Linear regression

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Contents

Review of vector/matrix notation and linear algebra

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Scalar and vectors

- A **scalar** is just a numeric value like 0.9 or -18.7.
- Scalars are usually denoted as lower case letters like x or a.
- A **vector** is an ordered list of scalar values. Sometimes we refer to these scalar values of the vector as *attributes* or *entries* of the vector.
- Vectors are usually denoted by bold lowercase letters like $\mathbf{x}$ or $\mathbf{y}$.

Vectors

- A vector can appear sometimes written as a row vector, e.g.

$$\mathbf{x} = [x_1, x_2, x_3, x_4, x_5]$$

  Or as a column vector

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix}$$

- In this module, ALL vectors will be column vectors by default. So, when you see a vector, e.g. $\mathbf{x}, \mathbf{y}, \mathbf{z}$ always think this vector has a column-wise shape.

Matrices

- A **matrix** is a rectangular array of scalars arranged in rows and columns.

- Matrices are usually denoted by bold uppercase letters, e.g. **X** or **Y**.

- The following matrix has three rows and two columns

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

- The entries in the matrix above are of the form x_{ij}, where the first subindex i indicates the row of the element and the second subindex j indicates the column.

Matrix transpose

- Let $\mathbf{X}$ be a matrix with elements x_{ij}.
- The transpose of a matrix $\mathbf{X}$ is a new matrix $\mathbf{X}^\top$ with elements x_{ji}.

$$\mathbf{X} = \begin{bmatrix} 4.1 & -5.6 \\ -2.6 & 7.9 \\ 3.5 & 1.8 \end{bmatrix}, \quad \mathbf{X}^\top = \begin{bmatrix} 4.1 & -2.6 & 3.5 \\ -5.6 & 7.9 & 1.8 \end{bmatrix}$$

Matrix multiplication

- Let **A** be a matrix with entries a_{ik} of dimensions $p \times q$.
- Let **B** be a matrix with entries b_{kj} of dimensions $t \times s$.
- Matrix multiplication of the form **AB** is only possible if $q = t$.
- If this is the case, the matrix $\mathbf{C} = \mathbf{AB}$ has dimensions $p \times s$ with entries

$$c_{ij} = \sum_k a_{ik} b_{kj}.$$

Transpose of a product

- Let $\mathbf{w}$ be a vector of dimensions $d \times 1$. Let $\mathbf{X}$ be a matrix with dimensions $n \times d$.

- The transpose of the product $\mathbf{Xw}$, $(\mathbf{Xw})^\top$ is

$$(\mathbf{Xw})^\top = \mathbf{w}^\top \mathbf{X}^\top.$$

- We can apply this result to a product of several matrices

$$\begin{aligned}
(\mathbf{ABCD})^\top &= ((\mathbf{AB})(\mathbf{CD}))^\top \\
&= (\mathbf{CD})^\top (\mathbf{AB})^\top \\
&= \mathbf{D}^\top \mathbf{C}^\top \mathbf{B}^\top \mathbf{A}^\top.
\end{aligned}$$

From a scalar operation to a vector operation

- It is usually desirable to transform a scalar operation into a vector operation.

- When coding scalar operations, we require making use of loops, which can be expensive.

- In contrast, vector operations are handled efficiently by low-level routines already included in modules like numpy.

Example

Write the following scalar operation into a vector/matrix form

$$\sum_{i=1}^{n}(y_i - \sum_{j=1}^{d} x_{ij} w_j)^2.$$

Answer (I)

- The sum above can be written as

$$
\begin{aligned}
\sum_{i=1}^{n}(y_i - \sum_{j=1}^{d} x_{ij}w_j)^2 = {} & (y_1 - \sum_{j=1}^{d} x_{1j}w_j)(y_1 - \sum_{j=1}^{d} x_{1j}w_j) \\
& + \cdots \\
& + (y_n - \sum_{j=1}^{d} x_{nj}w_j)(y_n - \sum_{j=1}^{d} x_{nj}w_j).
\end{aligned}
$$

- Let us define a vector $\mathbf{v}$ of dimensions $n \times 1$ with entries given as

$$
(y_i - \sum_{j=1}^{d} x_{ij}w_j).
$$

Answer (II)

- The product of vectors $\mathbf{v}^\top \mathbf{v}$ gives the same result than the required sum,

$$\mathbf{v}^\top \mathbf{v} = \begin{bmatrix} (y_1 - \sum_{j=1}^{d} x_{1j} w_j) & \cdots & (y_n - \sum_{j=1}^{d} x_{nj} w_j) \end{bmatrix} \begin{bmatrix} (y_1 - \sum_{j=1}^{d} x_{1j} w_j) \\ \vdots \\ (y_n - \sum_{j=1}^{d} x_{nj} w_j) \end{bmatrix}$$

$$= \sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} x_{ij} w_j)^2.$$

- How do we express the elements in $\mathbf{v}$ with vectors and matrices?

