Artificial Intelligence and Machine Learning

Barbara Caputo

Back to classification

1. Instance based classifiers
   - Use observation directly (no models)
   - e.g. K nearest neighbors

2. Generative:
   - build a generative statistical model
   - e.g., Bayesian networks

3. Discriminative
   - directly estimate a decision rule/boundary
   - e.g., decision tree

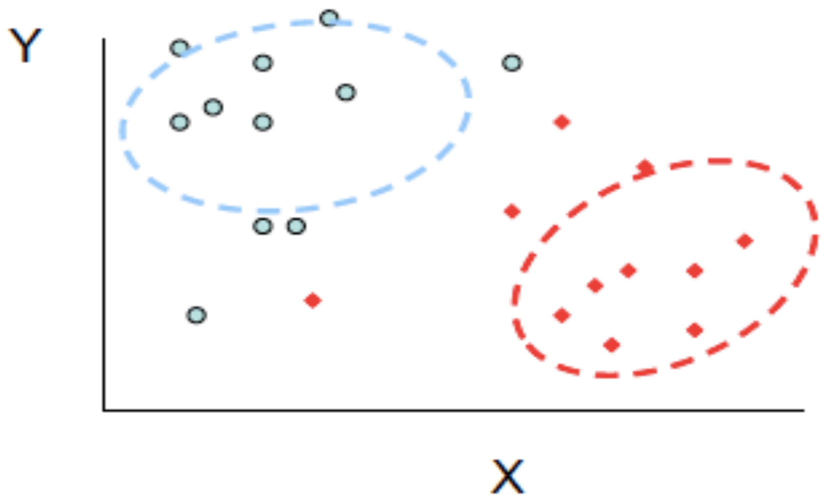
Generative vs. discriminative classifiers

- When using generative classifiers we relied on all points to learn the generative model
- When using discriminative classifiers we mainly care about the boundary

Generative vs. discriminative classifiers

- When using generative classifiers we relied on all points to learn the generative model
- When using discriminative classifiers we mainly care about the boundary

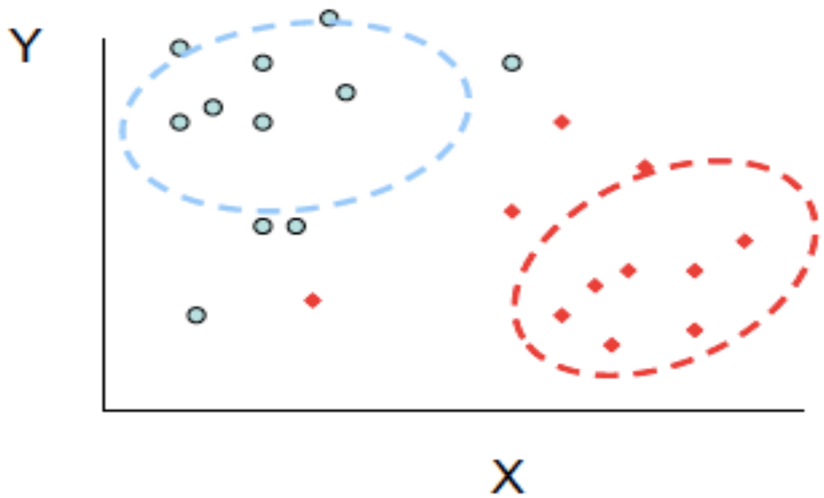
Generative model



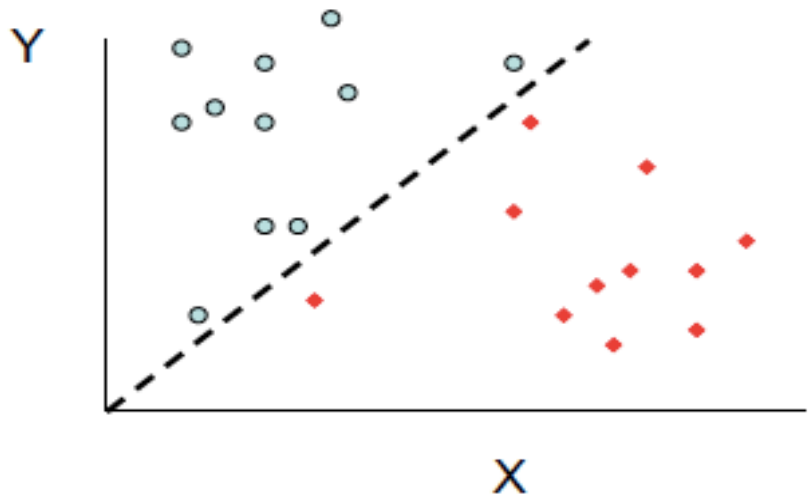
Generative vs. discriminative classifiers

- When using generative classifiers we relied on all points to learn the generative model
- When using discriminative classifiers we mainly care about the boundary

Generative model



Discriminative model



Regression for classification

- In some cases we can use linear regression for determining the appropriate boundary.
- However, since the output is usually binary or discrete there are more efficient regression methods

Regression for classification

- In some cases we can use linear regression for determining the appropriate boundary.
- However, since the output is usually binary or discrete there are more efficient regression methods
- Recall that for classification we are interested in the conditional probability $p(y \mid X ; \theta)$ where θ are the parameters of our model
- When using regression θ represents the values of our regression coefficients (w).

