Lecture 5: Introduction to Probabilistic (Bayesian) Modelling and Inference

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MATH60047/70047 - Stochastic Simulation

October 24, 2022

Imperial College London

Announcements

- ► Tomorrow, we are at HXLY 414, Maths Learning Centre. We will be coding exercises and some more things.
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 - Please bring your laptops.
 - Jupyter Notebooks (can you run it?)
- Assignment is to be posted this Wednesday (26 October).
 - ▶ Due 9 Nov. 2022
 - ▶ 10 percent

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We will introduce today *probabilistic* (Bayesian) inference which is a very general framework for inference.

We will see how to use rejection sampling for this purpose.

Probabilistic Inference

We have seen in past lectures that we could generate data from the model:

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However, in this course, our aim is not solely to simulate synthetic data.

We want to infer hidden states or parameters given observed data.

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 - Can be taken uninformative

Probabilistic Inference

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Another important quantity is p(y). In the continuous case:

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In the discrete case,

$$p(y) = \sum_x p(x,y) = \sum_x p(y|x)p(x).$$

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But can we sample from it?

A discrete inference example

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Consider the following discrete distribution:

$p(x_1,x_2)$	$X_1 = 1$	$X_1 = 2$	$X_1 = 3$	$X_1 = 4$	$X_1 = 5$	$X_1 = 6$
$X_2 = 1$	1/36	1/36	1/36	1/36	1/36	1/36
$X_2 = 2$	1/36	1/36	1/36	1/36	1/36	1/36
$X_2 = 3$	1/36	1/36	1/36	1/36	1/36	1/36
$X_2 = 4$	1/36	1/36	1/36	1/36	1/36	1/36
$X_2 = 5$	1/36	1/36	1/36	1/36	1/36	1/36
$X_2 = 6$	1/36	1/36	1/36	1/36	1/36	1/36

This is the probability distribution of a roll of a pair of dice.

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Can we figure out the probability distribution conditioned on this observation?

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So in essence,

$$p(y|x_1, x_2) = \begin{cases} 1 & \text{if } y = x_1 + x_2 \\ 0 & \text{otherwise} \end{cases}$$

A discrete inference example

We know that y = 9 (observed).

Let us write the Bayes rule:

$$p(x_1, x_2|y=9) = \frac{p(y=9|x_1, x_2)p(x_1, x_2)}{p(y=9)}.$$

We know that $p(y = 9|x_1, x_2)$ is an indicator function at 9.

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$$p(y|x_1, x_2) = \mathbf{1}(y = x_1 + x_2)$$

We can write it out explicitly for the values of x_1 and x_2 .

A discrete inference example

$p(y=9 x_1,x_2)$	$X_1 = 1$	$X_1 = 2$	$X_1 = 3$	$X_1 = 4$	$X_1 = 5$	$X_1 = 6$
$X_2 = 1$	0	0	0	0	0	0
$X_2 = 2$	0	0	0	0	0	0
$X_2 = 3$	0	0	0	0	0	1
$X_2 = 4$	0	0	0	0	1	0
$X_2 = 5$	0	0	0	1	0	0
$X_2 = 6$	0	0	1	0	0	0

What happens if we multiply this with $p(x_1)p(x_2)$?

A discrete inference example

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$p(x_1)p(x_2)$	$X_1 = 1$	$X_1 = 2$	$X_1 = 3$	$X_1 = 4$	$X_1 = 5$	$X_1 = 6$
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$X_2 = 4$	0	0	0	0	1/36	0
$X_2 = 5$	0	0	0	1/36	0	0
$X_2 = 6$	0	0	1/36	0	0	0

Now we know the numerator: $p(y = 9|x_1, x_2)p(x_1, x_2)$.

A discrete inference example

Recall:

$$p(x_1, x_2|y=9) = \frac{p(y=9|x_1, x_2)p(x_1, x_2)}{p(y=9)}.$$

Therefore, we need to compute p(y=9).

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How is it computed?

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Therefore, we need to compute p(y=9).

How is it computed?

