CS 2750 Machine Learning
Lecture 8-9

Linear regression

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Supervised learning

Data: $D = \{D_1, D_2, .., D_n\}$ **a set of *n* examples**

$D_i = < \mathbf{x}_i, y_i >$

$\mathbf{x}_i = (x_{i,1}, x_{i,2}, \cdots x_{i,d})$ is an input vector of size *d*

y_i is the desired output (given by a teacher)

Objective: learn the mapping $f : X \to Y$

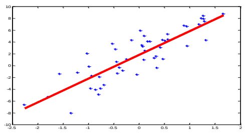
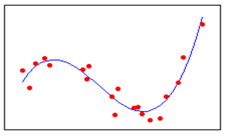
s.t. $y_i \approx f(\mathbf{x}_i)$ for all $i = 1, .., n$

- **Regression:** Y is **continuous**
  Example: earnings, product orders $\rightarrow$ company stock price
- **Classification:** Y is **discrete**
  Example: handwritten digit in binary form $\rightarrow$ digit label

Supervised learning examples

- **Regression:** Y is **continuous**

$$\left.\begin{array}{l}\text{Debt/equity}\\ \text{Earnings}\\ \text{Future product orders}\end{array}\right| \longrightarrow \text{Stock price}$$

Data:

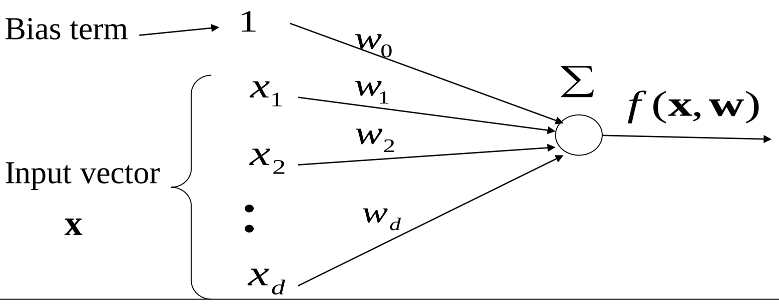
Debt/equity	Earnings	Future prod orders	Stock price
20	115	20	123.45
18	120	31	140.56
….			

Linear regression

- **Function** $f : X \rightarrow Y$
- Y is a linear combination of input components

$$f(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots w_d x_d = w_0 + \sum_{j=1}^{d} w_j x_j$$

$w_0, w_1, \ldots w_k$ - **parameters (weights)**



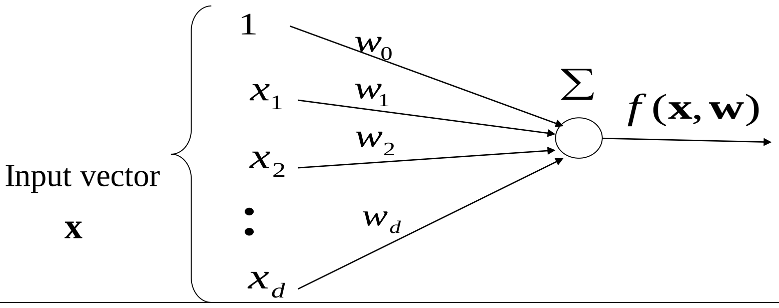
Linear regression

- **Shorter (vector) definition of the model**
  - Include bias constant in the input vector

$$\mathbf{x} = (1, x_1, x_2, \cdots x_d)$$

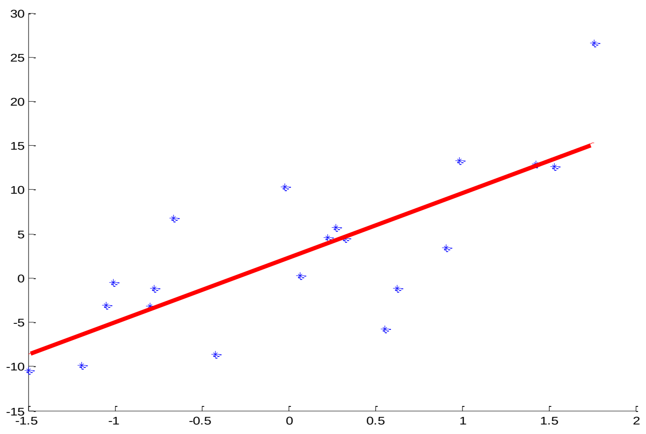
$$f(\mathbf{x}) = w_0 x_0 + w_1 x_1 + w_2 x_2 + \ldots w_d x_d = \mathbf{w}^T \mathbf{x}$$