Regression for classification

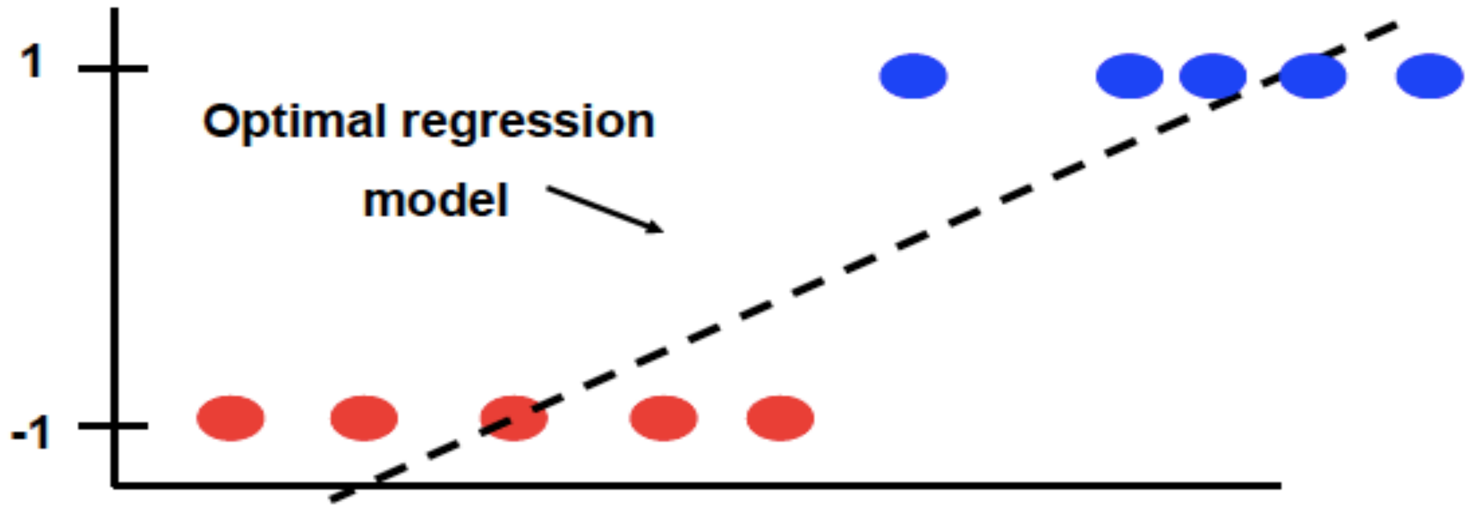
- Assume we would like to use linear regression to learn the parameters for $p(y \mid X ; \theta)$
- Problems?

Regression for classification

- Assume we would like to use linear regression to learn the parameters for p(y | X ; θ)
- Problems?

$\mathbf{w}^T\mathbf{X} \geq 0 \Rightarrow$ classify as 1

$\mathbf{w}^T\mathbf{X} < 0 \Rightarrow$ classify as -1



The sigmoid function

The sigmoid function

$$p(y \mid X; \theta)$$

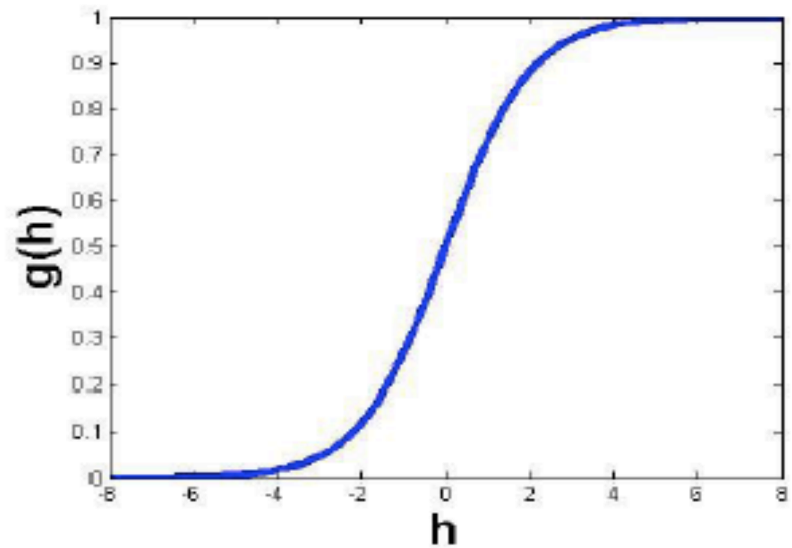
- To classify using regression models we replace the linear function with the sigmoid function:

The sigmoid function

$$p(y \mid X;\theta)$$

- To classify using regression models we replace the linear function with the sigmoid function:

Always between 0 and 1 $\longrightarrow$ $g(h) = \dfrac{1}{1+e^{-h}}$



The sigmoid function

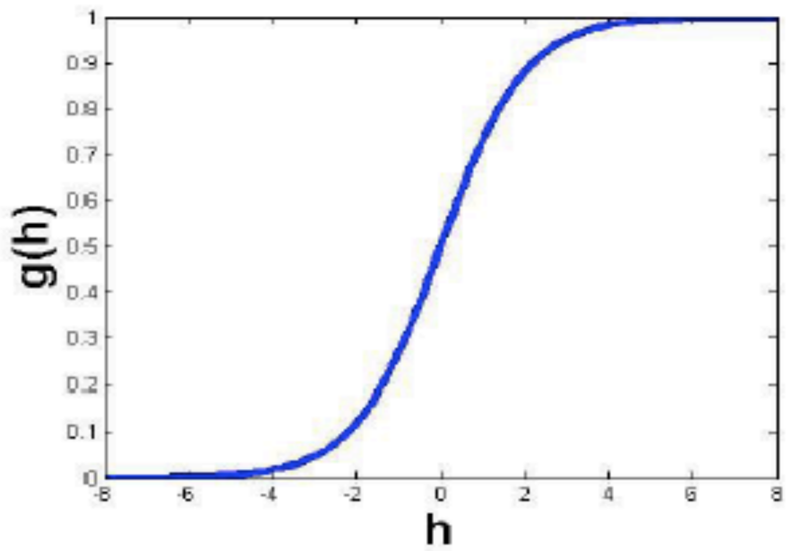
$$p(y \mid X;\theta)$$

- To classify using regression models we replace the linear function with the sigmoid function:

Always between 0 and 1 $\longrightarrow$ $$g(h) = \frac{1}{1+e^{-h}}$$

- Using the sigmoid we set (for binary classification problems)

$$p(y=0 \mid X;\theta) = g(\mathrm{w}^{\mathrm{T}}X) = \frac{1}{1+e^{\mathrm{w}^{\mathrm{T}}X}}$$

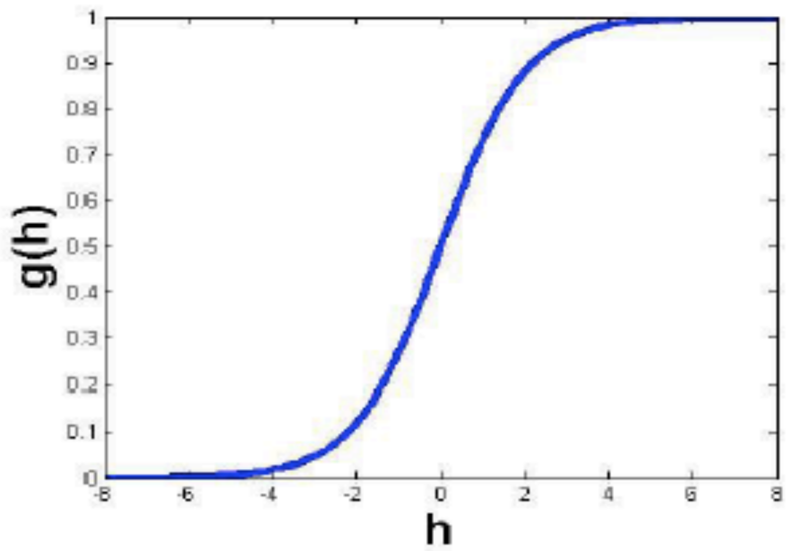


The sigmoid function

$$p(y \mid X;\theta)$$

- To classify using regression models we replace the linear function with the sigmoid function:

Always between 0 and 1 $\longrightarrow$ $$g(h)=\frac{1}{1+e^{-h}}$$



- Using the sigmoid we set (for binary classification problems)

$$p(y=0 \mid X;\theta)=g(\mathrm{w}^{\mathrm{T}}X)=\frac{1}{1+e^{\mathrm{w}^{\mathrm{T}}X}}$$

$$p(y=1 \mid X;\theta)=1-g(\mathrm{w}^{\mathrm{T}}X)=\frac{e^{\mathrm{w}^{\mathrm{T}}X}}{1+e^{\mathrm{w}^{\mathrm{T}}X}}$$

