Linear Modeling and Regression

Morteza H. Chehreghani
morteza.chehreghani@chalmers.se

Department of Computer Science and Engineering
Chalmers University of Technology

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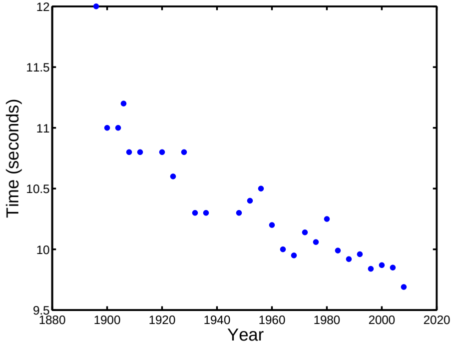
Reference

The content and the slides are adapted from

S. Rogers and M. Girolami, A First Course in Machine Learning (FCML), 2nd edition, Chapman & Hall/CRC 2016, ISBN: 9781498738484

Some data and a problem



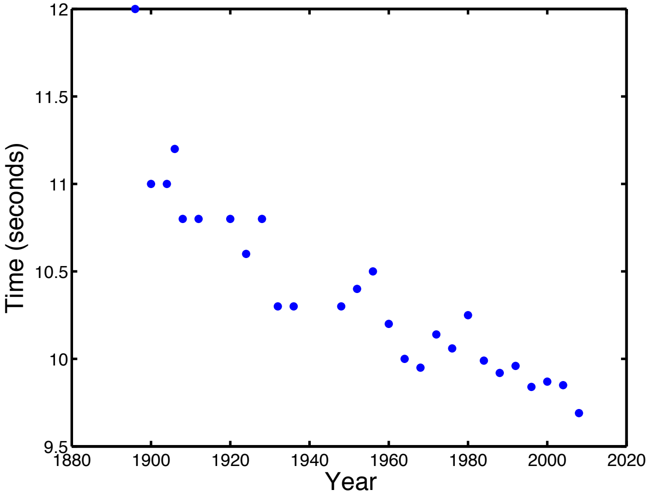
Winning times for the men's Olympic 100m sprint, 1896-2008.

In this lecture, we will use this data to predict the winning time in London 2012

Reading: Section 1.1 of FCML

Back of envelope calculation

Draw a line through it!



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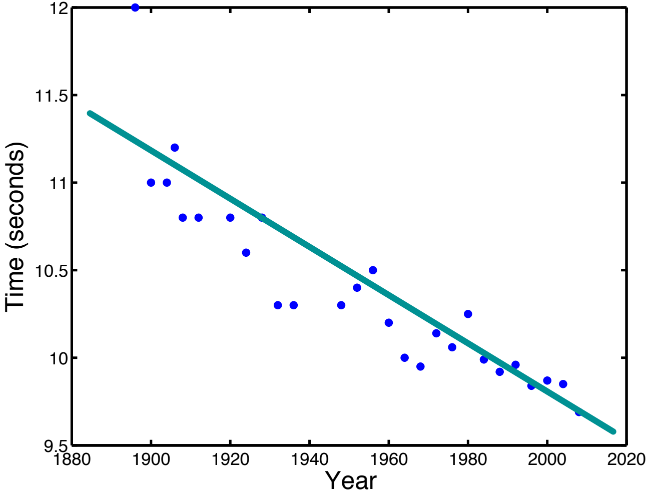

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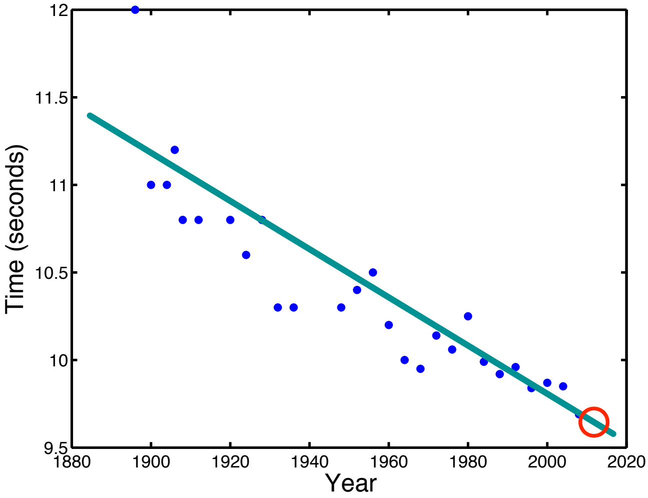

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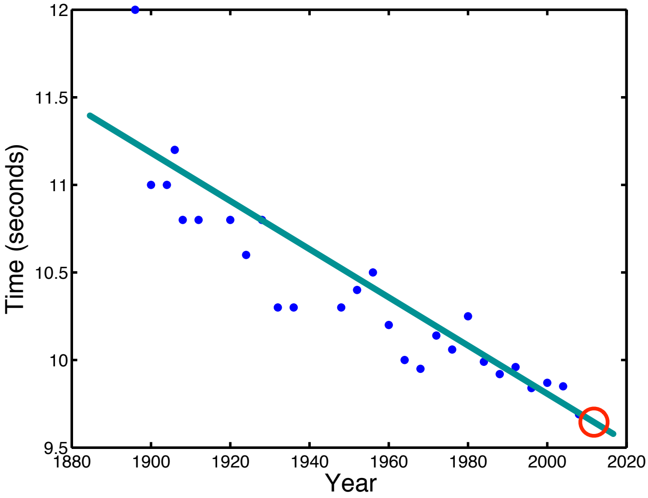

Our aim is to formalise this process.

What did we do?

Basically:

- **Decided to draw a line through our data.**
- Chose a straight line.
- Drew a good straight line.
- Extended the line to 2012.
- Read off the winning time for 2012.

Technically

- Decided we needed a model.
- Chose a linear model.
- Fitted a linear model.
- Evaluated the model at 2012.
- Used this as our prediction.

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3. That this relationship will continue into the future.

Are they any good?

Definitions

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- Olympic year: x.

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- Olympic year: x.
- Winning time: t.

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Our goal is to create a model.

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Data

We're going to create the model from data:

- N attribute-target pairs, (x_n, t_n)
- e.g. $(1896, 12s), (1900, 11s), \ldots, (2008, 9.69s)$
- $x_1 = 1896,\ t_1 = 12$, etc.

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Often called **training** data

A linear model

$$t = f(x)$$

A linear model

$$t = f(x) = w_0 + w_1 x$$

model parameters

A linear model

$$t = f(x) = w_0 + w_1 x = f(x; w_0, w_1)$$

- w_0 and w_1 are *parameters* of the model.

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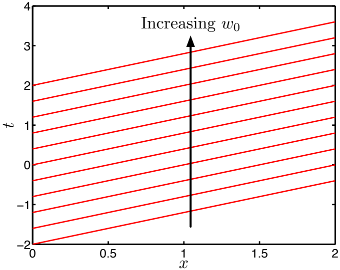

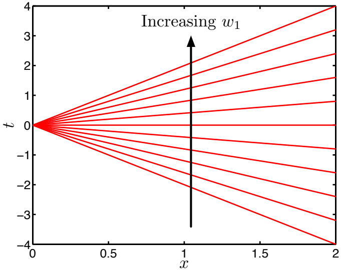

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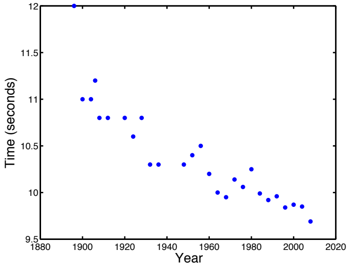
We have data and a family of models:



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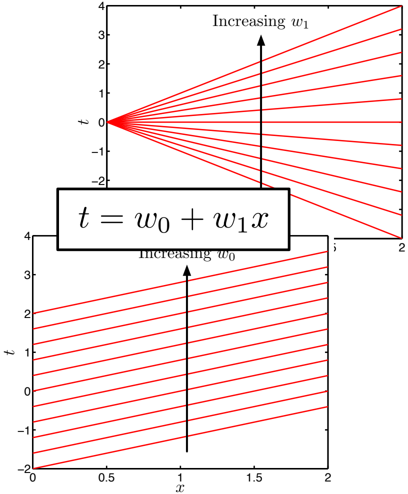

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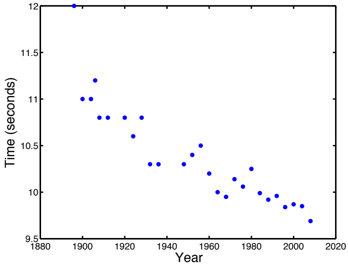

