

Machine Learning

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SAPIENZA
UNIVERSITÀ DI ROMA

Where we are



✓



Today

Choosing a restaurant

- In everyday life we need to make decisions by taking into account lots of factors
- The question is what weight we put on each of these factors (how important are they with respect to the others).

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Reviews (out of 5 stars)	\$	Distance	Cuisine (out of 10)
4	30	21	7
2	15	12	8
5	27	53	9
3	20	5	6

Choosing a restaurant

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- The question is what weight we put on each of these factors (how important are they with respect to the others).
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- If we have many observations we may be able to recover the weights

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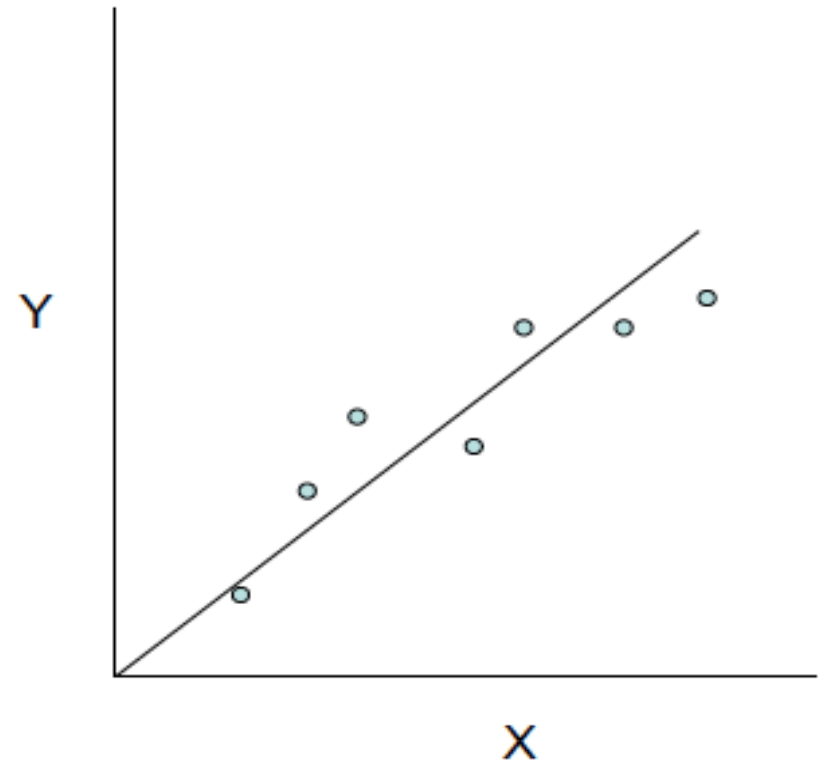
?



Linear regression

Linear regression

- Given an input x we would like to compute an output y
- For example:
 - Predict height from age
 - Predict Google's price from Yahoo's price
 - Predict distance from wall using sensor readings



Note that now Y can be **continuous**

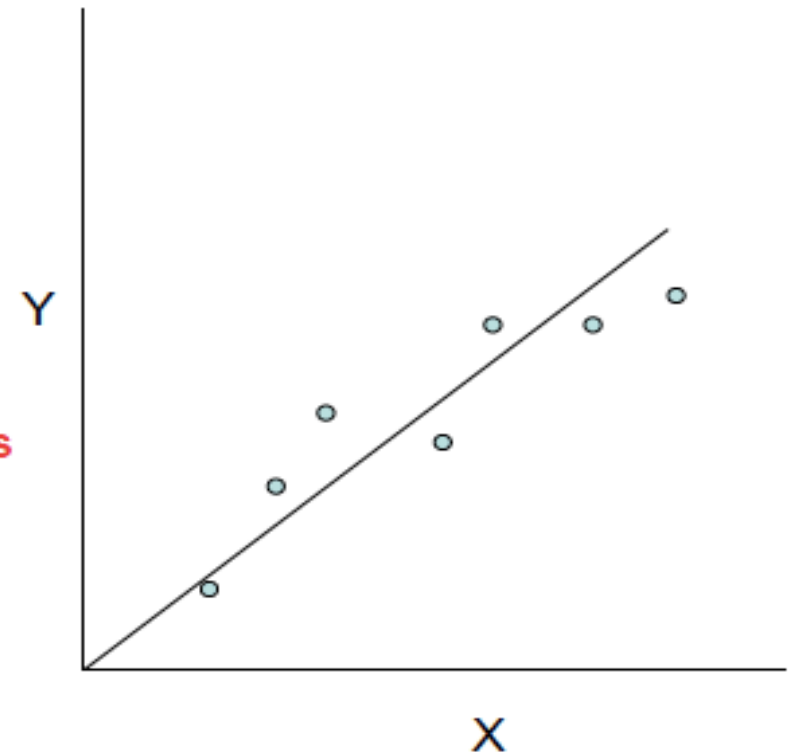
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What we are
trying to predict