The sigmoid function

$$p(y \mid X;\theta)$$

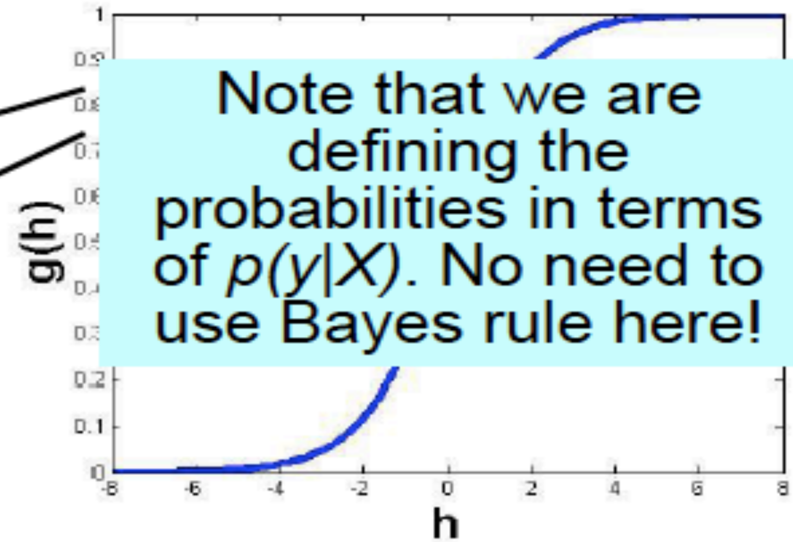
- To classify using regression models we replace the linear function with the sigmoid function:

$$g(h)=\frac{1}{1+e^{-h}}$$

- Using the sigmoid we set (for binary classification problems)

$$p(y=0 \mid X;\theta)=g(\mathrm{w}^{\mathrm{T}}X)=\frac{1}{1+e^{\mathrm{w}^{\mathrm{T}}X}}$$

$$p(y=1 \mid X;\theta)=1-g(\mathrm{w}^{\mathrm{T}}X)=\frac{e^{\mathrm{w}^{\mathrm{T}}X}}{1+e^{\mathrm{w}^{\mathrm{T}}X}}$$



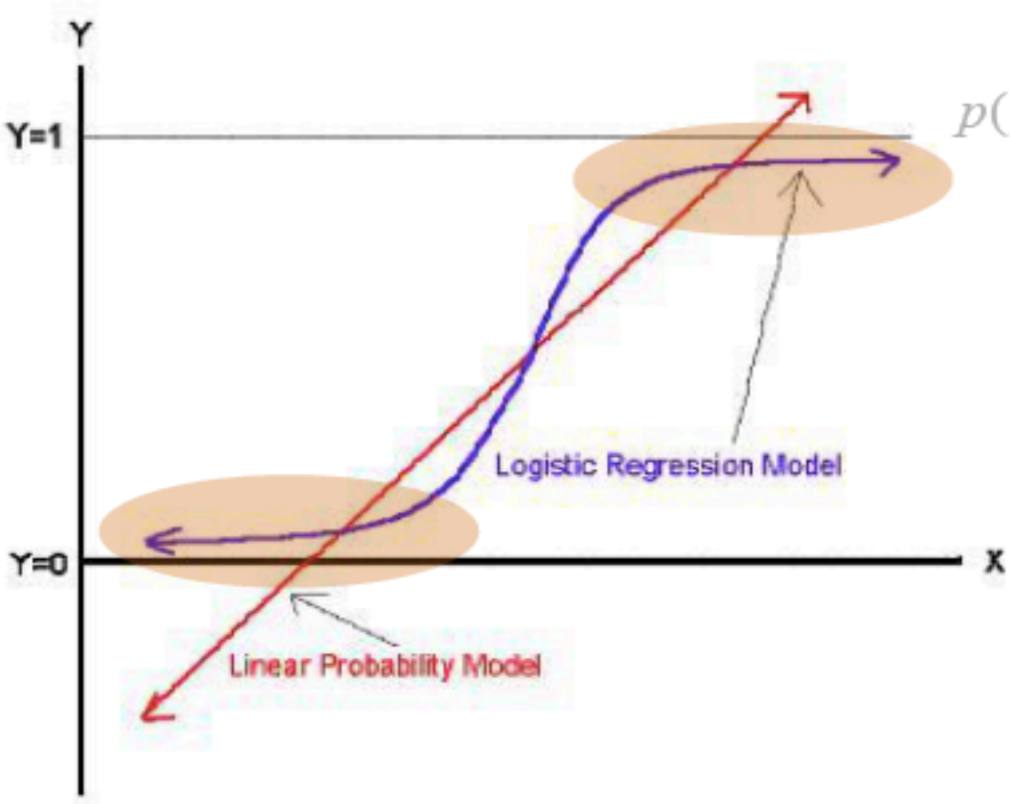
Note that we are defining the probabilities in terms of *p(y|X)*. No need to use Bayes rule here!

Logistic regression vs. Linear regression

Logistic regression vs. Linear regression

$$p(y=0 \mid X;\theta) = g(\mathrm{w}^{\mathrm{T}}X) = \frac{1}{1+e^{\mathrm{w}^{\mathrm{T}}X}}$$

$$p(y=1 \mid X;\theta) = 1 - g(\mathrm{w}^{\mathrm{T}}X) = \frac{e^{\mathrm{w}^{\mathrm{T}}X}}{1+e^{\mathrm{w}^{\mathrm{T}}X}}$$



Determining parameters for logistic regression problems

- So how do we learn the parameters?

