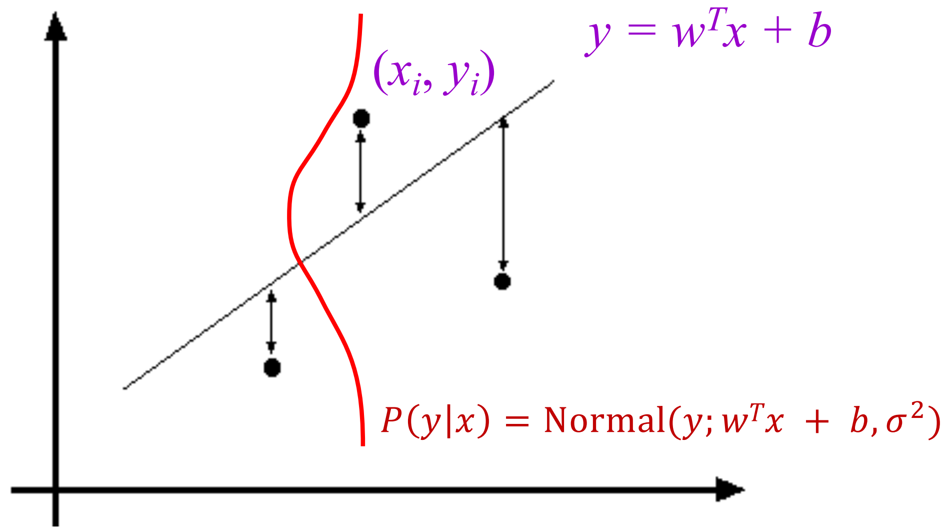
$$\log P_w(y|x) = \log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{\left(y - f_w(x)\right)^2}{2\sigma^2}\right]\right]$$

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

