COMS21202: Symbols, Patterns and Signals Probabilistic Data Models

Dima Damen

Dima.Damen@bristol.ac.uk

Bristol University, Department of Computer Science Bristol BS8 1UB, UK

February 5, 2016

Data Modelling

- Deterministic models do not explicitly model uncertainties or 'randomness' in data
- Variability of inferences derived from the data is not included

Data Modelling

- Deterministic models do not explicitly model uncertainties or 'randomness' in data
- Variability of inferences derived from the data is not included
- In many tasks, we benefit from modelling uncertainty and randomness

Data Modelling

- Deterministic models do not explicitly model uncertainties or 'randomness' in data
- Variability of inferences derived from the data is not included
- In many tasks, we benefit from modelling uncertainty and randomness
- ► This is explicit in Probabilistic Models

Back to Fish - Discrete

Discrete variable:

Example

A fisherman returns with the daily catch of fish. If we select a fish at random from the hold, what species will it be? $fish \in \{salmon, seabass, cod, ...\}$

Back to Fish - Discrete

Discrete variable:

Example

A fisherman returns with the daily catch of fish. If we select a fish at random from the hold, what species will it be? $fish \in \{salmon, seabass, cod, ...\}$

A deterministic model would give one value, the most likely

Back to Fish - Discrete

Discrete variable:

Example

A fisherman returns with the daily catch of fish. If we select a fish at random from the hold, what species will it be?

```
\textit{fish} \in \{\textit{salmon}, \textit{seabass}, \textit{cod}, ...\}
```

- A deterministic model would give one value, the most likely
- A probabilistic model quantifies the chance/probability of the selected fish being one of the possible species.
- ▶ Model the probability $P(x_i = q_i)$ where $q_i \in \{salmon, seabass, cod, \cdots\}$

Continuous variable:

Example

Predict the weight of fish from its length

Let us assume that we think the weight of fish is directly proportional to its length, i.e. $weight = b \times length + a$.

Continuous variable:

Example

Predict the weight of fish from its length

Let us assume that we think the weight of fish is directly proportional to its length, i.e. weight = $b \times length + a$.

A probabilistic approach would model weight as a random variable and hypothesize that

$$weight = b \times length + a + \epsilon$$

Continuous variable:

Example

Predict the weight of fish from its length

Let us assume that we think the weight of fish is directly proportional to its length, i.e. $weight = b \times length + a$.

A **probabilistic approach** would model weight as a **random variable** and hypothesize that

$$weight = b \times length + a + \epsilon$$

where ϵ is a random variable, usually close to zero

$$weight = b \times length + a + \epsilon$$

➤ To model the random variable, we measure the difference between the *predicted* and *measured* weight values

$$weight = b \times length + a + \epsilon$$

- ➤ To model the random variable, we measure the difference between the *predicted* and *measured* weight values
- ▶ Modelled using a probability distribution for ϵ ,
 - by a uniform distribution
 - by a normal distribution
 - · · · ·

$$weight = b \times length + a + \epsilon$$

- ➤ To model the random variable, we measure the difference between the *predicted* and *measured* weight values
- ▶ Modelled using a probability distribution for ϵ ,
 - by a uniform distribution
 - by a normal distribution
 - **...**
- In the next slides, we will make the *logical* simplification (weight = 0 when length = 0)

$$weight = b \times length + a + \epsilon$$

- ➤ To model the random variable, we measure the difference between the predicted and measured weight values
- ▶ Modelled using a probability distribution for ϵ ,
 - by a uniform distribution
 - by a normal distribution
 - **...**
- ► In the next slides, we will make the *logical* simplification (weight = 0 when length = 0)
- As a conclusion, the y-intercept can be set to zero, and

$$weight = a \times length + \epsilon$$

$$weight = a \times length + \epsilon$$

This is a model with one parameter, apart from the uncertainty

$$weight = a \times length + \epsilon$$

This is a model with one parameter, apart from the uncertainty

We can assume, for example, that ϵ is $\mathcal{N}(0, \sigma^2)$

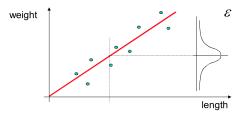
$$p(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\epsilon^2}{2\sigma^2}}$$

$$weight = a \times length + \epsilon$$

This is a model with one parameter, apart from the uncertainty

We can assume, for example, that ϵ is $\mathcal{N}(0, \sigma^2)$

$$p(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\epsilon^2}{2\sigma^2}}$$



- Similar to building deterministic models, probabilistic model parameters need to be tuned/trained
- Maximum-likelihood estimation (MLE) is a method of estimating the parameters of a probabilistic model.