We need to sum over all possible values of x_1 and x_2 :

$$p(y = 9) = \sum_{x_1, x_2} p(y = 9|x_1, x_2)p(x_1, x_2).$$

A discrete inference example

Let us write out the denominator:

$$p(y = 9) = \sum_{x_1, x_2} p(y = 9|x_1, x_2) p(x_1, x_2)$$

$$= \sum_{x_1, x_2} \mathbf{1}(y = x_1 + x_2) p(x_1) p(x_2)$$

$$= \sum_{x_1, x_2} \mathbf{1}(y = x_1 + x_2) \times \frac{1}{6} \times \frac{1}{6}$$

$$= \frac{1}{36} \sum_{x_1, x_2} \mathbf{1}(y = x_1 + x_2)$$

$$= 4/36$$

$$= 1/9.$$

A discrete inference example

We go back to our table of $p(y=9|x_1,x_2)p(x_1,x_2)$ and divide by p(y=9):

$p(x_1, x_2 y=9)$	$X_1 = 1$	$X_1 = 2$	$X_1 = 3$	$X_1 = 4$	$X_1 = 5$	$X_1 = 6$
$X_2 = 1$	0	0	0	0	0	0
$X_2 = 2$	0	0	0	0	0	0
$X_2 = 3$	0	0	0	0	0	1/4
$X_2 = 4$	0	0	0	0	1/4	0
$X_2 = 5$	0	0	0	1/4	0	0
$X_2 = 6$	0	0	1/4	0	0	0

This is our posterior distribution $p(x_1, x_2|y=9)!$

A continuous inference example

Let us consider the following model:

$$p(x) = \mathcal{N}(x; \mu_0, \sigma_0^2)$$
$$p(y|x) = \mathcal{N}(y; x, \sigma^2).$$

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What is the posterior density p(x|y)?

A continuous inference example

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In this example, we will derive the posterior density using the Bayes rule ourselves (not looking up).

A continuous inference example

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This is the notation which means proportional to.

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This is the notation which means proportional to. Therefore, we have

$$p(x|y) \propto \mathcal{N}(y; x, \sigma^2) \mathcal{N}(x; \mu_0, \sigma_0^2).$$

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$$= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-x)^2}{2\sigma^2}\right) \frac{1}{\sqrt{2\pi\sigma_0^2}} \exp\left(-\frac{(x-\mu_0)^2}{2\sigma_0^2}\right)$$

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$$= \frac{1}{\sqrt{2\pi\sigma^{2}\sigma_{0}^{2}}} \exp\left(-\frac{(y-x)^{2}}{2\sigma^{2}} - \frac{(x-\mu_{0})^{2}}{2\sigma_{0}^{2}}\right).$$

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So we've got:

$$p(x|y) \propto \exp\left(-\frac{(y-x)^2}{2\sigma^2} - \frac{(x-\mu_0)^2}{2\sigma_0^2}\right).$$

A continuous inference example

We can now use the help of the fact that the product of two Gaussians is a Gaussian. We can parameterise the posterior as

$$p(x|y) = \mathcal{N}(x; \mu_p, \sigma_p^2),$$

where μ_p and σ_p^2 are the posterior mean and variance, respectively.

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where μ_p and σ_p^2 are the posterior mean and variance, respectively. This means, we need to match

$$\exp\left(-\frac{(y-x)^2}{2\sigma^2} - \frac{(x-\mu_0)^2}{2\sigma_0^2}\right) = \exp\left(-\frac{(x-\mu_p)^2}{2\sigma_p^2}\right),\,$$

in terms of x (we can ignore the constants).

A continuous inference example

$$\frac{-y^2}{2\sigma^2} + \frac{yx}{\sigma^2} - \frac{x^2}{2\sigma^2} - \frac{x^2}{2\sigma_0^2} + \frac{x\mu_0}{\sigma_0^2} = \frac{-x^2}{2\sigma_p^2} + \frac{x\mu_p}{\sigma_p^2}$$

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Match the coefficients of x^2 :

$$\frac{1}{\sigma^2} + \frac{1}{\sigma_0^2} = \frac{1}{\sigma_p^2}.$$

which implies

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$$\sigma_p^2 = \frac{\sigma^2 \sigma_0^2}{\sigma^2 + \sigma_0^2}.$$

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which implies

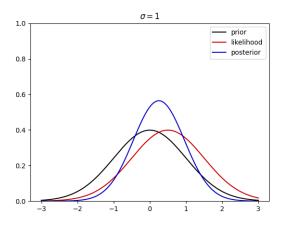
$$\mu_p = \frac{\sigma^2 \mu_0 + \sigma_0^2 y}{\sigma^2 + \sigma_0^2}.$$

A continuous inference example

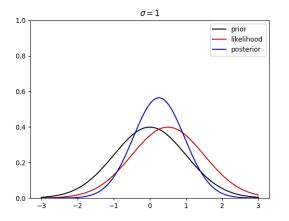
Finally, we obtain

$$\mu_p = \frac{\sigma^2 \mu_0 + \sigma_0^2 y}{\sigma^2 + \sigma_0^2}$$
$$\sigma_p^2 = \frac{\sigma^2 \sigma_0^2}{\sigma^2 + \sigma_0^2}.$$