Determining parameters for logistic regression problems

- So how do we learn the parameters?
- Similar to other regression problems we look for the MLE for w
- The likelihood of the data given the model is:

Determining parameters for logistic regression problems

- So how do we learn the parameters?
- Similar to other regression problems we look for the MLE for w
- The likelihood of the data given the model is:

$$L(y \mid X; w) = \prod_i (1 - g(X_i; w))^{y_i} g(X_i; w)^{(1-y_i)}$$

Determining parameters for logistic regression problems

- So how do we learn the parameters?
- Similar to other regression problems we look for the MLE for w
- The likelihood of the data given the model is:

Defining a new function, *g*

$$p(y=0 \mid X;\theta) = g(X;w) = \frac{1}{1+e^{w^T X}}$$

$$p(y=1 \mid X;\theta) = 1 - g(X;w) = \frac{e^{w^T X}}{1+e^{w^T X}}$$

$$L(y \mid X;w) = \prod_i (1-g(X_i;w))^{y_i} g(X_i;w)^{(1-y_i)}$$

Solving logistic regression problems

Solving logistic regression problems

$$g(X;w) = \frac{1}{1+e^{\mathbf{w}^T X}}$$

$$1 - g(X;w) = \frac{e^{\mathbf{w}^T X}}{1+e^{\mathbf{w}^T X}}$$

- The likelihood of the data is: $L(y \mid X;w) = \prod_i (1-g(X_i;w))^{y_i} g(X_i;w)^{(1-y_i)}$

Solving logistic regression problems

$$g(X;w) = \frac{1}{1+e^{\mathrm{w}^T X}}$$

$$1 - g(X;w) = \frac{e^{\mathrm{w}^T X}}{1+e^{\mathrm{w}^T X}}$$

- The likelihood of the data is: $L(y \mid X;w) = \prod_i (1-g(X_i;w))^{y_i} g(X_i;w)^{(1-y_i)}$

- Taking the log we get:

$$LL(y \mid X;w) = \sum_{i=1}^{N} y_i \ln(1-g(X_i;w)) + (1-y_i) \ln g(X_i;w)$$

Solving logistic regression problems

$$g(X;w) = \frac{1}{1+e^{w^T X}}$$

$$1 - g(X;w) = \frac{e^{w^T X}}{1+e^{w^T X}}$$

- The likelihood of the data is: $L(y \mid X;w) = \prod_i (1-g(X_i;w))^{y_i} g(X_i;w)^{(1-y_i)}$

- Taking the log we get:

$$LL(y \mid X;w) = \sum_{i=1}^{N} y_i \ln(1-g(X_i;w)) + (1-y_i)\ln g(X_i;w)$$

$$= \sum_{i=1}^{N} y_i \ln \frac{1-g(X_i;w)}{g(X_i;w)} + \ln g(X_i;w)$$

Solving logistic regression problems

$$g(X;w) = \frac{1}{1+e^{\mathrm{w}^T X}}$$

$$1-g(X;w) = \frac{e^{\mathrm{w}^T X}}{1+e^{\mathrm{w}^T X}}$$

- The likelihood of the data is: $L(y \mid X;w) = \prod_i (1-g(X_i;w))^{y_i} g(X_i;w)^{(1-y_i)}$

- Taking the log we get:

$$\begin{aligned} LL(y \mid X;w) &= \sum_{i=1}^{N} y_i \ln(1-g(X_i;w)) + (1-y_i) \ln g(X_i;w) \\ &= \sum_{i=1}^{N} y_i \ln \frac{1-g(X_i;w)}{g(X_i;w)} + \ln g(X_i;w) \\ &= \sum_{i=1}^{N} y_i \mathrm{w}^T X_i - \ln(1+e^{w^T X_i}) \end{aligned}$$

Maximum likelihood estimation

Maximum likelihood estimation

$$\frac{\partial}{\partial w^j} l(w) = \frac{\partial}{\partial w^j} \sum_{i=1}^{N} \{ y_i \mathrm{w}^{\mathrm{T}} X_i - \ln(1 + e^{\mathrm{w}^{\mathrm{T}} X_i}) \}$$

$$g(X; w) = \frac{1}{1 + e^{\mathrm{w}^{\mathrm{T}} X}}$$

$$1 - g(X; w) = \frac{e^{\mathrm{w}^{\mathrm{T}} X}}{1 + e^{\mathrm{w}^{\mathrm{T}} X}}$$

Maximum likelihood estimation

$$\frac{\partial}{\partial w^j} l(w) = \frac{\partial}{\partial w^j} \sum_{i=1}^{N} \{y_i \mathrm{w}^{\mathrm{T}} X_i - \ln(1 + e^{\mathrm{w}^{\mathrm{T}} X_i})\}$$

$$= \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i; w))\}$$

$$g(X; w) = \frac{1}{1 + e^{\mathrm{w}^{\mathrm{T}} X}}$$

$$1 - g(X; w) = \frac{e^{\mathrm{w}^{\mathrm{T}} X}}{1 + e^{\mathrm{w}^{\mathrm{T}} X}}$$