- Similar to building deterministic models, probabilistic model parameters need to be tuned/trained
- Maximum-likelihood estimation (MLE) is a method of estimating the parameters of a probabilistic model.
- ightharpoonup Assume heta is a vector of all parameters of the probabilistic model
- ▶ MLE is an extremum estimator obtained by maximising an objective function of θ

Definition

Assume $f(\theta)$ is an objective function to be optimised (e.g. maximised), the *arg max* corresponds to the value of θ that attains the maximum value of the objective function f

Definition

Assume $f(\theta)$ is an objective function to be optimised (e.g. maximised), the $arg\ max$ corresponds to the value of θ that attains the maximum value of the objective function f

$$\hat{\theta} = arg \max_{\theta} f(\theta)$$

Definition

Assume $f(\theta)$ is an objective function to be optimised (e.g. maximised), the $arg\ max$ corresponds to the value of θ that attains the maximum value of the objective function f

$$\hat{\theta} = arg \max_{\theta} f(\theta)$$

Note: this is different than maximising the function (i.e. finding the maximum value $[max f(\theta)]$)

Definition

Assume $f(\theta)$ is an objective function to be optimised (e.g. maximised), the *arg max* corresponds to the value of θ that attains the maximum value of the objective function f

$$\hat{\theta} = arg \max_{\theta} f(\theta)$$

- Note: this is different than maximising the function (i.e. finding the maximum value $[max f(\theta)]$)
- Tuning the parameter is then equal to finding the maximum argument arg max

Given a set of N data points - x_i is length and y_i is weight in our *fishy* example

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}$$

Given a set of N data points - x_i is length and y_i is weight in our *fishy* example

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}\$$

- The probabilistic approach would:
 - derive expression for conditional probability of observing data D given parameter a

Given a set of N data points - x_i is length and y_i is weight in our *fishy* example

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}\$$

- The probabilistic approach would:
 - derive expression for conditional probability of observing data D given parameter a

 using observed data, find paramter value which maximises the conditional probability (i.e. the likelihood)

$$a_{ML} = arg max_a p(D|a)$$

Given a set of N data points

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}$$

Given a set of N data points

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}\$$

Assume that observations are independent - a common assumption often referred to as **i.i.d. independent and identically distributed** - then :

$$p(D|a) = \prod_{i=1}^{N} p(y_i|x_i, a)$$

Given a set of N data points

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}\$$

Assume that observations are independent - a common assumption often referred to as **i.i.d. independent and identically distributed** - then :

$$p(D|a) = \prod_{i=1}^{N} p(y_i|x_i, a)$$

Given $y_i = a x_i + \epsilon$, and ϵ is $\mathcal{N}(0, \sigma^2)$, then

$$p(y_i|x_i,a) \sim \mathcal{N}(ax_i,\sigma^2)$$

Given a set of N data points

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}\$$

Assume that observations are independent - a common assumption often referred to as **i.i.d. independent and identically distributed** - then :

$$p(D|a) = \prod_{i=1}^{N} p(y_i|x_i, a)$$

Given $y_i = a x_i + \epsilon$, and ϵ is $\mathcal{N}(0, \sigma^2)$, then

$$p(y_i|x_i,a) \sim \mathcal{N}(ax_i,\sigma^2)$$

For a large sample:

The average of y_i value will be a x_i

Given a set of N data points

$$D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}\$$

Assume that observations are independent - a common assumption often referred to as i.i.d. independent and identically distributed - then :

$$p(D|a) = \prod_{i=1}^{N} p(y_i|x_i, a)$$

Given $y_i = ax_i + \epsilon$, and ϵ is $\mathcal{N}(0, \sigma^2)$, then

$$p(y_i|x_i,a) \sim \mathcal{N}(ax_i,\sigma^2)$$

For a large sample:

- ► The average of *y_i* value will be *a x_i*
- ▶ The 'spread' will be the same as for ϵ , defined by σ^2

The conditional probability (for all data) is thus formulated as

$$p(D|a) = \prod_{i=1}^{N} p(y_i|x_i, a)$$

$$= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}}$$

$$a_{ML} = arg \, max_a \, p(D|a)$$

$$a_{ML} = arg \max_{a} p(D|a)$$

$$= arg \max_{a} \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}}$$

$$\begin{aligned} a_{ML} &= arg \, max_a \, p(D|a) \\ &= arg \, max_a \prod_{i=1}^N \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}} \\ &= arg \, max_a \sum_{i=1}^N \ln \left(\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}} \right) \end{aligned}$$

$$\begin{aligned} a_{ML} &= arg \max_{a} p(D|a) \\ &= arg \max_{a} \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_{i} - ax_{i})^{2}}{\sigma^{2}}} \\ &= arg \max_{a} \sum_{i=1}^{N} \ln \left(\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_{i} - ax_{i})^{2}}{\sigma^{2}}} \right) \\ &= arg \max_{a} \sum_{i=1}^{N} \ln \frac{1}{\sqrt{2\pi}\sigma} - \frac{(y_{i} - ax_{i})^{2}}{2\sigma^{2}} \end{aligned}$$