$$w_{ML} = \text{argmin}_w \sum_i \left(y_i - f_w(x_i)\right)^2$$

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

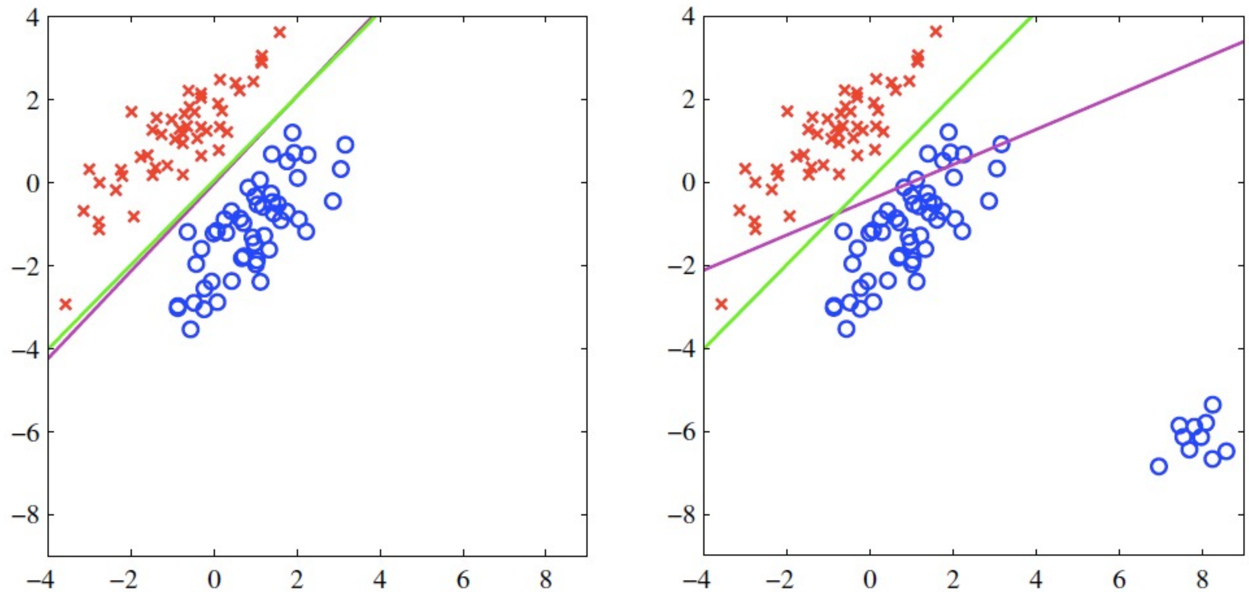
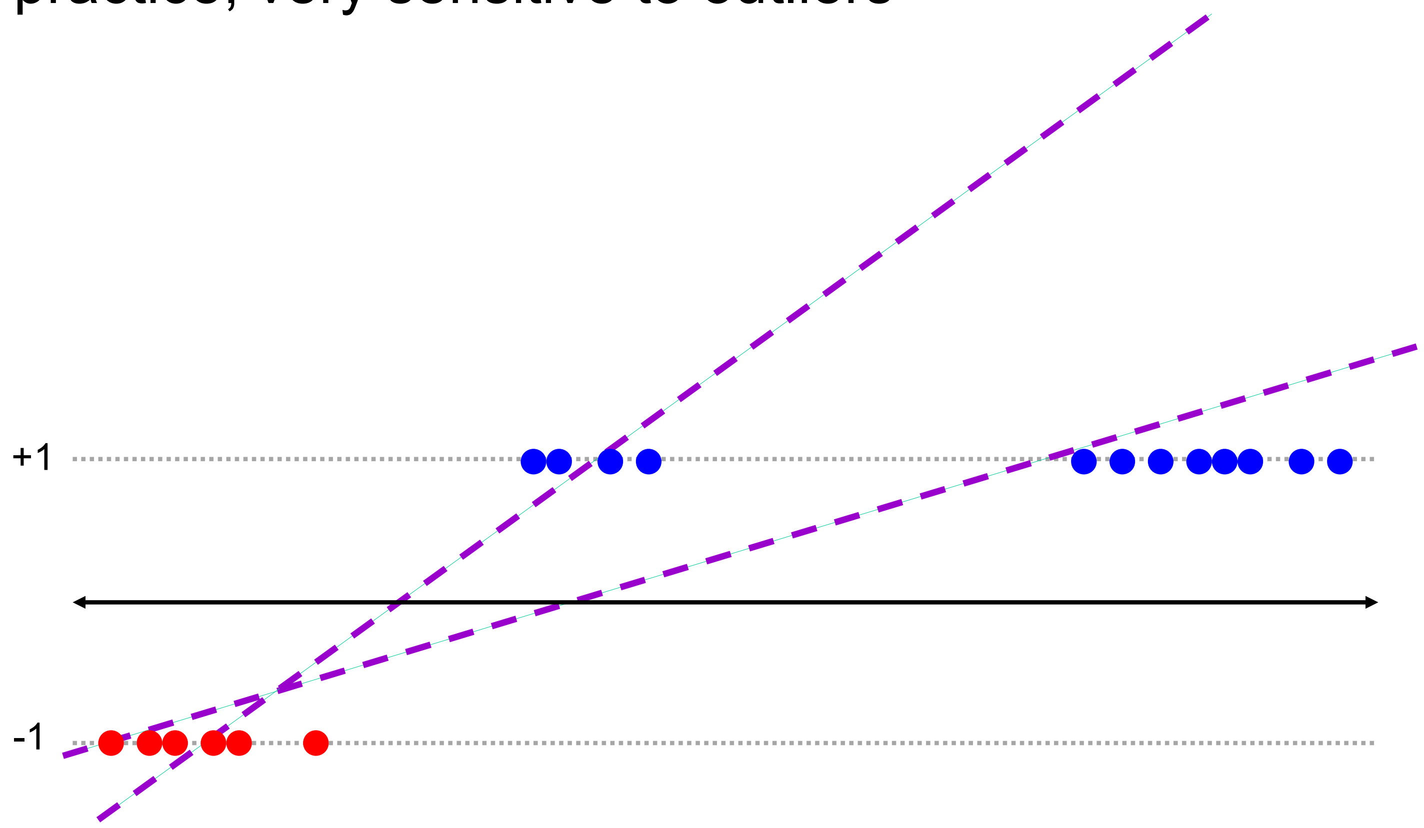