A continuous inference example

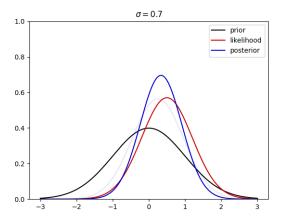


A continuous inference example



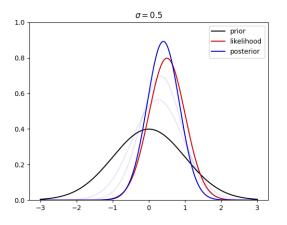
The likelihood is plotted for observation y = 0.5!

A continuous inference example



Peakier posterior for smaller likelihood variance.

A continuous inference example



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Rejection sampling for the Gaussian posterior

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We will use the same model and compare the samples to the exact posterior we computed.

Rejection sampling for the Gaussian posterior

Recall

$$p(x|y) \propto p(y|x)p(x)$$

 $\propto \mathcal{N}(y; x, \sigma^2)\mathcal{N}(x; \mu_0, \sigma_0^2).$

We denote this unnormalised posterior by $\bar{p}(x|y)$.

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Note that this is a function of x: y is observed data and is fixed!

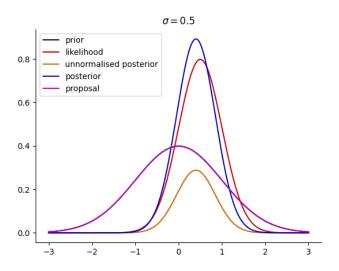
Rejection sampling for the Gaussian posterior

We need to choose a proposal. Let us choose

$$q(x) = \mathcal{N}(x; 0, 1).$$

and ${\cal M}=1.$ It turns out this is enough for us.

Rejection sampling for the Gaussian posterior



Rejection sampling for the Gaussian posterior

Rejection sampling:

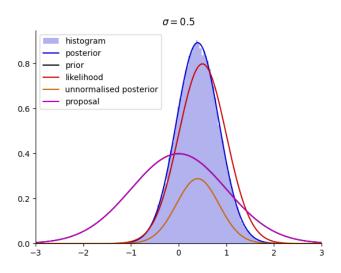
- ▶ Sample $X' \sim q(x)$.
- ▶ Sample $U \sim \mathsf{Unif}(0,1)$.
- Accept if

$$U \le \frac{p(y|X')p(X')}{Mq(X')},$$

otherwise reject.

Repeat.

Rejection sampling for the Gaussian posterior



Gamma-Poisson model

Another tractable example is the Gamma-Poisson model.

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and the likelihood is given as

$$p(y|x) = \mathsf{Poisson}(y;x) = \frac{x^y}{y!} \exp(-x).$$

This can be seen as an observation model of a count.

Gamma-Poisson model

Derive the posterior.

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This is another Gamma density, i.e.:

$$p(x|y) = \mathsf{Gamma}(x; \alpha + y, \beta + 1).$$

Rejection sampling for the Gamma-Poisson model

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Rejection sampling for the Gamma-Poisson model

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We will use the same model and compare the samples to the exact posterior we computed.

We choose a prior

$$p(x) = \mathsf{Gamma}(x;\alpha,1) = \frac{1}{\Gamma(\alpha)} x^{\alpha-1} \exp(-x),$$

and a likelihood

$$p(y|x) = \mathsf{Poisson}(y;x) = \frac{x^y}{y!} \exp(-x).$$

Rejection sampling for the Gamma-Poisson model

Recall that our unnormalised posterior is written as

$$\bar{p}(x|y) = x^{y+\alpha-1} \exp(-2x).$$

Rejection sampling for the Gamma-Poisson model

Recall that our unnormalised posterior is written as

$$\bar{p}(x|y) = x^{y+\alpha-1} \exp(-2x).$$

Let us choose an exponential proposal:

$$q_{\lambda}(x) = \lambda \exp(-\lambda x).$$

Rejection sampling for the Gamma-Poisson model

Let us compute

$$M_{\lambda} = \sup_{x} \frac{\bar{p}(x|y)}{q_{\lambda}(x)}.$$

Rejection sampling for the Gamma-Poisson model

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$$M_{\lambda} = \sup_{x} \frac{\bar{p}(x|y)}{q_{\lambda}(x)}.$$