To tune the parameter, i.e. find the ML parameter,

$$a_{ML} = arg \max_{a} p(D|a)$$

$$= arg \max_{a} \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_{i} - ax_{i})^{2}}{\sigma^{2}}}$$

$$= arg \max_{a} \sum_{i=1}^{N} \ln \left(\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_{i} - ax_{i})^{2}}{\sigma^{2}}} \right)$$

$$= arg \max_{a} \sum_{i=1}^{N} \ln \frac{1}{\sqrt{2\pi}\sigma} - \frac{(y_{i} - ax_{i})^{2}}{2\sigma^{2}}$$

$$= arg \max_{a} \sum_{i=1}^{N} -(y_{i} - ax_{i})^{2} \qquad \text{(remove constants)}$$

To tune the parameter, i.e. find the ML parameter,

$$a_{ML} = arg \max_{a} p(D|a)$$

$$= arg \max_{a} \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_{i} - ax_{i})^{2}}{\sigma^{2}}}$$

$$= arg \max_{a} \sum_{i=1}^{N} \ln \left(\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_{i} - ax_{i})^{2}}{\sigma^{2}}} \right)$$

$$= arg \max_{a} \sum_{i=1}^{N} \ln \frac{1}{\sqrt{2\pi}\sigma} - \frac{(y_{i} - ax_{i})^{2}}{2\sigma^{2}}$$

$$= arg \max_{a} \sum_{i=1}^{N} -(y_{i} - ax_{i})^{2} \qquad \text{(remove constants)}$$

$$= arg \min_{a} \sum_{i=1}^{N} (y_{i} - ax_{i})^{2}$$

Deterministic Least Squares:

$$a_{LS} = arg \min_a R(a) = arg \min_a \sum_i (y_i - a x_i)^2$$

Probabilistic Maximum Likelihood:

$$a_{ML} = arg \, min_a \sum_i (y_i - a \, x_i)^2$$

Deterministic Least Squares:

$$a_{LS} = arg \min_{a} R(a) = arg \min_{a} \sum_{i} (y_i - a x_i)^2$$

Probabilistic Maximum Likelihood:

$$a_{ML} = arg \, min_a \sum_i (y_i - a \, x_i)^2$$

same answer, different view

Deterministic Least Squares:

$$a_{LS} = arg \min_{a} R(a) = arg \min_{a} \sum_{i} (y_i - a x_i)^2$$

Probabilistic Maximum Likelihood:

$$a_{ML} = arg \, min_a \sum_i (y_i - a \, x_i)^2$$

- same answer, different view
- ▶ Note: ML answer here assumes uncertainty is normally distributed

In both cases,

$$a_{ML} = arg \, min_a \sum_i (y_i - a \, x_i)^2$$

In both cases,

$$a_{ML} = arg \, min_a \sum_i (y_i - a \, x_i)^2$$

To find the minimum, find the derivative

$$\frac{d}{da}\sum_{i}(y_{i}-ax_{i})^{2}=-2\sum_{i}x_{i}(y_{i}-ax_{i})$$

In both cases,

$$a_{ML} = arg \, min_a \sum_i (y_i - a \, x_i)^2$$

To find the minimum, find the derivative

$$\frac{d}{da}\sum_{i}(y_{i}-ax_{i})^{2}=-2\sum_{i}x_{i}(y_{i}-ax_{i})$$

and equate it to zero

$$-2\sum_{i} x_{i}(y_{i} - a_{ML}x_{i}) = 0$$

$$\sum_{i} x_{i}y_{i} - a_{ML}\sum_{i} x_{i}^{2} = 0$$

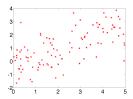
$$a_{ML} = \frac{\sum_{i} y_{i}x_{i}}{\sum_{i} x_{i}^{2}}$$

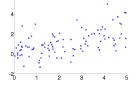
so why to take the probabilistic approach?

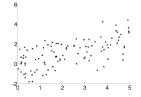
- so why to take the probabilistic approach?
- ▶ Probabilistic Models can tell us more

- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- ► For example: how much does *a_{ML}* vary if it is computed for many data samples? How reliable is it?