Answer (III)

- For a fixed i, $x_{i1}, \ldots, x_{id}$ can be grouped into a vector $\mathbf{x}_i^\top$.
- The internal sums in the entries of $\mathbf{v}$ can then be written as

$$\sum_{j=1}^{d} x_{ij} w_j = \mathbf{x}_i^\top \mathbf{w} = \begin{bmatrix} x_{i1} & x_{i2} & \cdots & x_{id} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix}$$

- We can now write $\mathbf{v}$ as

$$\mathbf{v} = \begin{bmatrix} y_1 - \mathbf{x}_1^\top \mathbf{w} \\ \vdots \\ y_n - \mathbf{x}_n^\top \mathbf{w}. \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \mathbf{x}_1^\top \mathbf{w} \\ \vdots \\ \mathbf{x}_n^\top \mathbf{w}. \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} \mathbf{w}$$

- We can group the scalars $y_1, \ldots, y_n$ into a vector $\mathbf{y}$.
- We can group the row vectors $\mathbf{x}_1^\top, \ldots, \mathbf{x}_n^\top$ into a matrix $\mathbf{X}$.

Answer (IV)

- It means that $\mathbf{v} = \mathbf{y} - \mathbf{X}\mathbf{w}$.

- Finally

$$\sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} x_{ij} w_j)^2 = \mathbf{v}^\top \mathbf{v} = (\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w}) .$$

Two common types of products

- **Inner product**. The inner product between two vectors results in a scalar.
- Let $\mathbf{x}$ and $\mathbf{y}$ be vectors of dimension $m \times 1$. The inner product is given as

$$\mathbf{x}^\top \mathbf{y} = \sum_{i=1}^{m} x_i y_i,$$

- **Outer product**. The outer product between two vectors results in a matrix.
- Let $\mathbf{x}$ be a vector of dimension $m \times 1$ and $\mathbf{y}$ a vector of dimension $p \times 1$. The outer product is given as

$$\mathbf{x}\mathbf{y}^\top = \begin{bmatrix} x_1 y_1 & \cdots & x_1 y_p \\ x_2 y_1 & \cdots & x_2 y_p \\ \vdots & \vdots & \vdots \\ x_m y_1 & \cdots & x_m y_p. \end{bmatrix}$$

Differentiating a function in a vector/matrix form (I)

- We will see cases in which a function $f(\mathbf{w})$ depends on some parameters grouped in a vector $\mathbf{w}$.
- We would like to find the vector of parameters $\mathbf{w}$ that maximise $f(\mathbf{w})$.
- For example, suppose $f(\mathbf{w})$ is defined as

$$f(\mathbf{w}) = \sum_{i=1}^{d} w_i x_i.$$

- We can group the scalars $x_1, \ldots, x_d$ into $\mathbf{x}$. Likewise for $\mathbf{w}$.
- According to what we saw before, we can write $f(\mathbf{w})$ as $f(\mathbf{w}) = \mathbf{x}^\top \mathbf{w}$.

Differentiating a function in a vector/matrix form (II)

- For a fixed $\mathbf{x}$, we are interested in computing the gradient of $f(\mathbf{w})$ with respect to $\mathbf{w}$

$$\frac{df(\mathbf{w})}{d\mathbf{w}} = \begin{bmatrix} \frac{\partial f(\mathbf{w})}{\partial w_1} \\ \vdots \\ \frac{\partial f(\mathbf{w})}{\partial w_d} \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ x_d. \end{bmatrix} = \mathbf{x}.$$

- Some useful identities when differentiating with respect to a vector

$f(\mathbf{w})$	$\frac{df(\mathbf{w})}{d\mathbf{w}}$
$\mathbf{w}^\top \mathbf{x}$	$\mathbf{x}$
$\mathbf{x}^\top \mathbf{w}$	$\mathbf{x}$
$\mathbf{w}^\top \mathbf{w}$	$2\mathbf{w}$
$\mathbf{w}^\top \mathbf{C}\mathbf{w}$	$2\mathbf{C}\mathbf{w}.$

Identity matrix and the inverse of a matrix

- The identity matrix of size N is a square matrix with ones on the main diagonal and zeros elsewhere, e.g.,

$$\mathbf{I}_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

- The inverse matrix of a matrix $\mathbf{A}$ of dimensions $d \times d$, denoted as $\mathbf{A}^{-1}$, satisfies

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

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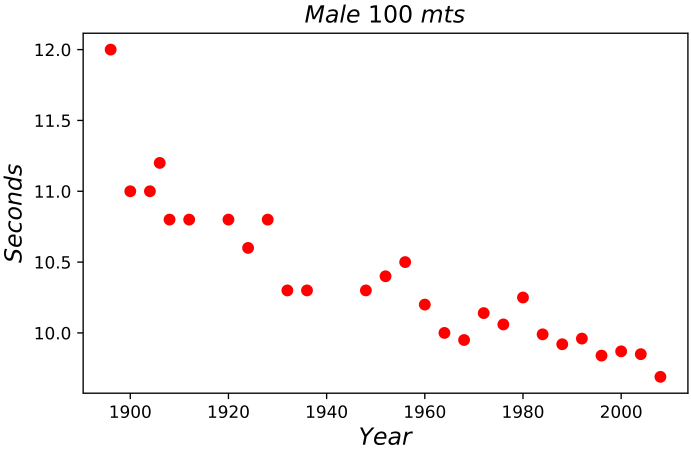
Olympic 100m Data

Image from Wikimedia Commons `http://bit.ly/191adDC`.