$$y = wx + \varepsilon$$

Observed values



Linear regression

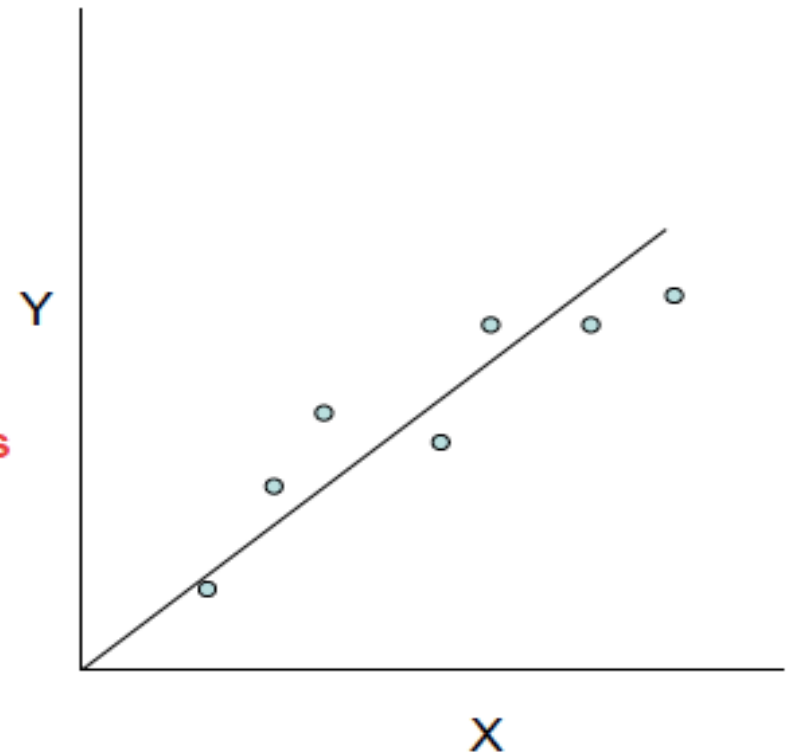
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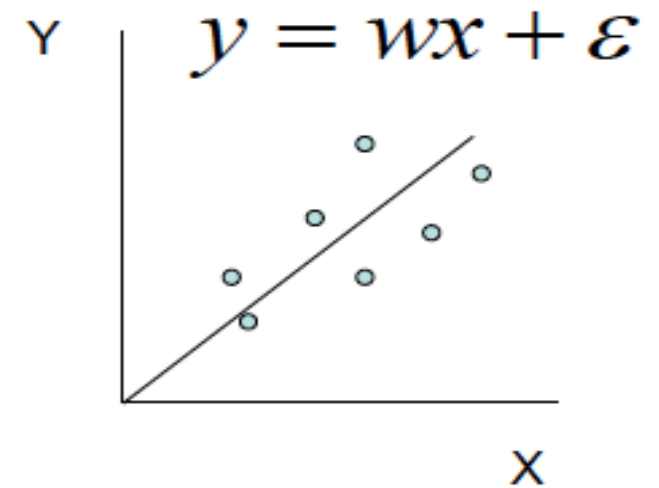
\nearrow Observed values

where w is a parameter and ε represents measurement or other noise



Linear regression

- Our goal is to estimate w from a training data of $\langle x_i, y_i \rangle$ pairs

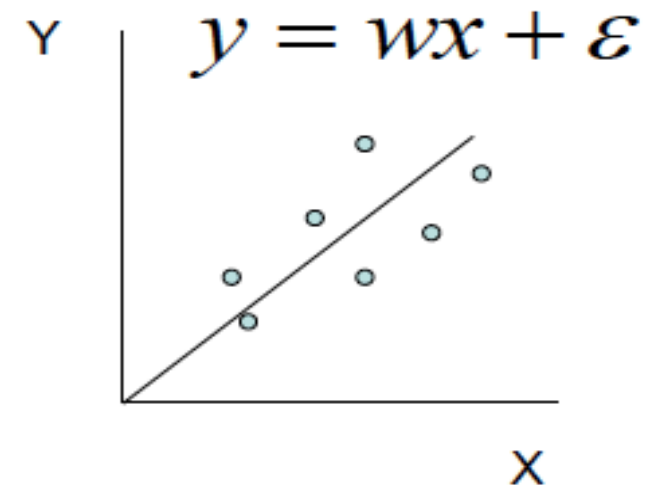


Linear regression

- Our goal is to estimate w from a training data of $\langle x_i, y_i \rangle$ pairs
- One way to find such relationship is to minimize the a least squares error:

$$\arg \min_w \sum_i (y_i - wx_i)^2$$

- Several other approaches can be used as well
- So why least squares?
 - minimizes squared distance between measurements and predicted line
 - has a nice probabilistic interpretation
 - easy to compute



If the noise is Gaussian with mean 0 then least squares is also the maximum likelihood estimate of w

Solving linear regression using least squares minimization

- We just take the derivative w.r.t. to w and set to 0:

Solving linear regression using least squares minimization

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$$\frac{\partial}{\partial w} \sum_i (y_i - wx_i)^2 = 2 \sum_i -x_i (y_i - wx_i) \Rightarrow$$

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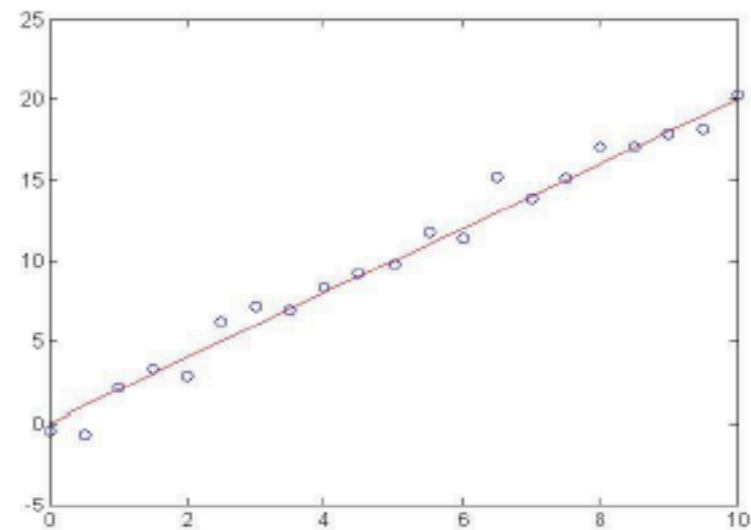
$$2 \sum_i x_i (y_i - wx_i) = 0 \Rightarrow$$