$w_0, w_1, \ldots w_k$ **- parameters (weights)**



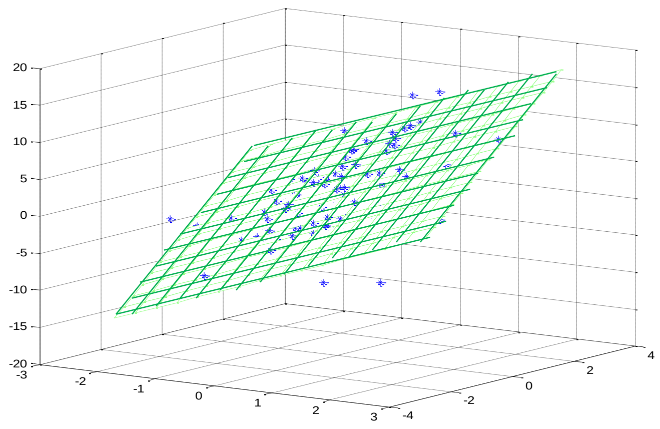
Linear regression. Example

- 1 dimensional input $\mathbf{x} = (x_1)$



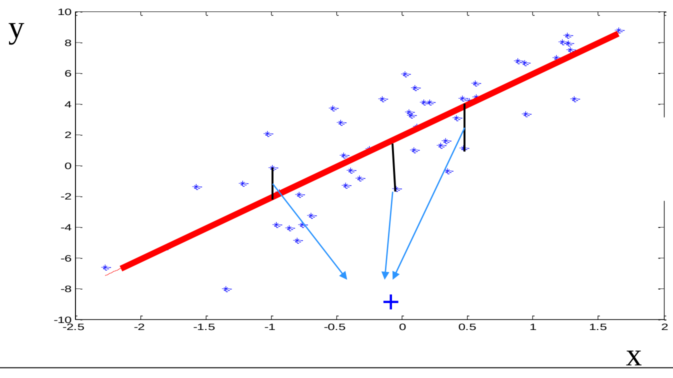
Linear regression. Example.

- 2 dimensional input $\mathbf{x} = (x_1, x_2)$



Linear regression: error

- **Data:** $D_i = < \mathbf{x}_i, y_i >$
- **Function:** $\mathbf{x}_i \rightarrow f(\mathbf{x}_i)$
- **Goal:** find the **best set** of model parameters
- **Error**: a measure of misfit of the model and the data



Linear regression: Error.

- **Data:** $D_i = < \mathbf{x}_i, y_i >$
- **Function:** $\mathbf{x}_i \rightarrow f(\mathbf{x}_i)$
- **Goal:** find the **best set** of model parameters
- **Error function**
  - a measure of misfit of the model and the data
  - in other words, it measures how much our predictions deviate from the desired answers

Mean-squared error: *Error(w, D)*

$$J_n = \frac{1}{n} \sum_{i=1,..n} (y_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

- **Learning:**

  We want to find the weights minimizing the error !

Linear regression: Optimization.

- We want the **weights minimizing the error**

$$J_n = \frac{1}{n} \sum_{i=1,..n} (y_i - f(\mathbf{x}_i, \mathbf{w}))^2 = \frac{1}{n} \sum_{i=1,..n} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

- For the optimal set of parameters, derivatives of the error with respect to each parameter must be 0

$$\frac{\partial}{\partial w_j} J_n(\mathbf{w}) = -\frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 x_{i,0} - w_1 x_{i,1} - \ldots - w_d x_{i,d}) x_{i,j} = 0$$

- **Vector of derivatives:**

$$\mathrm{grad}_{\mathbf{w}}(J_n(\mathbf{w})) = \nabla_{\mathbf{w}}(J_n(\mathbf{w})) = -\frac{2}{n} \sum_{i=1}^{n} (y_i - \mathbf{w}^T \mathbf{x}_i) \mathbf{x}_i = \bar{\mathbf{0}}$$

Linear regression: Optimization.

- $\text{grad}_{\mathbf{w}}(J_n(\mathbf{w})) = \bar{\mathbf{0}}$ defines a set of equations in **w**

$$\frac{\partial}{\partial w_j} J_n(\mathbf{w}) = \cancel{-\frac{2}{n}} \sum_{i=1}^{n} (y_i - w_0 x_{i,0} - w_1 x_{i,1} - \ldots - w_d x_{i,d}) x_{i,j} = 0$$

$$\frac{\partial}{\partial w_0} J_n(\mathbf{w}) = \sum_{i=1}^{n} (y_i - w_0 x_{i,0} - w_1 x_{i,1} - \ldots - w_d x_{i,d}) = 0$$

$$\frac{\partial}{\partial w_1} J_n(\mathbf{w}) = \sum_{i=1}^{n} (y_i - w_0 x_{i,0} - w_1 x_{i,1} - \ldots - w_d x_{i,d}) x_{i,1} = 0$$

$$\ldots$$

$$\frac{\partial}{\partial w_j} J_n(\mathbf{w}) = \sum_{i=1}^{n} (y_i - w_0 x_{i,0} - w_1 x_{i,1} - \ldots - w_d x_{i,d}) x_{i,j} = 0$$

$$\ldots$$

$$\frac{\partial}{\partial w_d} J_n(\mathbf{w}) = \sum_{i=1}^{n} (y_i - w_0 x_{i,0} - w_1 x_{i,1} - \ldots - w_d x_{i,d}) x_{i,d} = 0$$