Dataset


Male 100 mts
Seconds
Year
12.0
11.5
11.0
10.5
10.0
1900
1920
1940
1960
1980
2000

Model

- We will use a linear model $f(x, \mathbf{w})$ to predict y, where y is the time in seconds and x the year of the competition.

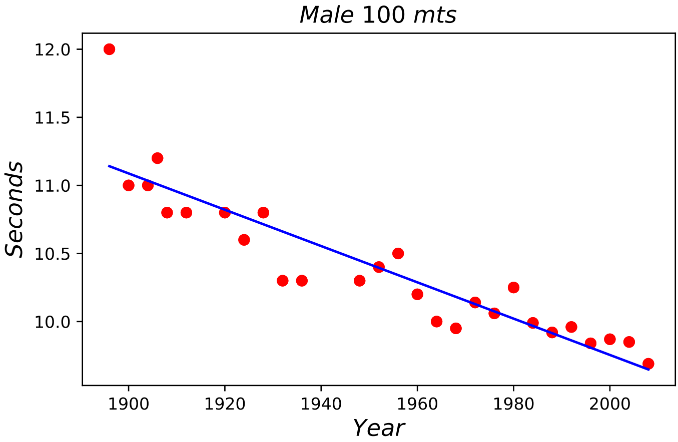
- The linear model is given as

$$f(x, \mathbf{w}) = w_0 + w_1 x,$$

  where w_0 is the intercept and w_1 is the slope.

- We use $\mathbf{w}$ to refer both to w_0 and w_1.

Data and model



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Linear model

- A simple model for regression consists in using a linear combination of the attributes to predict the output

$$f(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_D x_D,$$

where $w_0, w_1, \cdots, w_D$ are the parameters of the regression model.

- The term w_0 is the bias term or intercept, e.g. $f(\mathbf{0}, \mathbf{w}) = w_0$.

- The expression above can be written in a vectorial form

$$f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^\top \mathbf{x}.$$

where we have defined $\mathbf{w} = [w_0, w_1, \cdots, w_D]^\top$ and $\mathbf{x} = [1, x_1, \cdots, x_D]^\top$.

- Notice that $x_0 = 1$.

Parenthesis: Gaussian pdf

- The Gaussian pdf has the form

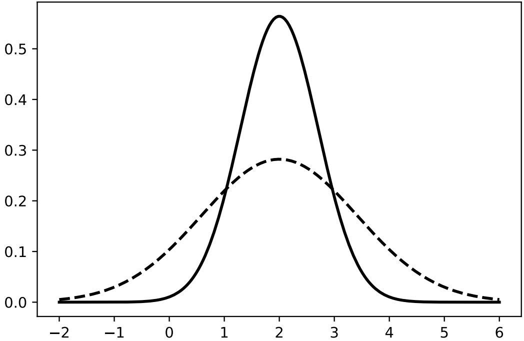
$$p(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(y-\mu)^2}{2\sigma^2}\right\}.$$

- A Gaussian pdf requires two parameters μ and σ^2, the mean and the variance of the RV Y.

- We denote the Gaussian pdf as $p(y|\mu, \sigma^2) = \mathcal{N}(y|\mu, \sigma^2)$ or $y \sim \mathcal{N}(\mu, \sigma^2)$.

Parenthesis: Gaussian pdf

The mean of the three Gaussians is $\mu = 2$ and the variances are $\sigma^2 = 0.5$ (solid), and $\sigma^2 = 2$ (dashed).



Gaussian regression model (I)

- We use a Gaussian regression model to relate the inputs and outputs

$$y = f(\mathbf{x}, \mathbf{w}) + \underbrace{\epsilon}_{\text{noises}},$$

  where $\epsilon \sim \mathcal{N}(0, \sigma^2)$.

- It assumes that each output y_i that we observe can be explained as the prediction of an underlying model, $f(\mathbf{x}_i, \mathbf{w})$ plus a noise term ϵ_i.
- For a fixed $\mathbf{x}$ and a fixed $\mathbf{w}$, $f(\mathbf{x}, \mathbf{w})$ is a constant, then

$$y = \text{constant} + \epsilon,$$

  where ϵ is a continuous RV.