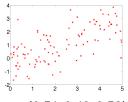
- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- For example: how much does a_{ML} vary if it is computed for many data samples? How reliable is it?

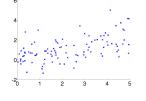


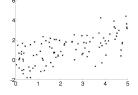




- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- For example: how much does a_{ML} vary if it is computed for many data samples? How reliable is it?



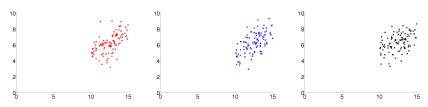




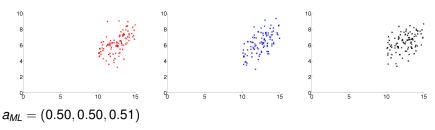
 $a_{ML} = (0.51, 0.49, 0.52)$

- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- ► For example: how much does *a_{ML}* vary if it is computed for many data samples? How reliable is it?

- so why to take the probabilistic approach?
- ► Probabilistic Models can tell us more
- ► For example: how much does a_{ML} vary if it is computed for many data samples? How reliable is it?



- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- ► For example: how much does a_{ML} vary if it is computed for many data samples? How reliable is it?



- so why to take the probabilistic approach?
- ▶ Probabilistic Models can tell us more
- ► For example: how much does *a_{ML}* vary if it is computed for many data samples? How reliable is it?

- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- For example: how much does a_{ML} vary if it is computed for many data samples? How reliable is it?
- ► For *M* different samples

$$Var(a_{ML}) = \frac{1}{M-1} \sum_{j=1}^{M} \left(a_{MLj} - \overline{a_{ML}} \right)$$

- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- ► For example: how much does *a_{ML}* vary if it is computed for many data samples? How reliable is it?
- ► For *M* different samples

$$Var(a_{ML}) = \frac{1}{M-1} \sum_{j=1}^{M} \left(a_{MLj} - \overline{a_{ML}} \right)$$

If

$$a_{ML} = \frac{\sum_{i} y_{i} x_{i}}{\sum_{i} x_{i}^{2}}$$

- so why to take the probabilistic approach?
- Probabilistic Models can tell us more
- ► For example: how much does *a_{ML}* vary if it is computed for many data samples? How reliable is it?
- ► For *M* different samples

$$Var(a_{ML}) = \frac{1}{M-1} \sum_{j=1}^{M} \left(a_{MLj} - \overline{a_{ML}} \right)$$

▶ If

$$a_{ML} = \frac{\sum_{i} y_{i} x_{i}}{\sum_{i} x_{i}^{2}}$$

ightharpoonup Then for the same values x_i

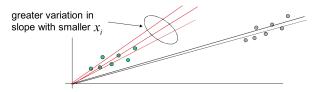
$$Var(a_{ML}) = \frac{\sigma^2}{\sum_i x_i^2}$$

$$Var(a_{ML}) = \frac{\sigma^2}{\sum_i x_i^2}$$

Variance is thus dependent on input variables

$$Var(a_{ML}) = \frac{\sigma^2}{\sum_i x_i^2}$$

Variance is thus dependent on input variables



 Maximum Likelihood Estimation (MLE) is a common method for solving such problems

```
\theta_{MLE} = \arg \max_{\theta} p(D|\theta)

= \arg \max_{\theta} \ln p(D|\theta)

= \arg \min_{\theta} - \ln p(D|\theta)
```

 Maximum Likelihood Estimation (MLE) is a common method for solving such problems

$$heta_{MLE} = arg \max_{\theta} p(D|\theta)$$

$$= arg \max_{\theta} \ln p(D|\theta)$$

$$= arg \min_{\theta} - \ln p(D|\theta)$$

 Maximum Likelihood Estimation (MLE) is a common method for solving such problems

$$heta_{MLE} = arg \max_{\theta} p(D|\theta)$$

$$= arg \max_{\theta} \ln p(D|\theta)$$

$$= arg \min_{\theta} - \ln p(D|\theta)$$

MLE Recipe

1. Determine θ , D and expression for likelihood $p(D|\theta)$

 Maximum Likelihood Estimation (MLE) is a common method for solving such problems

```
	heta_{MLE} = arg \max_{\theta} p(D|\theta)
= arg \max_{\theta} \ln p(D|\theta)
= arg \min_{\theta} - \ln p(D|\theta)
```

- 1. Determine θ , D and expression for likelihood $p(D|\theta)$
- 2. Take the natural logarithm of the likelihood