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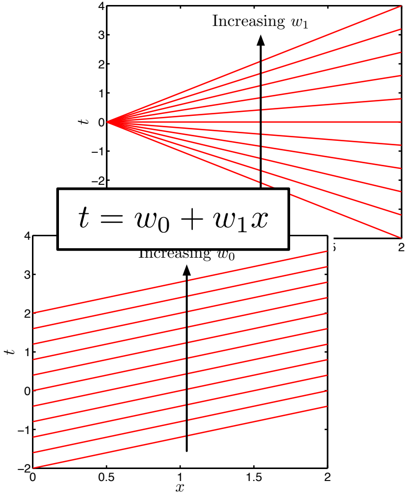

Need to find w_0, w_1 from $(x_1, t_1), (x_2, t_2), \ldots, (x_N, t_N)$

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- How good is a particular line (w_0, w_1)?
- We need to be able to provide a numerical value of goodness for any w_0, w_1.
  - How good is $w_0 = 5, w_1 = 0.1$?
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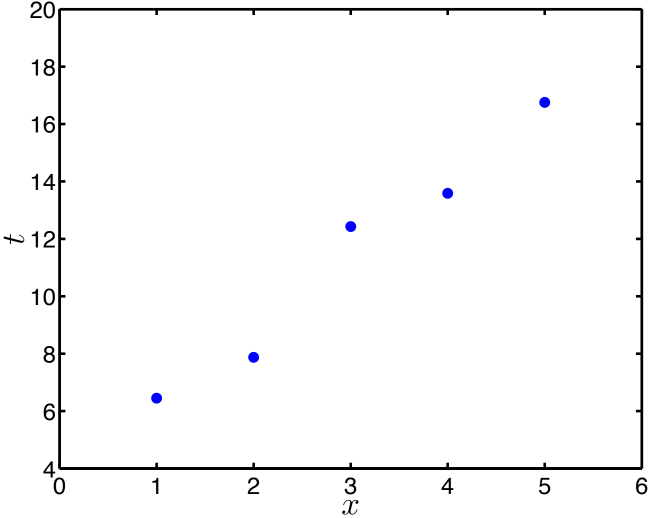
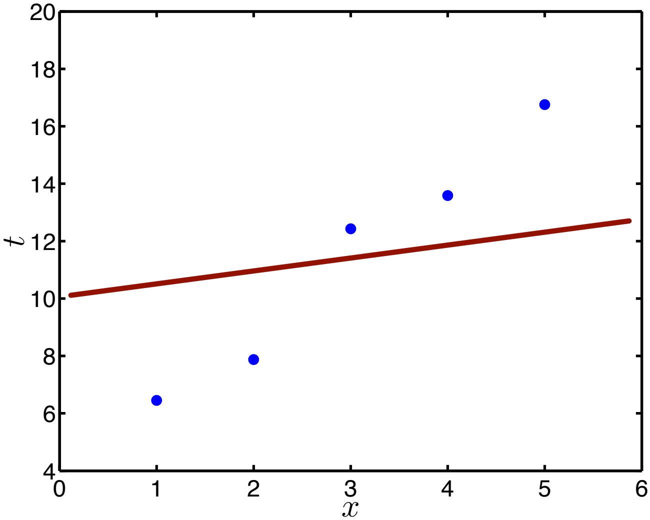
- Once we can answer these questions, we can search for the best w_0, w_1 pair.

Loss



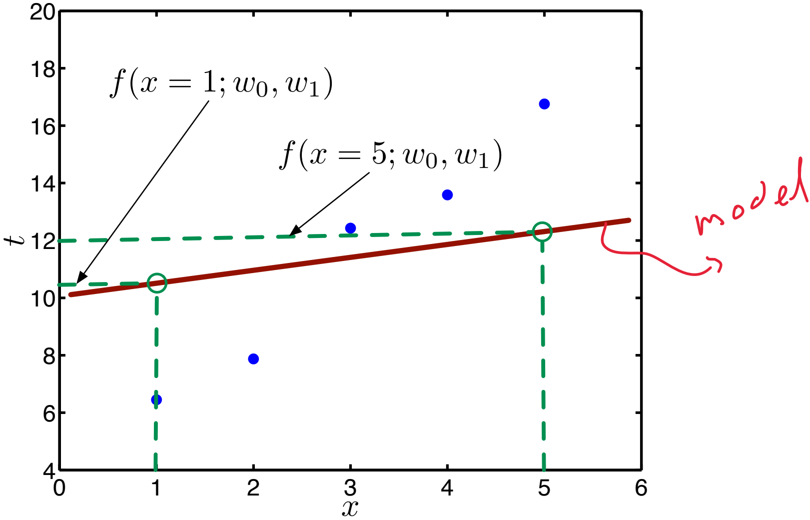
Some different data.

Loss



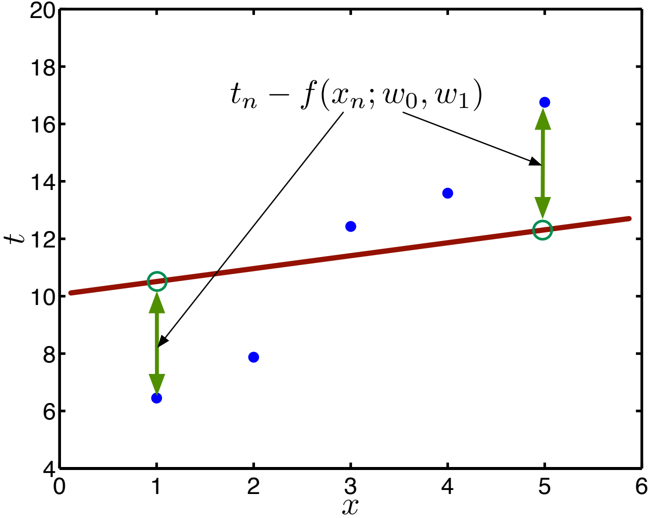
Given w_0 and w_1 you can draw a line.

Loss



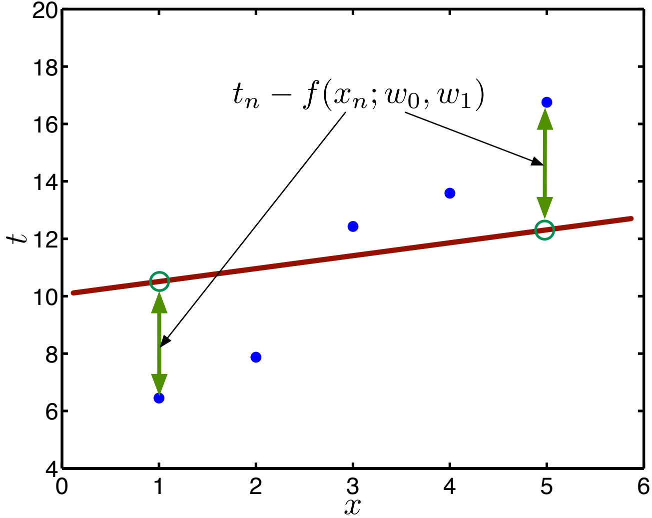
This means that we can compute $f(x_n; w_0, w_1)$ for each x_n.

Loss



$f(x_n; w_0, w_1)$ can be compared with the truth, t_n.

Loss



actual value

$f(x_n; w_0, w_1)$ can be compared with the truth, t_n.

$(t_n - \underbrace{f(x_n; w_0, w_1)}))^2$ tells us how *badly* we model (x_n, t_n).

→ model value

Squared loss

- The *Squared loss* of the n-th training point is defined as:

$$\mathcal{L}_n = (t_n - f(x_n; w_0; w_1))^2$$

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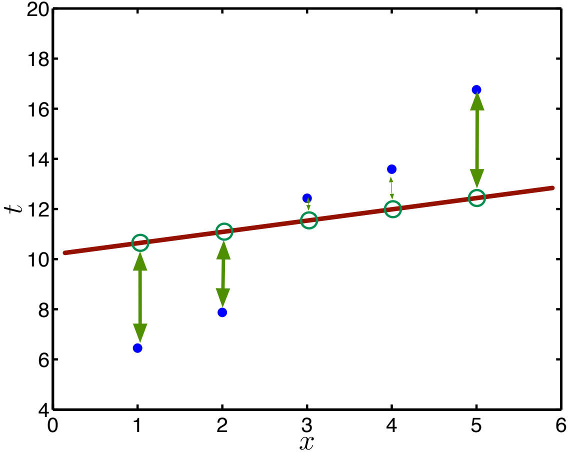
- The lower $\mathcal{L}_n$, the closer the line at x_n passes to t_n.