Maximum likelihood estimation

$$\frac{\partial}{\partial w^j} l(w) = \frac{\partial}{\partial w^j} \sum_{i=1}^{N} \{y_i \mathrm{w}^T X_i - \ln(1+e^{\mathrm{w}^T X_i})\}$$

$$= \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i; w))\}$$

$$= \sum_{i=1}^{N} X_i^j \{y_i - p(y^i = 1 | X_i; w)\}$$

$$g(X; w) = \frac{1}{1+e^{\mathrm{w}^T X}}$$

$$1 - g(X; w) = \frac{e^{\mathrm{w}^T X}}{1+e^{\mathrm{w}^T X}}$$

Taking the partial derivative w.r.t. each component of the **w** vector

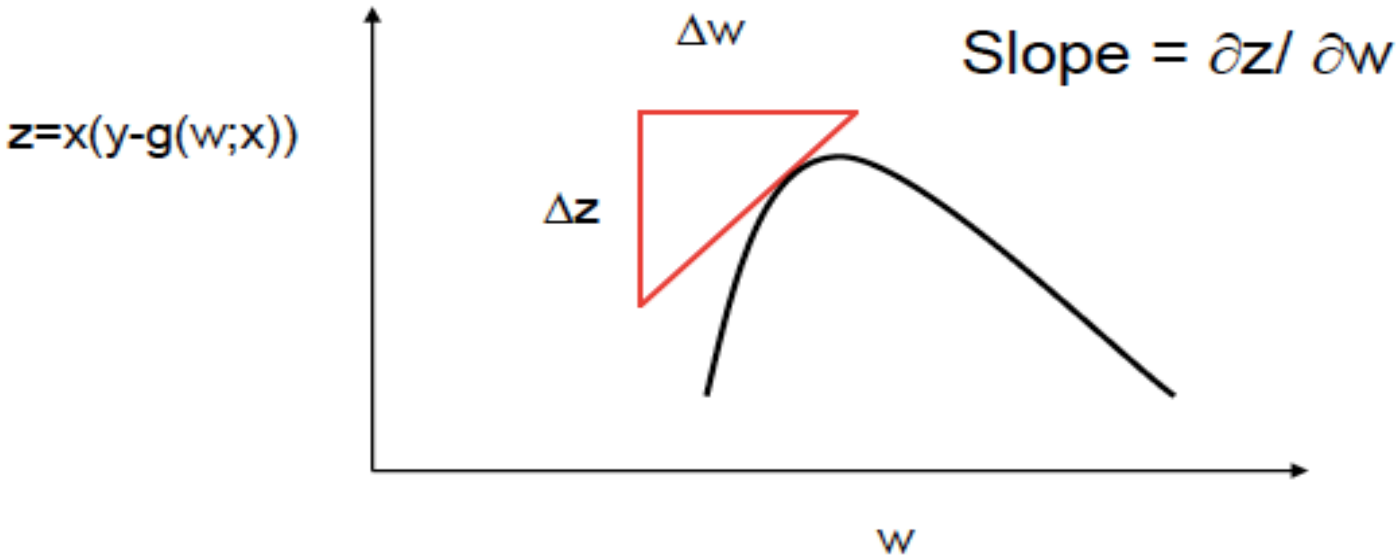
Bad news: No close form solution!

Good news: Concave function

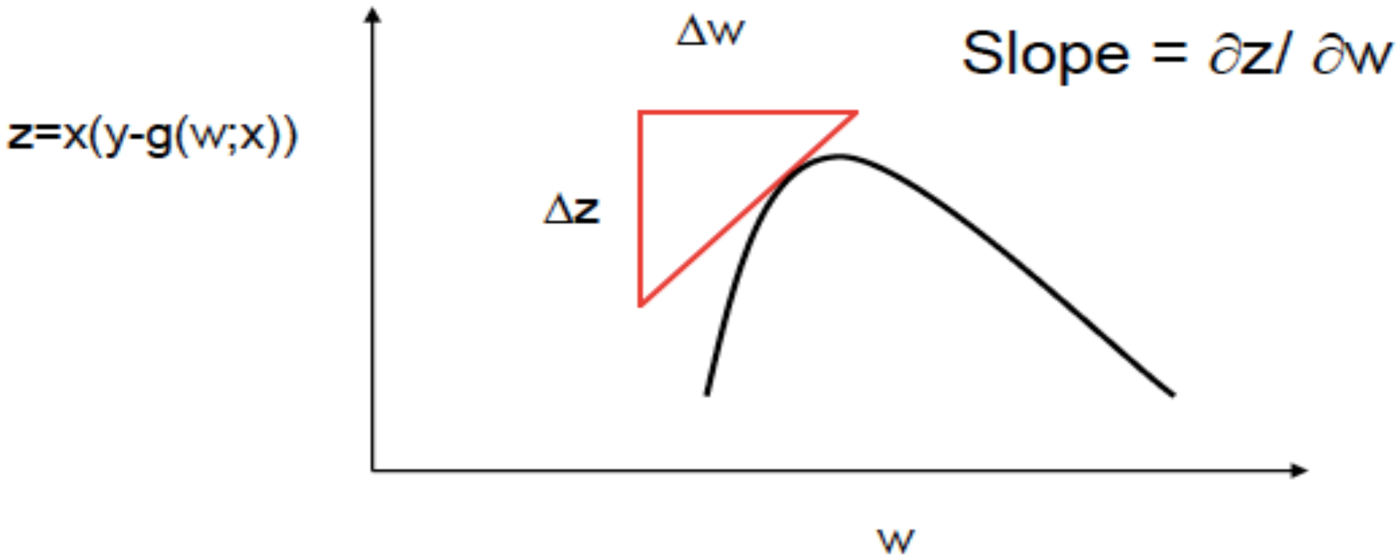
Five mins break!

