Basics of Model-Based Learning

Michael U. Gutmann

Probabilistic Modelling and Reasoning (INFR11134)
School of Informatics, The University of Edinburgh

Autumn Semester 2025

Recap

- Topic 1: Representation What reasonably weak assumptions can we make to efficiently represent $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$?
  - Directed and undirected graphical models
  - Factorisation and independencies
- Topic 2: Exact inference Can we further exploit the assumptions on $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$ to efficiently compute the posterior probability or derived quantities?
  - Yes! Factorisation can be exploited by using the distributive law and by caching computations.
  - Variable elimination and message passing algorithms
  - Inference for hidden Markov models

Recap

$$p(\mathbf{x}|\mathbf{y}_o) = \frac{\sum_{\mathbf{z}} p(\mathbf{x},\mathbf{y}_o,\mathbf{z})}{\sum_{\mathbf{x},\mathbf{z}} p(\mathbf{x},\mathbf{y}_o,\mathbf{z})}$$

- Topic 3: Actions and decision making How to predict the outcome of actions and choose optimal actions?
  - Actions as interventions in the data generating process.
  - Graph surgery and different ways to compute postinterventional distributions
  - Decision theory and common loss functions
  - Some loss functions were related to learning from data
- Issue 4: Where do the non-negative numbers $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$ come from?

  Topic 4: Learning How can we learn the numbers from data?

Program

1. Basic concepts
2. Learning by maximum likelihood estimation
3. Learning by Bayesian inference

Program

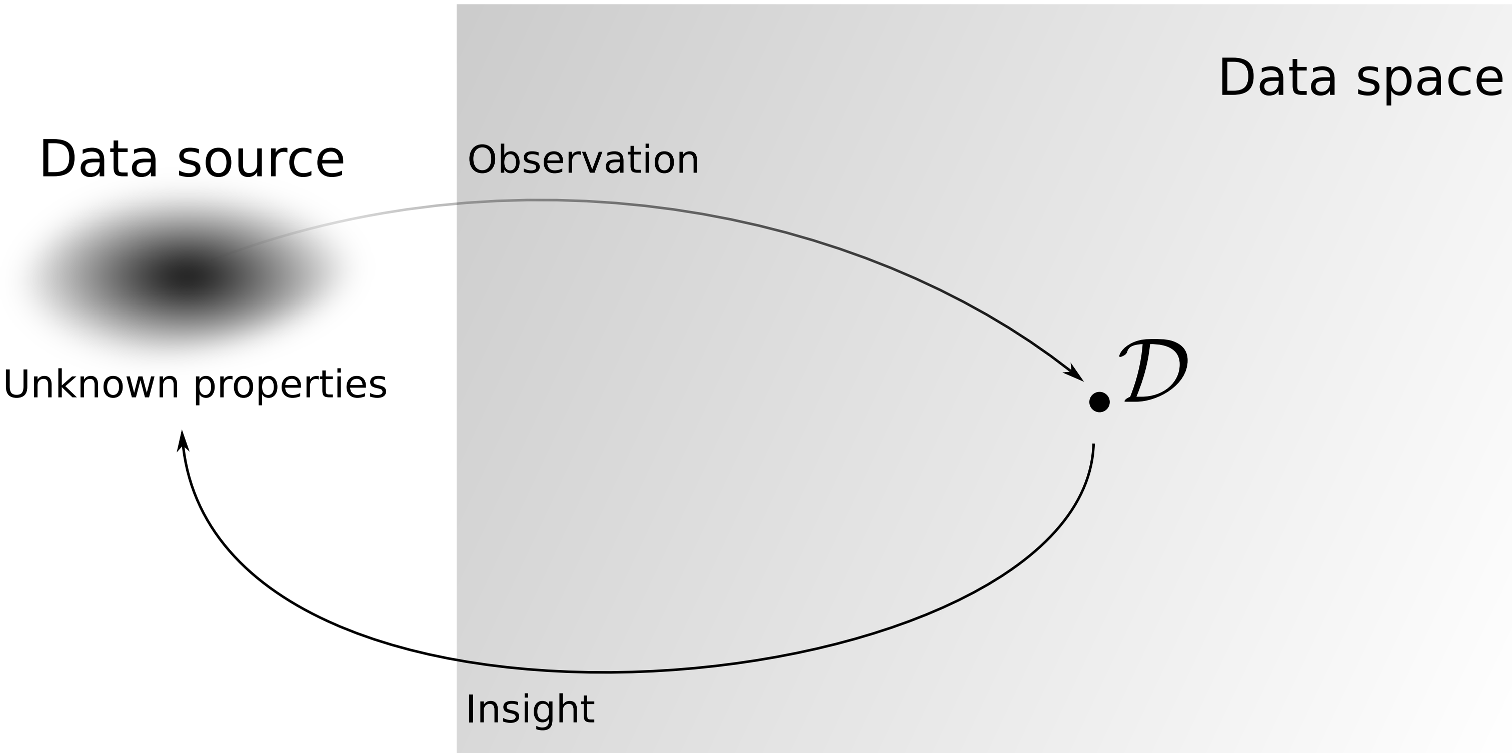
1. Basic concepts
   - Observed data as a sample drawn from an unknown data generating distribution
   - Probabilistic, statistical, and Bayesian models
   - Partition function and unnormalised statistical models
   - Learning = parameter estimation or learning = Bayesian inference

2. Learning by maximum likelihood estimation

3. Learning by Bayesian inference

Learning from data

- Use observed data $\mathcal{D}$ to learn about their source
- Enables probabilistic inference, decision making, ...



Data

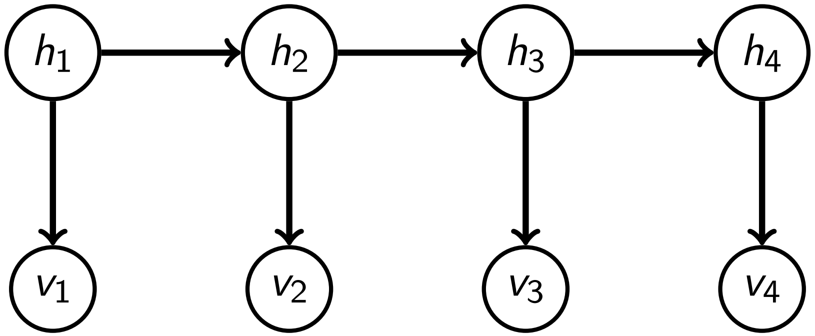
- We typically assume that the observed data $\mathcal{D}$ correspond to a random sample (draw) from an unknown distribution $p_*(\mathcal{D})$

$$\mathcal{D} \sim p_*(\mathcal{D})$$

- In other words, we consider the data $\mathcal{D}$ to be a realisation (observation) of a random variable with distribution p_*.

Data

- Example: You use some transition and emission distribution and generate data from the hidden Markov model.
  (e.g. via ancestral sampling)



- You know the visibles $(v_1, v_2, v_3, \ldots, v_T) \sim p(v_1, \ldots, v_T)$.
- You give the generated visibles to a friend who does not know about the distributions that you used, nor possibly that you used a HMM. For your friend:

$$\mathcal{D} = (v_1, v_2, v_3, \ldots, v_T) \qquad \mathcal{D} \sim p_*(\mathcal{D})$$

Independent and identically distributed (iid) data

- Let $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. If

$$p_*(\mathcal{D}) = \prod_{i=1}^{n} p_*(\mathbf{x}_i)$$

  then the data (or the corresponding random variables) are said to the iid. $\mathcal{D}$ is also said to be a random sample from p_*.
- In other words, the $\mathbf{x}_i$ were independently drawn from the same distribution $p_*(\mathbf{x})$.
- Example: n time series $(v_1, v_2, v_3, \ldots, v_T)$ each independently generated with the same transition and emission distribution.

