

Algorithms in Nature

Regression

Goal of regression



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).
- Assume we would like to build a recommender system based on an individuals' preferences
- If we have many observations we may be able to recover the weights

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



Linear regression

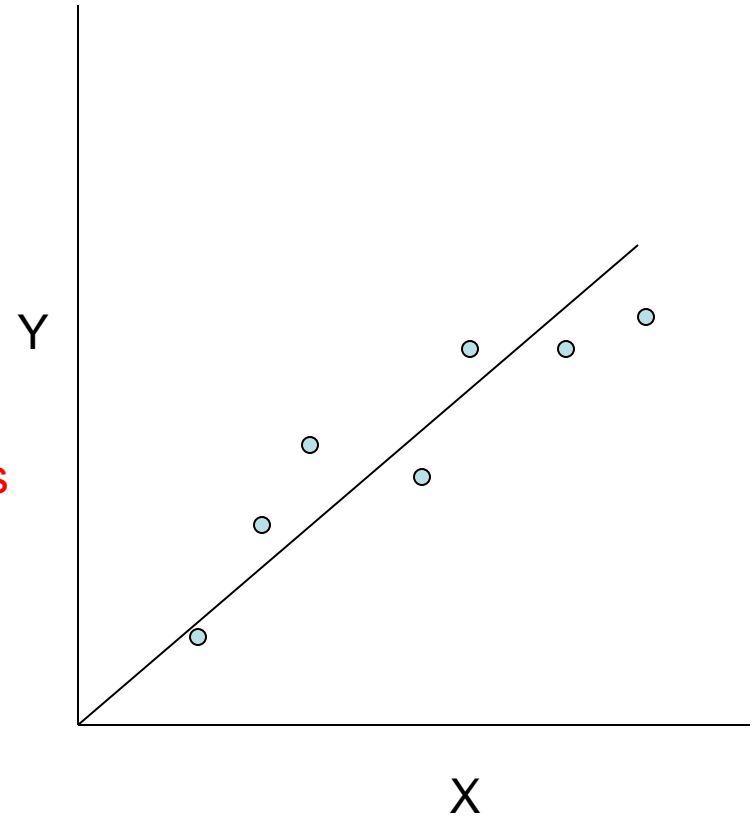
- Given an input x we would like to compute an output y
- In linear regression we assume that y and x are related with the following equation:

What we are trying to predict

$$y = wX + \varepsilon$$

Observed values

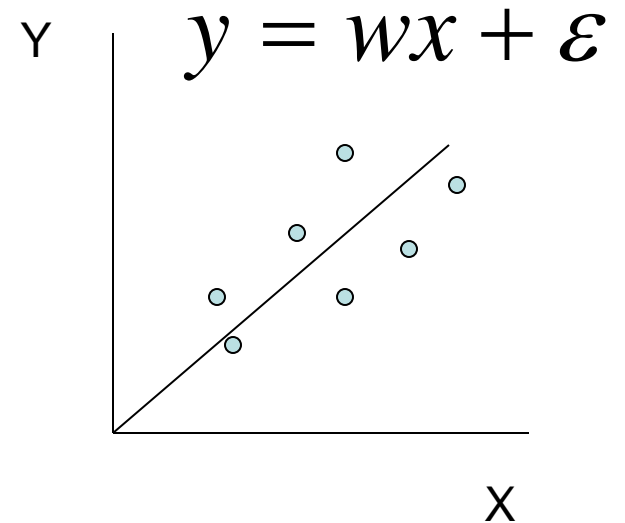
where w is a parameter and ε represents measurement or other noise



Linear regression

- Our goal is to estimate w from a training data of $\langle x_i, y_i \rangle$ pairs
- This could be done using a least squares approach

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



Solving linear regression

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

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

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

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

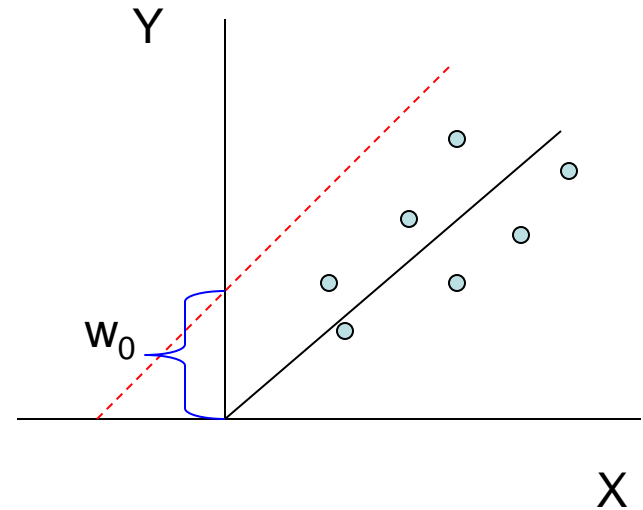
$$w = \frac{\sum_i x_i y_i}{\sum_i x_i^2}$$