The ratio is given by

$$\frac{\bar{p}(x|y)}{q_{\lambda}(x)} = \frac{x^{\alpha - 1 + y}e^{-2x}}{\lambda e^{-\lambda x}},$$
$$= \frac{x^{\alpha - 1 + y}e^{-(2 - \lambda)x}}{\lambda}.$$

Rejection sampling for the Gamma-Poisson model

We aim at optimising this w.r.t. x, so first compute \log :

$$\log \frac{\bar{p}(x|y)}{q_{\lambda}(x)} = \log x^{\alpha - 1 + y} + \log e^{-(2 - \lambda)x} - \log \lambda$$
$$= (\alpha - 1 + y) \log x - (2 - \lambda)x - \log \lambda.$$

Rejection sampling for the Gamma-Poisson model

We aim at optimising this w.r.t. x, so first compute \log :

$$\log \frac{\bar{p}(x|y)}{q_{\lambda}(x)} = \log x^{\alpha - 1 + y} + \log e^{-(2 - \lambda)x} - \log \lambda$$
$$= (\alpha - 1 + y) \log x - (2 - \lambda)x - \log \lambda.$$

We now take the derivative of this w.r.t. x:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(\alpha - 1 + y)\log x - (2 - \lambda)x - \log \lambda\right] = \frac{\alpha - 1 + y}{x} - (2 - \lambda),$$

Rejection sampling for the Gamma-Poisson model

and set it to zero:

$$\frac{\alpha - 1 + y}{x} - (2 - \lambda) = 0.$$

This gives us the maximiser

$$x^* = \frac{\alpha - 1 + y}{2 - \lambda}.$$

Rejection sampling for the Gamma-Poisson model

We can now compute $M_{\lambda} = \bar{p}(x^{\star}|y)/q_{\lambda}(x^{\star})$::

$$M_{\lambda} = \frac{\bar{p}(x^{*}|y)}{q_{\lambda}(x^{*})}$$

$$= \frac{x^{*\alpha-1+y}e^{-(2-\lambda)x^{*}}}{\lambda}$$

$$= \frac{1}{\lambda} \left(\frac{\alpha-1+y}{2-\lambda}\right)^{\alpha-1+y} e^{-(2-\lambda)\left(\frac{\alpha-1+y}{2-\lambda}\right)}$$

$$= \frac{1}{\lambda} \left(\frac{\alpha-1+y}{2-\lambda}\right)^{\alpha-1+y} e^{-(\alpha-1+y)}.$$

We can now optimise this further to choose our optimal proposal.

Rejection sampling for the Gamma-Poisson model

We will first compute the log of M_{λ} :

$$\log M_{\lambda} = \log \frac{1}{\lambda} + (\alpha - 1 + y) \log \left(\frac{\alpha - 1 + y}{2 - \lambda} \right) - (\alpha - 1 + y)$$
$$= -\log \lambda + (\alpha - 1 + y) \log \left(\frac{\alpha - 1 + y}{2 - \lambda} \right) - (\alpha - 1 + y).$$

Taking the derivative of this w.r.t. λ , we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\log M_{\lambda} = -\frac{1}{\lambda} + \frac{(\alpha - 1 + y)}{2 - \lambda}$$

Rejection sampling for the Gamma-Poisson model

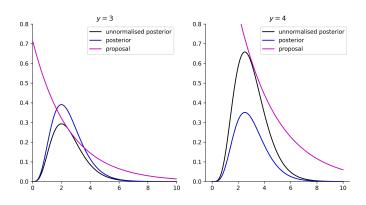
Setting this to zero, we obtain

$$\frac{1}{\lambda} = \frac{(\alpha - 1 + y)}{2 - \lambda},$$

which implies that

$$\lambda^* = \frac{2}{\alpha + y}.$$

Rejection sampling for the Gamma-Poisson model



Rejection sampling for the Gamma-Poisson model

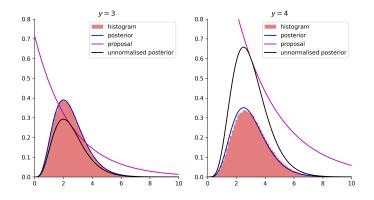


Figure: Histogram of the samples drawn using rejection sampling.

Today, we have covered:

- ► The Bayes rule and its applications
- Derivation of posterior distributions
- Rejection sampling for posterior distributions

We will look at more complex probabilistic models in next lectures. We will also look at more efficient sampling methods.

Imperial College London

See you tomorrow! (HXLY 414, Maths Learning Centre)

References I