Figure 4.4 The left plot shows data from two classes, denoted by red crosses and blue circles, together with the decision boundary found by least squares (magenta curve) and also by the logistic regression model (green curve), which is discussed later in Section 4.3.2. The right-hand plot shows the corresponding 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

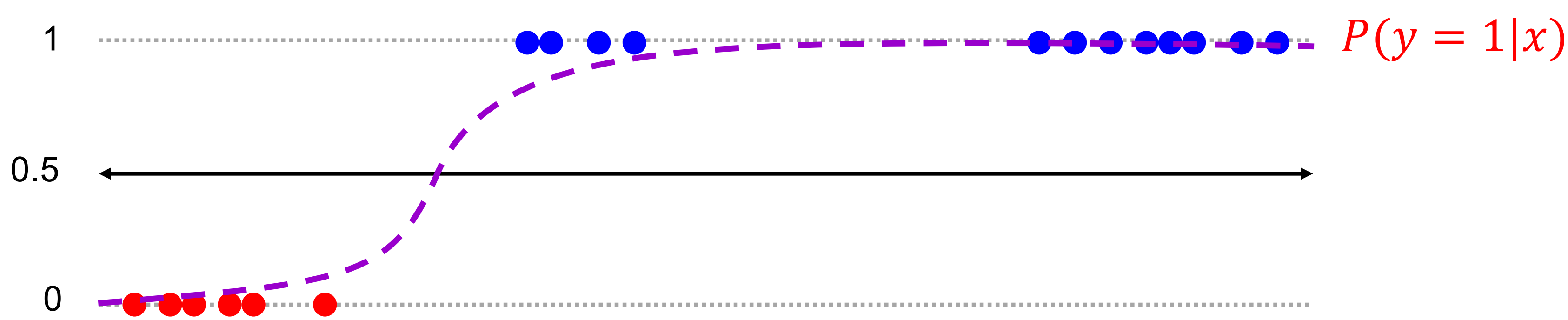
Problem with linear regression

- 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?