Solving linear regression

$$\frac{\partial}{\partial w_j} J_n(\mathbf{w}) = \sum_{i=1}^{n} (y_i - w_0 x_{i,0} - w_1 x_{i,1} - \ldots - w_d x_{i,d}) x_{i,j} = 0$$

By rearranging the terms we get a **system of linear equations** with *d+1* unknowns

$$\boxed{\mathbf{A}\mathbf{w} = \mathbf{b}}$$

$$w_0 \sum_{i=1}^{n} x_{i,0} 1 + w_1 \sum_{i=1}^{n} x_{i,1} 1 + \ldots + w_j \sum_{i=1}^{n} x_{i,j} 1 + \ldots + w_d \sum_{i=1}^{n} x_{i,d} 1 = \sum_{i=1}^{n} y_i 1$$

$$w_0 \sum_{i=1}^{n} x_{i,0} x_{i,1} + w_1 \sum_{i=1}^{n} x_{i,1} x_{i,1} + \ldots + w_j \sum_{i=1}^{n} x_{i,j} x_{i,1} + \ldots + w_d \sum_{i=1}^{n} x_{i,d} x_{i,1} = \sum_{i=1}^{n} y_i x_{i,1}$$

$$\bullet\bullet\bullet$$

$$w_0 \sum_{i=1}^{n} x_{i,0} x_{i,j} + w_1 \sum_{i=1}^{n} x_{i,1} x_{i,j} + \ldots + w_j \sum_{i=1}^{n} x_{i,j} x_{i,j} + \ldots + w_d \sum_{i=1}^{n} x_{i,d} x_{i,j} = \sum_{i=1}^{n} y_i x_{i,j}$$

$$\bullet\bullet\bullet$$

Solving linear regression

- The optimal set of weights satisfies:

$$\nabla_{\mathbf{w}}(J_n(\mathbf{w})) = -\frac{2}{n}\sum_{i=1}^{n}(y_i - \mathbf{w}^T\mathbf{x}_i)\mathbf{x}_i = \bar{\mathbf{0}}$$

Leads to a **system of linear equations (SLE)** with *d+1* unknowns of the form

$$\mathbf{A}\mathbf{w} = \mathbf{b}$$

$$w_0\sum_{i=1}^{n}x_{i,0}x_{i,j} + w_1\sum_{i=1}^{n}x_{i,1}x_{i,j} + \ldots + w_j\sum_{i=1}^{n}x_{i,j}x_{i,j} + \ldots + w_d\sum_{i=1}^{n}x_{i,d}x_{i,j} = \sum_{i=1}^{n}y_i x_{i,j}$$

Solution to SLE: $\boxed{\mathbf{w} = \mathbf{A}^{-1}\mathbf{b}}$

Assuming **X** is an *nxd* data matrix with rows corresponding to examples and columns to inputs, and ***y*** is nx1 vector of outputs, then $\mathbf{w} = (\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{y}$

Gradient descent solution

Objective: optimize the weights in the linear regression model

$$J_n = Error(\mathbf{w}) = \frac{1}{n}\sum_{i=1,..n}(y_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

An alternative to SLE solution:

- **Gradient descent**

  Idea:

  – Adjust weights in the direction that improves the Error

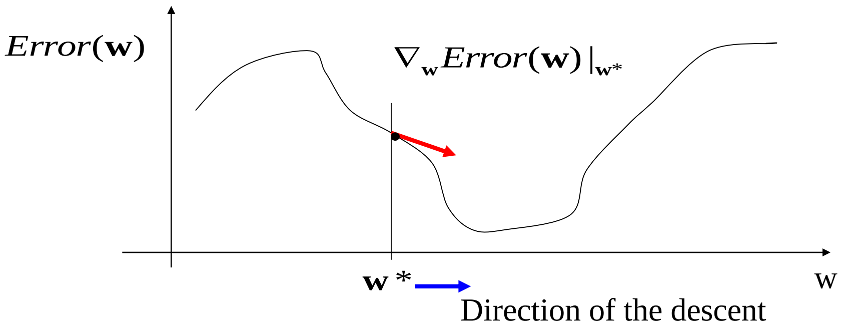
  – The gradient tells us what is the right direction

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha\nabla_{\mathbf{w}}Error_i(\mathbf{w})$$

$\alpha > 0$ - a **learning rate** (scales the gradient changes)

Gradient descent method

- Descend using the gradient information



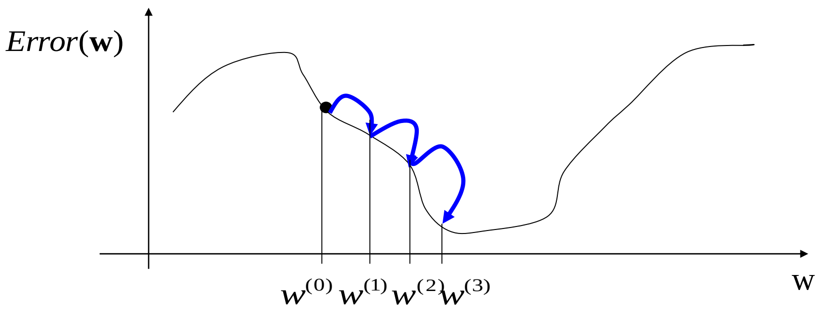
- Change the value of **w** according to the gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} Error_i(\mathbf{w})$$

