Closed-Form Inference

Mark van der Wilk

Department of Computing Imperial College London

>@markvanderwilk
m.vdwilk@imperial.ac.uk

January 24, 2022

Computing Posteriors

- Previous lecture investigated which computations we need to perform to find posteriors.
- ► Now, we focus on actually doing them.
- We focus on inference problems with two variables, one hidden (latent), one observed (data).

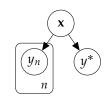
$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$
(1)

► As before, the model is specified by the full joint, often in terms of tractable densities, i.e.

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) \tag{2}$$

Terminology

$$p(\mathbf{y}, y^*, \mathbf{x}) = p(y^*|\mathbf{x}) \prod_{n=1}^{N} p(y_n|\mathbf{x}) p(\mathbf{x}) \quad (3)$$

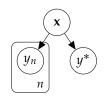


$$\underbrace{p(\mathbf{x}|\mathbf{y})}_{\text{posterior}} = \underbrace{\frac{p(\mathbf{y}|\mathbf{x})}{p(\mathbf{y})} \underbrace{p(\mathbf{y})}_{\text{posterior}}}_{\text{marginal likelihood}} = \underbrace{\frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{\int p(\mathbf{y}|\mathbf{x})p(\mathbf{x})d\mathbf{x}}}_{\text{posterior}} \tag{4}$$

- ▶ When solving an inference problem, what is fixed and what is variable in $p(\mathbf{x}|\mathbf{y})$? ▶ observation \mathbf{y} is fixed, \mathbf{x} varies.
- What variable is the likelihood a function of? ➤ x only!
 We say "likelihood of parameters / latent variable x".

Terminology

$$p(\mathbf{y}, y^*, \mathbf{x}) = p(y^*|\mathbf{x}) \prod_{n=1}^{N} p(y_n|\mathbf{x}) p(\mathbf{x}) \quad (5)$$



$$\underbrace{p(y^*|\mathbf{y})}_{\text{posterior}} \stackrel{\text{MA}}{=} \int p(y^*|\mathbf{x}) \underbrace{p(\mathbf{x}|\mathbf{y})}_{\text{posterior}} d\mathbf{x} = \int p(y^*|\mathbf{x}) \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})} d\mathbf{x} \qquad (6)$$

- ▶ If we aren't talking about a fixed observed dataset, we can investigate properties of distributions as a function of **y**. If we do so we may refer to $p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{x})p(\mathbf{x})d\mathbf{x}$ as the *prior predictive* distribution.
- ► We use different terminology for these settings to indicate whether **y** is observed and fixed, or whether we investigate how the probability changes for different possible outcomes **y**.

Example: One-Armed Bandit

- ► Each time you run a "one-armed bandit", you get a random return of *Y*_n.
- Y_n is distributed according to density $p(y_n|x)$, with $\mathbb{E}_{p(y_n|x)}[y_n] = x$.
- ► The mean return is assigned by the manufacturer by sampling from p(x).



Example: One-Armed Bandit

You are interested in computing for example:

• $p(x|\mathbf{y})$ to understand your belief about the average return. In particular

$$P(X > 0|\mathbf{y}) = \int_0^\infty p(x|\mathbf{y}) dx.$$
 (7)

• $p(y^*|\mathbf{y})$ to understand your belief in your potential return in the next run. In particular

$$p(\mathbf{y}^*|\mathbf{y}) = \int p(\mathbf{y}^*|x)p(x|\mathbf{y})dx$$
 (8)

$$P(Y^* > 0|\mathbf{y}) = \int_0^\infty p(\mathbf{y}^*|\mathbf{y}) dy^*.$$
 (9)

► In general, we are interested in **summary statistics** of posterior distributions **> integrals**.

How difficult is Bayesian inference?

- ► Let's think about *actually* computing some of these quantities.
- ► How difficult is this really?

$$P(X > 0|\mathbf{y}) = \int_0^\infty p(\mathbf{x}|\mathbf{y}) d\mathbf{x}, \qquad p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

Let's start with the posterior.

- ► Computing the numerator of $p(\mathbf{x}|\mathbf{y})$ is easy: multiplication.
- ► Denominator $p(y) = \int p(y|x)p(x)dx$ seems hard. Integrals are hard.
- ▶ Do we really need p(y)? It's just a constant... Are relative probabilities not enough?
- ▶ No hope of computing $p(X > 0|\mathbf{y})$ without $p(\mathbf{y})$.