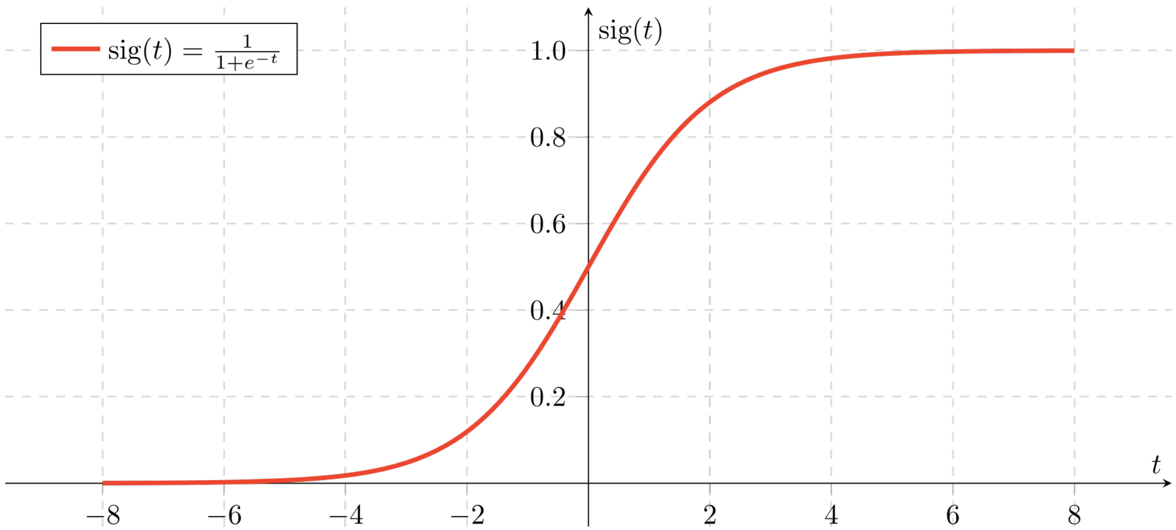
Linear classifiers: Outline

- 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 $w^T x$:

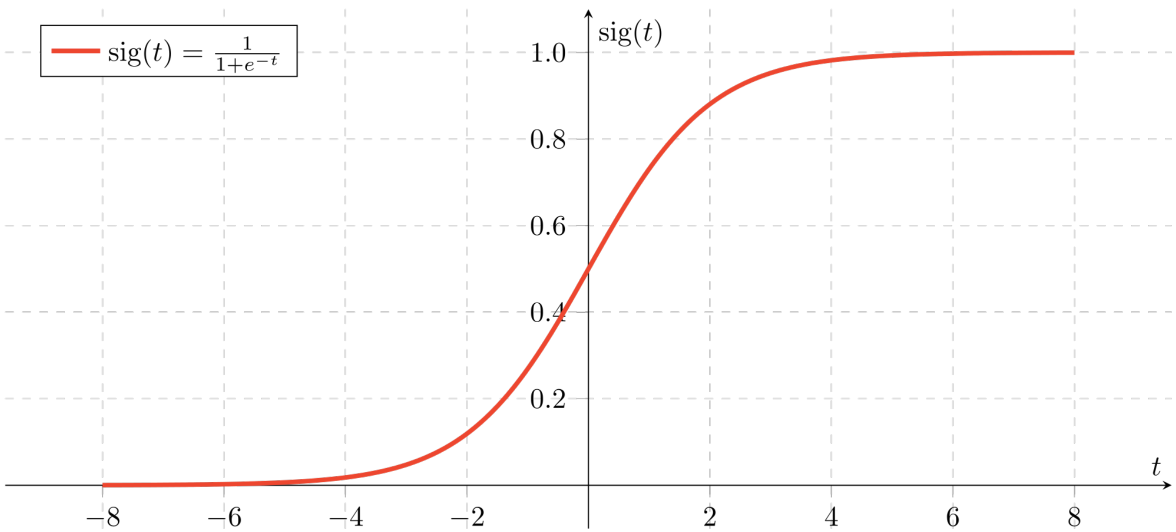
$$P_w(y = 1|x) = \sigma(w^T x) = \frac{1}{1+\exp(-w^T x)}$$



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



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

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

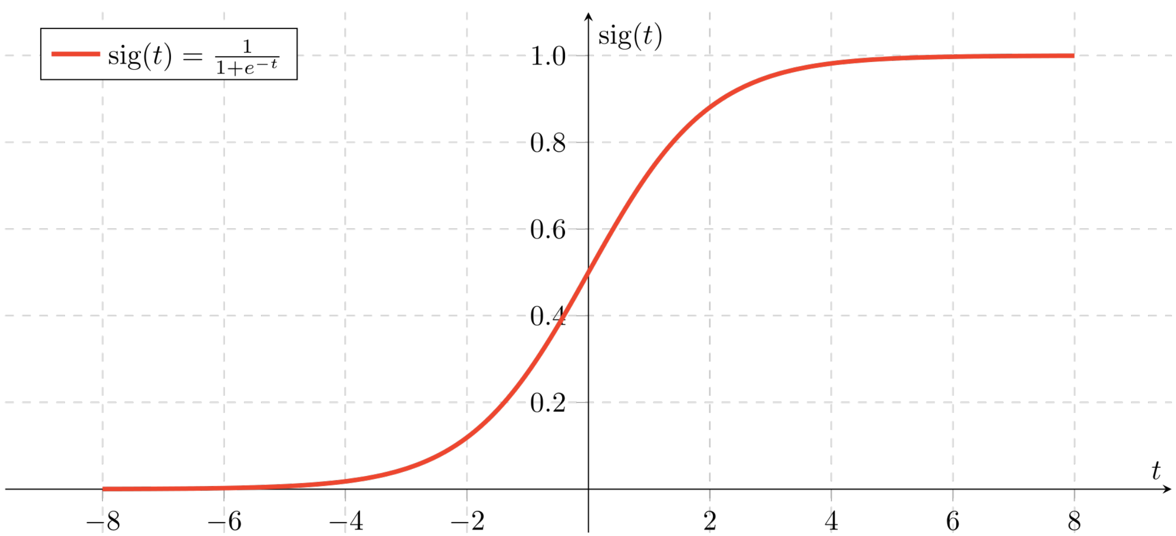
$$= \frac{1+\exp(-w^T x)-1}{1+\exp(-w^T x)} = \frac{\exp(-w^T x)}{1+\exp(-w^T x)} = \frac{1}{\exp(w^T x)+1}$$