Total squared loss



Average the loss at each training point to give single figure for all data:

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2$$

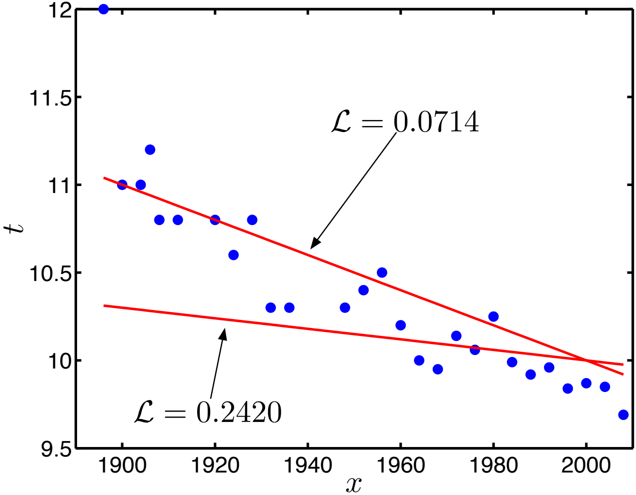
loss func.

- The average loss:

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - \underbrace{f(x_n; w_0, w_1)}_{w_0 + w_1 n})^2$$

- $\mathcal{L}$ tells us how good the model is as a function of w_0 and w_1.
  - Remember that lower is better!
  - How good is $w_0 = 5, w_1 = 0.1$?
  - How good is $w_0 = 6, w_1 = -0.2$?
  - Which is better?

Example



$\mathcal{L} = 0.0714$
$\mathcal{L} = 0.2420$
12
11.5
11
10.5
10
9.5
1900
1920
1940
1960
1980
2000
t
x

An optimisation problem

- We've derived an expression for how good the model is for any w_0 and w_1.

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2$$

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- Could use trial and error to find a good w_0, w_1 combination.
- Can we get a mathematical expression?

$$\underset{w_0,w_1}{\operatorname{argmin}} \ \mathcal{L} \quad = \quad \underset{w_0,w_1}{\operatorname{argmin}} \ \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2$$

Aside - finding maxima and minima

Say we want to find

$$\underset{z}{\operatorname{argmin}}\ f(z),\ \ f(z) = 2z^2 - 12z + 15.$$

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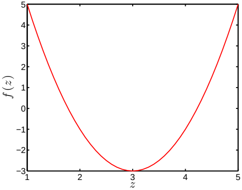

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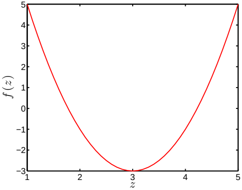

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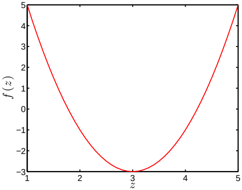

At a minimum (or a maximum), the gradient must be zero.

The gradient is given by the first derivative of the function:

$$\frac{df(z)}{dz} = 4z - 12$$

Setting to zero and solving for z

$$4z - 12 = 0,\ \ z = 12/4 = 3$$

Finding maxima and minima

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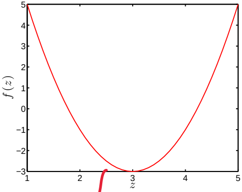
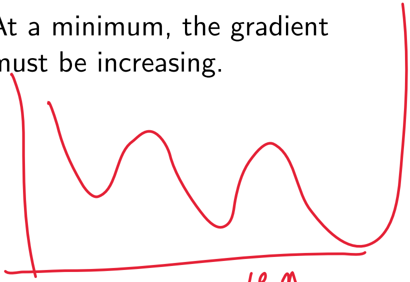


convex

At a minimum, the gradient must be increasing.



non convex

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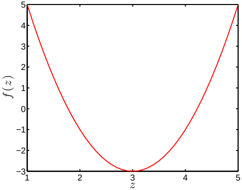

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Taking the second derivative:

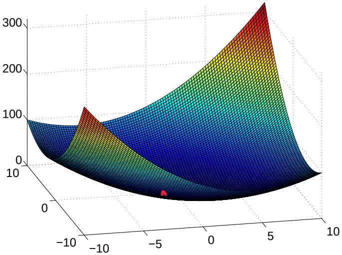
$$\frac{df(z)}{dz} = 4z - 12$$
$$\frac{d^2z}{dz^2} = 4$$

The gradient is always increasing. Therefore, we have found a minimum and it is the only minumum.

Finding maxima and minima

What about functions of more than one parameter?

$$\underset{y,z}{\operatorname{argmin}}\ f(y,z),\ \ f(y,z) = y^2 + z^2 + y + z + yz$$



We now use *partial derivatives*, $\frac{\partial f}{\partial z}$ and $\frac{\partial f}{\partial y}$

When calculating the partial derivative with respect to y we assume everything else (including z) is a constant.

$$\frac{\partial f}{\partial y} = 2y + 1 + z, \quad \frac{\partial f}{\partial z} = 2z + 1 + y$$

$$\frac{\partial f}{\partial y} = 2y + 1 + z = 0, \quad \frac{\partial f}{\partial z} = 2z + 1 + y = 0$$

To find a potential minimum, set both to zero and solve for y and z:

$$\begin{aligned} y &= -\frac{1}{3} \\ z &= -\frac{1}{3}. \end{aligned}$$

To make sure its a minimum, check second derivatives:

$$\frac{\partial^2 f}{\partial y^2} = 2, \quad \frac{\partial^2 f}{\partial z^2} = 2.$$

Both are positive so we have a minimum.

Back to our function

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2.$$

Now, recall that:

$$f(x_n; w_0, w_1) = w_0 + w_1 x$$

So:

$$\underset{w_0, w_1}{\operatorname{argmin}}\ \mathcal{L} = \underset{w_0, w_1}{\operatorname{argmin}}\ \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2$$

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We need to find $\frac{\partial \mathcal{L}}{\partial w_0}$ and $\frac{\partial \mathcal{L}}{\partial w_1}$, and use thoese to find the *best* values!

Differentiating the loss

- Taking partial derivatives with respect to w_0 and w_1:

$$
\begin{aligned}
\mathcal{L} &= \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2 \\
\frac{\partial \mathcal{L}}{\partial w_0} &= -\frac{2}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n) \\
\frac{\partial \mathcal{L}}{\partial w_1} &= -\frac{2}{N}\sum_{n=1}^{N}x_n(t_n - w_0 - w_1 x_n)
\end{aligned}
$$

Finding w_0:

$$\frac{\partial \mathcal{L}}{\partial w_0} = -\frac{2}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)$$

$$0 = -\frac{2}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)$$

$$w_0 \underbrace{\frac{1}{N}\sum_{n=1}^{N} 1}_{=1} = \qquad \frac{\cancel{2}}{N}\sum_{n=1}^{N} w_0 = \frac{\cancel{2}}{N}\sum_{n=1}^{N} t_n - \frac{\cancel{2}}{N}\sum_{n=1}^{N} w_1 x_n \qquad \frac{1}{N} w_1 \sum_{n=1}^{N} x_n$$

$$w_0 = \bar{t} - w_1 \bar{x}$$

Where

$$\bar{t} = \frac{1}{N}\sum_{n=1}^{N} t_n, \quad \bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

Finding w_1:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_1} &= -\frac{2}{N}\sum_{n=1}^{N} x_n(t_n - w_0 - w_1 x_n) \\
0 &= -\frac{2}{N}\sum_{n=1}^{N} x_n(t_n - w_0 - w_1 x_n) \\
w_1 \frac{1}{N}\sum_{n=1}^{N} x_n^2 &= \frac{1}{N}\sum_{n=1}^{N} x_n t_n - w_0 \frac{1}{N}\sum_{n=1}^{N} x_n \\
w_1 \overline{x^2} &= \overline{xt} - w_0 \overline{x}
\end{aligned}
$$

Where

$$
\overline{x^2} = \frac{1}{N}\sum_{n=1}^{N} x_n^2, \quad \overline{xt} = \frac{1}{N}\sum_{n=1}^{N} x_n t_n
$$

Substituting:

Substituting our expression for w_0 into that for w_1:

$$
\begin{aligned}
w_0 &= \bar{t} - w_1\bar{x} \\
w_1\overline{x^2} &= \overline{xt} - w_0\bar{x} \\
w_1\overline{x^2} &= \overline{xt} - \bar{x}(\bar{t} - w_1\bar{x}) \\
w_1 &= \frac{\overline{xt} - \bar{x}\bar{t}}{\overline{x^2} - (\bar{x})^2}
\end{aligned}
$$

$\bar{t} - w_0\bar{x}$

So, to summarise:

$$
w_1 = \frac{\overline{xt} - \bar{x}\bar{t}}{\overline{x^2} - (\bar{x})^2}, \quad w_0 = \bar{t} - w_1\bar{x}
$$

Note that $\overline{xt} \neq \bar{x}\bar{t}$ and $\overline{x^2} \neq (\bar{x})^2$.