Independent and identically distributed (iid) data

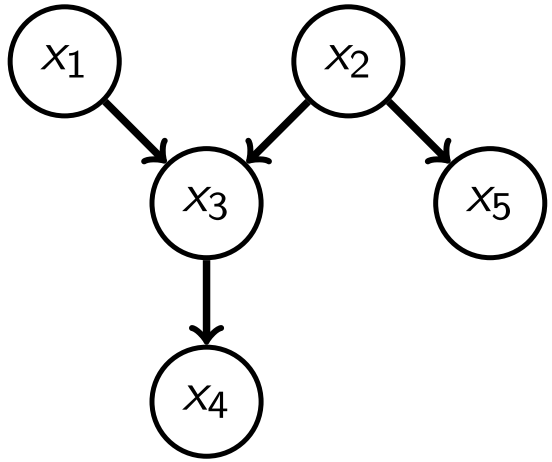
- Example: Generate n samples $(x_1^{(i)}, \ldots, x_5^{(i)})$ from

$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_2)p(x_3|x_1, x_2)p(x_4|x_3)p(x_5|x_2)$$

  with known conditionals, using e.g. ancestral sampling.
- You collect the n observed values of x_4, i.e.

$$x_4^{(1)}, \ldots, x_4^{(n)}$$

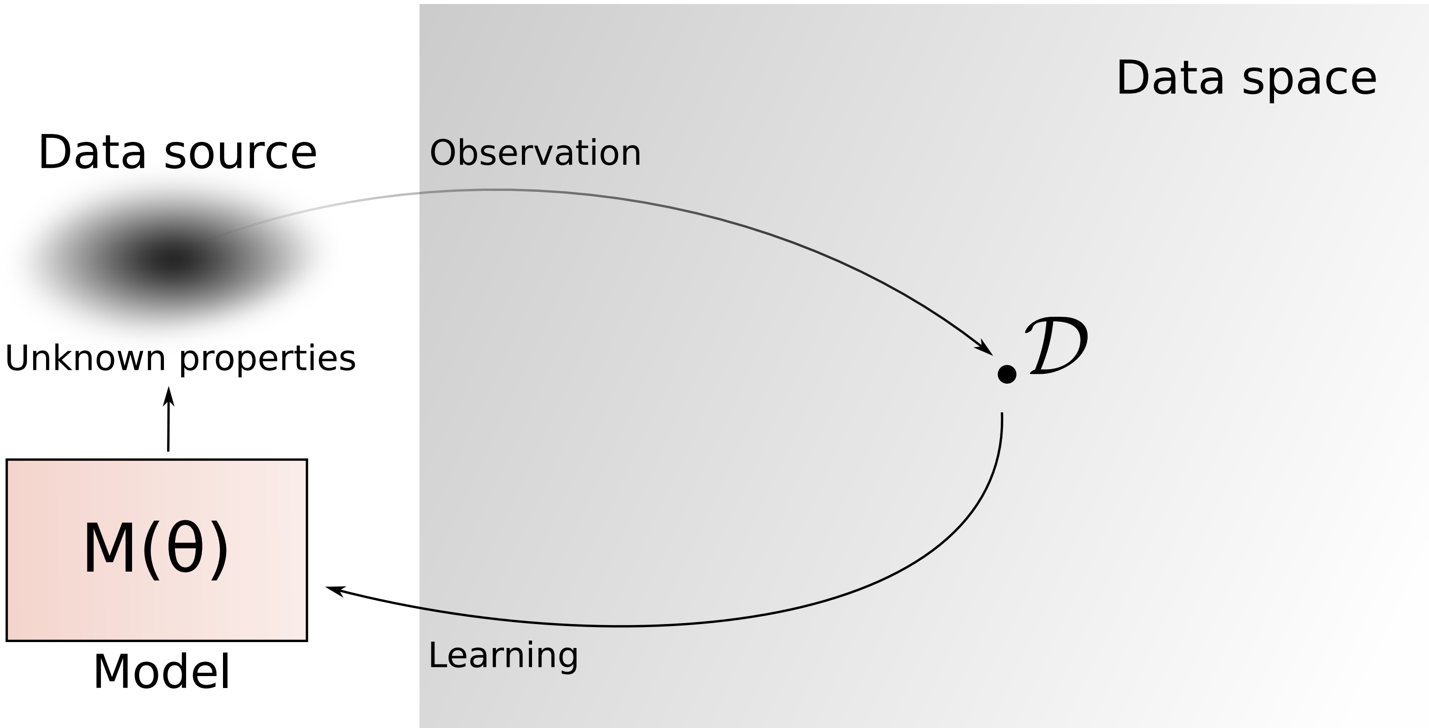
  and give them to a friend who does not know how you generated the data but that they are iid.



- For your friend, the $x_4^{(i)}$ are data points $x_i \sim p_*$.
- Remark: if the subscript index is occupied, we often use superscripts to enumerate the data points.

Using models to learn from data

- Set up a model with properties that the unknown data source might have.
- The potential properties are the parameters $\boldsymbol{\theta}$ of the model.
- Model may include independence and parametric family assumptions.
- Learning: Assess which $\boldsymbol{\theta}$ are in line with the observed data $\mathcal{D}$.



Models

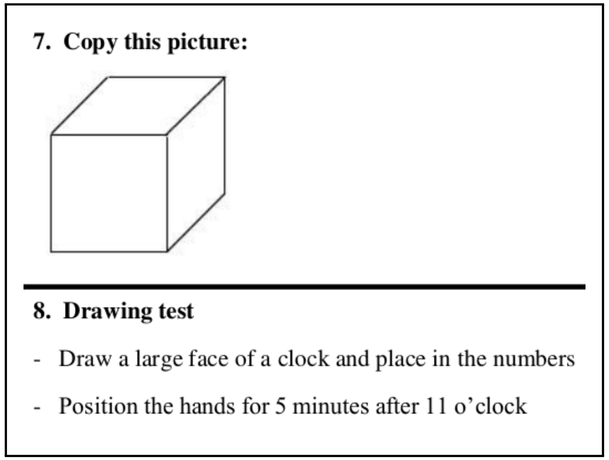
- The term “model” has multiple meanings, see e.g. `https://en.wikipedia.org/wiki/Model`
- In our course:
  - probabilistic model
  - statistical model
  - Bayesian model
- See Section 3 in the background document *Introduction to Probabilistic Modelling*
- Note: the three types are often confounded, and often just called probabilistic or statistical model, or just “model”.

Probabilistic model

Example from the first lecture: cognitive impairment test

- Sensitivity of 0.8 and specificity of 0.95 (Scharre, 2010)
- *Probabilistic* model for presence of impairment ($x = 1$) and detection by the test ($y = 1$):

$$\mathbb{P}(x = 1) = 0.11 \quad \text{(prior)}$$
$$\mathbb{P}(y = 1|x = 1) = 0.8 \quad \text{(sensitivity)}$$
$$\mathbb{P}(y = 0|x = 0) = 0.95 \quad \text{(specificity)}$$


7. Copy this picture:

8. Drawing test

- Draw a large face of a clock and place in the numbers
- Position the hands for 5 minutes after 11 o'clock

(Example from sagetest.osu.edu)

- From first lecture:
  A probabilistic model is an abstraction of reality that uses probability theory to quantify the chance of uncertain events.

Probabilistic model

- In brief: probabilistic model $\equiv$ probability distribution (pmf/pdf).
- Probabilistic model was written in terms of the probability $\mathbb{P}$. In terms of the pmf it is

$$
\begin{aligned}
p_x(1) &= 0.11 \\
p_{y|x}(1|1) &= 0.8 \\
p_{y|x}(0|0) &= 0.95
\end{aligned}
$$

- Commonly written as

$$
\begin{aligned}
p(x = 1) &= 0.11 \\
p(y = 1|x = 1) &= 0.8 \\
p(y = 0|x = 0) &= 0.95
\end{aligned}
$$

where the notation for probability measure $\mathbb{P}$ and pmf p are confounded.

Statistical model

- If we substitute the numbers with parameters, we obtain a (parametric) *statistical* model

$$
\begin{aligned}
p(x=1) &= \theta_1 \\
p(y=1|x=1) &= \theta_2 \\
p(y=0|x=0) &= \theta_3
\end{aligned}
$$

- For each value of the θ_i, we obtain a different pmf. Dependency highlighted by writing

$$
\begin{aligned}
p(x=1; \theta_1) &= \theta_1 \\
p(y=1|x=1; \theta_2) &= \theta_2 \\
p(y=0|x=0; \theta_3) &= \theta_3
\end{aligned}
$$

- Or: $p(x, y; \boldsymbol{\theta})$ where $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$ is a vector of parameters.
- A statistical model corresponds to a set/family of probabilistic models, here indexed by the parameters $\boldsymbol{\theta}$: $\{p(\mathbf{x}; \boldsymbol{\theta})\}_{\boldsymbol{\theta}}$

Bayesian model

- In *Bayesian* models, we combine statistical models with a (prior) probability distribution on the parameters $\boldsymbol{\theta}$.
- Each member of the family $\{p(\mathbf{x}; \boldsymbol{\theta})\}_{\boldsymbol{\theta}}$ is considered a conditional pmf/pdf of $\mathbf{x}$ given $\boldsymbol{\theta}$
- Use conditioning notation $p(\mathbf{x}|\boldsymbol{\theta})$
- The conditional $p(\mathbf{x}|\boldsymbol{\theta})$ and the pmf/pdf $p(\boldsymbol{\theta})$ for the (prior) distribution of $\boldsymbol{\theta}$ together specify the joint pmf/pdf via the product rule
$$p(\mathbf{x}, \boldsymbol{\theta}) = p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})$$
- Bayesian model for $\mathbf{x}$ = probabilistic model for $(\mathbf{x}, \boldsymbol{\theta})$.
- The prior may be parameterised, e.g. $p(\boldsymbol{\theta}; \boldsymbol{\alpha})$. The parameters $\boldsymbol{\alpha}$ are called "hyperparameters".