 Maximum Likelihood Estimation (MLE) is a common method for solving such problems

```
	heta_{MLE} = arg \max_{\theta} p(D|\theta)
= arg \max_{\theta} \ln p(D|\theta)
= arg \min_{\theta} - \ln p(D|\theta)
```

- 1. Determine θ , D and expression for likelihood $p(D|\theta)$
- 2. Take the natural logarithm of the likelihood
- 3. Take the derivative of $\ln p(D|\theta)$ w.r.t. θ . If θ is a multi-dimensional vector, take partial derivatives

 Maximum Likelihood Estimation (MLE) is a common method for solving such problems

```
	heta_{MLE} = arg \max_{\theta} p(D|\theta)
= arg \max_{\theta} \ln p(D|\theta)
= arg \min_{\theta} - \ln p(D|\theta)
```

- 1. Determine θ , D and expression for likelihood $p(D|\theta)$
- 2. Take the natural logarithm of the likelihood
- 3. Take the derivative of $\ln p(D|\theta)$ w.r.t. θ . If θ is a multi-dimensional vector, take partial derivatives
- 4. Set derivative(s) to 0 and solve for θ



MLE Recipe - Ex1

1. Determine θ , D and expression for likelihood $p(D|\theta)$

MLE Recipe - Ex1

1. Determine θ , D and expression for likelihood $p(D|\theta)$

$$p(D|a) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}}$$

MLE Recipe - Ex1

1. Determine θ , D and expression for likelihood $p(D|\theta)$

$$p(D|a) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}}$$

2. Take the natural logarithm of the likelihood

MLE Recipe - Ex1

1. Determine θ , D and expression for likelihood $p(D|\theta)$

$$p(D|a) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}}$$

2. Take the natural logarithm of the likelihood $a_{ML} = arg \min_{a} \sum_{i} (y_i - a x_i)^2$

MLE Recipe - Ex1

1. Determine θ , D and expression for likelihood $p(D|\theta)$

$$p(D|a) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_j)^2}{\sigma^2}}$$

- 2. Take the natural logarithm of the likelihood $a_{ML} = arg \min_{a} \sum_{i} (y_i a x_i)^2$
- 3. Take the derivative of $\ln p(D|\theta)$ w.r.t. θ . If θ is a multi-dimensional vector, take partial derivatives

MLE Recipe - Ex1

1. Determine θ , D and expression for likelihood $p(D|\theta)$

$$p(D|a) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}}$$

- 2. Take the natural logarithm of the likelihood $a_{ML} = arg \min_{a} \sum_{i} (y_i a x_i)^2$
- 3. Take the derivative of $\ln p(D|\theta)$ w.r.t. θ . If θ is a multi-dimensional vector, take partial derivatives $\frac{d}{da}\sum_{i}(y_{i}-ax_{i})^{2}=-2\sum_{i}x_{i}(y_{i}-ax_{i})$
- 4. Set derivative(s) to 0 and solve for θ

MLE Recipe - Ex1

1. Determine θ , D and expression for likelihood $p(D|\theta)$

$$p(D|a) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \frac{(y_i - ax_i)^2}{\sigma^2}}$$

- 2. Take the natural logarithm of the likelihood $a_{MI} = arg \min_{a} \sum_{i} (y_i a x_i)^2$
- 3. Take the derivative of $\ln p(D|\theta)$ w.r.t. θ . If θ is a multi-dimensional vector, take partial derivatives

$$\frac{d}{da}\sum_{i}(y_{i}-ax_{i})^{2}=-2\sum_{i}x_{i}(y_{i}-ax_{i})$$

4. Set derivative(s) to 0 and solve for θ

$$a_{ML} = \frac{\sum_{i} y_{i} x_{i}}{\sum_{i} x_{i}^{2}}$$

Example

Example

- Data: head/tail binary attempts (of size N)
- ▶ Model:
- Model Parameters:

Example

- Data: head/tail binary attempts (of size N)
- Model: Binomial distribution
- Model Parameters:

Example

- Data: head/tail binary attempts (of size N)
- Model: Binomial distribution
- Model Parameters: head probability α

Definition

The **binomial distribution** gives the probability distribution for a discrete variable to obtain exactly D successes out of N trials, where the probability of the success is α and the probability of failure is $(1 - \alpha)$ and $0 \le \alpha \le 1$

The binomial distribution probability density function is given by

$$P(D|N) = {N \choose D} \alpha^{D} (1 - \alpha)^{N-D}$$
$$= \frac{N!}{D!(N-D)!} \alpha^{D} (1 - \alpha)^{N-D}$$