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

Sigmoid: Properties

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

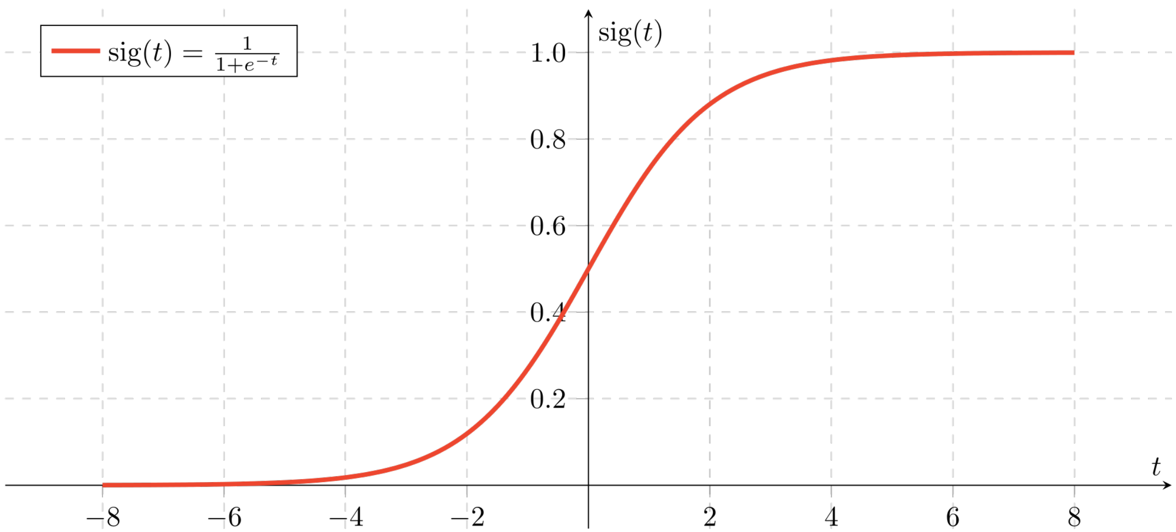
- Sigmoid is *symmetric*: $1 - \sigma(t) = \sigma(-t)$



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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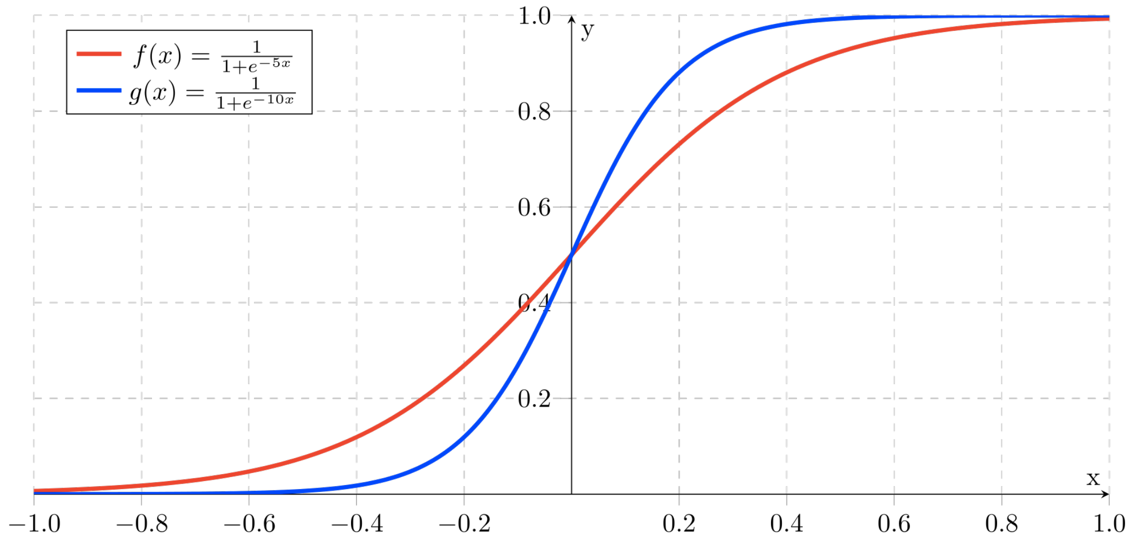


Image source

Sigmoid: Interpretation

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

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

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

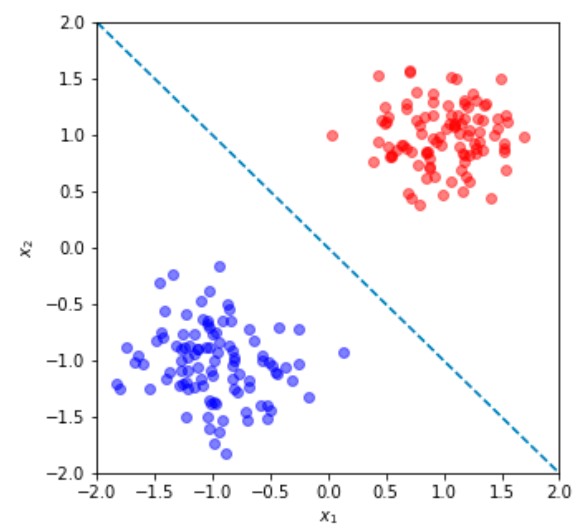
$$= \frac{1}{1+\exp(-a)} = \sigma(a), \qquad a = \log\frac{P(y=1|x)}{P(y=-1|x)}$$