Graphical models as statistical models

- Directed or undirected graphical models are sets of probability distributions, e.g. all p that factorise as

$$p(\mathbf{x}) = \prod_i p(x_i|\mathrm{pa}_i) \quad \text{or} \quad p(\mathbf{x}) \propto \prod_i \phi_i(\mathcal{X}_i)$$

  They are thus statistical models.

- If we consider parametric families for $p(x_i|\mathrm{pa}_i)$ and $\phi_i(\mathcal{X}_i)$, they correspond to parametric statistical models

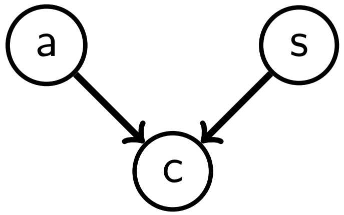
$$p(\mathbf{x};\boldsymbol{\theta}) = \prod_i p(x_i|\mathrm{pa}_i;\boldsymbol{\theta}_i) \quad \text{or} \quad p(\mathbf{x};\boldsymbol{\theta}) \propto \prod_i \phi_i(\mathcal{X}_i;\boldsymbol{\theta}_i)$$

  where $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots)$.

Cancer-asbestos-smoking example (Barber Figure 9.4)

- Very simple toy example about the relationship between lung Cancer, Asbestos exposure, and Smoking

DAG:



Factorisation:
$p(c, a, s) = p(c|a, s)p(a)p(s)$

Parametric models: (for binary vars)

$$p(a = 1; \theta_a) = \theta_a$$
$$p(s = 1; \theta_s) = \theta_s$$

$p(c = 1 \mid a, s; \boldsymbol{\theta}_c)$	a	s
θ_c^1	0	0
θ_c^2	1	0
θ_c^3	0	1
θ_c^4	1	1

All parameters are ≥ 0

- Factorisation + parametric models for the factors gives the parametric statistical model

$$p(c, a, s; \boldsymbol{\theta}) = p(c|a, s; \boldsymbol{\theta}_c)p(a; \theta_a)p(s; \theta_s) \qquad \boldsymbol{\theta} = (\theta_a, \theta_s, \boldsymbol{\theta}_c)$$

Cancer-asbestos-smoking example

- The model specification $p(a = 1; \theta_a) = \theta_a$ is equivalent to

$$
\begin{aligned}
p(a; \theta_a) &= (\theta_a)^a (1 - \theta_a)^{1-a} \\
&= \theta_a^{\mathbb{1}(a=1)} (1 - \theta_a)^{\mathbb{1}(a=0)}
\end{aligned}
$$

  Note: $(\theta_a)^a$ means parameter θ_a to the power of a.
- a is a Bernoulli random variable with "success" probability θ_a.
- Equivalently for s.

Cancer-asbestos-smoking example

- Table parameterisation $p(c|a, s; \boldsymbol{\theta}_c)$, with $\boldsymbol{\theta}_c = (\theta_c^1, \ldots, \theta_c^4)$, can be written more compactly in similar form.
- Enumerate the states of the parents of c so that

$$\mathrm{pa}_c = 1 \Leftrightarrow (a = 0, s = 0) \quad \ldots \quad \mathrm{pa}_c = 4 \Leftrightarrow (a = 1, s = 1)$$

- We then have

$$\begin{aligned} p(c|a, s; \boldsymbol{\theta}_c) &= \prod_{j=1}^{4} \left[(\theta_c^j)^c (1 - \theta_c^j)^{1-c} \right]^{\mathbb{1}(\mathrm{pa}_c = j)} \\ &= \prod_{j=1}^{4} (\theta_c^j)^{\mathbb{1}(c=1, \mathrm{pa}_c = j)} (1 - \theta_c^j)^{\mathbb{1}(c=0, \mathrm{pa}_c = j)} \end{aligned}$$

  Product over the possible states of the parents and the possible states of c.
- Equivalent to the table but more convenient to manipulate.

Cancer-asbestos-smoking example

- Working with the table representation does not shrink the set of probabilistic models.
- Set of $p(c, a, s)$ defined by the DAG = parametric family $\{p(c, a, s; \boldsymbol{\theta})\}_{\boldsymbol{\theta}}$, where $\boldsymbol{\theta}$ are the parameters in the table.
- Other parametric models are possible too:
  - As before but some parameters are tied, e.g. $\theta_c^2 = \theta_c^3$
  - $p(c = 1|a, s) = \sigma\left(w_0 + w_1 a + w_2 s\right)$ where $\sigma()$ is the sigmoid function $\sigma(u) = 1/(1 + \exp(-u))$.

In both cases, the parameterisation limits the space of possible probabilistic models.

(see slides *Basic Assumptions for Efficient Model Representation*)

Cancer-asbestos-smoking example

- We can turn the table-based parametric model into a Bayesian model by assigning a (prior) probability distribution to $\boldsymbol{\theta}$
- Often: we assume independence of the parameters so that the prior pdf/pmf factorises, e.g.

$$p(\boldsymbol{\theta}) = p(\theta_a)p(\theta_s)\prod_{j=1}^{4} p(\theta_c^j)$$

- With correspondence $p(\mathbf{x};\boldsymbol{\theta}) = p(\mathbf{x}|\boldsymbol{\theta})$, the Bayesian model is

$$\begin{aligned} p(\mathbf{x},\boldsymbol{\theta}) &= p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \\ &= \theta_a^{\mathbb{1}(a=1)}(1-\theta_a)^{\mathbb{1}(a=0)}p(\theta_a)\theta_s^{\mathbb{1}(s=1)}(1-\theta_s)^{\mathbb{1}(s=0)}p(\theta_s) \\ &\quad \prod_{j=1}^{4}(\theta_c^j)^{\mathbb{1}(c=1,\mathrm{pa}_c=j)}(1-\theta_c^j)^{\mathbb{1}(c=0,\mathrm{pa}_c=j)}\prod_{j=1}^{4} p(\theta_c^j) \end{aligned}$$

- Note the factorisation.

Partition function

- pdfs/pmfs integrate/sum to one.
- Parameterised Gibbs distributions

$$p(\mathbf{x};\boldsymbol{\theta}) \propto \prod_i \phi_i(\mathcal{X}_i;\boldsymbol{\theta}_i)$$

  do typically not integrate/sum one.
- For normalisation, we can divide the unnormalised model $\tilde{p}(\mathbf{x};\boldsymbol{\theta}) = \prod_i \phi_i(\mathcal{X}_i;\boldsymbol{\theta}_i)$ by the partition function $Z(\boldsymbol{\theta})$,

$$Z(\boldsymbol{\theta}) = \int \tilde{p}(\mathbf{x};\boldsymbol{\theta})\mathrm{d}\mathbf{x} \quad \text{or} \quad Z(\boldsymbol{\theta}) = \sum_{\mathbf{x}} \tilde{p}(\mathbf{x};\boldsymbol{\theta}).$$

- By construction,

$$p(\mathbf{x};\boldsymbol{\theta}) = \frac{\tilde{p}(\mathbf{x};\boldsymbol{\theta})}{Z(\boldsymbol{\theta})}$$

  sums/integrates to one for all values of $\boldsymbol{\theta}$.

Unnormalised statistical models

- If each element of $\{p(\mathbf{x};\boldsymbol{\theta})\}_{\boldsymbol{\theta}}$ integrates/sums to one

$$\int p(\mathbf{x};\boldsymbol{\theta})\mathrm{d}\mathbf{x} = 1 \quad \text{or} \quad \sum_{\mathbf{x}} p(\mathbf{x};\boldsymbol{\theta}) = 1$$

  for all $\boldsymbol{\theta}$, we say that the statistical model is normalised.
- If not, the statistical model is unnormalised.
- Undirected graphical models generally correspond to unnormalised models.
- But: partition function $Z(\boldsymbol{\theta})$ may be hard to evaluate, which is an issue for likelihood-based learning.