- What is the pdf for y? (we are adding a constant to a Gaussian RV)
  - $E\{y\} = E\{\text{constant} + \epsilon\} = \text{constant}$
  - $\text{var}\{y\} = \text{var}\{\text{constant}\} + \text{var}\{\epsilon\} = \sigma^2$.

Gaussian regression model (II)

- This means that

$$y \sim \mathcal{N}(constant, \sigma^2),$$

where we said constant was $f(\mathbf{x}, \mathbf{w})$, this is,

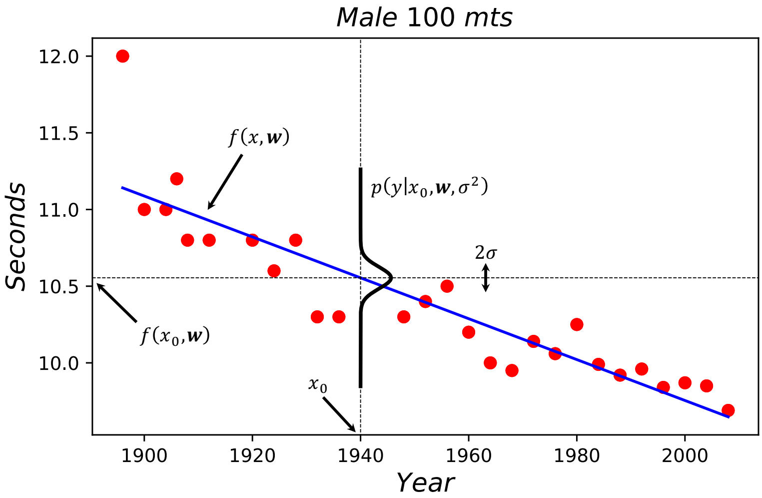
$$y \sim \mathcal{N}(f(\mathbf{x}, \mathbf{w}), \sigma^2).$$

- Because we assumed that $\mathbf{x}$ and $\mathbf{w}$ are given, we can also write

$$p(y|\mathbf{x}, \mathbf{w}, \sigma^2) = \mathcal{N}(y|f(\mathbf{x}, \mathbf{w}), \sigma^2).$$

- If we knew the value for $\mathbf{w}$, once we have a new $\mathbf{x}_*$, we can predict the output as $f(\mathbf{x}_*, \mathbf{w})$.
- σ^2 tells us the noise variance.

Gaussian regression model (III)



How do we estimate $\mathbf{w}$? (I)

- We start with a training dataset $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$.

- We assume that the random variables $Y_1, \cdots, Y_N$ are *independent*,

$$p(y_1, \cdots, y_N | \mathbf{x}_1, \cdots, \mathbf{x}_N) = p(y_1|\mathbf{x}_1) \cdots p(y_N|\mathbf{x}_N) = \prod_{n=1}^{N} p(y_n|\mathbf{x}_n).$$

- We also assume that the RVs $Y_1, \cdots, Y_N$ follow an *identical* distribution, Gaussian in this case

$$p(y_n|\mathbf{x}_n, \mathbf{w}, \sigma^2) = \mathcal{N}(y_n|f(\mathbf{x}_n, \mathbf{w}), \sigma^2) = \mathcal{N}(y_n|\mathbf{w}^\top \mathbf{x}_n, \sigma^2).$$

- Both assumptions go by the name of the *iid* assumption, *independent and identically distributed*.

How do we estimate $\mathbf{w}$? (II)

- Putting both assumptions together, we get

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N} p(y_n|\mathbf{x}_n, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(y_n|\mathbf{w}^\top \mathbf{x}_n, \sigma^2),$$

where $\mathbf{y} = [y_1, \cdots, y_N]^\top \in \mathbb{R}^{N\times 1}$ and $\mathbf{X} = [\mathbf{x}_1, \cdots, \mathbf{x}_N]^\top \in \mathbb{R}^{N\times(D+1)}$.

- The expression above can then be written as

$$\begin{aligned} p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) &= \prod_{n=1}^{N} \mathcal{N}(y_n|\mathbf{w}^\top \mathbf{x}_n, \sigma^2), \\ &= \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(y_n - \mathbf{w}^\top \mathbf{x}_n)^2}{2\sigma^2}\right\}. \\ &= \frac{1}{(2\pi\sigma^2)^{\frac{N}{2}}} \exp\left\{-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \mathbf{w}^\top \mathbf{x}_n)^2\right\}. \end{aligned}$$

How do we estimate $\mathbf{w}$? (III)

- When we look at a Gaussian pdf, like

$$p(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(y-\mu)^2}{2\sigma^2}\right\},$$

  we assume that both μ and σ^2 are given. In this case, the pdf follows all the properties we reviewed before.
- The same is true for

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N} p(y_n|\mathbf{x}_n, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(y_n|\mathbf{w}^\top \mathbf{x}_n, \sigma^2).$$

- Given $\mathbf{w}^\top \mathbf{x}_n$ and σ^2, then each $p(y_n|\mathbf{x}_n, \mathbf{w}, \sigma^2)$ is a pdf.
- A different approach would be to say: I have some data for $\{y_n\}_{n=1}^N$ and $\{\mathbf{x}_n\}_{n=1}^N$ but
  - "I don't know what is $\mathbf{w}^\top$ (therefore I don't know what is $\mathbf{w}^\top \mathbf{x}_n$)"
  - "I don't know what is σ^2".