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)



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

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

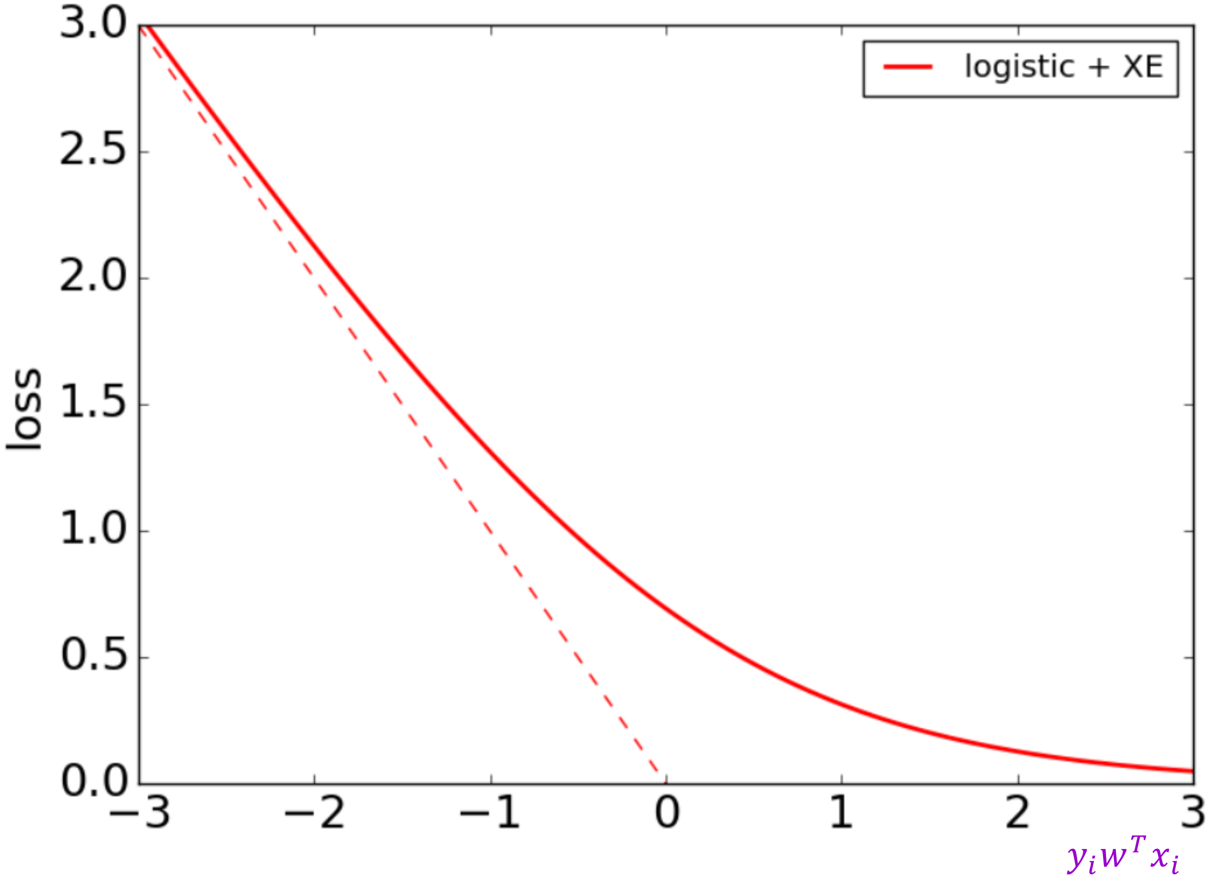


Figure source

Logistic loss: Optimization

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

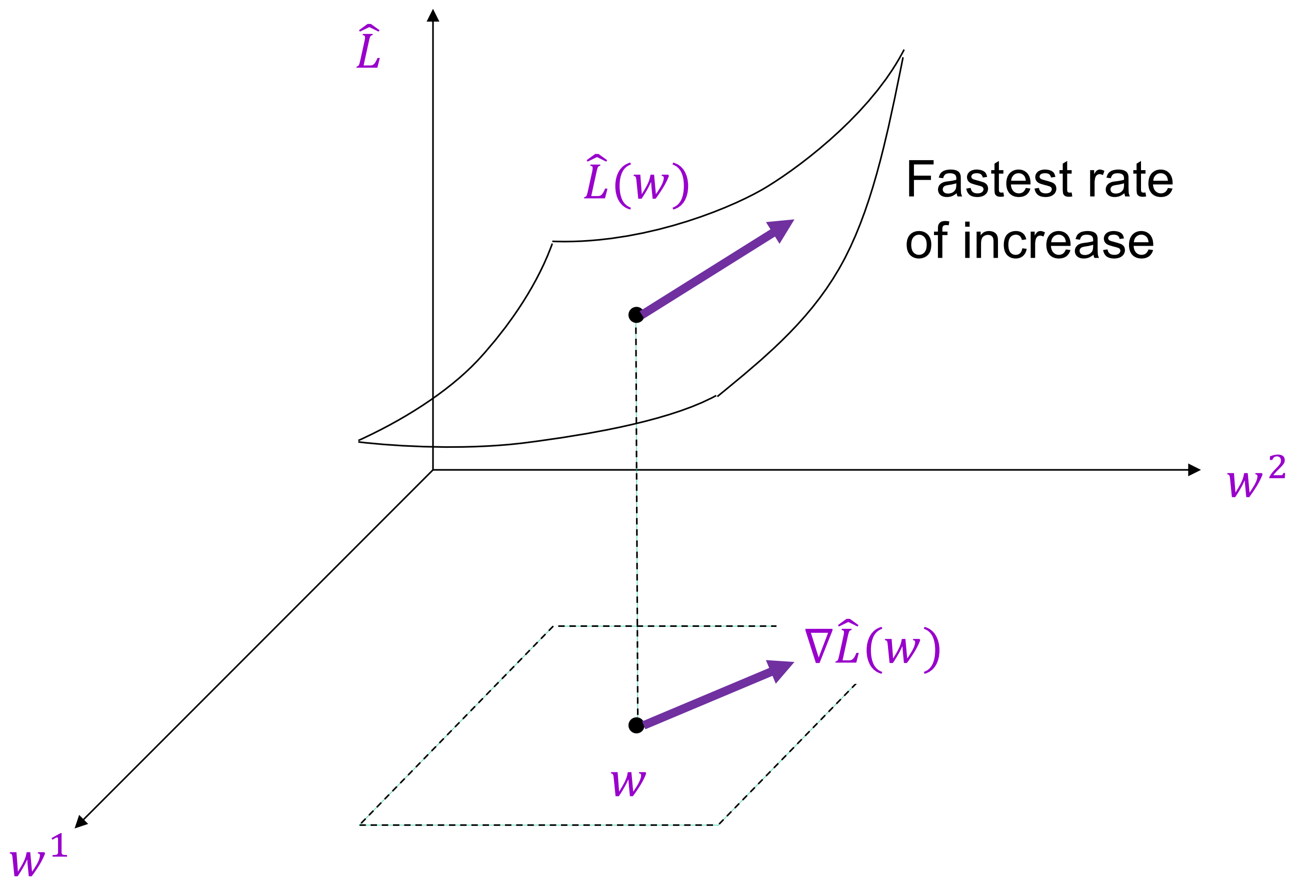
$$\hat{L}(w) = -\frac{1}{n}\sum_{i=1}^{n} \log P_w(y_i|x_i)$$