$$\sum_i x_i y_i = \sum_i wx_i^2 \Rightarrow$$

$$w = \frac{\sum_i x_i y_i}{\sum_i x_i^2}$$

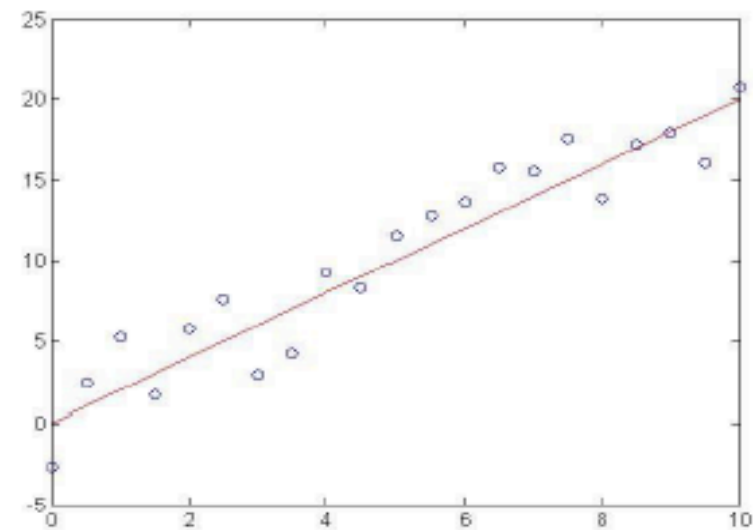
Regression example

- Generated: $w=2$
- Recovered: $w=2.03$
- Noise: $\text{std}=1$



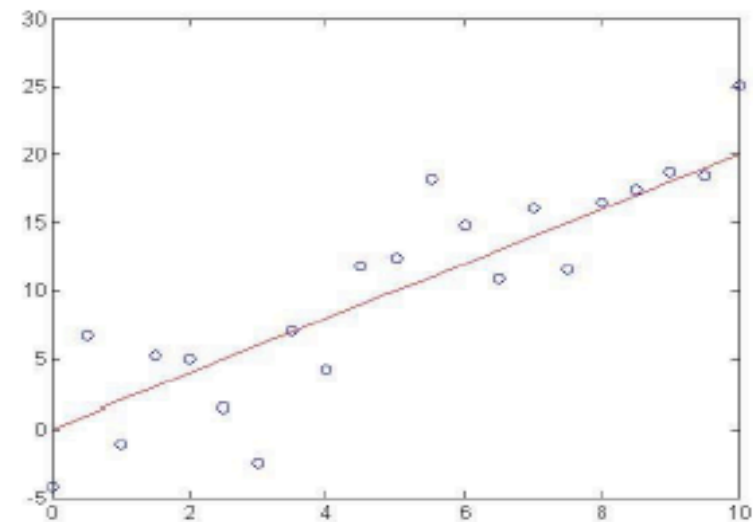
Regression example

- Generated: $w=2$
- Recovered: $w=2.05$
- Noise: $\text{std}=2$



Regression example

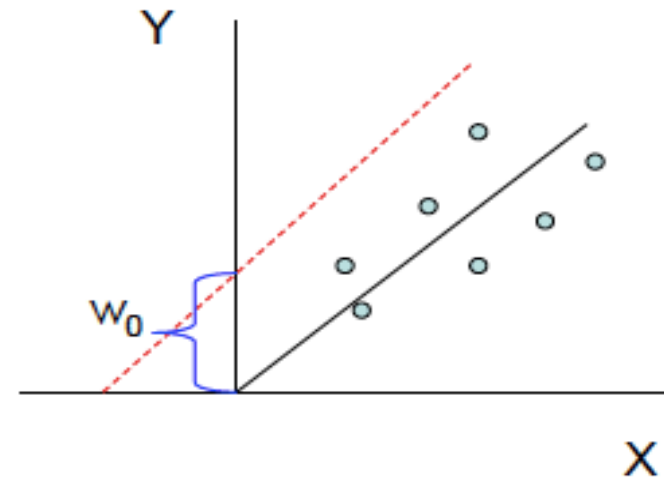
- Generated: $w=2$
- Recovered: $w=2.08$
- Noise: $\text{std}=4$



Bias term

- So far we assumed that the line passes through the origin
- What if the line does not?
- No problem, simply change the model to

$$y = w_0 + w_1x + \varepsilon$$



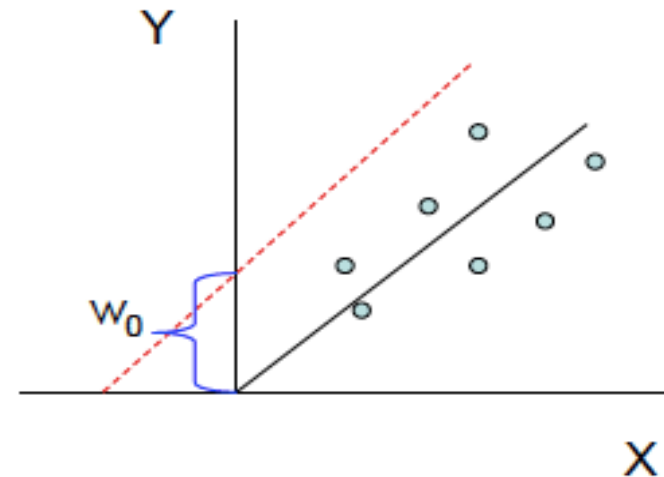
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- Can use least squares to determine w_0 , w_1

$$w_0 = \frac{\sum_i y_i - w_1 x_i}{n}$$

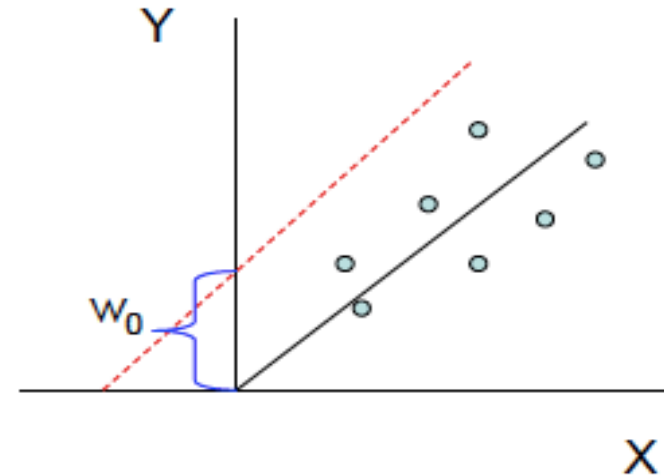


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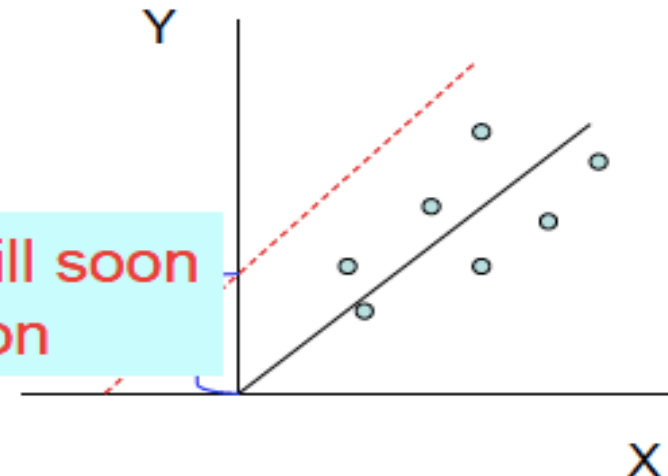
$$w_1 = \frac{\sum_i x_i (y_i - w_0)}{\sum_i x_i^2}$$

Bias term

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$y = w_0 + w_1x$ Just a second, we will soon give a simpler solution

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$$w_0 = \frac{\sum_i y_i - w_1 x_i}{n}$$