$\alpha > 0$ a learning rate (scales the gradient changes)

Gradient descent method

- Iteratively approaches the optimum of the Error function



Batch vs online gradient algorithm

- The error function defined on the complete dataset *D*

$$J_n = Error(\mathbf{w}) = \frac{1}{n}\sum_{i=1,..n}(y_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

- We say we are learning the model in **the batch mode**:
  - All examples are available at the time of learning
  - Weights are optimizes with respect to all training examples

- An alternative is to learn the model in **the online mode**
  - Examples are arriving sequentially
  - Model weights are updated after every example
  - If needed examples seen can be forgotten

-

Online gradient algorithm

- **The error function** for the complete dataset *D*

$$J_n = Error(\mathbf{w}, D) = \frac{1}{n}\sum_{i=1,..n}(y_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

- **Error for one example** $D_i = < \mathbf{x}_i, y_i >$

$$J_{\text{online}} = Error_i(\mathbf{w}, \mathbf{x}_i) = \frac{1}{2}(y_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

- **Online gradient method: changes weights after every example**

$$w_j \leftarrow w_j - \alpha \frac{\partial}{\partial w_j} Error_i(\mathbf{w})$$

- **vector form:**

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} Error_i(\mathbf{w})$$

$\alpha > 0$ - Learning rate that depends on the number of updates

Online gradient method

Linear model $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$

On-line error $J_{online} = Error_i(\mathbf{w}) = \frac{1}{2}(y_i - f(\mathbf{x}_i, \mathbf{w}))^2$

On-line algorithm: generates a sequence of online updates

(i)-th update step with : $D_i =< \mathbf{x}_i, y_i >$

j-th weight:

$$w_j^{(i)} \leftarrow w_j^{(i-1)} - \alpha(i) \frac{\partial Error_i(\mathbf{w})}{\partial w_j} |_{\mathbf{w}^{(i-1)}}$$

$$\boxed{w_j^{(i)} \leftarrow w_j^{(i-1)} + \alpha(i)(y_i - f(\mathbf{x}_i, \mathbf{w}^{(i-1)}))x_{i,j}}$$

Fixed learning rate: $\alpha(i) = C$
- Use a small constant

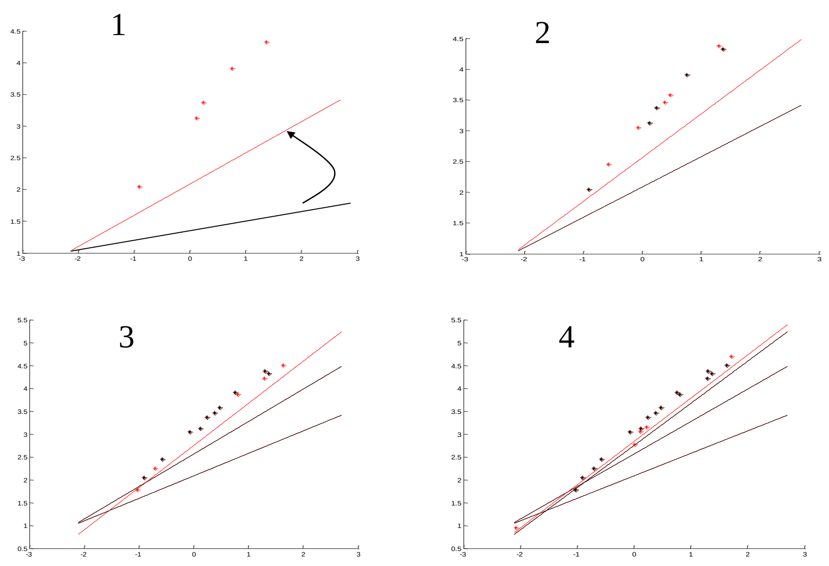
Annealed learning rate: $\alpha(i) \approx \frac{1}{i}$
- Gradually rescales changes

Online regression algorithm

```
Online-linear-regression (stopping_criterion)
   Initialize weights  $\mathbf{w} = (w_0, w_1, w_2 \ldots w_d)$
   initialize i=1;
   while stopping_criterion = FALSE
       select the next data point  $D_i = (\mathbf{x}_i, y_i)$
       set learning rate  $\alpha(i)$
       update weight vector  $\mathbf{w} \leftarrow \mathbf{w} + \alpha(i)(y_i - f(\mathbf{x}_i, \mathbf{w}))\mathbf{x}_i$
   end
return weights
```