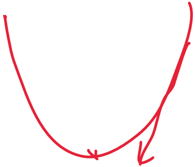
Gradient Descent: an alternative approach

numerical optimization

Repeatedly move in the direction of the gradient using *step size* η:

$$w_0 \leftarrow w_0 - \eta \frac{\partial \mathcal{L}}{\partial w_0}$$

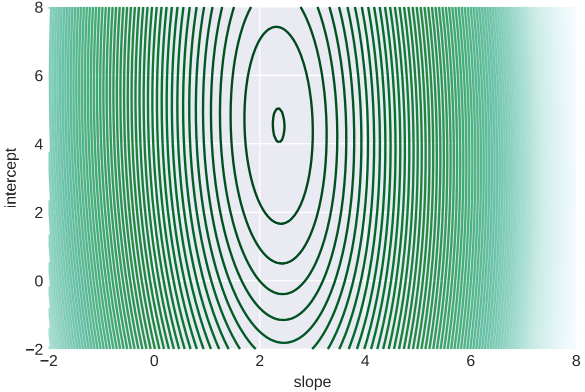
$$w_1 \leftarrow w_1 - \eta \frac{\partial \mathcal{L}}{\partial w_1}$$



For *convex* functions, this is guaranteed to *converge* to the *global optimum*.

There are many *accelerated* variations to speed up convergence.

Searching for the best parameters

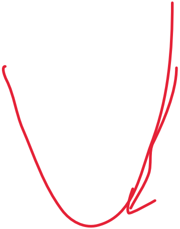


“Climbing down” formally: gradient descent

1. define a “learning rate” η
2. initialize the parameters w_0, w_1 (slope and intercept)
3. compute the gradients (steepest direction)
4. update the parameters as

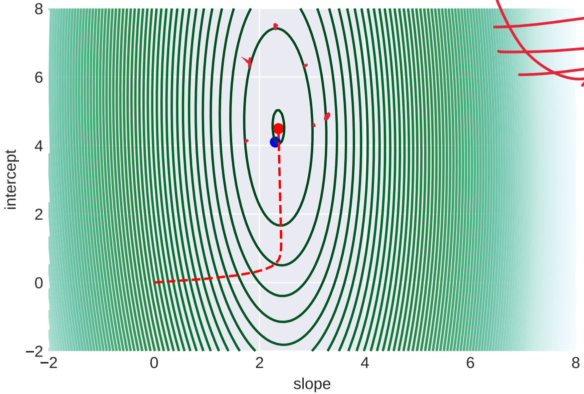
$$w_0 \leftarrow w_0 - \eta \frac{\partial \mathcal{L}}{\partial w_0}$$

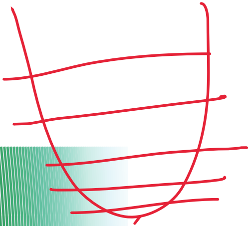
$$w_1 \leftarrow w_1 - \eta \frac{\partial \mathcal{L}}{\partial w_1}$$



5. is the gradient close to zero? if no, go back to 3

gradient descent example





w_0

w_1

Olympic data

n	x_n	t_n	$x_n t_n$	x_n^2
1	1896	12.00	22752.0	3.5948e+06
2	1900	11.00	20900.0	3.6100e+06
3	1904	11.00	20944.0	3.6252e+06
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
26	2004	9.85	19739.4	4.0160e+06
27	2008	9.69	19457.5	4.0321e+06
$(1/N)\sum_{n=1}^{N}$	1952.37	10.39	20268.1	3.8130e+06
	$\overline{x}$	$\overline{t}$	$\overline{xt}$	$\overline{x^2}$

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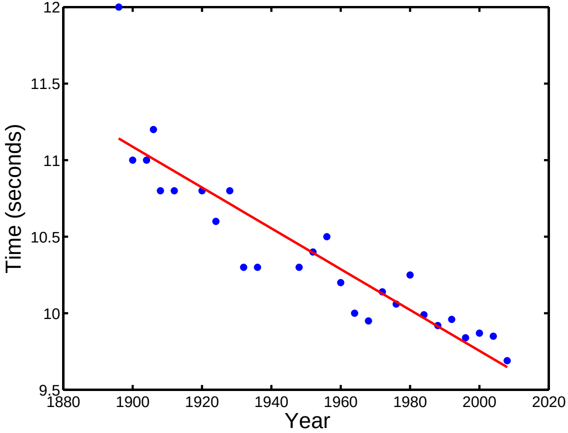
	$\overline{x}$	$\overline{t}$	$\overline{xt}$	$\overline{x^2}$

Substituting these values into our expressions gives:

$$w_1 = -0.0133, \ \ w_0 = 36.416$$

The model



$$t = 36.416 - 0.0133x \rightarrow 201$$

w_0 w_1

Our prediction

- We want to predict the winning time at London 2012.
- Substitute $x = 2012$ into our model.

$$\begin{aligned} t &= 36.416 - 0.0133x \\ t_{2012} &= 36.416 - 0.0133 \times 2012 \\ t_{2012} &= 9.5947\ s \end{aligned}$$

- Based on our modelling assumptions and the previous data, we predict a winning time of 9.5947 seconds.

Assumptions

Our Assumptions

1. **That there exists a relationship between Olympic year and winning time.**

Are they any good?

1. Is the relationship really between Olympic year and time?

Assumptions

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2. **That this relationship is linear (i.e. a straight line).**

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2. Seems a bit simple? Does the line go through all of the points?

Assumptions

Our Assumptions

1. That there exists a relationship between Olympic year and winning time.
2. That this relationship is linear (i.e. a straight line).
3. **This this relationship will continue into the future.**

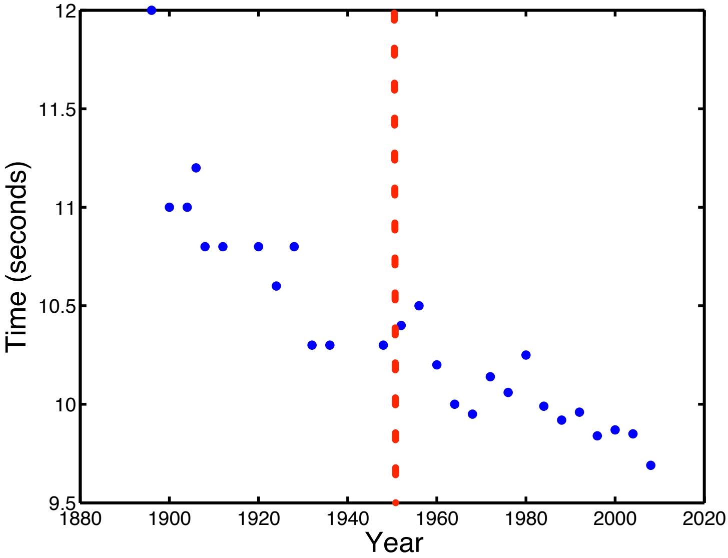
Are they any good?

1. Is the relationship really between Olympic year and time?
2. Seems a bit simple? Does the line go through all of the points?
3. Forever? Negative winning times?