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Multivariate regression

- What if we have several inputs?
 - Stock prices for Yahoo, Microsoft and Ebay for the Google prediction task

Multivariate regression

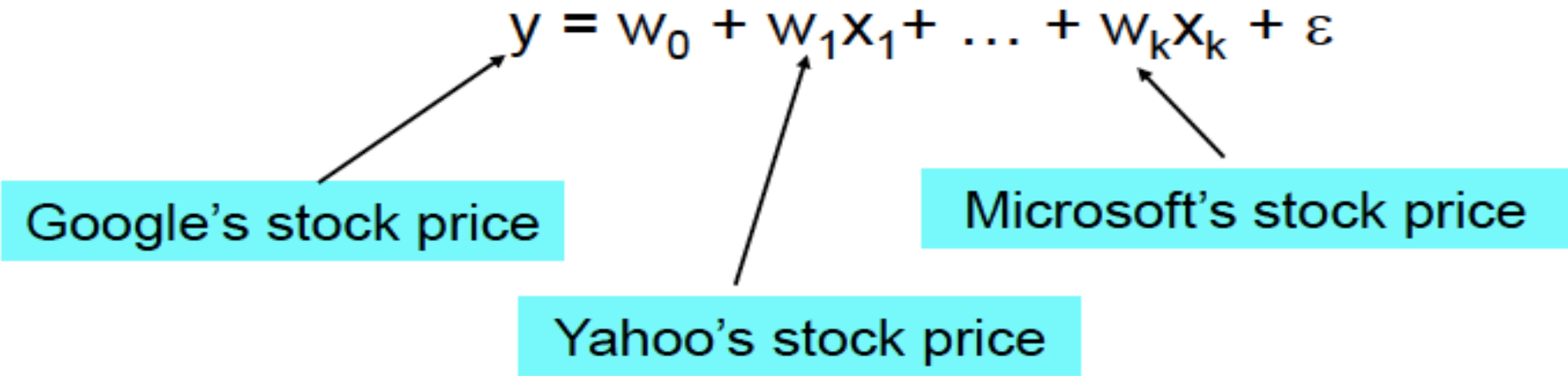
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$$y = w_0 + w_1x_1 + \dots + w_kx_k + \varepsilon$$

Google's stock price



Yahoo's stock price

Microsoft's stock price

Multivariate regression

- What if we have several inputs?
 - Stock prices for Yahoo, Microsoft and Ebay for the Google
- This becomes a regression problem
- Again, its easy to model:

Not all functions can be approximated using the input values directly

$$y = w_0 + w_1x_1 + \dots + w_kx_k + \varepsilon$$

$$y=10+3x_1^2-2x_2^2+\varepsilon$$

In some cases we would like to use polynomial or other terms based on the input data, are these still linear regression problems?

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In some cases we would like to use polynomial or other terms based on the input data, are these still linear regression problems?

Yes. As long as the coefficients are linear the equation is still a linear regression problem!

Five mins break!

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- Polynomial: $\phi_j(x) = x^j$ for $j=0 \dots n$

- Gaussian: $\phi_j(x) = \frac{(x - \mu_j)}{2\sigma_j^2}$

- Sigmoid: $\phi_j(x) = \frac{1}{1 + \exp(-s_j x)}$

Any function of the input values can be used. The solution for the parameters of the regression remains the same.

General linear regression problem

- Using our new notations for the basis function linear regression can be written as

$$y = \sum_{j=0}^n w_j \phi_j(x)$$

- Where $\phi_j(x)$ can be either x_j for multivariate regression or one of the non linear basis we defined

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- Once again we can use 'least squares' to find the optimal solution.

LMS for the general linear regression problem

Our goal is to minimize the following loss function:

$$J(\mathbf{w}) = \sum_i (y^i - \sum_j w_j \phi_j(x^i))^2$$

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Moving to vector notations we get:

$$J(\mathbf{w}) = \sum_i (y^i - \mathbf{w}^T \phi(x^i))^2$$

$$y = \sum_{j=0}^n w_j \phi_j(x)$$

\mathbf{w} – vector of dimension $k+1$

$\phi(x^i)$ – vector of dimension $k+1$

y^i – a scalar

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$$\sum_i y^i \phi(x^i)^T = w^T \left[\sum_i \phi(x^i) \phi(x^i)^T \right]$$

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Define:

$$\Phi = \begin{pmatrix} \phi_0(x^1) & \phi_1(x^1) & \cdots & \phi_m(x^1) \\ \phi_0(x^2) & \phi_1(x^2) & \cdots & \phi_m(x^2) \\ \vdots & \vdots & \cdots & \vdots \\ \phi_0(x^n) & \phi_1(x^n) & \cdots & \phi_m(x^n) \end{pmatrix}$$

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Then deriving \mathbf{w}
we get:

$$\mathbf{w} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}$$

LMS for general linear regression problem

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Deriving \mathbf{w} we get: $\mathbf{w} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}$

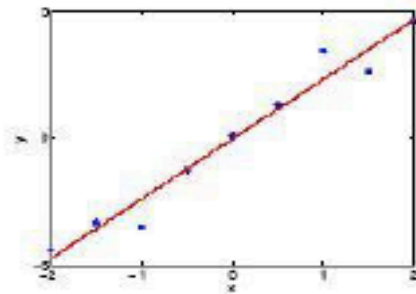
k+1 entries vector

n by k+1 matrix

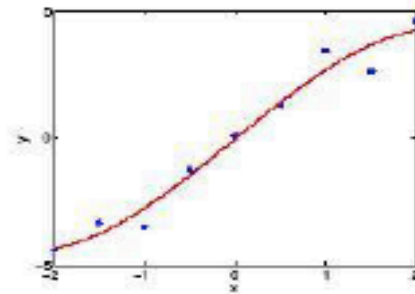
n entries vector

This solution is
also known as
'psuedo inverse'