How do we estimate $\mathbf{w}$? (IV)

- With y_n and $\mathbf{x}_n$ given but with unknown values for $\mathbf{w}$ and σ^2, each $p(y_n|\mathbf{x}_n, \mathbf{w}, \sigma^2)$ is not a pdf anymore.
- In that case, the function

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(y_n|\mathbf{w}^\top \mathbf{x}_n, \sigma^2),$$

  receives the name of a *likelihood function*.
- We can think of a likelihood function as a function of the parameters $\mathbf{w}$ and σ^2,

$$g(\mathbf{w}, \sigma^2) = p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2),$$

- And subsequently, we can use *multivariate calculus* to find the values of $\mathbf{w}, \sigma^2$ that maximise $g(\mathbf{w}, \sigma^2)$.
- In statistics, this is known as the *maximum-likelihood* (ML) criterion to estimate parameters.

How do we estimate $\mathbf{w}$? (V)

- Given $\mathbf{y}, \mathbf{X}$, we use the ML criterion to find the parameters $\mathbf{w}$ and σ^2 that maximise

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{\frac{N}{2}}} \exp\left\{-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \mathbf{w}^\top \mathbf{x}_n)^2\right\}.$$

- In practice, we prefer to maximise the log of the likelihood $p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2)$,

$$\begin{aligned} LL(\mathbf{w}, \sigma^2) &= \log p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) \\ &= -\frac{N}{2}\log(2\pi) - \frac{N}{2}\log\sigma^2 - \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \mathbf{w}^\top \mathbf{x}_n)^2. \end{aligned}$$

- **Consistency of the ML criterion** If data was really generated according to the probability we specified, the correct parameters will be recovered in the limit as $N \to \infty$.

Connection with the sum of squared errors

- If we multiply $LL(\mathbf{w}, \sigma^2)$ by minus one, we get

$$E(\mathbf{w}, \sigma^2) = -\log p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) \propto \sum_{n=1}^{N} (y_n - \mathbf{w}^\top \mathbf{x}_n)^2.$$

- The ML criterion for this model has a close connection with the sum-of-squared errors used in non-probabilistic formulations of linear regression.

- Maximising the log-likelihood function is equivalent to minimising the sum-of-squares errors.

- Notice that the $\log$ is a monotonic function, meaning that if we find $\mathbf{w}, \sigma^2$ that maximise $g(\mathbf{w}, \sigma^2)$, those will also maximise $\log(g(\mathbf{w}, \sigma^2))$.

Normal equation (I)

- Let us find an estimate for $\mathbf{w}$.
- From what we saw before,

$$LL(\mathbf{w}, \sigma^2) = -\frac{N}{2}\log(2\pi) - \frac{N}{2}\log\sigma^2 - \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \mathbf{w}^\top \mathbf{x}_n)^2.$$

- Using what we reviewed in the section on vector/matrix notation, it can be shown that this expression can be written in a vectorial form as

$$LL(\mathbf{w}, \sigma^2) = -\frac{N}{2}\log(2\pi) - \frac{N}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w})$$

- Let us focus on the term $(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w})$,

$$(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{y}^\top\mathbf{y} - \mathbf{w}^\top\mathbf{X}^\top\mathbf{y} - \mathbf{y}^\top\mathbf{X}\mathbf{w} + \mathbf{w}^\top\mathbf{X}^\top\mathbf{X}\mathbf{w}$$

Normal equation (II)

- We can find the $\mathbf{w}$ that maximises $LL(\mathbf{w}, \sigma^2)$ by taking the gradient $\frac{dLL(\mathbf{w},\sigma^2)}{d\mathbf{w}}$, equating to zero and solving for $\mathbf{w}$.