Some things to think about

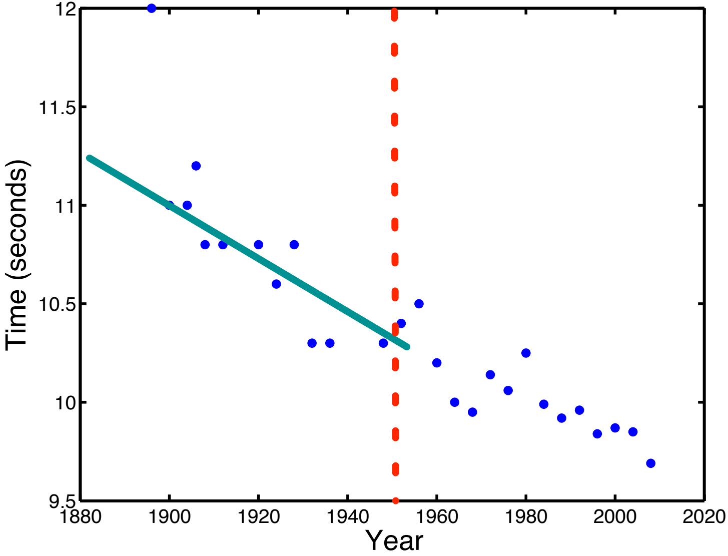
- Is this a good prediction?
- Would you go to the bookmakers and place a bet on the winning time being exactly 9.547 s?
- Are we asking the correct question? Being too precise?

A question we could have answered in 1950



Will the winning time be sub 10s in 2000?

A question we could have answered in 1950



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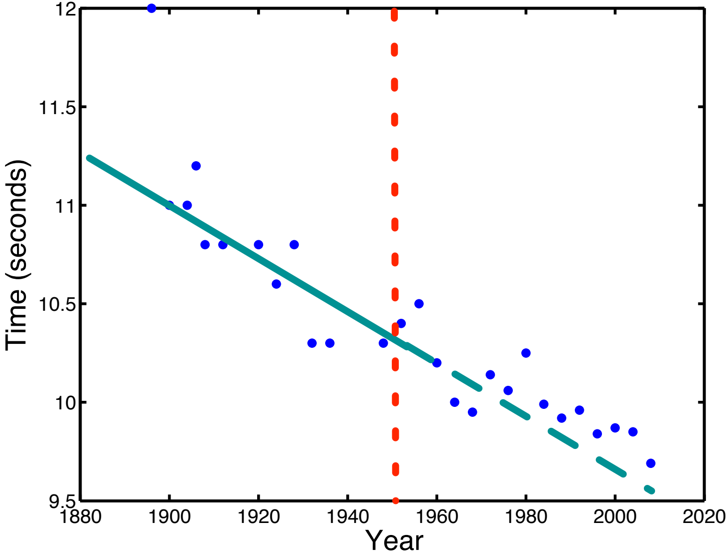

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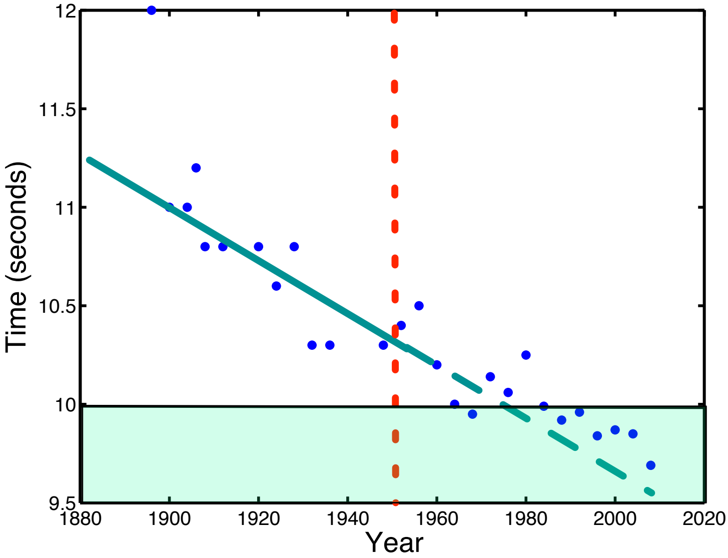

Will the winning time be sub 10s in 2000?

Regression in statistics and machine learning

- regression models are among the most widely used tools in statistics
- but regression is also an important problem in machine learning
- difference in emphasis:
  - in statistics, the purpose is often *explanation*: "how does x affect t?" "is x important for t?"
  - in machine learning, the purpose is typically *prediction*: "what's the most likely t, given x?"

Multivariate Data

- Olympic winning time may depend also on weather, track conditions etc.
- Each data point is thus represented by a *vector* of dimension D of *features* or *attributes*, $\mathbf{x}$.
- Our problem thus is to find a function $t = f(\mathbf{x})$.
- *Multi-linear* function:

$$t = f(x, w_0, w_1, \cdots, w_D) := w_0 + w_1 x_1 + \cdots + w_D x_D.$$

Squared loss

- The squared loss of the *n*-th training point is:

$$\mathcal{L}_n = (t_n - f(\mathbf{x}_n; w_0; w_1 \cdots, w_D))^2$$

- The *averaged squared loss* is:

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(\mathbf{x}_n; w_0, w_1, \cdots, w_D))^2$$

Squared loss

$x_n = \begin{bmatrix} 1 \\ x_{1,n} \\ x_{2,n} \\ \vdots \\ x_{D,n} \end{bmatrix}, \quad w = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix}$

- The *averaged squared loss* is:

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$w^T x_n = 1 \times w_0 + w_1 x_{1,n} + \ldots + w_D x_{D,n}$

- Then

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - \boxed{\mathbf{w}^\top \mathbf{x}_n})^2.$$

Note that: (we append 1 to the begining of $\mathbf{x}_n$)

$$\mathbf{x}_n \leftarrow [1 \quad \mathbf{x}_n]$$

- Therefore

$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^\top(\mathbf{t} - \mathbf{X}\mathbf{w})$$

Recipe

- Put data and parameters into vectors/matrix.
- Write the model in vector form.
- Write the loss in vector/matrix form.

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Why?

More features: $t = w_0 + w_1 x_1 + \cdots + w_D x_D$
More complex models: $t = w_0 + w_1 x + w_2 x^2 + \ldots + w_D x^D$

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$$\mathbf{x}_n = \begin{bmatrix} 1 \\ x_{n,1} \\ x_{n,2} \\ \vdots \\ x_{n,D} \end{bmatrix},$$

Recipe

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$\tilde{w}^T x_n = x_n^T w$

Xw

a vector of $N \times 1$

Why?

More features: $t = w_0 + w_1 x_1 + \cdots + w_D x_D$

More complex models: $t = w_0 + w_1 x + w_2 x^2 + \ldots + w_D x^D$

$$\mathbf{x}_n = \begin{bmatrix} 1 \\ x_{n,1} \\ x_{n,2} \\ \vdots \\ x_{n,D} \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \ldots & x_{1,D} \\ 1 & x_{2,1} & x_{2,2} & \ldots & x_{2,D} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N,1} & x_{N,2} & \ldots & x_{N,D} \end{bmatrix}, \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{bmatrix}$$

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$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^\mathsf{T}(\mathbf{t} - \mathbf{X}\mathbf{w}), \texttt{ where } \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_D \end{bmatrix}.$$

Different models, same loss

- We have a single loss that corresponds to many different models, with different $\mathbf{w}$ and $\mathbf{X}$

$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^\mathsf{T}(\mathbf{t} - \mathbf{X}\mathbf{w}).$$

- We can get an expression for the $\mathbf{w}$ that minimises $\mathcal{L}$, that will work for any of these models.

Minimising the loss

- When minimising the scalar loss

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2,$$

- we took partial derivatives with respect to each parameter and set to zero.

Minimising the loss

- When minimising the scalar loss

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2,$$

- we took partial derivatives with respect to each parameter and set to zero.
- We now have a vector/matrix loss

$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^{\mathsf{T}}(\mathbf{t} - \mathbf{X}\mathbf{w}),$$

- and will take partial derivatives with respect to the vector $\mathbf{w}$ and set to zero:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{0}$$

Partial diff. wrt vector

The result of taking the partial derivative with respect to a vector is a vector where each element is the partial derivative with respect to one parameter:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial w_0} \\ \frac{\partial \mathcal{L}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{L}}{\partial w_D} \end{bmatrix}$$

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Useful identites:

$f(\mathbf{w})$	$\frac{\partial f}{\partial \mathbf{w}}$
$\mathbf{w}^T\mathbf{x}$	$\mathbf{x}$
$\mathbf{x}^T\mathbf{w}$	$\mathbf{x}$
$\mathbf{w}^T\mathbf{w}$	$2\mathbf{w}$
$\mathbf{w}^T\mathbf{C}\mathbf{w}$	$2\mathbf{C}\mathbf{w}$

$w_0 + w_1 x_1 + \cdots + w_D x_D$

$x = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_D \end{bmatrix}$

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Computing $\frac{\partial \mathcal{L}}{\partial \mathbf{w}}$

$$\frac{\partial}{\partial \mathbf{w}} \left(\frac{1}{N} (\mathbf{t} - \mathbf{X}\mathbf{w})^{\mathsf{T}} (\mathbf{t} - \mathbf{X}\mathbf{w}) \right) \quad = \quad \frac{1}{N} (2\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{w} - 2\mathbf{X}^{\mathsf{T}}\mathbf{t})$$