- 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



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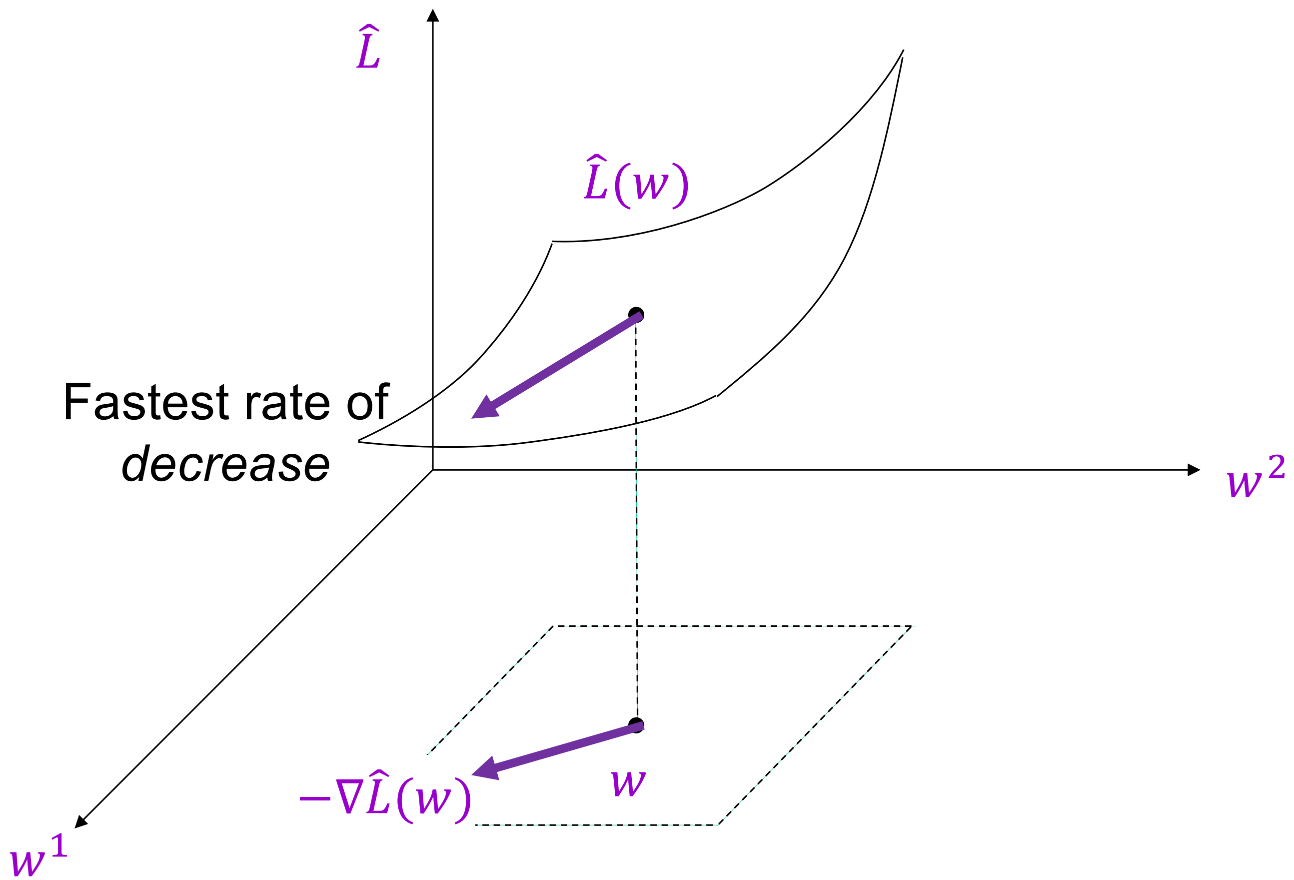
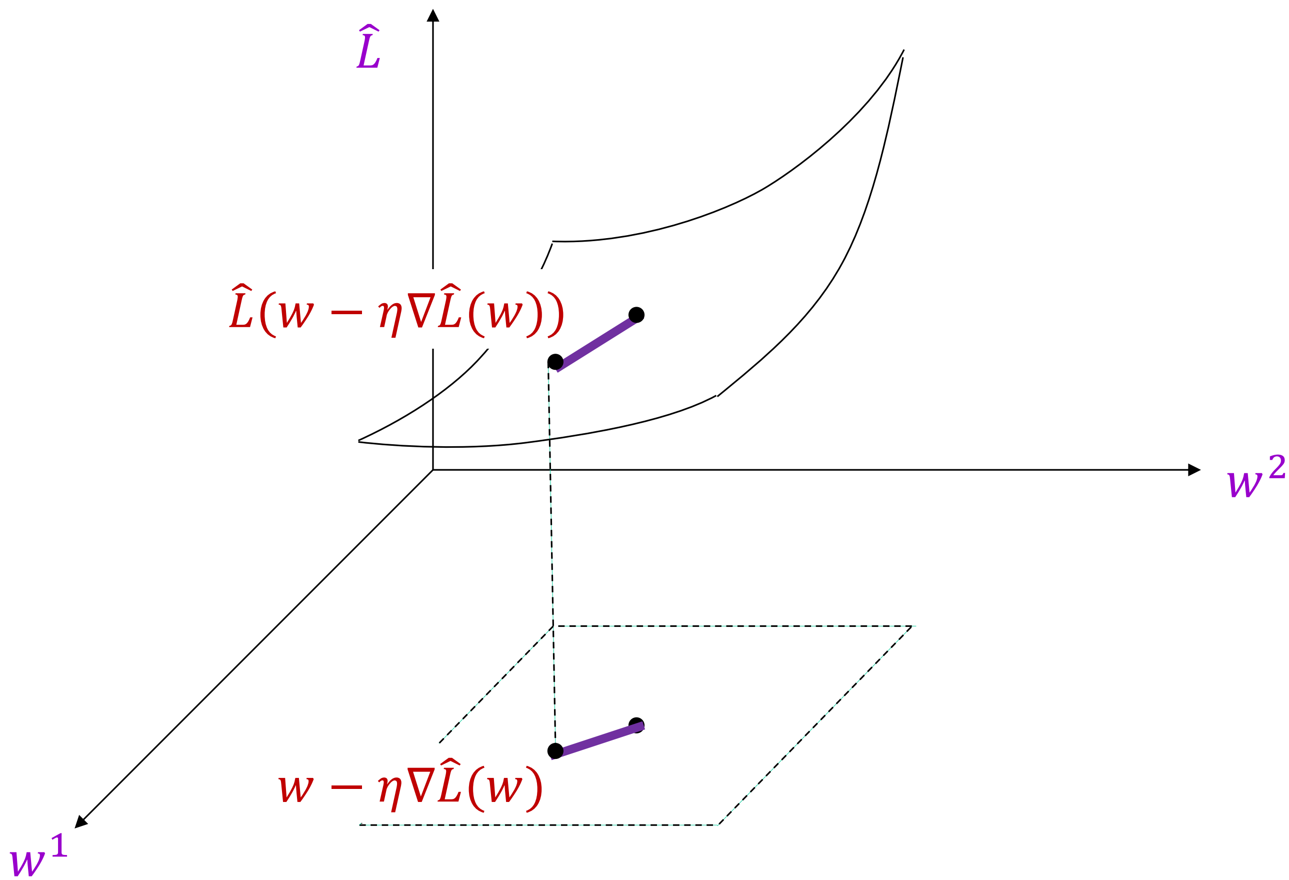