Gradient ascent

Gradient ascent

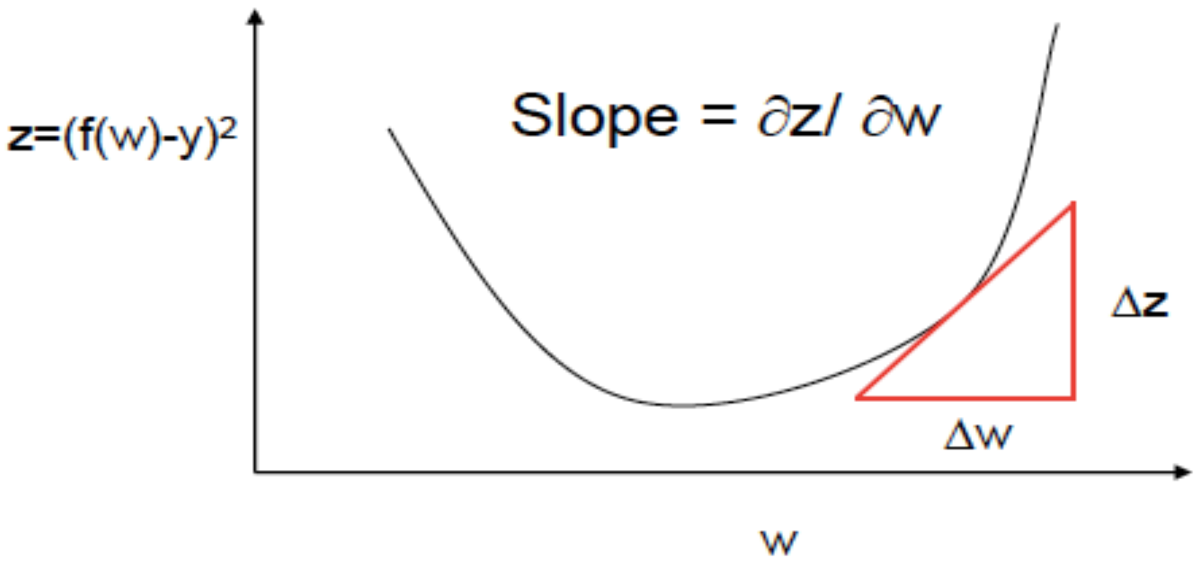


Gradient ascent

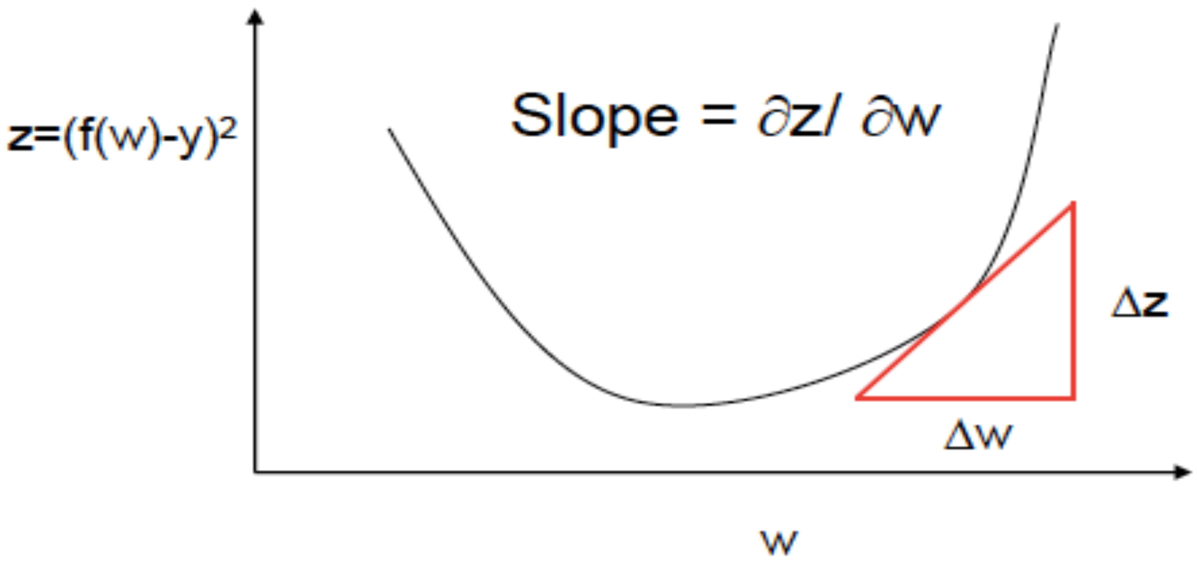


- Going in the direction to the slope will lead to a larger z
- But not too much, otherwise we would go beyond the optimal w