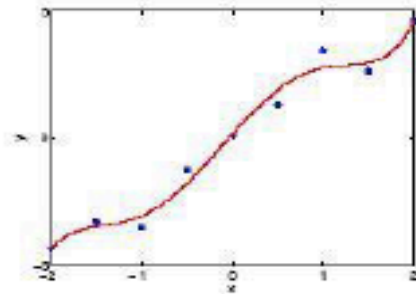
Example: Polynomial regression



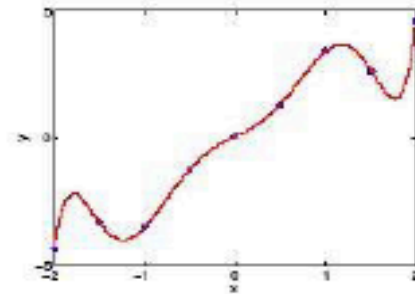
degree = 1, CV = 0.6



degree = 3, CV = 1.5



degree = 5, CV = 6.0



degree = 7, CV = 15.6

A probabilistic interpretation

Our least squares minimization solution can also be motivated by a probabilistic interpretation of the regression problem: $y = \mathbf{w}^T \phi(x) + \varepsilon$

A probabilistic interpretation

Our least squares minimization solution can also be motivated by a probabilistic interpretation of the regression problem: $y = \mathbf{w}^T \phi(x) + \varepsilon$

The MLE for \mathbf{w} in this model is the same as the solution we derived for least squares criteria:

$$\mathbf{w} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}$$

Other types of linear regression

- Linear regression is a useful model for many problems
- However, the parameters we learn for this model are **global**; they are the same regardless of the value of the input x
- Extension to linear regression adjust their parameters based on the region of the input we are dealing with

Five mins break!

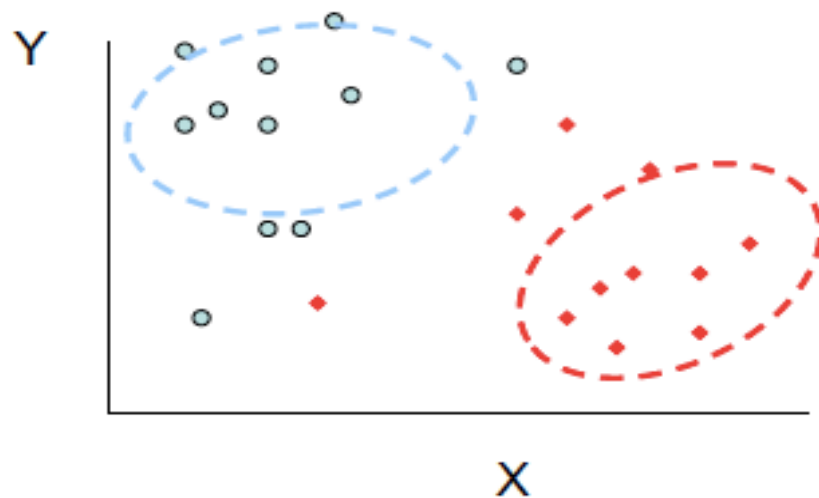
Back to classification

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

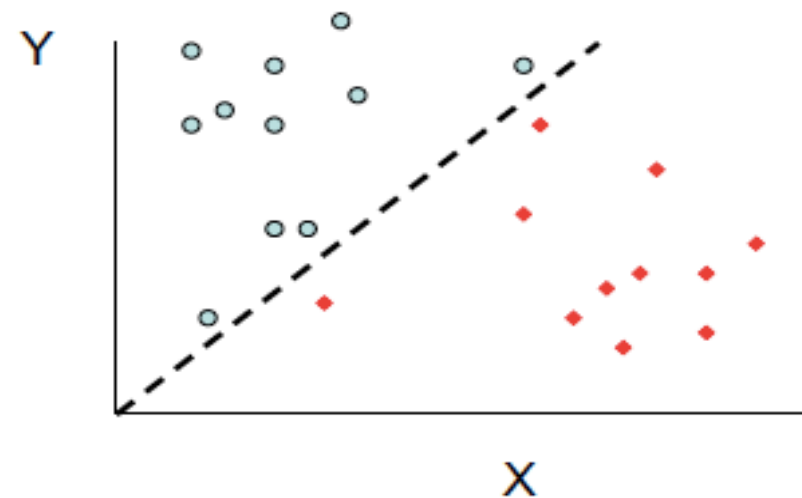
Generative vs. discriminative classifiers

- 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 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 $p(y | X ; \theta)$ where θ are the parameters of our model
- When using regression θ represents the values of our regression coefficients (w).

Regression for classification

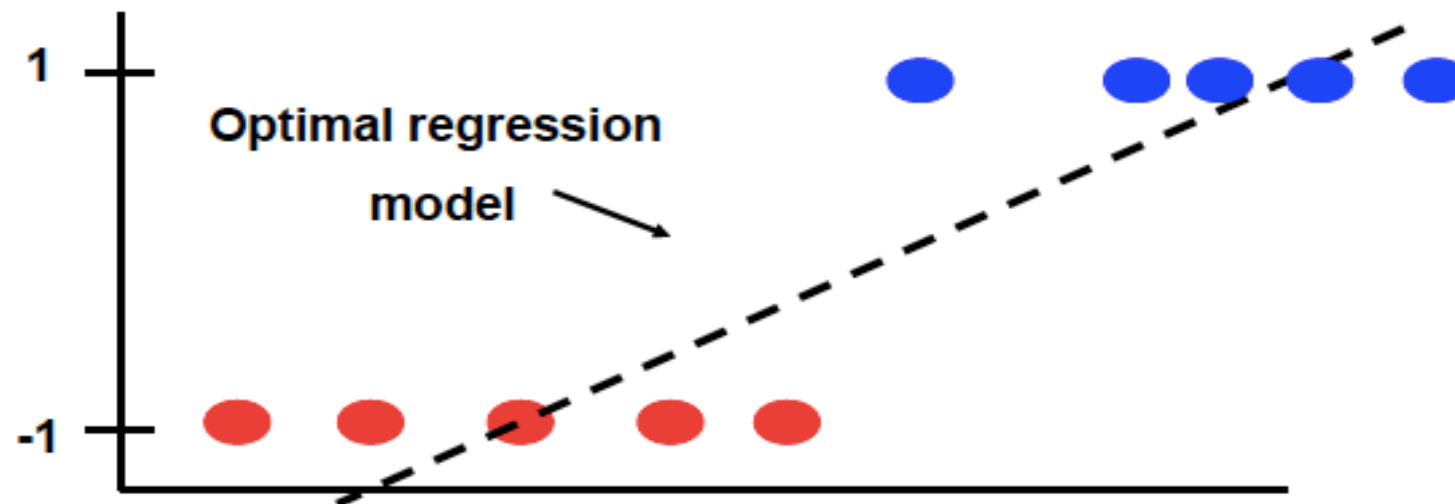
- Assume we would like to use linear regression to learn the parameters for $p(y | X; \theta)$
- Problems?