Gradient descent



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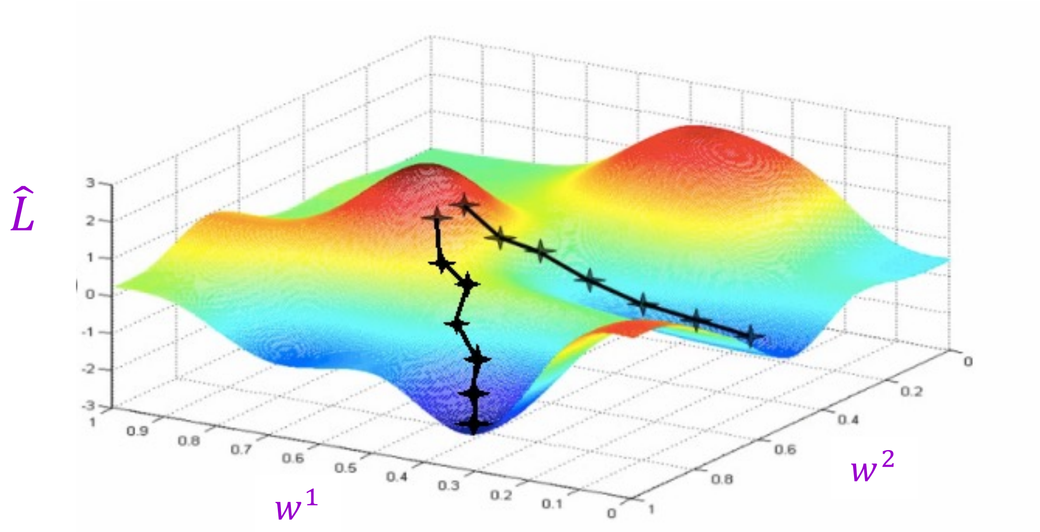

Gradient descent

- 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: $w \leftarrow w - \eta \nabla \hat{L}(w)$
  - 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 $(x_1, y_1), \ldots, (x_b, y_b)$:

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

    - 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:

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

SGD for logistic regression

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

Derivative of sigmoid:

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

SGD for logistic regression

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- 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*: $\left[g_2\big(g_1(a)\big)\right]' = g_2'\big(g_1(a)\big) g_1'(a)$

SGD for logistic regression

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

- Let's find the gradient:

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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 closer 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

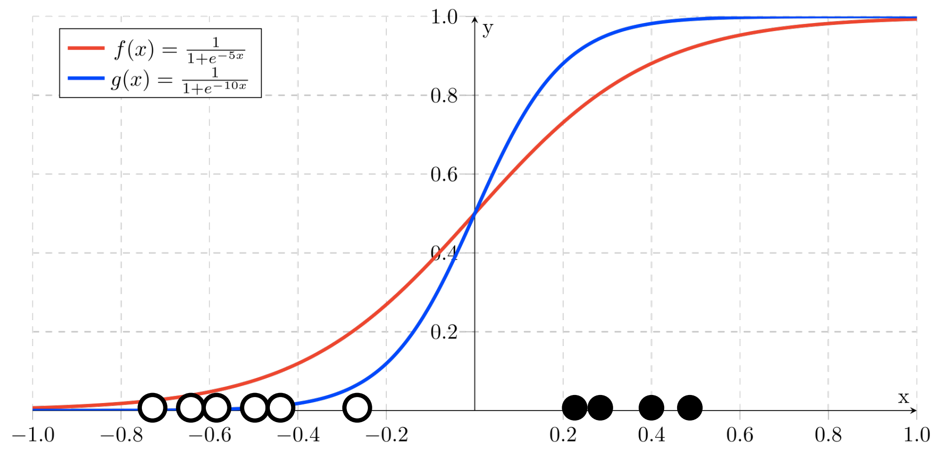

Image source

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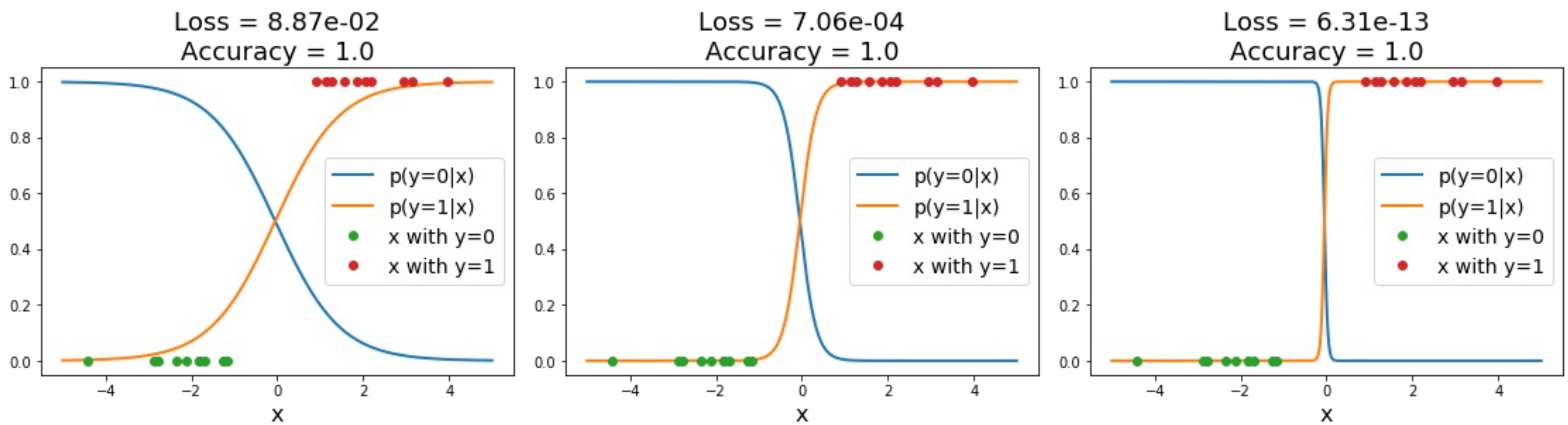

Source: [J. Johnson]