Matrix transpose

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \end{bmatrix}, \ \mathbf{X}^{\mathsf{T}} = \begin{bmatrix} x_{11} & x_{21} & x_{31} \\ x_{12} & x_{22} & x_{32} \end{bmatrix}$$

Transpose of sum/product

$$(\mathbf{a} + \mathbf{b})^{\mathsf{T}} = \mathbf{a}^{\mathsf{T}} + \mathbf{b}^{\mathsf{T}}, \ (\mathbf{X}\mathbf{w})^{\mathsf{T}} = \mathbf{w}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}$$

Computing $\frac{\partial \mathcal{L}}{\partial \mathbf{w}}$

$$
\begin{aligned}
\frac{\partial}{\partial \mathbf{w}} \left(\frac{1}{N} (\mathbf{t} - \mathbf{X}\mathbf{w})^\mathsf{T} (\mathbf{t} - \mathbf{X}\mathbf{w}) \right) &= \cancel{\frac{1}{N}} (\cancel{2}\mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{w} - \cancel{2}\mathbf{X}^\mathsf{T}\mathbf{t}) = \mathbf{0} \\
\mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{w} &= \mathbf{X}^\mathsf{T}\mathbf{t}
\end{aligned}
$$

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Matrix inverse

Inverse is defined (for a square matrix $\mathbf{A}$) as the matrix $\mathbf{A}^{-1}$ that satisfies:

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$$

Where $\mathbf{I}$ is the *identity* matrix,

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}, \text{ and } \mathbf{I}\mathbf{A} = \mathbf{A}, \text{ for any } \mathbf{A}$$

Computing $\frac{\partial \mathcal{L}}{\partial \mathbf{w}}$

$$
\begin{aligned}
\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{w} &= \mathbf{X}^{\mathsf{T}}\mathbf{t} \\
\underbrace{\underbrace{(\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}}_{A^{-1}}\underbrace{\mathbf{X}^{\mathsf{T}}\mathbf{X}}_{A}}_{I w = w}\mathbf{w} &= (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{t}
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Computing $\frac{\partial \mathcal{L}}{\partial \mathbf{w}}$

$$\begin{aligned} \mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{w} &= \mathbf{X}^\mathsf{T}\mathbf{t} \\ (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{w} &= (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t} \\ \mathbf{w} &= (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t} \end{aligned}$$

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An alternative optimization: Gradient Descent

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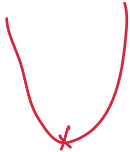

Linear model - Olympic data

$t = w_0 + w_1 x$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & 1896 \\ 1 & 1900 \\ \vdots & \\ 1 & 2008 \end{bmatrix}, \quad \mathbf{t} = \begin{bmatrix} 12.00 \\ 11.00 \\ \vdots \\ 9.85 \end{bmatrix}$$

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$$\widehat{\mathbf{w}} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t} = \begin{bmatrix} 36.416 \\ -0.0133 \end{bmatrix} \begin{array}{l} \to \hat{w}_0 \\ \to \hat{w}_1 \end{array}$$

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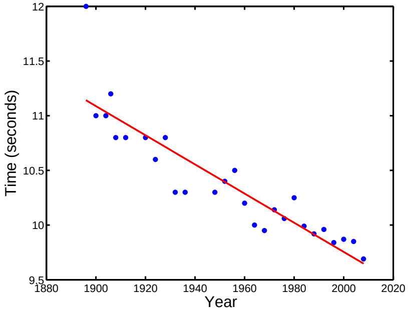
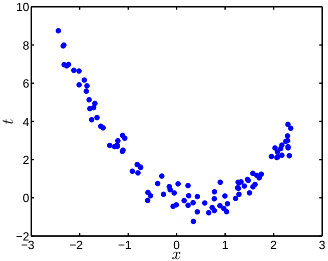


Quadratic model - synthetic data

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 \end{bmatrix}$$

$\cancel{t = w_0 + w_1 x}$ $\rightarrow$ $t = w_0 + w_1 x + w_2 x^2$



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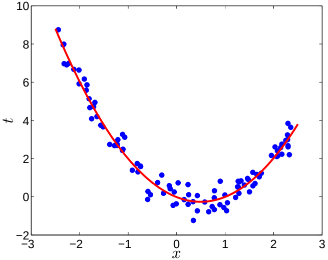
$$\widehat{\mathbf{w}} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t} = \begin{bmatrix} -0.0149 \\ -0.9987 \\ 1.0098 \end{bmatrix}$$

$$t_n = -0.0149 - 0.9987x_n + 1.0098x_n^2$$



8th order model - Olympic data

$$t = w_0 + w_1 x + w_2 x^2 + \ldots + w_8 x^8$$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_8 \end{bmatrix}, \; \mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^8 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \ldots & x_N^8 \end{bmatrix}$$

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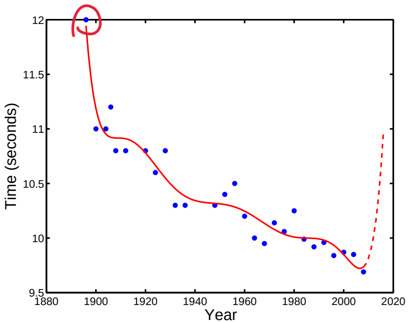

More general models

- So far, we've only considered functions of the form

$$t = w_0 + w_1 x + w_2 x^2 + \ldots + w_D x^D$$

- In fact, each term can be any function of x (or even $\mathbf{x}$)

$$t = w_0 \underline{h_0(x)} + w_1 \underline{h_1(x)} + \ldots + w_D \underline{h_D(x)}$$

- For example,

$$t = w_0 + w_1 x + w_2 \sin(x) + w_3 x^{-1} + \ldots$$

More general models

- So far, we've only considered functions of the form

$$t = w_0 + w_1 x + w_2 x^2 + \ldots + w_D x^D$$

- In fact, each term can be any function of x (or even $\mathbf{x}$)

$$t = w_0 h_0(x) + w_1 h_1(x) + \ldots + w_D h_D(x)$$

- For example,

$$t = w_0 + w_1 x + w_2 \sin(x) + w_3 x^{-1} + \ldots$$

- In General:

$\cos(x)$
$|x_{n,1} - x_{n,2}|$

$$\mathbf{X} = \begin{bmatrix} h_0(x_1) & h_1(x_1) & \ldots & h_D(x_1) \\ h_0(x_2) & h_1(x_2) & \ldots & h_D(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ h_0(x_N) & h_1(x_N) & \ldots & h_D(x_N) \end{bmatrix}$$

Example – Olympic data

$$t = w_0 + w_1 x + w_2 \sin\left(\frac{x-a}{b}\right)$$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_1 & \sin((x_1 - a)/b) \\ \vdots & \vdots & \vdots \\ 1 & x_N & sin((x_N - a)/b) \end{bmatrix}$$

$h_0 = 1$

$h_1 = x$

$h_2 = \sin\left(\frac{x-a}{b}\right)$

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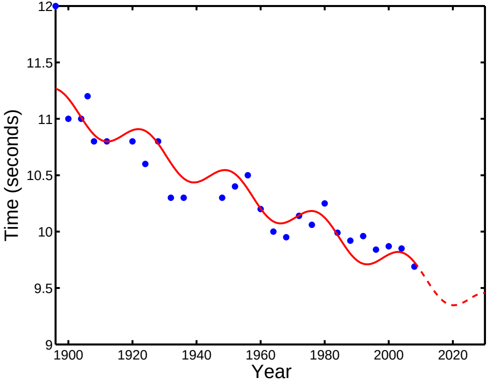

Summary

- Formulated our loss in terms of vectors and matrices.
- Differentiated it with respect to the parameter vector.
- Used this to find a general expression for $\widehat{\mathbf{w}}$ - the parameters that minimise the loss.
- Shown examples of models with differing numbers of terms.
- Not restricted to x^D - can have any function of x (or even $\mathbf{x}$).
- Shown example of model including a sin term.