Gradient descent



Gradient descent



- Going in the *opposite* direction to the slope will lead to a smaller z
- But not too much, otherwise we would go beyond the optimal w

Gradient ascent for logistic regression

Gradient ascent for logistic regression

$$\frac{\partial}{\partial w^j} l(w) = \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i; w))\}$$

Gradient ascent for logistic regression

$$\frac{\partial}{\partial w^j} l(w) = \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i; w))\}$$

We use the gradient to adjust the value of w:

$$w^j \leftarrow w^j + \varepsilon \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i; w))\}$$

Where ε is a (small) constant

Algorithm for logistic regression

Algorithm for logistic regression

1. Chose λ

Algorithm for logistic regression

1. Chose λ
2. Start with a guess for $\mathbf{w}$

Algorithm for logistic regression

1. Chose λ
2. Start with a guess for **w**
3. For all j set $$w^j \leftarrow w^j + \varepsilon \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i; w))\}$$

Algorithm for logistic regression

1. Chose λ
2. Start with a guess for **w**
3. For all j set $$w^j \leftarrow w^j + \varepsilon \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i;w))\}$$
4. If no improvement for

$$LL(y \mid X;w) = \sum_{i=1}^{N} y_i \ln(1 - g(X_i;w)) + (1 - y_i) \ln g(X_i;w)$$

stop. Otherwise go to step 3

Example

Regularization

- Similar to other data estimation problems, we may not have enough samples to learn good models for logistic regression classification
- One way to overcome this is to 'regularize' the model, impose additional constraints on the parameters we are fitting.

d

Regularization

- Similar to other data estimation problems, we may not have enough samples to learn good models for logistic regression classification
- One way to overcome this is to 'regularize' the model, impose additional constraints on the parameters we are fitting.
- For example, lets assume that w^j comes from a Gaussian distribution with mean 0 and variance σ^2 (where σ^2 is a user defined parameter): $w^j \sim N(0, \sigma^2)$
- In that case we have **a prior** on the parameters and so:

$$p(y=1,\theta \mid X) \propto p(y=1 \mid X;\theta)\, p(\theta)$$

Regularization

- If we regularize the parameters we need to take the prior into account when computing the posterior for our parameters

$$p(y=1,\theta \mid X) \propto p(y=1 \mid X;\theta)\,p(\theta)$$

Regularization

- If we regularize the parameters we need to take the prior into account when computing the posterior for our parameters

$$p(y=1,\theta \mid X) \propto p(y=1 \mid X;\theta)\, p(\theta)$$

- Here we use a Gaussian model for the prior.
- Thus, the log likelihood changes to :

$$LL(y;w \mid X) = \sum_{i=1}^{N} y_i \mathrm{w}^{\mathrm{T}} X_i - \ln(1+e^{w^T X_i}) - \sum_j \frac{(w^j)^2}{2\sigma^2}$$

Assuming mean of 0 and removing terms that are not dependent on w

Regularization

- If we regularize the parameters we need to take the prior into account when computing the posterior for our parameters

$$p(y=1,\theta \mid X) \propto p(y=1 \mid X;\theta)\, p(\theta)$$

- Here we use a Gaussian model for the prior.
- Thus, the log likelihood changes to :

$$LL(y;w \mid X) = \sum_{i=1}^{N} y_i \mathrm{w}^{\mathrm{T}} X_i - \ln(1+e^{w^T X_i}) - \sum_j \frac{(w^j)^2}{2\sigma^2}$$

Assuming mean of 0 and removing terms that are not dependent on w

- And the new update rule (after taking the derivative w.r.t. w^j) is:

$$w^j \leftarrow w^j + \varepsilon \sum_{i=1}^{N} X_i^j \{y_i - (1 - g(X_i;w))\} - \varepsilon \frac{w^j}{\sigma^2}$$

Also known as the MAP estimate

The variance of our prior model

Regularization

- There are many other ways to regularize logistic regression
- The Gaussian model leads to an L2 regularization (we are trying to minimize the square value of w)
- Another popular regularization is an L1 which tries to minimize $|w|$

Important points

- Advantage of logistic regression over linear regression for classification
- Sigmoid function
- Gradient ascent / descent
- Regularization
- Logistic regression for multiple classes

Logistic regression

- The name comes from the **logit** transformation:

$$\log \frac{p(y=i \mid X;\theta)}{p(y=k \mid X;\theta)} = \log \frac{g(z_i)}{g(z_k)} = w_i^0 + w_i^1 x^1 + \ldots + w_i^d x^d$$

That’s all!