Closed-Form Inference

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Computing Posteriors

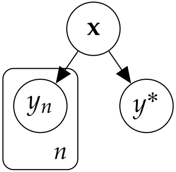
- Previous lecture investigated **which** computations we need to perform to find posteriors.
- Now, we focus on **actually doing them**.
- We focus on inference problems with two variables, one hidden (**latent**), one observed (**data**).

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

- 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

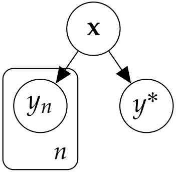


$$p(\mathbf{y}, y^*, \mathbf{x}) = p(y^*|\mathbf{x}) \prod_{n=1}^{N} p(y_n|\mathbf{x}) p(\mathbf{x}) \quad (3)$$

$$\underbrace{p(\mathbf{x}|\mathbf{y})}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{y}|\mathbf{x})}^{\text{likelihood}} \; \overbrace{p(\mathbf{x})}^{\text{prior}}}{\underbrace{p(\mathbf{y})}_{\substack{\text{marginal likelihood} \\ \text{/ evidence}}}} = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{\int p(\mathbf{y}|\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x}} \quad (4)$$

- 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? ⏩ $\mathbf{x}$ only!
  We say "likelihood of parameters / latent variable $\mathbf{x}$".

Terminology



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

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

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

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

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

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

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

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

- 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?

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

Let's start with the posterior.

- Computing the numerator of $p(\mathbf{x}|\mathbf{y})$ is easy: multiplication.
- Denominator $p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x}$ seems hard.
  Integrals are hard.
- Do we really need $p(\mathbf{y})$? 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 $p(y_n|x) = \mathcal{N}\left(y_n; x, \sigma^2\right)$ and $p(x) = \mathcal{N}(x; 0, v)$.

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

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

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

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

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

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

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.

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

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

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

- This was the case because $p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$ as a function of $\mathbf{x}$ 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 $y_n \in \{0, 1\}$.

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

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

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

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

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

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

Intractable Inference

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

- 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:

$$L(x) = p(\mathbf{y}|x) = \prod_n \mathcal{N}\left(y_n; x, \sigma^2\right) \tag{28}$$

- Prior from the Gaussian family of distributions:

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

- Posterior is also Gaussian!

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

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

Exponential Family

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

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

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

Example: Gaussian

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

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

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

Exponential Family

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

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

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

Example: Bernoulli

$$p(x) = \theta^x \cdot (1-\theta)^{1-x} \qquad x \in \{0, 1\} \tag{37}$$

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

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

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

Conjugate Prior for Exponential Family

Exponential families have conjugate priors!
For the likelihood:

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

We have the conjugate prior:

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

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.