- Taking the gradient of each term in $LL(\mathbf{w}, \sigma^2)$ wrt $\mathbf{w}$, we get

$$\frac{d}{d\mathbf{w}}\left[-\frac{N}{2}\log(2\pi)\right] = 0, \quad \frac{d}{d\mathbf{w}}\left[-\frac{N}{2}\log\sigma^2\right] = 0, \quad \frac{d}{d\mathbf{w}}\left[-\frac{1}{2\sigma^2}\mathbf{y}^\top\mathbf{y}\right] = 0,$$

$$\frac{d}{d\mathbf{w}}\left[\frac{1}{2\sigma^2}\mathbf{w}^\top\mathbf{X}^\top\mathbf{y}\right] = \frac{1}{2\sigma^2}\mathbf{X}^\top\mathbf{y},$$

$$\frac{d}{d\mathbf{w}}\left[\frac{1}{2\sigma^2}\mathbf{y}^\top\mathbf{X}\mathbf{w}\right] = \frac{1}{2\sigma^2}\mathbf{X}^\top\mathbf{y}$$

$$\frac{d}{d\mathbf{w}}\left[-\frac{1}{2\sigma^2}\mathbf{w}^\top\mathbf{X}^\top\mathbf{X}\mathbf{w}\right] = -\frac{1}{2\sigma^2}2\mathbf{X}^\top\mathbf{X}\mathbf{w}$$

Normal equation (III)

- Putting these terms together, we get

$$\begin{aligned}\frac{d}{d\mathbf{w}}LL(\mathbf{w},\sigma^2) &= \frac{1}{2\sigma^2}\mathbf{X}^\top\mathbf{y} + \frac{1}{2\sigma^2}\mathbf{X}^\top\mathbf{y} - \frac{1}{2\sigma^2}2\mathbf{X}^\top\mathbf{X}\mathbf{w}\\ &= \frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{y} - \frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{X}\mathbf{w}\end{aligned}$$

- Now, equating to zero and solving for **w**, we get

$$\begin{aligned}\frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{y} - \frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{X}\mathbf{w} &= \mathbf{0}\\ \mathbf{X}^\top\mathbf{X}\mathbf{w} &= \mathbf{X}^\top\mathbf{y}\\ \mathbf{w}_* &= \left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{y}.\end{aligned}$$

- The expression for $\mathbf{w}_*$ is known as the *normal equation*.
- The solution for $\mathbf{w}^*$ exists if we can compute $\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}$.
- The inverse can be computed as long as $\mathbf{X}^\top\mathbf{X}$ is non-singular (e.g. determinant different from zero, or has full-rank).

Solving for σ_*^2

- Following a similar procedure, it can be shown that the ML solution for σ_*^2 is given as

$$\sigma_*^2 = \frac{1}{N}(\mathbf{y} - \mathbf{X}\mathbf{w}_*)^\top(\mathbf{y} - \mathbf{X}\mathbf{w}_*).$$

Basis functions

- The model that is linear in $\mathbf{x}$ only allows linear relationships between $\mathbf{x}$ and y.

- We can extend the model to describe non-linear relationships between the inputs and the output by using basis functions, non-linear mappings from inputs to outputs.

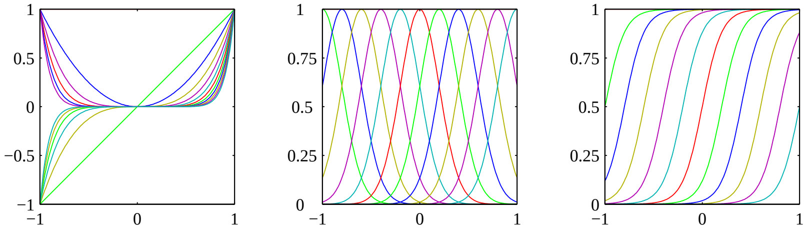
- However, we keep the linear relationship of y wrt $\mathbf{w}$ for tractability.

- The predictive model follows as $f(\mathbf{x}, \mathbf{w})$

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

  where $\phi_i(\mathbf{x})$ are basis functions and we have $M + 1$ parameters for the vector $\mathbf{w}$ and $\phi(\mathbf{x}) = [1, \phi_1(\mathbf{x}), \cdots, \phi_M(\mathbf{x})]^\top$.

Examples of basis functions



Polynomial: $\phi_i(x) = x^i$.
Exponential: $\phi_i(x) = \exp\left\{ -\frac{(x-\mu_i)^2}{2s^2} \right\}$
Sigmoidal: $\phi_i(x) = \sigma\left(\frac{x-\mu_i}{s}\right),\ \sigma(a) = 1/(1+\exp(-a))$.

Transforming the input using the basis functions

- As an example, let us use polynomial basis functions to predict y, the time in seconds in the 100 mt Olympics competition.

- For each x (year of the competition), we now compute the vector of polynomial basis functions

$$\phi(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \\ \vdots \\ x^M \end{bmatrix}$$

- We have converted the unidimensional input feature x into a higher dimensional feature representation $\phi(x) \in R^{M+1}$.