Advantages: very easy to implement, works on continuous data streams

On-line learning. Example

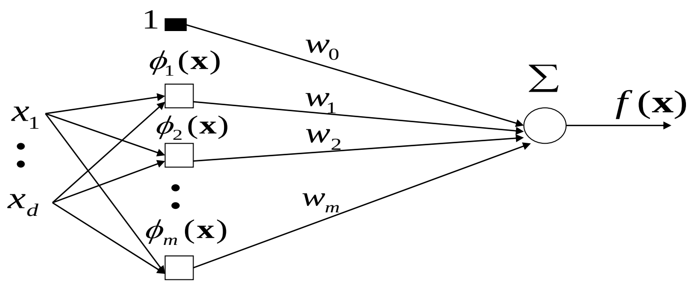


Extensions of simple linear model

Replace inputs to linear units with *m* **feature (basis) functions** to model **nonlinearities**

$$f(\mathbf{x}) = w_0 + \sum_{j=1}^{m} w_j \phi_j(\mathbf{x})$$

$\phi_j(\mathbf{x})$ - an arbitrary function of $\mathbf{x}$



Original input ⇨ **New input** ⇨ **Linear model**

Extensions of simple linear model

- **Models linear in the parameters we want to fit**

$$f(\mathbf{x}) = w_0 + \sum_{k=1}^{m} w_k \phi_k(\mathbf{x})$$

$w_0, w_1 \ldots w_m$ - parameters

$\phi_1(\mathbf{x}), \phi_2(\mathbf{x}) \ldots \phi_m(\mathbf{x})$ - **feature or basis functions**

- **Basis functions examples:**
  - **a higher order polynomial, one-dimensional input** $\mathbf{x} = (x_1)$

$\phi_1(x) = x \quad \phi_2(x) = x^2 \quad \phi_3(x) = x^3$

Extensions of simple linear model

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$$f(\mathbf{x}) = w_0 + \sum_{k=1}^{m} w_k \phi_k(\mathbf{x})$$

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- **Basis functions examples:**
  - a higher order polynomial, one-dimensional input $\mathbf{x} = (x_1)$

$\phi_1(x) = x \quad \phi_2(x) = x^2 \quad \phi_3(x) = x^3$

  - **Multidimensional quadratic** $\mathbf{x} = (x_1, x_2)$

$\phi_1(\mathbf{x}) = x_1 \quad \phi_2(\mathbf{x}) = x_1^2 \quad \phi_3(\mathbf{x}) = x_2 \quad \phi_4(\mathbf{x}) = x_2^2 \quad \phi_5(\mathbf{x}) = x_1 x_2$

Extensions of simple linear model

- **Models linear in the parameters we want to fit**

$$f(\mathbf{x}) = w_0 + \sum_{k=1}^{m} w_k \phi_k(\mathbf{x})$$

$w_0, w_1 \ldots w_m$ - parameters

$\phi_1(\mathbf{x}), \phi_2(\mathbf{x}) \ldots \phi_m(\mathbf{x})$ - **feature or basis functions**

- **Basis functions examples:**
  - a higher order polynomial, one-dimensional input $\mathbf{x} = (x_1)$

    $\phi_1(x) = x \quad \phi_2(x) = x^2 \quad \phi_3(x) = x^3$
  - Multidimensional quadratic $\mathbf{x} = (x_1, x_2)$

    $\phi_1(\mathbf{x}) = x_1 \quad \phi_2(\mathbf{x}) = x_1^2 \quad \phi_3(\mathbf{x}) = x_2 \quad \phi_4(\mathbf{x}) = x_2^2 \quad \phi_5(\mathbf{x}) = x_1 x_2$
  - **Other types of basis functions**

    $\phi_1(x) = \sin x \quad \phi_2(x) = \cos x$

Extensions of simple linear model

The same techniques as for the linear model to learn the weights

- **Error function** $J_n = 1/n \sum_{i=1,..n} (y - f(\mathbf{x}_i, \mathbf{w}))^2$

Assume: $\boldsymbol{\varphi}(\mathbf{x}_i) = (1, \phi_1(\mathbf{x}_i), \phi_2(\mathbf{x}_i), \ldots, \phi_m(\mathbf{x}_i))$

$$\nabla_{\mathbf{w}} J_n(\mathbf{w}) = -\frac{2}{n} \sum_{i=1,..n} (y_i - f(\mathbf{x}_i)) \boldsymbol{\varphi}(\mathbf{x}_i) = \bar{\mathbf{0}}$$

- Leads to a **system of *m* linear equations**

$$w_0 \sum_{i=1}^{n} 1 \phi_j(\mathbf{x}_i) + \ldots + w_j \sum_{i=1}^{n} \phi_j(\mathbf{x}_i) \phi_j(\mathbf{x}_i) + \ldots + w_m \sum_{i=1}^{n} \phi_m(\mathbf{x}_i) \phi_j(\mathbf{x}_i) = \sum_{i=1}^{n} y_i \phi_j(\mathbf{x}_i)$$

- Can be solved exactly like the linear case

Example. Regression with polynomials.