Reading off the partition function from a normalised model

- Consider $\tilde{p}(\mathbf{x};\boldsymbol{\theta}) = \exp\left(-\frac{1}{2}\mathbf{x}^\top\boldsymbol{\Sigma}^{-1}\mathbf{x}\right)$ where $\mathbf{x} \in \mathbb{R}^m$ and $\boldsymbol{\Sigma}$ is symmetric.
- Parameters $\boldsymbol{\theta}$ are the lower (or upper) triangular part of $\boldsymbol{\Sigma}$ including the diagonal.
- Corresponds to an unnormalised Gaussian.
- Partition function can be computed in closed form

$$Z(\boldsymbol{\theta}) = |\det 2\pi\boldsymbol{\Sigma}|^{1/2} \qquad p(\mathbf{x};\boldsymbol{\theta}) = \frac{1}{|\det 2\pi\boldsymbol{\Sigma}|^{1/2}}\exp\left(-\frac{1}{2}\mathbf{x}^\top\boldsymbol{\Sigma}^{-1}\mathbf{x}\right)$$

- Given a normalised model $p(\mathbf{x};\boldsymbol{\theta})$, you can read off the partition function as the inverse of the part that does not depend on $\mathbf{x}$, i.e. you can split a normalised $p(\mathbf{x};\boldsymbol{\theta})$ into an unnormalised model and the partition function:

$$p(\mathbf{x};\boldsymbol{\theta}) \longrightarrow p(\mathbf{x};\boldsymbol{\theta}) = \frac{\tilde{p}(\mathbf{x};\boldsymbol{\theta})}{Z(\boldsymbol{\theta})}$$

The domain matters

- Consider $\tilde{p}(\mathbf{x}; \boldsymbol{\theta}) = \exp\left(-\frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x}\right)$ where $\mathbf{x} \in \{0, 1\}^m$ and $\mathbf{A}$ is symmetric.
- Parameters $\boldsymbol{\theta}$ are the lower (or upper) triangular part of $\mathbf{A}$ including the diagonal.
- Model is known as Ising model or Boltzmann machine.
- Difference to previous slide:
  - Notation/parameterisation: $\mathbf{A}$ vs $\boldsymbol{\Sigma}^{-1}$ (does not matter)
  - $\mathbf{x} \in \{0, 1\}^m$ vs $\mathbf{x} \in \mathbb{R}^m$ (does matter!)
- Partition function defined via sum rather than integral

$$Z(\boldsymbol{\theta}) = \sum_{\mathbf{x} \in \{0,1\}^m} \exp\left(-\frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x}\right)$$

- There is no analytical closed-form expression for $Z(\boldsymbol{\theta})$. Expensive to compute if m is large.

Learning

We consider two approaches to learning:

1. Learning with statistical models = parameter estimation
   (or: estimation of the model)
2. Learning with Bayesian models = Bayesian inference

Learning with statistical models = parameter estimation

- We use use data to pick one element $p(\mathbf{x}; \hat{\boldsymbol{\theta}})$ from the set of probabilistic models $\{p(\mathbf{x}; \boldsymbol{\theta})\}_{\boldsymbol{\theta}}$.

$$\{p(\mathbf{x}; \boldsymbol{\theta})\}_{\boldsymbol{\theta}} \qquad \xrightarrow{\text{data } \mathcal{D}} \qquad p(\mathbf{x}; \hat{\boldsymbol{\theta}})$$

- In other words, we use data to select the estimate $\hat{\boldsymbol{\theta}}$ from the possible values of the parameters $\boldsymbol{\theta}$.
- Using data to pick a value of $\boldsymbol{\theta}$ corresponds to a mapping (function) from data to parameters. The mapping is called an estimator.
- Overloading of notation for the estimate and estimator:
  - $\hat{\boldsymbol{\theta}}$ as selected parameter value is the estimate of $\boldsymbol{\theta}$.
  - $\hat{\boldsymbol{\theta}}$ as mapping $\hat{\boldsymbol{\theta}}(\mathcal{D})$ is the estimator of $\boldsymbol{\theta}$.

  This overloading of notation is often done. For example, when writing $y = x^2 + 1$, y can be considered to be the output of the function ($\equiv$ estimate) or the function $y(x)$ itself ($\equiv$ estimator).

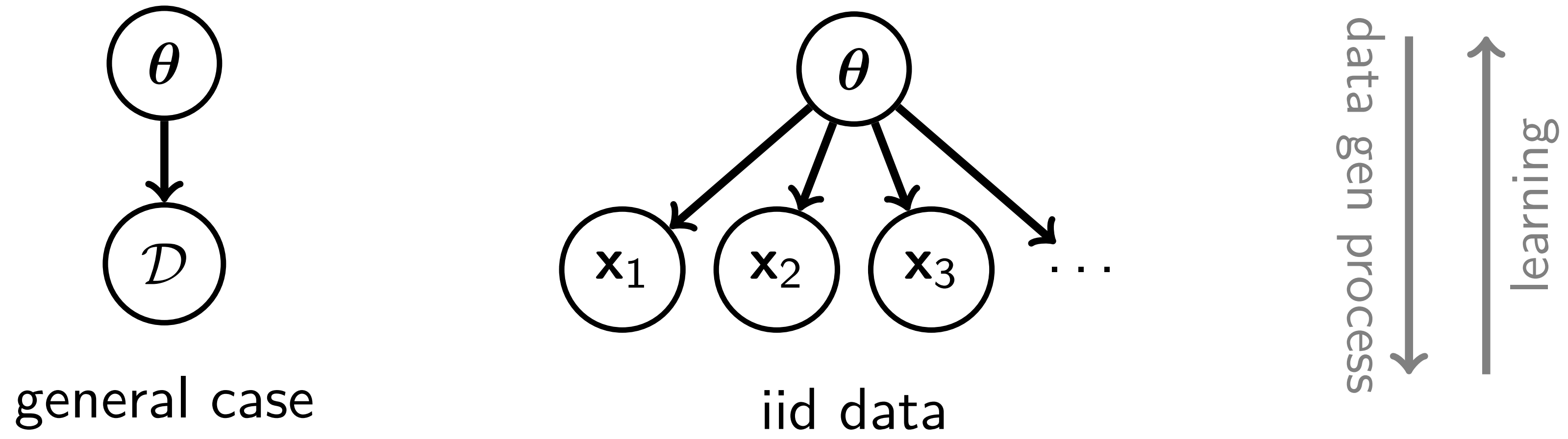
Learning with Bayesian models = Bayesian inference

- We use data to determine the plausibility (posterior pdf/pmf) of all possible values of the parameters $\boldsymbol{\theta}$.

$$p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \qquad \xrightarrow{\text{data } \mathcal{D}} \qquad p(\boldsymbol{\theta}|\mathcal{D})$$

- Instead of picking one value from the set of possible values of $\boldsymbol{\theta}$, we here assess all of them.
- Reduces learning to inference.
- "Inverts" the data generating process

DAGs:



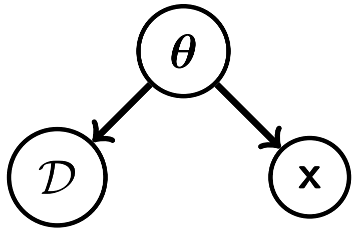
Predictive distribution

- Given data $\mathcal{D}$, we would like to predict the next value $\mathbf{x}$.
- If we take the parameter estimation approach, the predictive distribution is $p(\mathbf{x}; \hat{\boldsymbol{\theta}})$.
- In the Bayesian inference approach, we compute

$$
\begin{aligned}
p(\mathbf{x}|\mathcal{D}) &= \int p(\mathbf{x}, \boldsymbol{\theta}|\mathcal{D})\mathrm{d}\boldsymbol{\theta} \\
&= \int p(\mathbf{x}|\boldsymbol{\theta}, \mathcal{D})p(\boldsymbol{\theta}|\mathcal{D})\mathrm{d}\boldsymbol{\theta} \\
&= \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathcal{D})\mathrm{d}\boldsymbol{\theta}
\end{aligned}
$$

(if $\mathbf{x} \perp\!\!\!\perp \mathcal{D} \mid \boldsymbol{\theta}$ as e.g. in the iid case)

Visualisation as a DAG:



Average of predictions $p(\mathbf{x}|\boldsymbol{\theta})$, weighted by $p(\boldsymbol{\theta}|\mathcal{D})$.

There are many methods for parameter estimation

- There is a multitude of methods to estimate the parameters.
- Many methods can be framed in terms of a decision problem.
- More broadly, they often correspond to solving an optimisation problem, e.g. $\hat{\boldsymbol{\theta}} = \mathrm{argmax}_{\boldsymbol{\theta}} J(\boldsymbol{\theta}, \mathcal{D})$ for some objective function J. Called M-estimation in the statistics literature.
- Maximum likelihood estimation (MLE) is popular (see next).
- Maximum-a-posteriori estimation where we estimate $\boldsymbol{\theta}$ by computing the maximiser of the posterior $\hat{\boldsymbol{\theta}} = \mathrm{argmax}_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathcal{D})$.