Example: One-Armed Bandit (doing integrals)

Take
$$p(y_n|x) = \mathcal{N}(y_n; x, \sigma^2)$$
 and $p(x) = \mathcal{N}(x; 0, v)$.

$$p(x|\mathbf{y}) = \frac{\prod_{n} \mathcal{N}(y_n; x, \sigma^2) \mathcal{N}(x; 0, v)}{p(\mathbf{y})}$$
(10)

$$= \frac{(2\pi\sigma^2)^{-\frac{N}{2}}(2\pi v)^{-\frac{1}{2}}}{p(\mathbf{y})} \exp\left[-\frac{1}{2\sigma^2} \sum_{n} (y_n - x)^2 - \frac{1}{2v} x^2\right]$$
(11)

$$= \frac{(2\pi)^{-\frac{N+1}{2}}\sigma^{-N}v^{-\frac{1}{2}}}{p(\mathbf{y})} \exp \left[-\frac{1}{2\tau}(x-\mu)^2 - \frac{1}{2}(\sum_n y_n^2 - \frac{\mu^2}{\tau}) \right]$$
(12)

$$= c \exp\left[-\frac{1}{2\tau}(x-\mu)^2\right] \tag{13}$$

Equate coefficients to obtain

$$\tau = \frac{v\sigma^2}{vN + \sigma^2}, \qquad \mu = \frac{v}{vN + \sigma^2} \sum_n y_n. \tag{14}$$

Example: One-Armed Bandit (doing integrals)

From previous slide we know:

$$p(x|\mathbf{y}) = c \exp\left[-\frac{1}{2\tau}(x-\mu)^2\right],\tag{15}$$

$$\tau = \frac{v\sigma^2}{vN + \sigma^2}, \qquad \mu = \frac{v}{vN + \sigma^2} \sum_n y_n. \tag{16}$$

How to find *c*? Two options:

1. We know that $\int p(x|\mathbf{y})dx = 1$. Do the integral using $\int e^{-x^2}dx = \sqrt{\pi}$.

$$\int c \exp\left[-\frac{1}{2\tau}(x-\mu)^2\right] dx = c \cdot \sqrt{2\pi\tau} = 1 \implies c = \frac{1}{\sqrt{2\pi\tau}} \quad (17)$$

2. Let someone else do the integral, by using knowledge that

$$\mathcal{N}(x;\mu,\tau) = \frac{1}{\sqrt{2\pi\tau}} \exp\left[-\frac{1}{2\tau}(x-\mu)^2\right]. \tag{18}$$

Why could we compute the posterior?

One reason: We could integrate the unnormalised posterior.

$$p(x|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$$
 (19)

$$Z = \int p(\mathbf{y}|\mathbf{x})p(\mathbf{x})d\mathbf{x} \qquad \text{in this case} \qquad (20)$$

$$p(x|\mathbf{y}) = \frac{1}{Z}p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$$
 in this case (21)

- ► This was the case because p(y|x)p(x) as a function of **x** implies a Gaussian distribution.
- ▶ We know how to do the integral to normalise a Gaussian.

Intractable Inference

Example where things don't work out so nicely. Take $y_n \in \{0, 1\}$.

$$p(x) = \mathcal{N}(x; 0, v) \tag{22}$$

$$\ell(x) = \frac{1}{1 + e^{-x}}$$
 Logistic function (23)

$$p(y_n|x) = \ell(x)^{y_n} \cdot (1 - \ell(x))^{1 - y_n}.$$
(24)

I.e. Y_n is Bernoulli distributed with probability $\ell(x)$.

$$p(x|\mathbf{y}) = \frac{1}{Z} \frac{e^{-N_1 x - \frac{1}{2v}x^2}}{(1 + e^{-x})^N}$$
 (25)

$$Z = \int \frac{e^{-N_1 x - \frac{1}{2v}x^2}}{(1 + e^{-x})^N} dx$$
 (26)

Intractable Inference

$$Z = \int \frac{e^{-N_1 x - \frac{1}{2v} x^2}}{(1 + e^{-x})^N} dx$$
 (27)

- ► No known "closed-form" solution to this integral.
- ► Closed-form: Combination of finite number of terms of standard functions (exp, sin, log, sqrt...). Sometimes includes special functions (e.g. Gamma, Bessel...)
- If no closed-form solution is known, a quantity is also said to be intractable.
- Inference is intractable if it requires computing intractable quantities.

Tractable Inference

- ► In general it is hard to tell when inference is tractable.
- ► There is a set of distributions for which you can tell that inference is tractable.

Definition

A prior and likelihood are **conjugate** if their resulting posterior is of the same family as the prior.

If your prior was tractable, then your posterior will be as well!

Example: Gaussian-Gaussian conjugacy

The Gaussian example we saw earlier was an example of conjugacy.