Regression for classification

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- Problems?

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

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



The sigmoid function

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

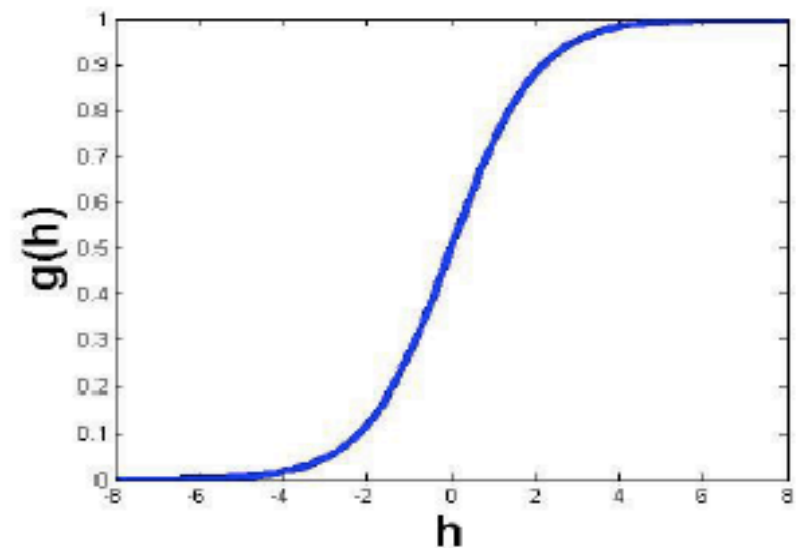
- To classify using regression models we replace the linear function with the sigmoid function:

The sigmoid function

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



1

The sigmoid function

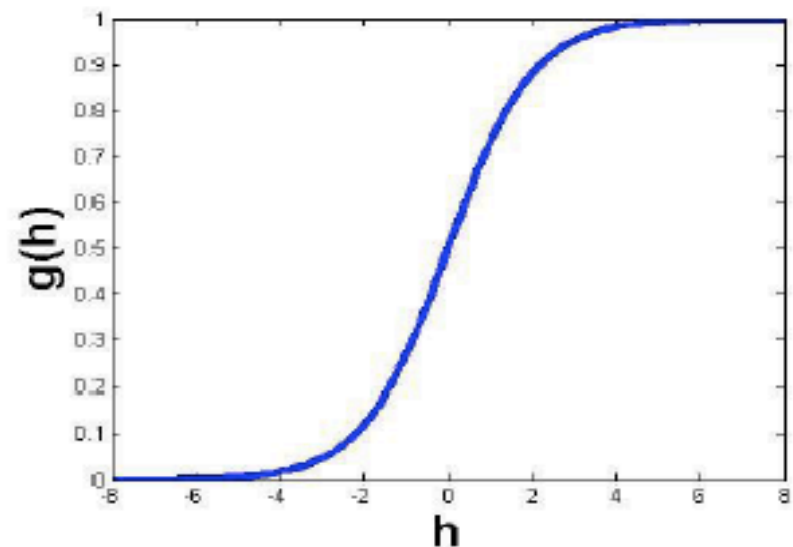
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Always between 0 and 1 $\rightarrow g(h) = \frac{1}{1 + e^{-h}}$

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

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



The sigmoid function

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

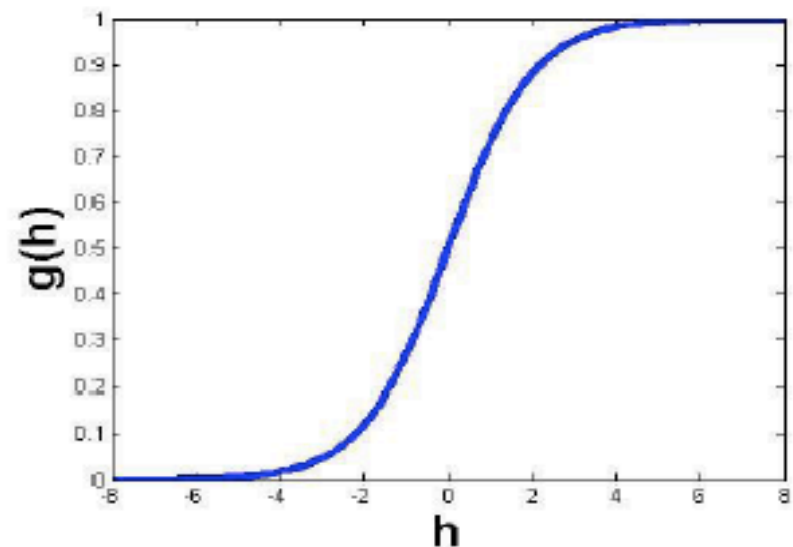
- To classify using regression models we replace the linear function with the sigmoid function:

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

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

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The sigmoid function

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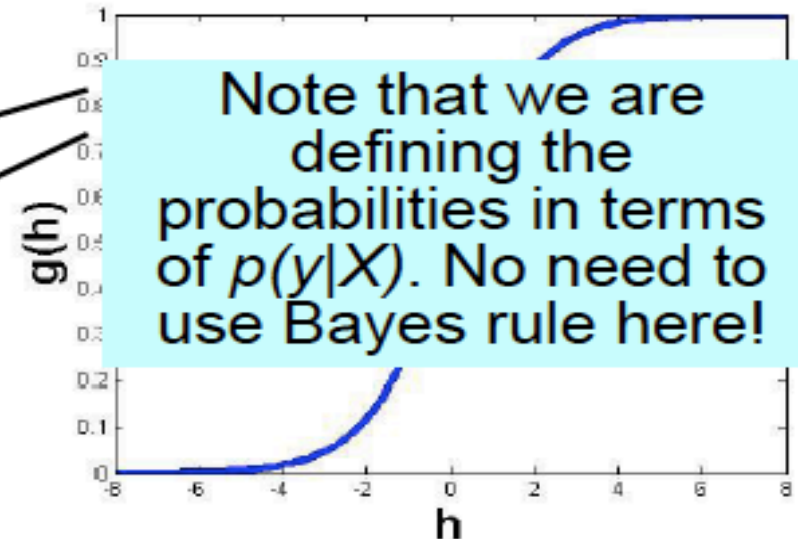
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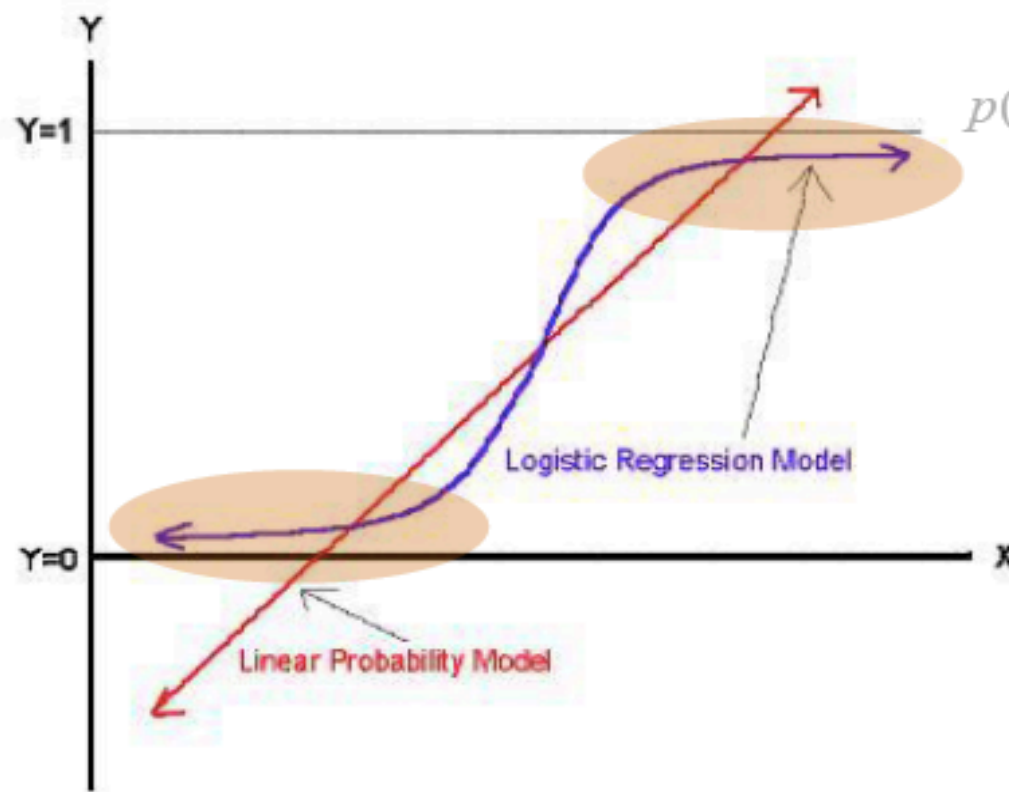
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Logistic regression vs. Linear regression

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

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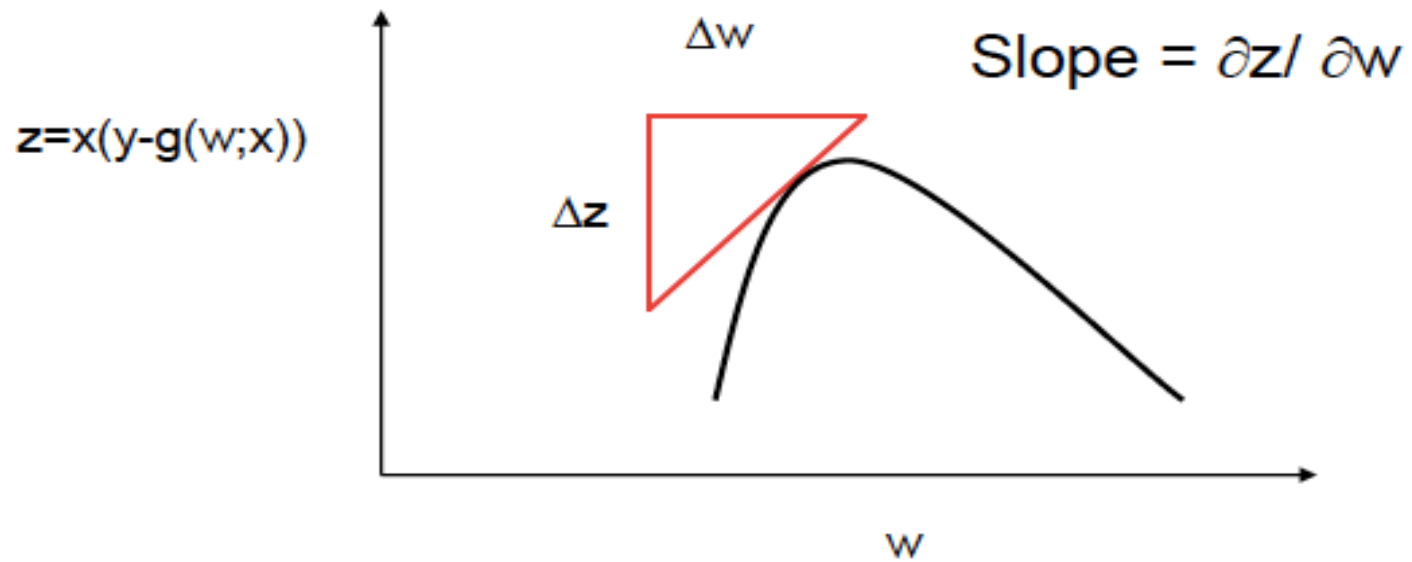
Taking the partial derivative w.r.t. each component of the w vector

Bad news: No close form solution!