Program

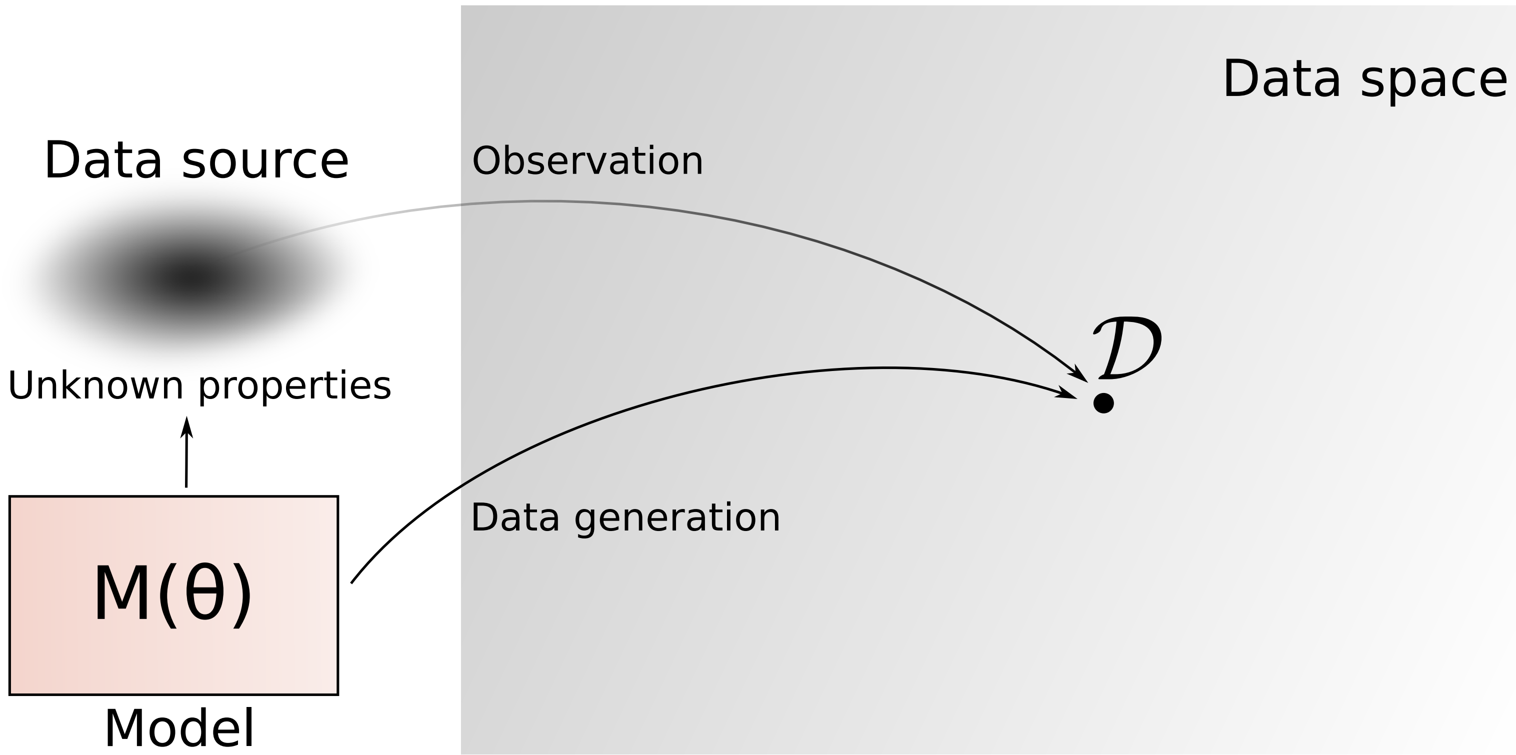
1. Basic concepts
   - Observed data as a sample drawn from an unknown data generating distribution
   - Probabilistic, statistical, and Bayesian models
   - Partition function and unnormalised statistical models
   - Learning = parameter estimation or learning = Bayesian inference
2. Learning by maximum likelihood estimation
3. Learning by Bayesian inference

Program

1. Basic concepts
2. Learning by maximum likelihood estimation
   - The likelihood function and the maximum likelihood estimate
   - MLE for Gaussian, Bernoulli, and fully observed directed graphical models of discrete random variables
   - The likelihood function is informative and more than just an objective function to optimise
3. Learning by Bayesian inference

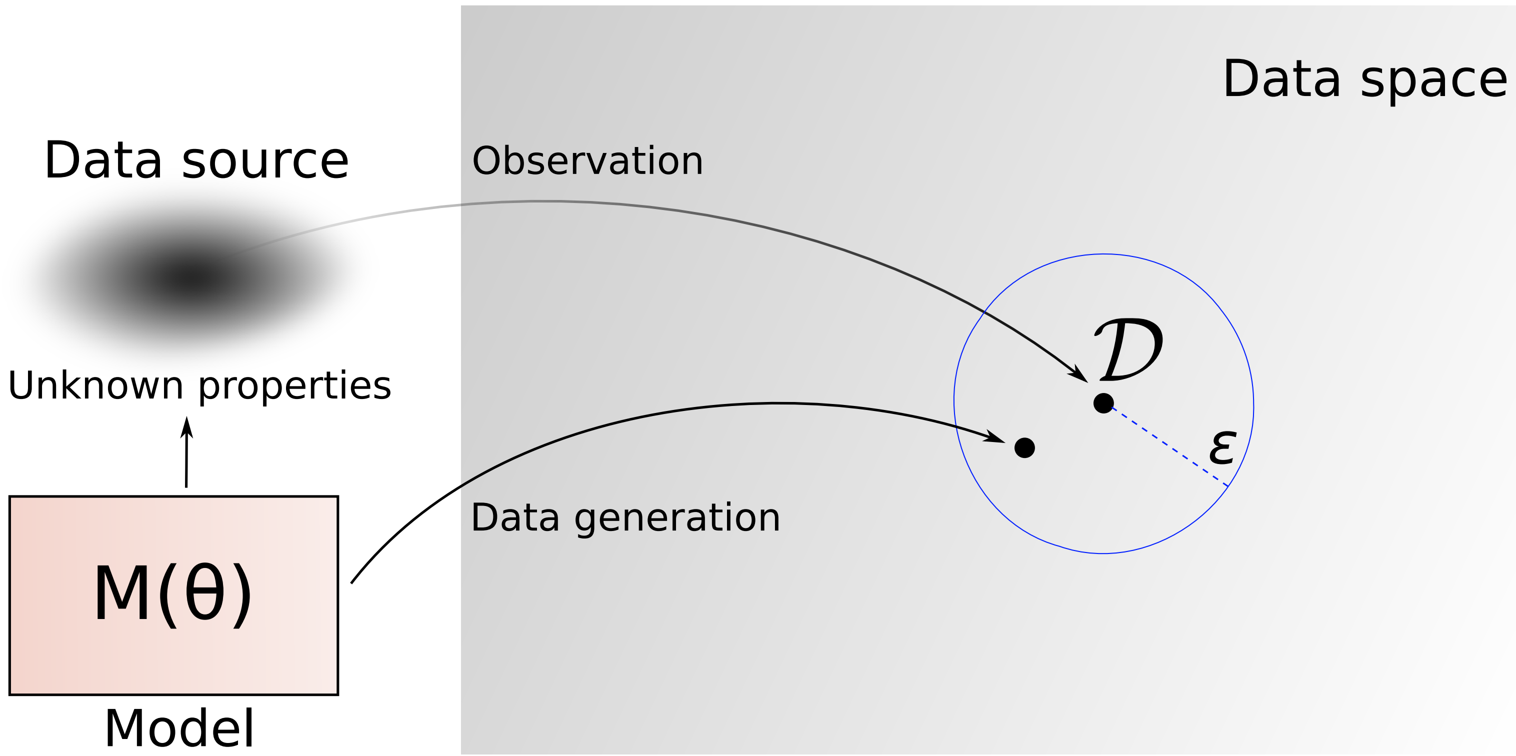
The likelihood function $L(\boldsymbol{\theta})$

- Measures agreement between $\boldsymbol{\theta}$ and the observed data $\mathcal{D}$
- Probability that sampling from the model with parameter value $\boldsymbol{\theta}$ generates data like $\mathcal{D}$.
- Exact match for discrete random variables



The likelihood function $L(\boldsymbol{\theta})$

- Measures agreement between $\boldsymbol{\theta}$ and the observed data $\mathcal{D}$
- Probability that sampling from the model with parameter value $\boldsymbol{\theta}$ generates data like $\mathcal{D}$.
- Small neighbourhood for continuous random variables



The likelihood function $L(\boldsymbol{\theta})$

- Probability that the model generates data like $\mathcal{D}$ for parameter value $\boldsymbol{\theta}$,

$$L(\boldsymbol{\theta}) = p(\mathcal{D}; \boldsymbol{\theta})$$

where $p(\mathcal{D}; \boldsymbol{\theta})$ is the parameterised model pdf/pmf.
- The likelihood function indicates the likelihood of the parameter values, and not of the data.
- For iid data $\mathbf{x}_1, \ldots, \mathbf{x}_n$

$$L(\boldsymbol{\theta}) = p(\mathcal{D}; \boldsymbol{\theta}) = p(\mathbf{x}_1, \ldots, \mathbf{x}_n; \boldsymbol{\theta}) = \prod_{i=1}^{n} p(\mathbf{x}_i; \boldsymbol{\theta})$$

- Log-likelihood function $\ell(\boldsymbol{\theta}) = \log L(\boldsymbol{\theta})$. For iid data:

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log p(\mathbf{x}_i; \boldsymbol{\theta})$$

Maximum likelihood estimate

- The maximum likelihood estimate (MLE) is

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \ell(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, L(\boldsymbol{\theta})$$

- Is the optimal decision for different common losses (see slides on decision making).
- Numerical methods are usually needed for the optimisation.
- We typically only find local optima (sub-optimal but often useful)
- In simple cases, closed form solution possible.