Accordingly, using the binomial probability distribution where D is the number of heads in N coin tosses and θ is the probability of getting heads in a single toss,

$$P(D|\theta) = \binom{N}{D} \theta^{D} (1-\theta)^{N-D}$$

Accordingly, using the binomial probability distribution where D is the number of heads in N coin tosses and θ is the probability of getting heads in a single toss,

$$P(D|\theta) = \binom{N}{D} \theta^D (1-\theta)^{N-D}$$

Maximum Likelihood Estimation (MLE) would then be looking for

$$\theta_{ML} = arg \max_{\theta} p(D|\theta)$$

► Take the natural logarithm

$$P(D|\theta) = \binom{N}{D} \theta^D (1-\theta)^{N-D}$$

Take the natural logarithm

$$P(D|\theta) = \binom{N}{D} \theta^{D} (1-\theta)^{N-D}$$

$$\ln P(D|\theta) = \ln \binom{N}{D} + D \ln \theta + (N-D) \ln (1-\theta)$$

Take the natural logarithm

$$P(D|\theta) = \binom{N}{D} \theta^{D} (1-\theta)^{N-D}$$

$$\ln P(D|\theta) = \ln \binom{N}{D} + D \ln \theta + (N-D) \ln (1-\theta)$$

Take the derivative w.r.t θ

Take the natural logarithm

$$P(D|\theta) = \binom{N}{D} \theta^{D} (1 - \theta)^{N-D}$$

$$\ln P(D|\theta) = \ln \binom{N}{D} + D \ln \theta + (N - D) \ln(1 - \theta)$$

▶ Take the derivative w.r.t θ

$$\frac{d}{d\theta}\ln P(D|\theta) = D\frac{1}{\theta} + (N-D)\frac{1}{1-\theta}(-1)$$

Take the natural logarithm

$$P(D|\theta) = \binom{N}{D} \theta^{D} (1 - \theta)^{N-D}$$

$$\ln P(D|\theta) = \ln \binom{N}{D} + D \ln \theta + (N - D) \ln(1 - \theta)$$

Take the derivative w.r.t θ

$$\frac{d}{d\theta} \ln P(D|\theta) = D\frac{1}{\theta} + (N - D)\frac{1}{1 - \theta}(-1)$$
$$= \frac{D}{\theta} - \frac{N - D}{1 - \theta}$$

$$\frac{D}{\theta_{ML}} - \frac{N - D}{1 - \theta_{ML}} = 0$$

$$\begin{split} \frac{D}{\theta_{ML}} - \frac{N - D}{1 - \theta_{ML}} &= 0\\ \frac{D(1 - \theta_{ML}) - (N - D)\theta_{ML}}{\theta_{ML}(1 - \theta_{ML})} &= 0 \end{split}$$

 \blacktriangleright Set the derivative to 0 and solve for θ

$$\begin{aligned} \frac{D}{\theta_{ML}} - \frac{N - D}{1 - \theta_{ML}} &= 0\\ \frac{D(1 - \theta_{ML}) - (N - D)\theta_{ML}}{\theta_{ML}(1 - \theta_{ML})} &= 0\\ D - N\theta_{ML} &= 0 \end{aligned}$$

 \blacktriangleright Set the derivative to 0 and solve for θ

$$\frac{D}{\theta_{ML}} - \frac{N - D}{1 - \theta_{ML}} = 0$$

$$\frac{D(1 - \theta_{ML}) - (N - D)\theta_{ML}}{\theta_{ML}(1 - \theta_{ML})} = 0$$

$$D - N\theta_{ML} = 0$$

$$\theta_{ML} = \frac{D}{N}$$

 \blacktriangleright Set the derivative to 0 and solve for θ

$$\begin{split} \frac{D}{\theta_{ML}} - \frac{N - D}{1 - \theta_{ML}} &= 0\\ \frac{D(1 - \theta_{ML}) - (N - D)\theta_{ML}}{\theta_{ML}(1 - \theta_{ML})} &= 0\\ D - N\theta_{ML} &= 0\\ \theta_{ML} &= \frac{D}{N} \end{split}$$

In conclusion, the probability of heads is the relative frequency of heads to the sample

Example

- Data: head/tail binary attempts (of size N)
- ▶ Model:
- Model Parameters:

Example

Given a coin, you were assigned the task of figuring out whether the coin will land on its head or tails. You were asked to build a probabilistic model (i.e. with confidence)

What if you chose another model?

- Data: head/tail binary attempts (of size N)
- ▶ Model:
- ► Model Parameters:

Example

Given a coin, you were assigned the task of figuring out whether the coin will land on its head or tails. You were asked to build a probabilistic model (i.e. with confidence)

What if you chose another model?