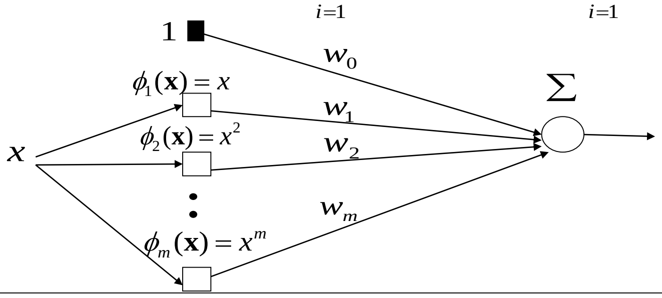
Regression with polynomials of degree m

- **Data instances:** pairs of $< x, y >$
- **Feature functions:** m feature functions

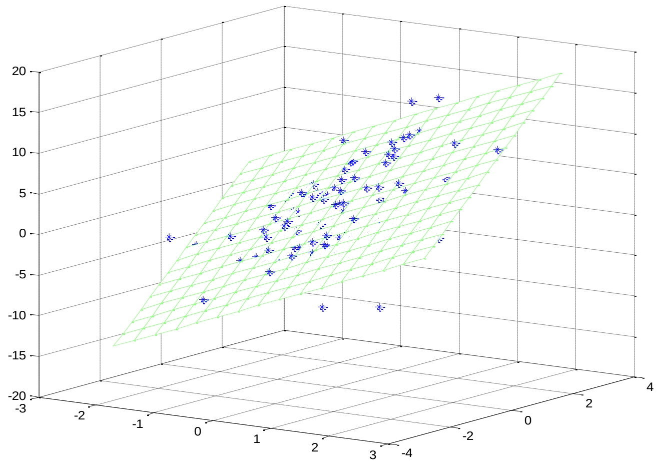
$$\phi_i(x) = x^i \qquad i = 1, 2, \ldots, m$$

- **Function to learn:**

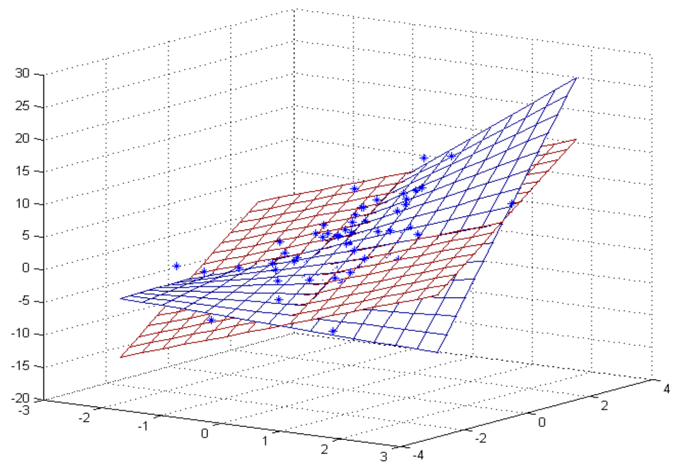
$$f(x, \mathbf{w}) = w_0 + \sum_{i=1}^{m} w_i \phi_i(x) = w_0 + \sum_{i=1}^{m} w_i x^i$$



Linear model example

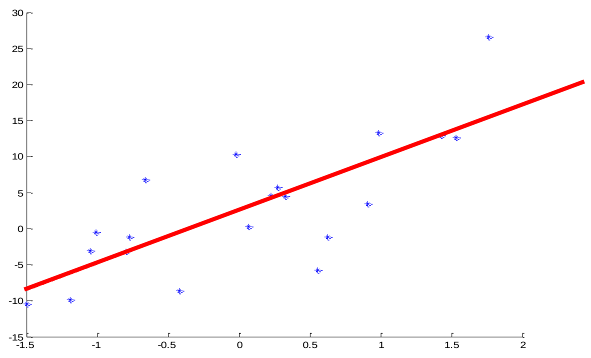


Non-linear (quadratic) model



Linear regression model

- **Linear model:** $y = f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x}$



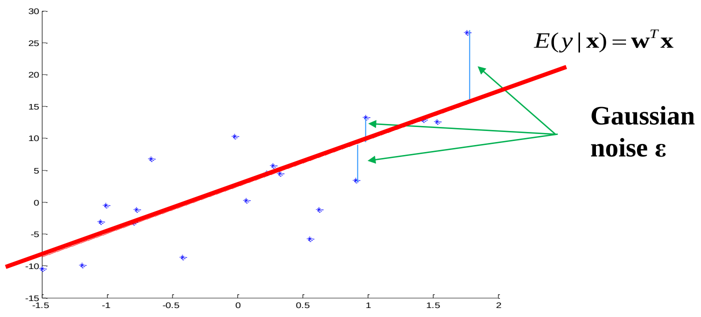
- **Notice: the above model does not try to explain variation in observed** y**s for the data**

Statistical model of regression

A statistical model of linear regression:

$$y = \mathbf{w}^T\mathbf{x} + \varepsilon \qquad \varepsilon \sim \mathrm{N}(0,\sigma^2)$$