Gaussian example

- Model

$$p(x;\boldsymbol{\theta}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \qquad \boldsymbol{\theta} = (\mu, \sigma^2) \qquad x \in \mathbb{R}$$

- Data $\mathcal{D}$: n iid observations $x_1, \ldots, x_n$
- Log-likelihood function

$$\begin{aligned} \ell(\boldsymbol{\theta}) &= \sum_{i=1}^{n} \log p(x_i;\boldsymbol{\theta}) \\ &= -\frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2 - \frac{n}{2}\log(2\pi\sigma^2) \end{aligned}$$

- Maximum likelihood estimates (see exercises)

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})^2$$

Bernoulli example

- Model

$$p(x;\theta) = \theta^x(1-\theta)^{1-x} = \theta^{\mathbb{1}(x=1)}(1-\theta)^{\mathbb{1}(x=0)}$$

  with $\theta \in [0,\ 1]$, $x \in \{0, 1\}$
- Equivalent to $p(x = 1;\theta) = \theta$, or the table

$p(x;\theta)$	x
$1-\theta$	0
θ	1

- Data $\mathcal{D}$: n iid observations $x_1, \ldots, x_n$
- Log-likelihood function

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^{n} \log p(x_i;\theta) \\ &= \sum_{i=1}^{n} x_i \log(\theta) + (1-x_i)\log(1-\theta)\end{aligned}$$

Bernoulli example

Log-likelihood function:

$$
\begin{aligned}
\ell(\theta) &= \sum_{i=1}^{n} x_i \log(\theta) + (1 - x_i) \log(1 - \theta) \\
&= n_{x=1} \log(\theta) + n_{x=0} \log(1 - \theta)
\end{aligned}
$$

where $n_{x=1}$ is the number of times $x_i = 1$, i.e.

$$
n_{x=1} = \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \mathbb{1}(x_i = 1)
$$

and $n_{x=0} = n - n_{x=1}$ is the number of times $x_i = 0$, i.e.

$$
n_{x=0} = \sum_{i=1}^{n} (1 - x_i) = \sum_{i=1}^{n} \mathbb{1}(x_i = 0)
$$

Bernoulli example

- Constraint optimisation problem:

$$\hat{\theta} = \underset{\theta \in [0,1]}{\operatorname{argmax}} \, n_{x=1} \log(\theta) + n_{x=0} \log(1 - \theta)$$

- Constraint is not needed as the unconstrained optimal θ turns out to satisfy it.
- First and second derivatives of $\ell(\theta)$ are

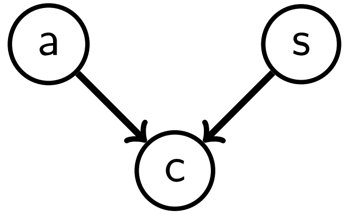
$$\ell(\theta)' = \frac{n_{x=1}}{\theta} - \frac{n_{x=0}}{1-\theta} \qquad \ell(\theta)'' = -\frac{n_{x=1}}{\theta^2} - \frac{n_{x=0}}{(1-\theta)^2} \tag{1}$$

- Setting $\ell(\theta)'$ to zero and solving for θ gives

$$\frac{n_{x=1}}{n_{x=0}} = \frac{\theta}{1-\theta} \qquad \Rightarrow \hat{\theta} = \frac{n_{x=1}}{n_{x=1} + n_{x=0}} = \frac{n_{x=1}}{n} \tag{2}$$

- $\ell''(\hat{\theta}) < 0$, hence $\hat{\theta}$ is a maximum.
- $\hat{\theta}$ is the fraction of ones in the data.

Cancer-asbestos-smoking example



- Statistical model

$$p(c, a, s; \boldsymbol{\theta}) = p(c|a, s; \theta_c^1, \ldots, \theta_c^4)p(a; \theta_a)p(s; \theta_s)$$

with $p(a = 1; \theta_a) = \theta_a \quad p(s = 1; \theta_s) = \theta_s$ and

$p(c = 1\|a, s; \theta_c^1, \ldots, \theta_c^4))$	a	s
θ_c^1	0	0
θ_c^2	1	0
θ_c^3	0	1
θ_c^4	1	1

- Data $\mathcal{D}$:: n iid observations $\mathbf{x}_1, \ldots, \mathbf{x}_n$, where $\mathbf{x}_i = (a_i, s_i, c_i)$

Cancer-asbestos-smoking example

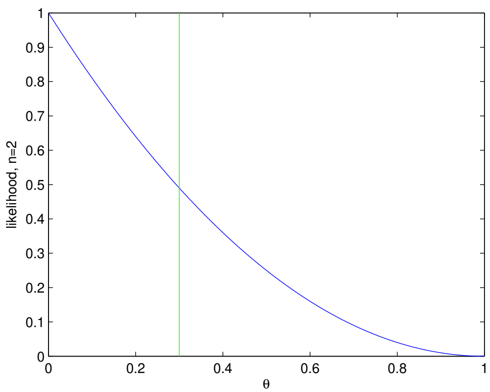
- The random variables a and s are Bernoulli distributed so that the parameters are estimated as before.
- For parameters of the conditional $p(c|a, s)$,

$$\hat{p}(c = 1|a = 0, s = 0) = \hat{\theta}_c^1 = \frac{\sum_{i=1}^n \mathbb{1}(c_i = 1, a_i = 0, s_i = 0)}{\sum_{i=1}^n \mathbb{1}(a_i = 0, s_i = 0)}$$

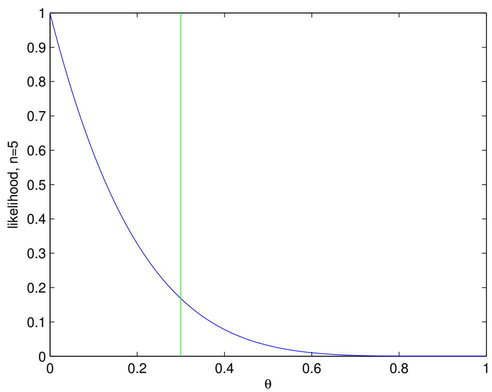
  and equivalently for the other parameters. (see exercises)
- Denominator: number of data points that satisfy the specifications (constraints) given by the conditioning set.
- Estimate is the fraction of times $c = 1$ among the data points that satisfy the constraints given by the conditioning set.

What we miss with maximum likelihood estimation

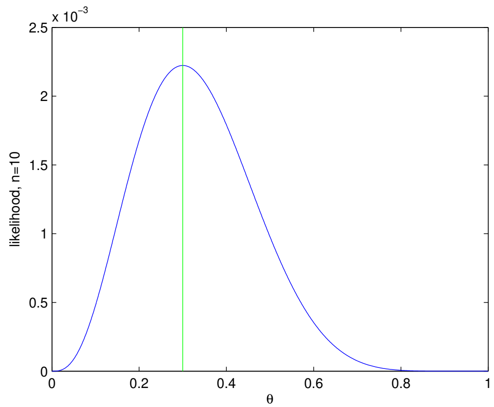
- The likelihood function indicates to which extent various parameter values are congruent with the observed data.
- Establishes an ordering of relative preferences for different parameter values, i.e. $\boldsymbol{\theta}_1$ is preferred over $\boldsymbol{\theta}_2$ if $L(\boldsymbol{\theta}_1) > L(\boldsymbol{\theta}_2)$.
- Max. lik. estimation ignores information contained in the data.
- Example: Likelihood for Bernoulli model with $\mathcal{D} = (0, 0, 0, 0, 0, 0, 0, 1, 1, 1, \ldots)$ generated with parameter value $1/3$ (green line)



(a) $n = 2$ observations



(b) $n = 5$ observations



(c) $n = 10$ observations

What we miss with maximum likelihood estimation

- A compromise between considering the whole (log) likelihood function and only its maximum is the computation of the curvature (Hessian) at the maximum.
- strong curvature: max lik estimate clearly to be preferred
- shallow curvature: several other parameter values are nearly equally in line with the data.