Data: head/tail binary attempts (of size N)

Model: Normal distribution

Model Parameters:

Example

Given a coin, you were assigned the task of figuring out whether the coin will land on its head or tails. You were asked to build a probabilistic model (i.e. with confidence)

What if you chose another model?

- Data: head/tail binary attempts (of size N)
- Model: Normal distribution
- ▶ Model Parameters: mean μ assume σ is a constant

Assume $D = \{d_1, d_2, \cdots d_N\}$ are *noisy* measurements of an actual signal $\theta = \mu$, where noise is Gaussian,

$$p(D|\theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(d_i-\theta)^2}{2\sigma^2}}$$

i.e. $D = \{0, 0, 1, 1, 1, \cdots\}$ where 0 represents tails and 1 represents heads...

$$\rho(D|\theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(d_i-\theta)^2}{2\sigma^2}}$$

$$p(D|\theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(d_i-\theta)^2}{2\sigma^2}}$$

$$\ln p(D|\theta) = N \ln \frac{1}{\sqrt{2\pi}\sigma} + \sum_{i=1}^{N} -\frac{(d_i - \theta)^2}{2\sigma^2}$$

$$p(D|\theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(d_i - \theta)^2}{2\sigma^2}}$$

$$\ln p(D|\theta) = N \ln \frac{1}{\sqrt{2\pi}\sigma} + \sum_{i=1}^{N} -\frac{(d_i - \theta)^2}{2\sigma^2}$$

$$\frac{d}{d\theta} \ln p(D|\theta) = \sum_{i=1}^{N} -\frac{2(d_i - \theta)(-1)}{2\sigma^2}$$

$$\sum_{i=1}^{N} \frac{(d_i - \theta_{ML})}{\sigma^2} = 0$$

$$\sum_{i=1}^{N} d_i - N\theta_{ML} = 0$$

$$\theta_{ML} = \frac{1}{N} \sum_{i=1}^{N} d_i$$

$$\theta_{ML} = \overline{d}$$

Example

Given a coin, you were assigned the task of figuring out whether the coin will land on its head or tails. You were asked to build a probabilistic model (i.e. with confidence)

Use binomial distribution for likelihood.

$$\theta_{ML} = \frac{D}{N}$$

where D is the number of success (i.e. heads)

Use Gaussian distribution for likelihood

$$\theta_{ML} = \frac{1}{N} \sum_{i=1}^{N} d_i$$

where $d_i = 1$ if success (i.e. heads) or $d_i = 0$ if failure (i.e. tails)

same answer, different view

Probabilistic Model - Likelihood and Prior

- MLE ignores any prior knowledge we may have about θ
- ▶ If we have prior knowledge about values that θ is likely to have, then we can built this into MLE

$$\theta_{ML} = arg \max_{\theta} p(D|\theta) p(\theta)$$

Probabilistic Model - Likelihood and Prior

- MLE ignores any prior knowledge we may have about θ
- If we have prior knowledge about values that θ is likely to have, then we can built this into MLE

$$\theta_{ML} = arg \max_{\theta} p(D|\theta) p(\theta)$$

This is known as Maximum a Posteriori (MAP) estimation

Example

Given a coin, you were assigned the task of figuring out whether the coin will land on its head or tails. You were asked to build a probabilistic model (i.e. with confidence)

Suppose we want to utilise our prior belief that coins are typically fair

Example

- Suppose we want to utilise our prior belief that coins are typically fair
- ▶ $p(\theta)$ would peak around $\theta = 0.5$

Example

- Suppose we want to utilise our prior belief that coins are typically fair
- ▶ $p(\theta)$ would peak around $\theta = 0.5$
- Let's use

$$p(\theta) = \theta (1 - \theta)$$

Example

- Suppose we want to utilise our prior belief that coins are typically fair
- ▶ $p(\theta)$ would peak around $\theta = 0.5$
- Let's use

$$p(\theta) = \frac{b}{\theta} \theta (1 - \theta)$$

Example

Given a coin, you were assigned the task of figuring out whether the coin will land on its head or tails. You were asked to build a probabilistic model (i.e. with confidence)