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

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

- Can use least squares to determine w_0 , w_1



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

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

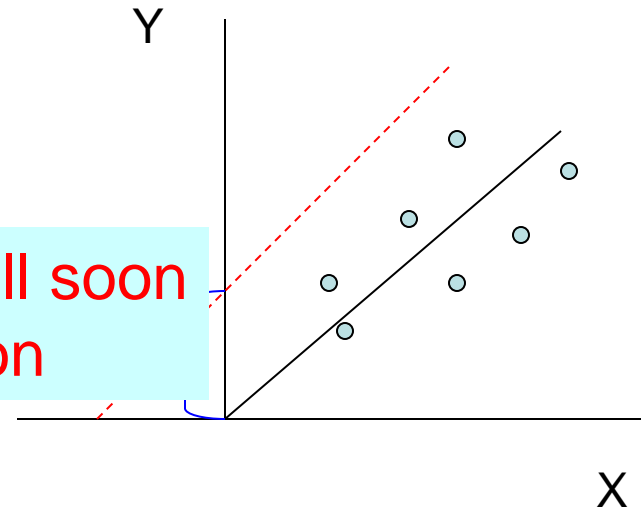
Bias term

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- What if the line does not?
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Just a second, we will soon give a simpler solution

- Can use least squares to determine w_0 , w_1



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

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

Multivariate regression

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

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

Google's stock price

Microsoft's stock price

Yahoo'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?

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

Non-Linear basis function

- So far we only used the observed values
- However, linear regression can be applied in the same way to functions of these values
- As long as these functions can be directly computed from the observed values the parameters are still linear in the data and the problem remains a linear regression problem

$$y = w_0 + w_1 x_1^2 + \dots + w_k x_k^2 + \varepsilon$$

Non-Linear basis function

- What type of functions can we use?
- A few common examples:

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

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

- 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
- 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:

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

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

w – vector of dimension $k+1$
 $\phi(x^i)$ – vector of dimension $k+1$
 y^i – a scalar

Moving to vector notations we get:

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

We take the derivative w.r.t \mathbf{w}

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

Equating to 0 we get $2 \sum_i (y^i - \mathbf{w}^T \boldsymbol{\phi}(x^i)) \boldsymbol{\phi}(x^i)^T = 0 \Rightarrow$

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

LMS for general linear regression problem

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Equating to 0 we get

$$2 \sum_i (y^i - \mathbf{w}^T \phi(x^i)) \phi(x^i)^T = 0 \Rightarrow$$
$$\sum_i y^i \phi(x^i)^T = \mathbf{w}^T \left[\sum_i \phi(x^i) \phi(x^i)^T \right]$$

Define:

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

Then deriving \mathbf{w}
we get:

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

LMS for general linear regression problem

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

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

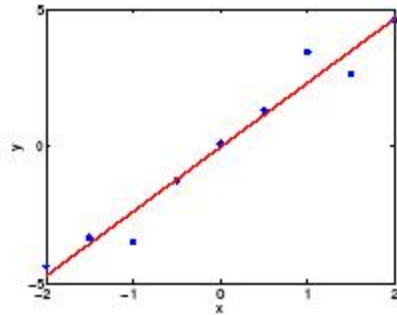
k+1 entries vector

n by k+1 matrix

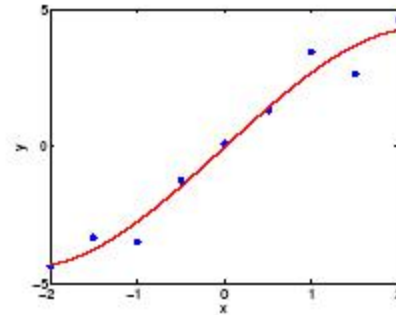
n entries vector

This solution is also known as 'psuedo inverse'

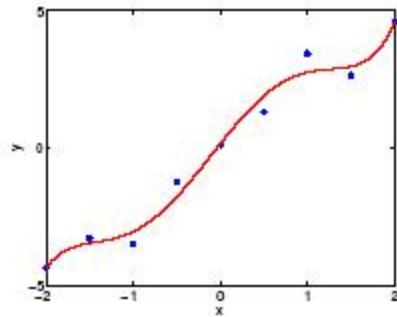
Example: Polynomial regression



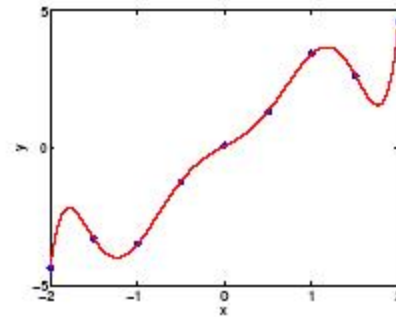
degree = 1, CV = 0.6



degree = 3, CV = 1.5



degree = 5, CV = 6.0



degree = 7, CV = 15.6