Making predictions

$$\widehat{\mathbf{w}} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t}$$

Where $\mathbf{X}$ depends on the choice of model:

$$\mathbf{X} = \begin{bmatrix} h_0(x_1) & h_1(x_1) & \dots & h_D(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ h_0(x_N) & h_1(x_N) & \dots & h_D(x_N) \end{bmatrix}$$

$$t = h_0(x)w_0 + h_1(x)w_1 + \dots + h_D(x)w_D$$

Making predictions

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To predict t at a new value of x, we first create $\mathbf{x}_{\mathrm{new}}$:

$$\mathbf{x}_{\mathrm{new}} = \begin{bmatrix} h_0(x_{\mathrm{new}}) \\ \vdots \\ h_D(x_{\mathrm{new}}) \end{bmatrix},$$

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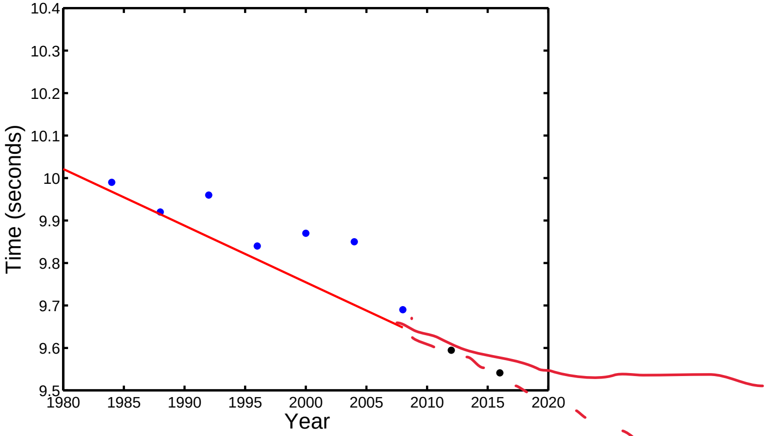
and then compute

$$t_{\text{new}} = \widehat{\mathbf{w}}^\mathsf{T}\mathbf{x}_{\text{new}}$$

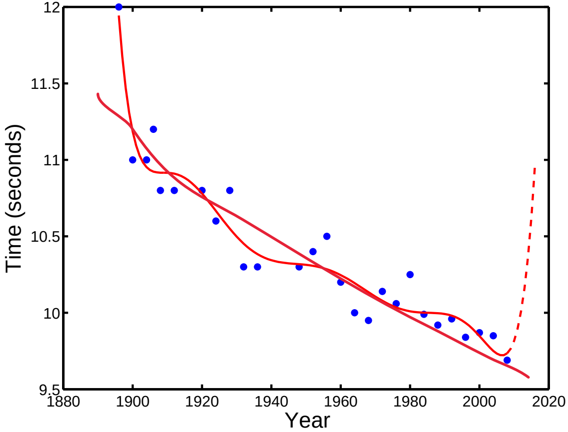
Example - Olympic data



Linear model – predictions OK?

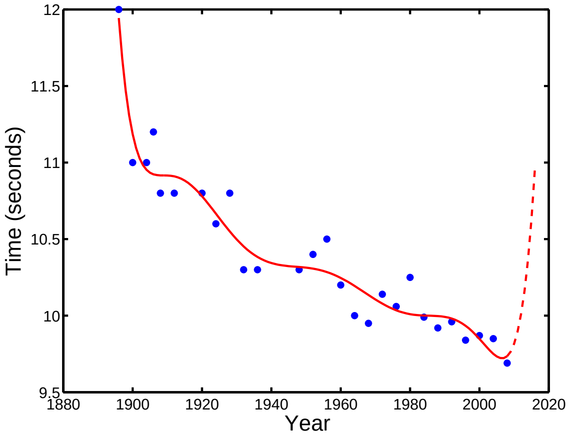
$w_0 + w_1 x$

Example - Olympic data



8th order model – predictions terrible!

Example - Olympic data



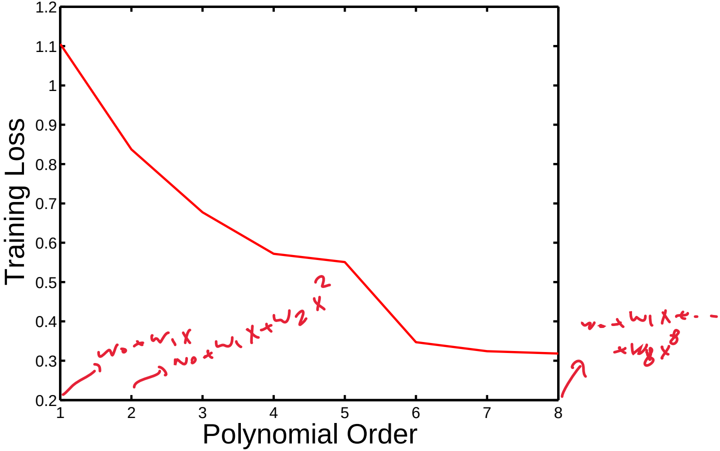
8th order model – predictions terrible!

Choice of model is **very** important.

Possible ways of choosing

- Lowest loss, $\mathcal{L}$?

How does loss change?



Loss, L, on the Olympic 100m data as additional terms (x^D) are added to the model.

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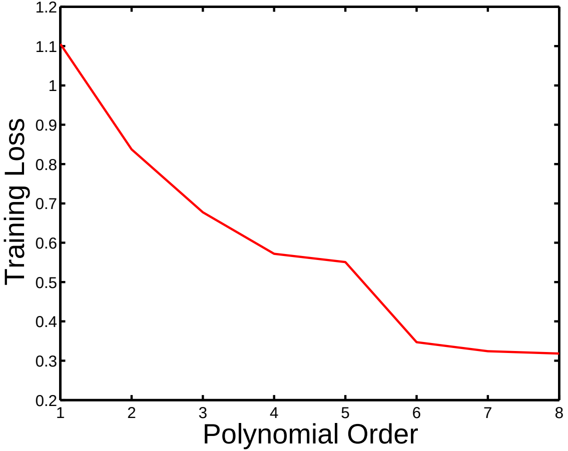
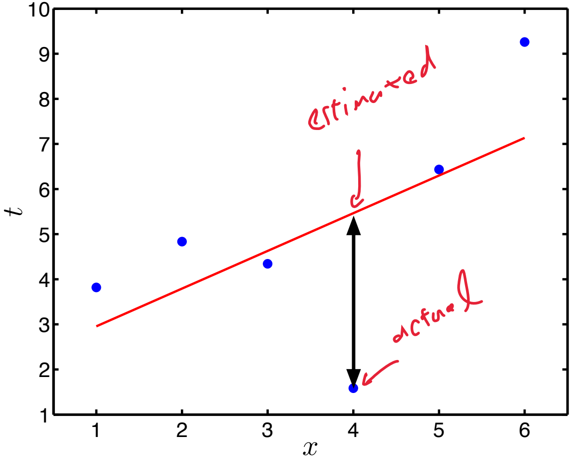


Loss, L, on the Olympic 100m data as additional terms (x^D) are added to the model.

Loss **always** decreases as the model is made more complex (i.e. higher order terms are added)

Loss always decreases with model complexity

Data comes from $t = x$ with some *noise* added:



Linear model $t = w_0 + w_1 x$.

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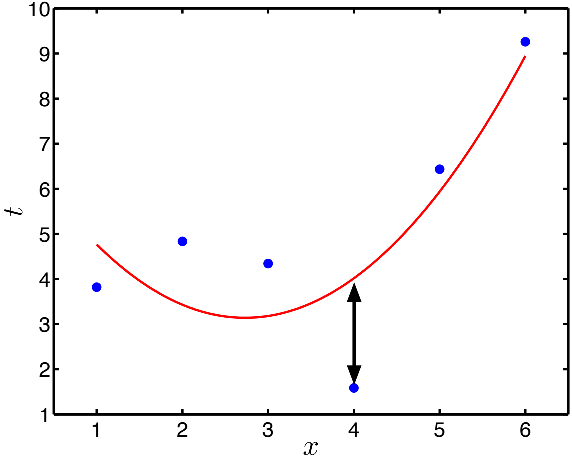

Quadratic model $t = w_0 + w_1 x + w_2 x^2$.

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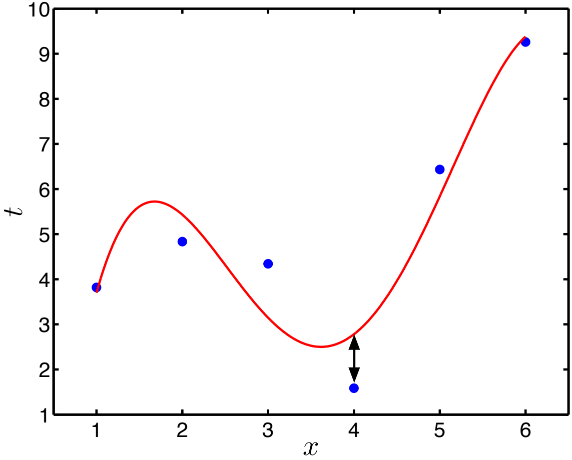

Fourth order $t = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4$.