- Suppose we want to utilise our prior belief that coins are typically fair
- ▶ $p(\theta)$ would peak around $\theta = 0.5$
- Let's use

$$p(\theta) = \frac{b}{\theta} \theta (1 - \theta)$$

where *b* is a normalising factor so the area under the curve is equal to 1

Likelihood:

$$p(D|\theta) = \binom{N}{D} \theta^D (1-\theta)^{N-D}$$

Prior:

$$p(\theta) = b\theta(1-\theta)$$

Posterior:

$$p(D|\theta) p(\theta) = \binom{N}{D} \theta^{D} (1-\theta)^{N-D} b \theta (1-\theta)$$

$$p(D|\theta) p(\theta) = \binom{N}{D} \theta^{D} (1-\theta)^{N-D} b \theta (1-\theta)$$

$$p(D|\theta) p(\theta) = \binom{N}{D} \theta^{D} (1-\theta)^{N-D} b \theta (1-\theta)$$

$$\ln p(D|\theta) p(\theta) = \ln \binom{N}{D} + D \ln \theta + (N-D) \ln(1-\theta) + \ln b + \ln \theta + \ln(1-\theta)$$

$$p(D|\theta) p(\theta) = \binom{N}{D} \theta^{D} (1-\theta)^{N-D} b \theta (1-\theta)$$

$$\ln p(D|\theta) p(\theta) = \ln \binom{N}{D} + D \ln \theta + (N-D) \ln(1-\theta) + \ln b + \ln \theta + \ln(1-\theta)$$

$$\frac{d}{d\theta}\ln p(D|\theta)\,p(\theta) = D\frac{1}{\theta} - (N-D)\frac{1}{1-\theta} + \frac{1}{\theta} - \frac{1}{(1-\theta)}$$

$$D\frac{1}{\theta_{MAP}} - (N-D)\frac{1}{1-\theta_{MAP}} + \frac{1}{\theta_{MAP}} - \frac{1}{(1-\theta_{MAP})} = 0$$

$$D\frac{1}{\theta_{MAP}} - (N - D)\frac{1}{1 - \theta_{MAP}} + \frac{1}{\theta_{MAP}} - \frac{1}{(1 - \theta_{MAP})} = 0$$

$$\frac{D + 1}{\theta_{MAP}} - (N - D + 1)\frac{1}{1 - \theta_{MAP}} = 0$$

$$D\frac{1}{\theta_{MAP}} - (N - D)\frac{1}{1 - \theta_{MAP}} + \frac{1}{\theta_{MAP}} - \frac{1}{(1 - \theta_{MAP})} = 0$$

$$\frac{D + 1}{\theta_{MAP}} - (N - D + 1)\frac{1}{1 - \theta_{MAP}} = 0$$

$$\frac{(D + 1)(1 - \theta_{MAP}) - (N - D + 1)\theta_{MAP}}{\theta_{MAP}(1 - \theta_{MAP})} = 0$$

$$D\frac{1}{\theta_{MAP}} - (N - D)\frac{1}{1 - \theta_{MAP}} + \frac{1}{\theta_{MAP}} - \frac{1}{(1 - \theta_{MAP})} = 0$$

$$\frac{D + 1}{\theta_{MAP}} - (N - D + 1)\frac{1}{1 - \theta_{MAP}} = 0$$

$$\frac{(D + 1)(1 - \theta_{MAP}) - (N - D + 1)\theta_{MAP}}{\theta_{MAP}(1 - \theta_{MAP})} = 0$$

$$\theta_{MAP} = \frac{D + 1}{N + 2}$$

▶ Set the derivative to 0 and solve for θ_{MAP}

$$\begin{split} & D \frac{1}{\theta_{MAP}} - (N - D) \frac{1}{1 - \theta_{MAP}} + \frac{1}{\theta_{MAP}} - \frac{1}{(1 - \theta_{MAP})} = 0 \\ & \frac{D + 1}{\theta_{MAP}} - (N - D + 1) \frac{1}{1 - \theta_{MAP}} = 0 \\ & \frac{(D + 1)(1 - \theta_{MAP}) - (N - D + 1)\theta_{MAP}}{\theta_{MAP}(1 - \theta_{MAP})} = 0 \\ & \theta_{MAP} = \frac{D + 1}{N + 2} \end{split}$$

 The prior added two 'virtual' coin tosses, one with heads and one with tails

Conclusion

- Probabilistic models encode randomness in the data
- They enable predicting confidence (as a probability)
- Parameters of the model are tuned
- Maximum Likelihood Estimation (MLE) is a recipe used for training model parameters
- MLE does not encode our prior knowledge of possible parameters
- Maximum a Posteriori (MAP) maximises likelihood along with prior

Further Reading

- Probability and Statistics for Engineers and Scientists
 Walpole et al (2007)
 - Section 3.1
 - Section 3.2
 - Section 4.1
 - Section 4.2
- Statistical Learning Methods Russell and Norvig (2003)
 - Chapter 20 (p. 712 720)