▶ Likelihood formed from Gaussian with unknown mean:

$$L(x) = p(\mathbf{y}|x) = \prod_{n} \mathcal{N}(y_n; x, \sigma^2)$$
 (28)

► Prior from the Gaussian family of distributions:

$$p(x) = \mathcal{N}(x; 0, v) \tag{29}$$

► Posterior is also Gaussian!

$$p(x|\mathbf{y}) \propto L(x)p(x)$$
 (30)

$$p(x|\mathbf{y}) = \mathcal{N}\left(x; \frac{v\sum_{n} y_{n}}{vN + \sigma^{2}}, \frac{v\sigma^{2}}{vN + \sigma^{2}}\right)$$
(31)

Exponential Family

This is no coincidence. The Gaussian distributions are part of the **exponential family**:

$$p(x|\eta) = h(x) \exp(\eta^{\mathsf{T}} t(x) - A(\eta)) \qquad \eta, t \in \mathbb{R}^{D}$$
 (32)

Different t(x) (and therefore $A(\eta)$), give different distributions.

Example: Gaussian

$$p(x) = (2\pi\sigma^2)^{-\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$
 (33)

$$t(x) = [x \quad x^2]^{\mathsf{T}}, \qquad \eta = [\mu/\sigma^2 \quad -\frac{1}{2\sigma^2}]^{\mathsf{T}},$$
 (34)

$$A(\eta) = -\frac{\eta_1^2}{4\eta_2^2} - \frac{1}{2}\log(-2\eta_2), \qquad h(x) = (2\pi)^{-\frac{1}{2}}.$$
 (35)

Exponential Family

This is no coincidence. The Gaussian distributions are part of the **exponential family**:

$$p(x|\eta) = h(x) \exp(\eta^{\mathsf{T}} t(x) - A(\eta)) \qquad \eta, t \in \mathbb{R}^{D}$$
 (36)

Different t(x) (and therefore $A(\eta)$), give different distributions.

Example: Bernoulli

$$p(x) = \theta^{x} \cdot (1 - \theta)^{1 - x} \qquad x \in \{0, 1\}$$

$$= \exp(x(\log \theta - \log 1 - \theta) + \log 1 - \theta)$$
(38)

$$= \exp(x(\log \theta - \log 1 - \theta) + \log 1 - \theta) \tag{38}$$

$$t(x) = x, \eta = \log \frac{p}{1-p}, (39)$$

$$A(\eta) = \log 1 - p$$
, $h(x) = 1$. (40)

Conjugate Prior for Exponential Family

Exponential families have conjugate priors! For the likelihood:

$$\ell(\eta) = p(x|\eta) = h(x) \exp(\eta^{\mathsf{T}} t(x) - A(\eta)) \qquad \eta, t \in \mathbb{R}^D$$
 (41)

We have the conjugate prior:

$$p(\eta|\tau, n_0) = H(\tau, n_0) \exp(\tau^{\mathsf{T}} \eta - n_0 A(\eta))$$
 (42)

Exam skills (NOT THIS YEAR)

Previous years:

- Convert distributions that are exponential families into their **natural form** (i.e. parameterised by η).
- ► Recognise when a likelihood and prior are conjugate, and when they are not.
- ► Find conjugate prior to a likelihood in exponential family.

See examples sheet for practice.

Exam skills (THIS YEAR)

You must be able to:

- ▶ do closed-form inference when distributions are Gaussian,
- do closed-form inference for discrete distributions,
- ► recognise when integrals w.r.t. Gaussians are possible,
- ▶ do integrals if an identity is given.

Summary

Inference

The procedure of drawing conclusions from observations.

In Bayesian statistics: Computing some conditional distribution (posterior).

Closed-form Expressions

A mathematical expression consisting of a finite number of standard operations (pow, exp, log, trig, etc).

See https://en.wikipedia.org/wiki/Closed-form_expression.

Closed-form Inference

An inference problem where all relevant quantities (e.g. posteriors) can be computed in closed-form.

Summary

- Integrals appear when finding the posterior (normalising constant / marginal likelihood)
- Integrals appear when making predictions
- ► Integrals can only be done in special cases
- Conjugate models is a (big) family of these special cases, which helps you recognise when you can do the closed-form inference (but this isn't examined this year)

Reading

Recommended reading:

▶ §6.6 of Mathematics for Machine Learning [1].

Further reading:

▶ §9.2 of ML: a Probabilistic Perspective [2].

References I

- [1] M. P. Deisenroth, A. A. Faisal, and C. S. Ong. Mathematics for machine learning. Cambridge University Press, 2020.
- [2] K. P. Murphy. Machine learning: a probabilistic perspective. MIT press, 2012.