ε is a random noise, represents things we cannot capture with $\mathbf{w}^T\mathbf{x}$



$$y \sim N(\mathbf{w}^T\mathbf{x}, \sigma^2)$$

Statistical model of regression

A statistical model of linear regression:

$$y = \mathbf{w}^T\mathbf{x} + \varepsilon \qquad \varepsilon \sim \mathrm{N}(0,\sigma^2)$$

$$y \sim N(\mathbf{w}^T\mathbf{x}, \sigma^2)$$

- **The conditional distribution of y given x**

$$p(y \mid \mathbf{x}, \mathbf{w}, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^2}(y - \mathbf{w}^T\mathbf{x})^2\right]$$

$$E(y \mid \mathbf{x}) = \mathbf{w}^T\mathbf{x}$$

ML estimation of the parameters

- **likelihood of predictions** = the probability of observing outputs y in D given $\mathbf{w}, \sigma$

$$L(D, \mathbf{w}, \sigma) = \prod_{i=1}^{n} p(y_i \mid \mathbf{x}_i, \mathbf{w}, \sigma)$$

- **Maximum likelihood estimation of parameters** w
  - parameters maximizing the likelihood of predictions

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \prod_{i=1}^{n} p(y_i \mid \mathbf{x}_i, \mathbf{w}, \sigma)$$

- **Log-likelihood** trick for the ML optimization
  - Maximizing the log-likelihood is equivalent to maximizing the likelihood

$$l(D, \mathbf{w}, \sigma) = \log(L(D, \mathbf{w}, \sigma)) = \log \prod_{i=1}^{n} p(y_i \mid \mathbf{x}_i, \mathbf{w}, \sigma)$$

ML estimation of the parameters

- **Using conditional density**

$$p(y \mid \mathbf{x}, \mathbf{w}, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp[-\frac{1}{2\sigma^2}(y - f(\mathbf{x}, \mathbf{w}))^2]$$

- **We can rewrite the log-likelihood as**

$$l(D, \mathbf{w}, \sigma) = \log(L(D, \mathbf{w}, \sigma)) = \log \prod_{i=1}^{n} p(y_i \mid \mathbf{x}_i, \mathbf{w}, \sigma)$$

$$= \sum_{i=1}^{n} \log p(y_i \mid \mathbf{x}_i, \mathbf{w}, \sigma) = \sum_{i=1}^{n} \left[-\frac{1}{2\sigma^2}(y_i - \mathbf{w}^T \mathbf{x}_i)^2 - c(\sigma) \right]$$

$$\boxed{= -\frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \mathbf{w}^T \mathbf{x}_i)^2} + C(\sigma)$$

Did we see a similar expression before?

ML estimation of the parameters

- **Using conditional density**

$$p(y \mid \mathbf{x},\mathbf{w},\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp[-\frac{1}{2\sigma^2}(y - f(\mathbf{x},\mathbf{w}))^2]$$

- **We can rewrite the log-likelihood as**

$$l(D,\mathbf{w},\sigma) = \log(L(D,\mathbf{w},\sigma)) = \log \prod_{i=1}^{n} p(y_i \mid \mathbf{x}_i,\mathbf{w},\sigma)$$

$$= \sum_{i=1}^{n} \log p(y_i \mid \mathbf{x}_i,\mathbf{w},\sigma) = \sum_{i=1}^{n} \left\{ -\frac{1}{2\sigma^2}(y_i - \mathbf{w}^T\mathbf{x}_i)^2 - c(\sigma) \right\}$$

$$\boxed{= -\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2} + C(\sigma)$$

- **Maximizing the predictive log likelihood** with regard to **w**, is **equivalent to minimizing the mean squared error function**

ML estimation of parameters

- **Criteria based on the mean squares error function and the log likelihood of the output are related**

$$J_{online}(y_i,\mathbf{x}_i) = \frac{1}{2\sigma^2} \log p(y_i \mid \mathbf{x}_i,\mathbf{w},\sigma) + c(\sigma)$$

- **We know how to optimize parameters *w***
  – the same approach as used for the least squares fit
- **But what is the ML estimate of the variance of the noise?**
- Maximize $l(D,\mathbf{w},\sigma)$ with respect to variance

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(\mathbf{x}_i,\mathbf{w}^*))^2$$

= **mean square prediction error for the best predictor**

Regularized linear regression

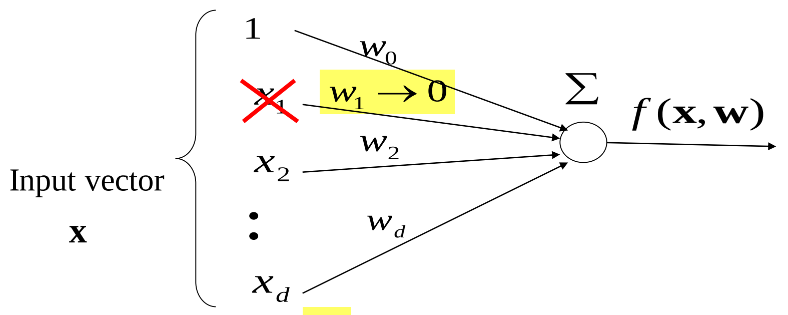
- If the number of parameters is large relative to the number of data points used to train the model, we face the threat of overfitting (generalization error of the model goes up)
- The prediction accuracy can be often improved by setting some coefficients to zero
  - Increases the bias, reduces the variance of estimates
- **Solutions:**
  - **Subset selection**
  - **Ridge regression**
  - **Lasso regression**
  - **Principal component regression**