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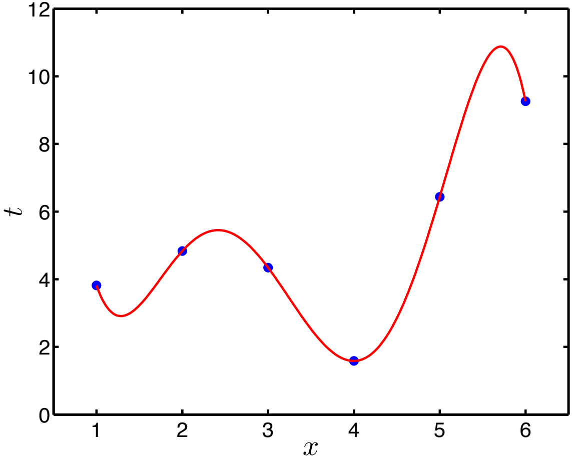

Fifth order $t = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$.

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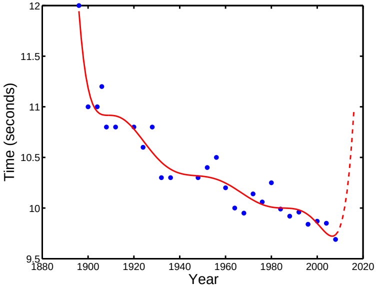

Noise

Not necessarily 'noise', just things we can't, or don't need to model.

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- We have N input-response pairs for training:

$$(x_1, t_1), (x_2, t_2), \ldots, (x_N, t_N).$$

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new training data

training data

validation data

unseen by the model

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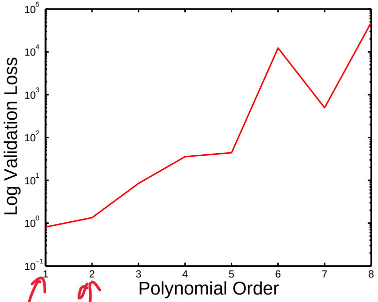
  - The M pairs are known as *validation data*.
- Example – use Olympics pre 1980 to train and post 1980 to validate.

Validation example



$w_0 + w_1 x$

$w_0 + w_1 x + w_2 x^2$

...

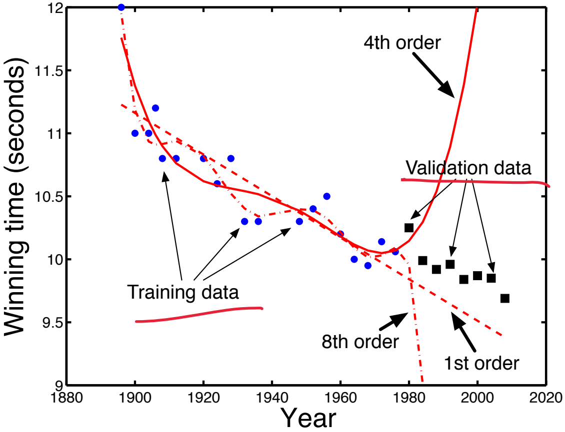
Predictions evaluated using validation loss:

$$\boxed{\mathcal{L}_v = \frac{1}{M}\sum_{m=1}^{M}(t_m - \mathbf{w}^\mathsf{T}\mathbf{x}_m)^2}$$

Best model?

Results suggest that a first order (linear) model ($t = w_0 + w_1 x$) is best.

Validation example



Best model

First order (linear) model generalises best.

How should we choose which data to hold back?

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- In some applications it will be clear.
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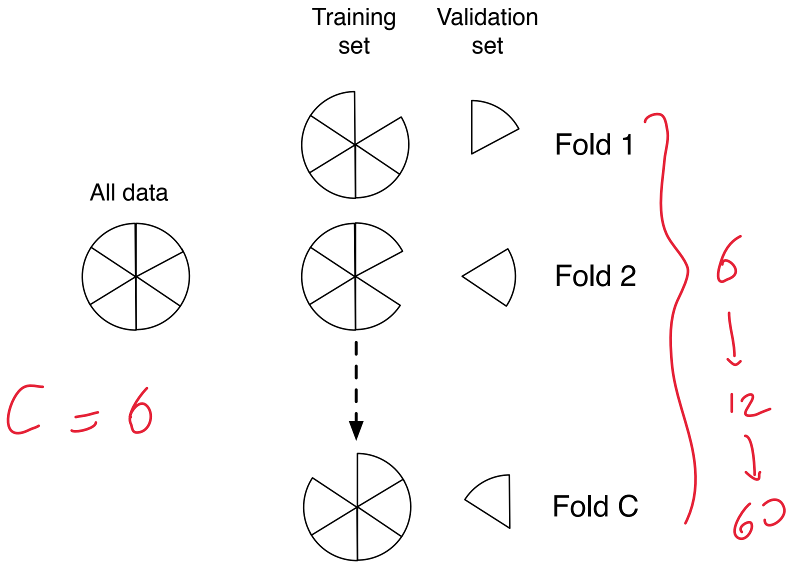
- Do it more than once – average the results.
- Do cross-validation.
  - Split the data into C equal sets. Train on $C - 1$, test on remaining.

Cross-validation



Average performance over the C ‘folds’.

Leave-one-out Cross-validation

- Cross-validation can be repeated to make results more accurate.
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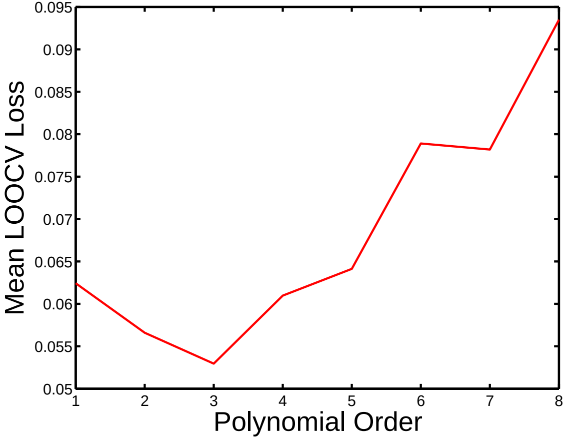
- e.g. Doing 10-fold CV 10 times gives us 100 performance values to average over.
- Extreme example is when $C = N$ so each fold includes one input-response pair.
    - Leave-one-out (LOO) CV.
- Example....

LOOCV – Olympic data



Best model?

LOO CV suggests a 3rd order model. Previous method suggests 1st order. Who knows which is right!

LOOCV – synthetic data (we know the answer!)

- Generate some data from a 3rd order model

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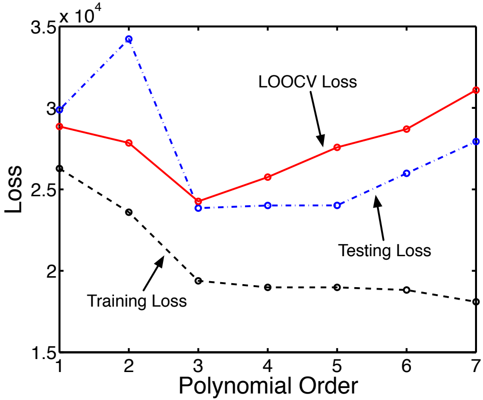
- Use LOOCV to compare models from first to 7th order:



(Testing loss comes from another dataset)

Computational issues

- CV and LOOCV let us choose from a set of models based on predictive performance.
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$$
\begin{aligned}
t &= \sum_{d=0}^{D} w_d h_d(x) \\
\widehat{\mathbf{w}} &= \underbrace{(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}}_{(D+1) \times (D+1)}\mathbf{X}^\mathsf{T}\mathbf{t}
\end{aligned}
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$$

- For some models we will need to use $C \ll N$.

Summary

- Showed how we can make predictions with our ‘linear’ model.
- Saw how choice of model has big influence in quality of predictions.
- Saw how the loss on the training data, $\mathcal{L}$, cannot be used to choose models.
  - Making model more complex always decreases the loss.
- Introduced the idea of using some data for validation.
- Introduced cross validation and leave-one-out cross validation.