Normal equations with a design matrix

- Given $\mathbf{X}$, we first compute a new design matrix $\mathbf{\Phi}$,

$$\mathbf{\Phi} = \begin{bmatrix} \phi(\mathbf{x}_1)^\top \\ \phi(\mathbf{x}_2)^\top \\ \vdots \\ \phi(\mathbf{x}_N)^\top \end{bmatrix} = \begin{bmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_M(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_M(\mathbf{x}_2) \\ \vdots & & & \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_M(\mathbf{x}_N) \end{bmatrix}$$

- We now can use $(\mathbf{y}, \mathbf{\Phi})$ and write the Gaussian linear regression problem

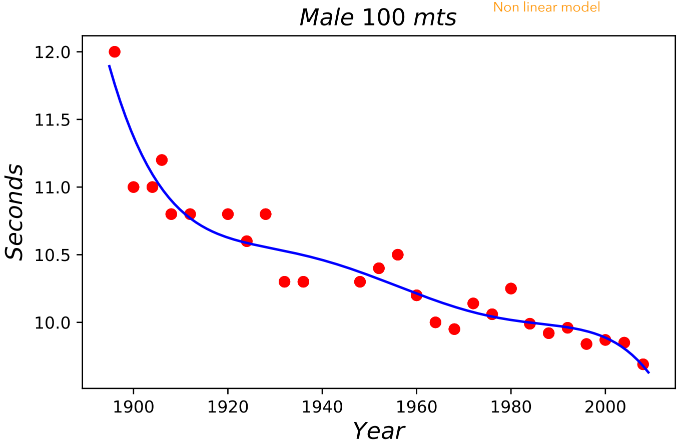
$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(y_n|\mathbf{w}^\top \phi_n, \sigma^2),$$

  where $\phi_n = \phi(\mathbf{x}_n)$.

- Using the ML criterion, we arrive to the following normal equation

$$\mathbf{w}_* = \left(\mathbf{\Phi}^\top \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^\top \mathbf{y}.$$

Olympic 100-mt data with $M = 5$



Alternative to find $\mathbf{w}$

different ways of finding w

- For solving the normal equation, we need to invert $\mathbf{X}^\top \mathbf{X}$.
- This inversion has a computational complexity between $\mathcal{O}((D+1)^{2.4})$ to $\mathcal{O}((D+1)^3)$ (depending on the implementation).
- The normal equation is linear regarding the number of instances in the training data, $\mathcal{O}(N)$.
- It can handle a large training set as long as it fits in memory.
- Alternatively, we can use iterative optimisation in cases with a large number of features and too many instances to fit in memory.

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General problem

- We are given a function $h(\mathbf{w})$, where $\mathbf{w} \in \mathbb{R}^p$.

- Aim: to find a value for $\mathbf{w}$ that minimises $h(\mathbf{w})$.

- Use an iterative procedure

$$\mathbf{w}_{k+1} = \mathbf{w}_k + \eta \mathbf{d}_k,$$

  where $\mathbf{d}_k$ is known as the search direction and it is such that

$$h(\mathbf{w}_{k+1}) < h(\mathbf{w}_k).$$

- The parameter η is known as the **step size** or **learning rate**.

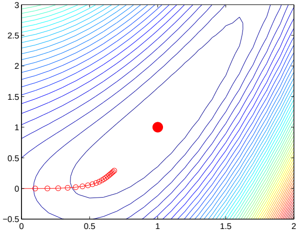
Gradient descent

- Perhaps, the simplest algorithm for unconstrained optimisation.
- It assumes that $\mathbf{d}_k = -\mathbf{g}_k$, where $\mathbf{g}_k = \mathbf{g}(\mathbf{w}_k)$.
- Also known as **steepest descent**.
- It can be written like

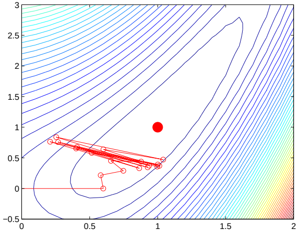
$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \mathbf{g}_k.$$

Step size

- The main issue in gradient descent is how to set the step size.
- If it is too small, convergence will be very slow. If it is too large, the method can fail to converge at all.



(a)



(b)

Figure: The function to optimise is $h(w_1, w_2) = 0.5(w_1^2 - w_2)^2 + 0.5(w_1 - 1)^2$. The minimum is at $(1, 1)$. In (a) $\eta = 0.1$. In (b) $\eta = 0.6$.

Alternatives to choose the step size η

- Line search methods (there are different alternatives).
- Line search methods may use search directions other than the steepest descent direction.
- Conjugate gradient (method of choice for quadratic objectives $g(\mathbf{w}) = \mathbf{w}^\top \mathbf{A}\mathbf{w}$).
- Use a *Newton* search direction.

Gradient descent for linear regression (I)

- For simplicity, let us assume that the objective function $h(\mathbf{w})$ corresponds to the mean squared error

$$E(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(y_n - \mathbf{w}^\top \mathbf{x}_n)^2.$$

- We could also minimise the negative $LL(\mathbf{w})$ instead.