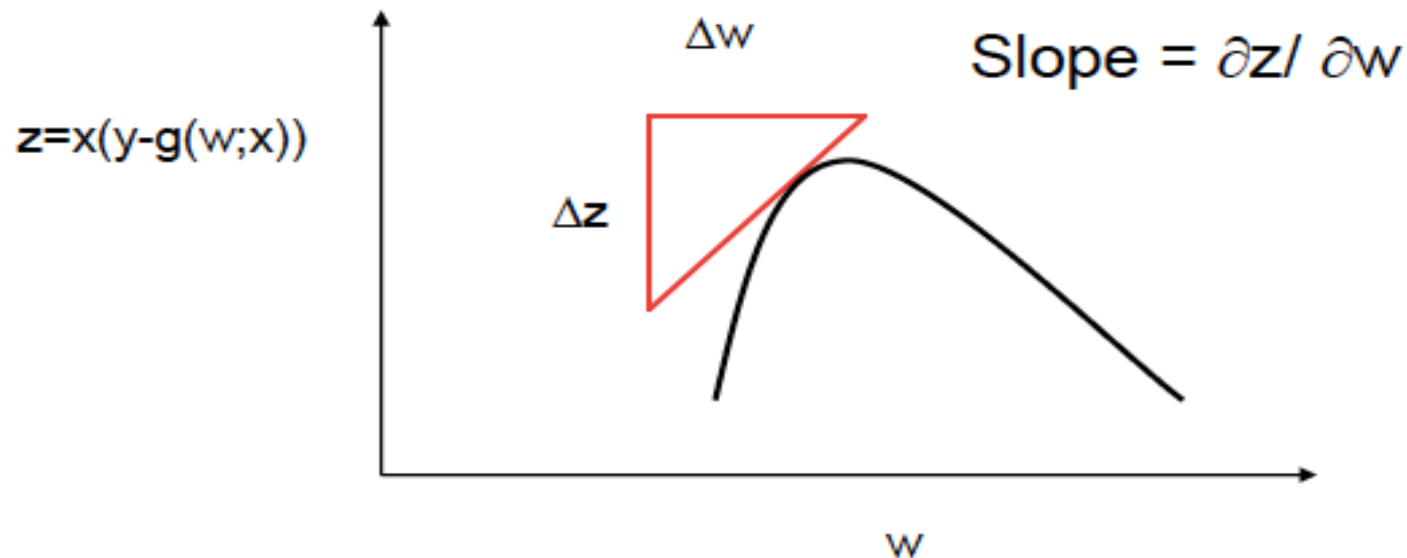
Good news: Concave function

Five mins break!

Gradient ascent

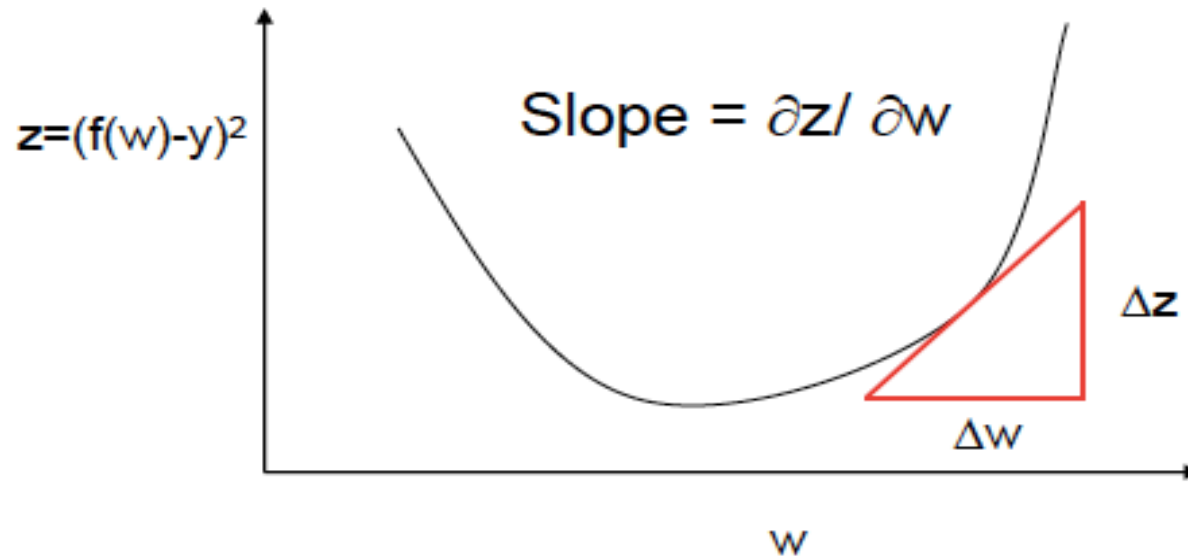


Gradient ascent

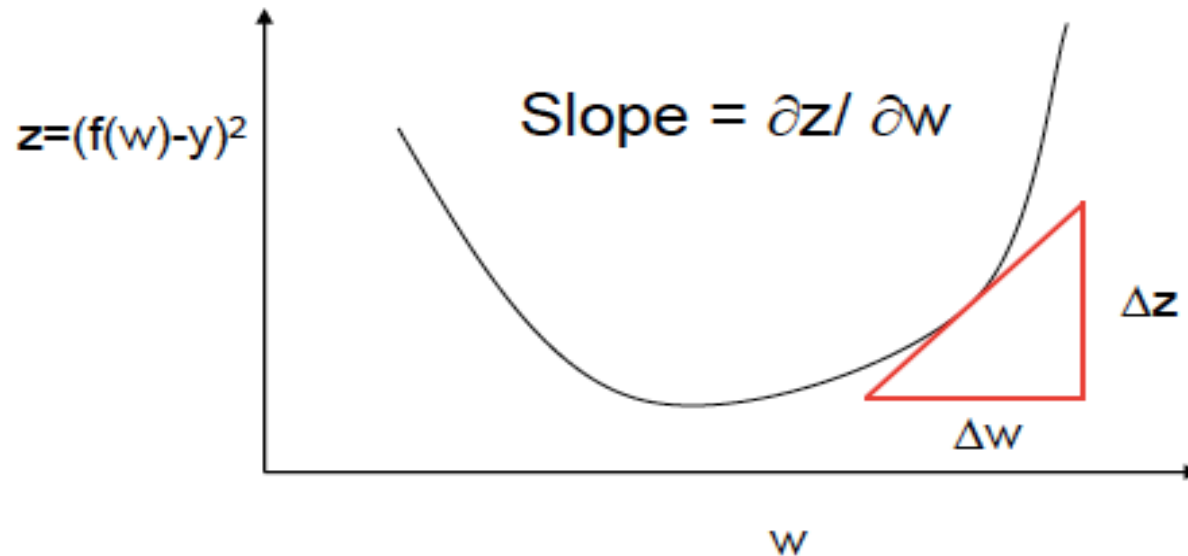


- Going in the direction to the slope will lead to a larger z
- But not too much, otherwise we would go beyond the optimal w

Gradient descent



Gradient descent



- Going in the *opposite* direction to the slope will lead to a smaller z
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Gradient ascent for logistic regression

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Gradient ascent for logistic regression

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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

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

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

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^i comes from a Gaussian distribution with mean 0 and variance σ^2 (where σ^2 is a user defined parameter): $w^i \sim N(0, \sigma^2)$
- In that case we have **a prior** on the parameters and so:

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

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

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

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

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

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- 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:

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

That's all!