Regularization: motivation

- If the model is too complex and can cause overfitting, its prediction accuracy can be improved by **removing some inputs from the model = setting their coefficients to zero**

$$f(\mathbf{x}) = w_0x_0 + w_1x_1 + w_2x_2 + w_3x_3 + \ldots w_dx_d = \mathbf{w}^T\mathbf{x}$$

$w_0, w_1, \ldots w_k$ **- parameters (weights)**



$$f(\mathbf{x}) = w_0x_0 + 0x_1 + w_2x_2 + w_3x_3 + \ldots w_dx_d = \mathbf{w}^T\mathbf{x}$$

Ridge regression

Question: how to force the weights to 0 ?

- Error function for the standard least squares estimates:

$$J_n(\mathbf{w}) = \boxed{\frac{1}{n}\sum_{i=1,..n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2}$$

- **We seek:** $\mathbf{w}^* = \arg\min_{\mathbf{w}} \frac{1}{n}\sum_{i=1,..n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2$

- **Ridge regression:**

$$J_n(\mathbf{w}) = \underbrace{\boxed{\frac{1}{n}\sum_{i=1,..n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2}}_{\textbf{Fit to data}} + \underbrace{\boxed{\lambda\|\mathbf{w}\|_{L2}^{\ 2}}}_{\textbf{Model complexity penalty}}$$

- Where $\|\mathbf{w}\|_{L2}^{\ 2} = \sum_{i=0}^{d} w_i^2$ and $\lambda \geq 0$

- What does the new error function do?

Ridge regression

Ridge regression:

$$J_n(\mathbf{w}) = \frac{1}{n}\sum_{i=1,..n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2 + \lambda\|\mathbf{w}\|_{L2}^2$$

Term $\|\mathbf{w}\|_{L2}^2 = \sum_{i=0}^{d} w_i^2$

- penalizes non-zero weights with the cost that is proportional to λ (a **shrinkage coefficient**)
- If an input attribute x_j has a small effect on improving the error function it is "shut down" by the penalty term
- Inclusion of a shrinkage penalty is often referred to as **regularization.**

  (ridge regression is related to Tikhonov regularization**)**

Regularized linear regression

How to solve the least squares problem if the error function is enriched by the regularization term $\lambda\|\mathbf{w}\|^2$?

Answer: The solution to the optimal set of weights w is obtained again by solving a set of linear equation.

Standard linear regression:

$$\nabla_{\mathbf{w}}(J_n(\mathbf{w})) = -\frac{2}{n}\sum_{i=1}^{n}(y_i - \mathbf{w}^T\mathbf{x}_i)\mathbf{x}_i = \bar{\mathbf{0}}$$

Solution: $\mathbf{w}^* = (\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{y}$

where **X** is an *nxd* matrix with rows corresponding to examples and columns to inputs

Regularized linear regression:

$$\mathbf{w}^* = (\lambda\mathbf{I} + \mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{y}$$

Lasso regression

- **Standard regression:**

$$J_n(\mathbf{w}) = \frac{1}{n}\sum_{i=1,..n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2$$

- **Lasso regression/regularization:**

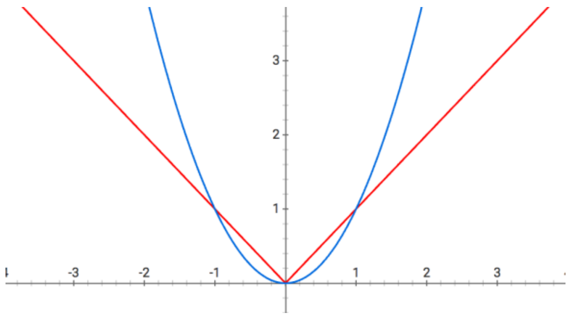
$$J_n(\mathbf{w}) = \underbrace{\boxed{\frac{1}{n}\sum_{i=1,..n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2}}_{\textbf{Fit to data}} + \underbrace{\boxed{\lambda\|\mathbf{w}\|_{L1}}}_{\textbf{Model complexity penalty}}$$

$$\|\mathbf{w}\|_{L1} = \sum_{i=0}^{d}|w_i| \qquad \text{and} \qquad \lambda \geq 0$$

- L1 is more aggressive pushing the weights to 0 compared to L2

Lasso vs Ridge penalty

- Lasso (L1) penalty $\|\mathbf{w}\|_{L1} = \sum_{i=0}^{d} | w_i |$
- Ridge (L2) penalty $\|\mathbf{w}\|_{L2}^2 = \sum_{i=0}^{d} w_i^2$



- L1 is more aggressive pushing the weights to 0 compared to L2