Program

1. Basic concepts
2. Learning by maximum likelihood estimation
   - The likelihood function and the maximum likelihood estimate
   - MLE for Gaussian, Bernoulli, and fully observed directed graphical models of discrete random variables
   - The likelihood function is informative and more than just an objective function to optimise
3. Learning by Bayesian inference

Program

1. Basic concepts
2. Learning by maximum likelihood estimation
3. Learning by Bayesian inference
   - Bayesian approach reduces learning to probabilistic inference
   - Different views of the posterior distribution
   - Conjugate priors
   - Posterior for Gaussian, Bernoulli, and fully observed directed graphical models of discrete random variables

Reduces learning to probabilistic inference

- We use data to determine the plausibility (posterior pdf/pmf) of all possible values of the parameters $\boldsymbol{\theta}$.

$$p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \qquad \xrightarrow{\text{data } \mathcal{D}} \qquad p(\boldsymbol{\theta}|\mathcal{D})$$

- Same framework for learning and inference.
- Decision that minimises the posterior expected log-loss.
- In some cases, closed-form solutions can be obtained (e.g. for conjugate priors).
- In some cases, exact inference methods that we discussed earlier can be used.
- If closed form solutions are not possible and exact inference is computationally too costly, we have to resort to approximate inference via e.g. sampling or variational methods.

The posterior combines likelihood function and prior

- Bayesian inference takes the whole likelihood function into account

$$
\begin{aligned}
p(\boldsymbol{\theta}|\mathcal{D}) &= \frac{p(\boldsymbol{\theta}, \mathcal{D})}{p(\mathcal{D})} \\
&= \frac{p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{D})} \\
&\propto p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \\
&\propto L(\boldsymbol{\theta})p(\boldsymbol{\theta})
\end{aligned}
$$

- $L(\boldsymbol{\theta})$ tilts the prior $p(\boldsymbol{\theta})$ to the posterior $p(\boldsymbol{\theta}|\mathcal{D})$.
- For iid data $\mathcal{D} = (\mathbf{x}_1, \ldots \mathbf{x}_n)$

$$
p(\boldsymbol{\theta}|\mathcal{D}) \propto \left[\prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta})\right] p(\boldsymbol{\theta})
$$

- For large n, likelihood dominates: $\operatorname{argmax}_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathcal{D}) \approx$ MLE (assuming the prior is non-zero at the MLE)

The posterior distribution is a conditional

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\boldsymbol{\theta},\mathcal{D})}{p(\mathcal{D})}$$

- For simplicity, consider discrete-valued data so that

$$p(\boldsymbol{\theta}|\mathcal{D}) = p(\boldsymbol{\theta}|\mathbf{x} = \mathcal{D}) = \frac{p(\boldsymbol{\theta}, \mathbf{x} = \mathcal{D})}{p(\mathcal{D})}$$

- Assume we can sample tuples $(\boldsymbol{\theta}^{(i)}, \mathbf{x}^{(i)})$ from the joint $p(\boldsymbol{\theta}, \mathbf{x})$

$$\boldsymbol{\theta}^{(i)} \sim p(\boldsymbol{\theta}) \qquad \mathbf{x}^{(i)} \sim p(\mathbf{x}|\boldsymbol{\theta}^{(i)})$$

- Conditioning on $\mathbf{x} = \mathcal{D}$ then corresponds to only retaining those samples $(\boldsymbol{\theta}^{(i)}, \mathbf{x}^{(i)})$ where $\mathbf{x}^{(i)} = \mathcal{D}$.
- Samples from the posterior = samples from the prior that produce data equal to the observed one.
- Remark: This view of Bayesian inference forms the basis of a class of approximate methods known as approximate Bayesian computation.

Conjugate priors

- Assume the prior is part of a parametric family with hyperparameters $\boldsymbol{\alpha}$, i.e. the prior is an element of $\{p(\boldsymbol{\theta}; \boldsymbol{\alpha})\}_{\boldsymbol{\alpha}}$, so that
$$p(\boldsymbol{\theta}) = p(\boldsymbol{\theta}; \boldsymbol{\alpha}_0)$$
for some fixed $\boldsymbol{\alpha}_0$.
- If the posterior $p(\boldsymbol{\theta}|\mathcal{D})$ is part of the same family as the prior,
  - the prior and posterior are called conjugate distributions
  - the prior is said to be a conjugate prior for $p(\mathbf{x}|\boldsymbol{\theta})$ or for the likelihood function.
- Learning then corresponds to updating the hyperparameters.
$$\boldsymbol{\alpha}_0 \qquad \xrightarrow{\text{data } \mathcal{D}} \qquad \boldsymbol{\alpha}(\mathcal{D})$$
- Models $p(\mathbf{x}|\boldsymbol{\theta})$ that a part of the exponential family always have a conjugate prior (see Barber 8.5).

Gaussian example (posterior of the mean for known variance)

- Denote pdf of a Gaussian random variable x with mean μ and variance σ^2 by $\mathcal{N}(x; \mu, \sigma^2)$.
- Bayesian model

$$p(x|\theta) = \mathcal{N}(x|\theta, \sigma^2) \qquad p(\theta; \boldsymbol{\alpha}_0) = \mathcal{N}(\theta; \mu_0, \sigma_0^2)$$

Hyperparameters $\boldsymbol{\alpha}_0 = (\mu_0, \sigma_0^2)$

- Data $\mathcal{D}$: n iid observations $x_1, \ldots, x_n$
- Posterior for θ (see exercises)

$$p(\theta|\mathcal{D}) = \mathcal{N}(\theta; \mu_n, \sigma_n^2)$$

$$\mu_n = \frac{\sigma_0^2}{\sigma_0^2 + \sigma^2/n}\bar{x} + \frac{\sigma^2/n}{\sigma_0^2 + \sigma^2/n}\mu_0 \quad \frac{1}{\sigma_n^2} = \frac{1}{\sigma^2/n} + \frac{1}{\sigma_0^2}$$

where $\bar{x} = 1/n \sum_i x_i$ is the sample average (the MLE).

Gaussian example (posterior of the mean for known variance)

$$\mu_n = \frac{\sigma_0^2}{\sigma_0^2+\sigma^2/n}\bar{x} + \frac{\sigma^2/n}{\sigma_0^2+\sigma^2/n}\mu_0$$

- Introduce

$$w_n = \frac{\sigma_0^2}{\sigma_0^2+\sigma^2/n} \tag{3}$$

  For $n = 0$, $w_n \to 0$. For $n \to \infty$, $w_n \to 1$

- Moreover:

$$\frac{\sigma^2/n}{\sigma_0^2+\sigma^2/n} = 1 - w_n \tag{4}$$

- Hence

$$\mu_n = w_n\bar{x} + (1-w_n)\mu_0 \tag{5}$$

  As the number of data points increases, μ_n travels from prior mean μ_0 to the MLE $\bar{x}$ along a straight line.

- The posterior mean of θ linearly interpolates between prior mean μ_0 and MLE $\hat{x}$.

Bernoulli example

- Recall: Beta distribution with parameters α, β

$$\mathcal{B}(f; \alpha, \beta) \propto f^{\alpha-1}(1-f)^{\beta-1} \qquad f \in [0, 1]$$

see the background document *Introduction to Probabilistic Modelling*

- Bayesian model

$$p(x|\theta) = \theta^x(1-\theta)^{1-x} \qquad p(\theta; \boldsymbol{\alpha}_0) = \mathcal{B}(\theta; \alpha_0, \beta_0)$$

where $x \in \{0, 1\}$, $\theta \in [0, 1]$, and $\boldsymbol{\alpha}_0 = (\alpha_0, \beta_0)$

- Data $\mathcal{D}$: n iid observations $x_1, \ldots, x_n$
- Posterior for θ (see exercises)