- We write the update equation as

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \frac{d}{d\mathbf{w}} E(\mathbf{w})\Big|_{\mathbf{w}=\mathbf{w}_k}.$$

Gradient descent for linear regression (II)

- Computing the gradient for $E(\mathbf{w})$, we get

$$\frac{d}{d\mathbf{w}}E(\mathbf{w}) = \frac{2}{N}\sum_{n=1}^{N}\left(\mathbf{w}^\top\mathbf{x}_n - y_n\right)\mathbf{x}_n = \frac{2}{N}\mathbf{X}^\top\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right).$$

- The update equation follows as

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta\frac{2}{N}\mathbf{X}^\top\left(\mathbf{X}\mathbf{w}_k - \mathbf{y}\right).$$

- The computation of the gradient involves using the whole dataset $(\mathbf{X}, \mathbf{y})$ at every step.

- For this reason, this algorithm is known as *batch gradient descent*.

Gradient descent and feature scaling

- Always normalise the features if using gradient descent.
- Gradient descent converges faster if all features have a similar scale.
- If the attributes are in very different scales, it may take a long time to converge.

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Online learning and large datasets

- Traiditionally in machine learning, the gradient $\mathbf{g}_k$ is computed using the whole dataset $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^{N}$.
- There are settings, though, where only a subset of the data can be used.
- **Online learning**: the instances $(\mathbf{x}_n, y_n)$ appear one at a time.
- **Large datasets**: computing the exact value for $\mathbf{g}_k$ would be expensive, if not impossible.

Stochastic gradient descent (I)

- In stochastic gradient descent (SGD), the gradient $\mathbf{g}_k$ is computed using a subset of the instances available.

update when new instances added

- The word stochastic refers to the fact that the value for $\mathbf{g}_k$ will depend on the subset of the instances chosen for computation.

Stochastic gradient descent (II)

- In the stochastic setting, a better estimate can be found if the gradient is computed using

$$\mathbf{g}_k = \frac{1}{|S|} \sum_{i \in S} \mathbf{g}_{k,i},$$

where $S \in \mathcal{D}$, $|S|$ is the cardinality of S, and $\mathbf{g}_{k,i}$ is the gradient at iteration k computed using the instance $(\mathbf{x}_i, y_i)$.

- This setting is called *mini-batch gradient descent*.

Step size in SGD

- Choosing the value of η is particularly important in SGD since there is no easy way to compute it.
- Usually the value of η will depend on the iteration k, η_k.
- It should follow the **Robbins-Monro** conditions

$$\sum_{k=1}^{\infty} \eta_k = \infty, \quad \sum_{k=1}^{\infty} \eta_k^2 < \infty.$$

- Various formulas for η_k can be used

$$\eta_k = \frac{1}{k}, \quad \eta_k = \frac{1}{(\tau_0 + k)^\kappa},$$

where τ_0 slows down early interations and $\kappa \in (0.5, 1]$.

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What is regularisation?

- It refers to a technique used for preventing overfitting in a predictive model.

- It consists in adding a term (a regulariser) to the objective function that encourages simpler solutions.

- With regularisation, the objective function for linear regression would be

$$h(\mathbf{w}) = E(\mathbf{w}) + \lambda R(\mathbf{w}),$$

  where $R(\mathbf{w})$ is the regularisation term and λ the regularisation parameter.

- In the expression for $h(\mathbf{w})$, we can use the negative $LL(\mathbf{w})$ instead of $E(\mathbf{w})$.

- If $\lambda = 0$, we get $h(\mathbf{w}) = E(\mathbf{w})$.

Different types of regularisation

- The objective function for linear regression would be

$$h(\mathbf{w}) = E(\mathbf{w}) + \lambda R(\mathbf{w}),$$

where $R(\mathbf{w})$ follows as

$$R(\mathbf{w}) = \alpha\|\mathbf{w}\|_1 + (1-\alpha)\frac{1}{2}\|\mathbf{w}\|_2^2,$$

where $\|\mathbf{w}\|_1 = \sum_{m=1}^{p} |w_m|$, and $\|\mathbf{w}\|_2^2 = \sum_{m=1}^{p} w_m^2$.

lawso relularisation

- If $\alpha = 1$, we get ℓ_1 regularisation.

- If $\alpha = 0$, we get ℓ_2 regularisation. Rich regression

- If $0 < \alpha < 1$, we get the elastic net regularisation.

Ridge regression or ℓ_2 regularisation

- In ridge regression, $\alpha = 0$,

$$h(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(y_n - \mathbf{w}^\top \mathbf{x}_n)^2 + \frac{\lambda}{2}\mathbf{w}^\top \mathbf{w},$$

- It can be shown that an optimal solution for $\mathbf{w}_*$ is given as

$$\mathbf{w}_* = \left(\mathbf{X}^\top \mathbf{X} + \frac{\lambda N}{2}\mathbf{I}\right)^{-1} \mathbf{X}^\top \mathbf{y}.$$

- Notice that we can also use iterative procedure for optimising $h(\mathbf{w})$ either through batch gradient decent, SGD or mini-batch SGD.