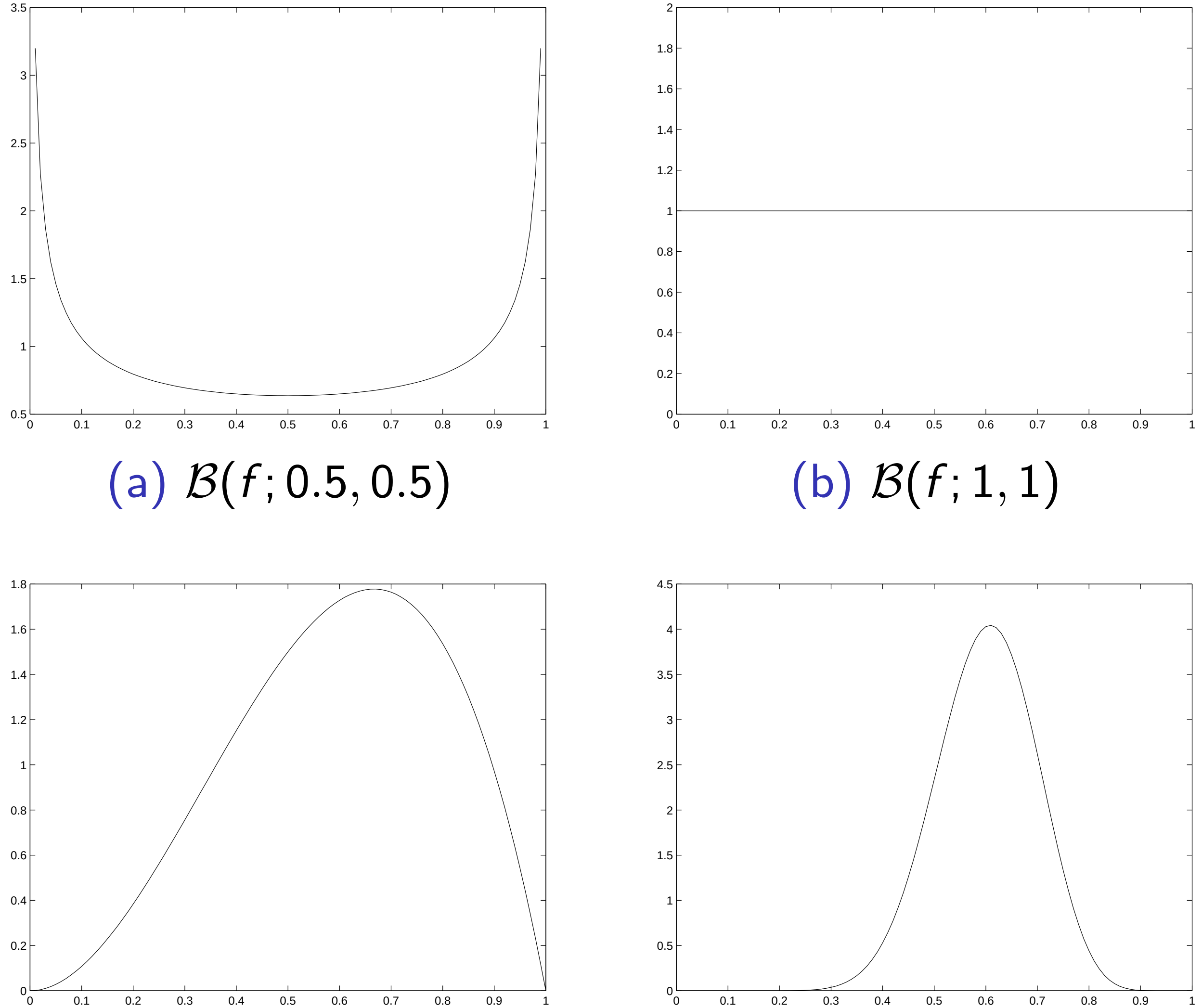
$$p(\theta|\mathcal{D}) = \mathcal{B}(\theta; \alpha_n, \beta_n)$$

$$\alpha_n = \alpha_0 + n_{x=1} \qquad \beta_n = \beta_0 + n_{x=0}$$

where $n_{x=1}$ were the number of ones and $n_{x=0}$ the number of zeros in the data.

Examples of the beta distribution $\mathcal{B}(f; \alpha, \beta)$ (Figures courtesy C. Williams)

Expected value: $\frac{\alpha}{\alpha+\beta}$, Variance: $\frac{\alpha}{\alpha+\beta}\frac{\beta}{\alpha+\beta}\frac{1}{\alpha+\beta+1}$

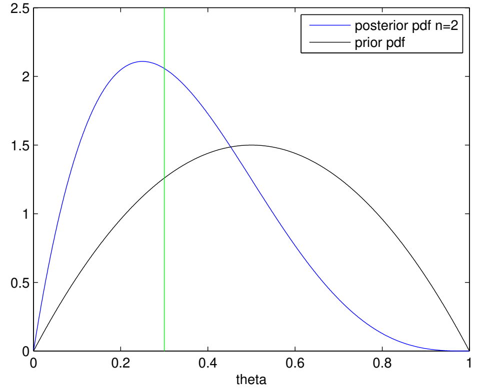


(a) $\mathcal{B}(f; 0.5, 0.5)$ (b) $\mathcal{B}(f; 1, 1)$

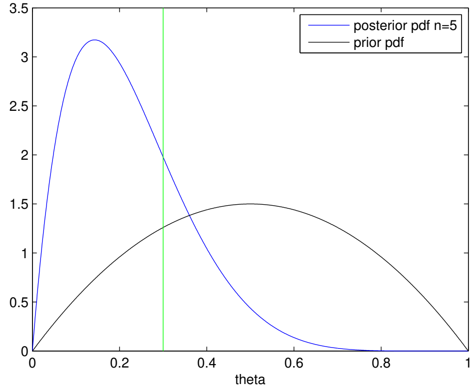
(c) $\mathcal{B}(f; 3, 2)$ (d) $\mathcal{B}(f; 15, 10)$

Bernoulli example

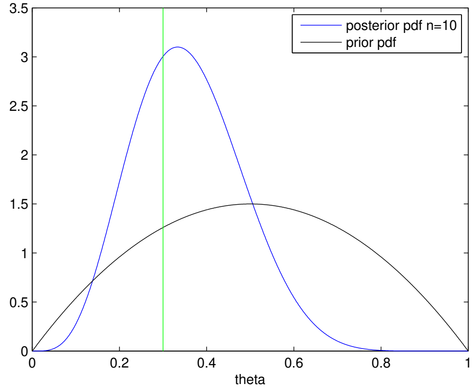
- Bernoulli model with $\mathcal{D} = (0, 0, 0, 0, 0, 0, 0, 1, 1, 1, \ldots)$ generated with parameter value 1/3 (green line)
- Posterior in blue, $\mathcal{B}(2, 2)$ prior in black
- Compare with earlier likelihood plots. Note the "pull" towards the prior when n is small.



(a) $n = 2$ observations



(b) $n = 5$ observations



(c) $n = 10$ observations

Cancer-asbestos-smoking example

- Bayesian model

$$p(c, a, s|\boldsymbol{\theta}) = p(c|a, s, \theta_c^1, \ldots, \theta_c^4)p(a|\theta_a)p(s|\theta_s)$$
$$= \prod_{j=1}^{4} (\theta_c^j)^{\mathbb{1}(c=1, \mathrm{pa}_c=j)}(1-\theta_c^j)^{\mathbb{1}(c=0, \mathrm{pa}_c=j)}$$
$$\theta_a^{\mathbb{1}(a=1)}(1-\theta_a)^{\mathbb{1}(a=0)}\theta_s^{\mathbb{1}(s=1)}(1-\theta_s)^{\mathbb{1}(s=0)}$$

- Assume the prior factorises (independence assumptions):

$$p(\theta_a, \theta_s, \theta_c^1, \ldots, \theta_c^4; \boldsymbol{\alpha}_0) = \prod_j \mathcal{B}(\theta_c^j; \alpha_{c,0}^j, \beta_{c,0}^j)$$
$$\mathcal{B}(\theta_a; \alpha_{a,0}, \beta_{a,0})\mathcal{B}(\theta_s; \alpha_{s,0}, \beta_{s,0})$$

- Data $\mathcal{D}$: n iid observations $\mathbf{x}_1, \ldots, \mathbf{x}_n$, where $\mathbf{x}_i = (a_i, s_i, c_i)$
- The parameters are independent under the posterior and follow a beta distribution (see exercises)

Program recap

1. Basic concepts
   - Observed data as a sample drawn from an unknown data generating distribution
   - Probabilistic, statistical, and Bayesian models
   - Partition function and unnormalised statistical models
   - Learning = parameter estimation or learning = Bayesian inference
2. Learning by maximum likelihood estimation
   - The likelihood function and the maximum likelihood estimate
   - MLE for Gaussian, Bernoulli, and fully observed directed graphical models of discrete random variables
   - The likelihood function is informative and more than just an objective function to optimise
3. Learning by Bayesian inference
   - Bayesian approach reduces learning to probabilistic inference
   - Different views of the posterior distribution
   - Conjugate priors
   - Posterior for Gaussian, Bernoulli, and fully observed directed graphical models of discrete random variables