

# MS&E 226: Fundamentals of Data Science

## Lecture 12: Bayesian inference

Ramesh Johari

# Priors

# Frequentist vs. Bayesian inference

- ▶ Frequentists treat the *parameters* as fixed (deterministic).
  - ▶ Considers the training data to be a random draw from the population model.
  - ▶ Uncertainty in estimates is quantified through the *sampling distribution*: what is seen if the estimation procedure is repeated over and over again, over many sets of training data (“parallel universes”).

# Frequentist vs. Bayesian inference

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  - ▶ Considers the training data to be a random draw from the population model.
  - ▶ Uncertainty in estimates is quantified through the *sampling distribution*: what is seen if the estimation procedure is repeated over and over again, over many sets of training data (“parallel universes”).
- ▶ Bayesians treat the *parameters* as random.
  - ▶ Key element is a *prior* distribution on the parameters.
  - ▶ Using Bayes’ theorem, combine prior with data to obtain a *posterior* distribution on the parameters.
  - ▶ Uncertainty in estimates is quantified through the posterior distribution.

## Bayes' rule: Discrete case

Suppose that we generate discrete data  $Y_1, \dots, Y_n$ , given a parameter  $\theta$  that can take one of finitely many values.

Recall that the distribution of the data given  $\theta$  is the *likelihood*  $\mathbb{P}(\mathbf{Y} = \mathbf{y} | \theta = t)$ .

The Bayesian adds to this a *prior distribution*  $\mathbb{P}(\theta = t)$ , expressing the belief that  $\theta$  takes on a given value. Then Bayes' rule says:

$$\begin{aligned} \text{POSTERIOR} \\ \mathbb{P}(\theta = t | \mathbf{Y} = \mathbf{y}) &= \frac{\mathbb{P}(\theta = t, \mathbf{Y} = \mathbf{y})}{\mathbb{P}(\mathbf{Y} = \mathbf{y})} \\ &= \frac{\mathbb{P}(\mathbf{Y} = \mathbf{y} | \theta = t) \mathbb{P}(\theta = t)}{\mathbb{P}(\mathbf{Y} = \mathbf{y})}. \\ &= \frac{\mathbb{P}(\mathbf{Y} = \mathbf{y} | \theta = t) \mathbb{P}(\theta = t)}{\sum_{\tau} \mathbb{P}(\mathbf{Y} = \mathbf{y} | \theta = \tau) \mathbb{P}(\theta = \tau)}. \end{aligned}$$

LIKELIHOOD

PRIOR

POSTERIOR  $\propto$

LIKELIHOOD  $\times$  PRIOR

"PROPORTIONAL TO"

## Bayes' rule: Continuous case

If data and/or parameters are continuous, we use densities instead of distributions. E.g., if both data and parameters are continuous, Bayes' rule says:

$$f(\boldsymbol{\theta}|\mathbf{Y}) = \frac{f(\mathbf{Y}|\boldsymbol{\theta})f(\boldsymbol{\theta})}{f(\mathbf{Y})},$$

where

$$f(\mathbf{Y}) = \int f(\mathbf{Y}|\tilde{\boldsymbol{\theta}})f(\tilde{\boldsymbol{\theta}})d\tilde{\boldsymbol{\theta}}.$$

## Bayes' rule: In words

The *posterior* is the distribution of the parameter, given the data.

Bayes' rule says:

$$\text{posterior} \propto \text{likelihood} \times \text{prior}.$$

Here “ $\propto$ ” means “proportional to”; the missing constant is  $1/f(\mathbf{Y})$ , the <sup>inverse of</sup> unconditional probability of the data.

Note that this constant *does not depend on the parameter  $\theta$* .

## Example: Biased coin flipping

We flip a biased coin 5 times, and get  $H, H, T, H, T$ . What is your estimate of the bias  $q$ ?

A Bayesian starts with a *prior* for  $q$ :  $f(q)$  (pdf).

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The posterior is the distribution of  $q$ , given the data we saw; we get this using Bayes' rule:

$$f(q|\mathbf{Y}) = \frac{\mathbb{P}(\mathbf{Y}|q)f(q)}{\int_0^1 \mathbb{P}(\mathbf{Y}|q')f(q')dq'}.$$

## Example: Biased coin flipping

As an example, suppose that  $f(q)$  was the uniform distribution on  $[0, 1]$ .

Then the posterior after  $n$  flips with  $k$   $H$ 's and  $n - k$   $T$ 's is:

$$f(q|\mathbf{Y}) = \frac{1}{B(k+1, n-k+1)} q^k (1-q)^{n-k},$$

the  $\text{Beta}(k+1, n-k+1)$  distribution.

In fact: if the *prior is a  $\text{Beta}(a, b)$  distribution, the posterior is a  $\text{Beta}(a+k, b+n-k)$  distribution.*<sup>1</sup> (The uniform distribution is a  $\text{Beta}(1, 1)$  distribution.)

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<sup>1</sup>We say the beta distribution (the prior on the parameter) is *conjugate* to the binomial distribution (the likelihood).

# Bayesian inference

# The goals of inference

Recall the two main goals of inference:

- ▶ What is a good guess of the population model (the true parameters)?
- ▶ How do I quantify my uncertainty in the guess?

Bayesian inference answers both questions directly through the posterior.

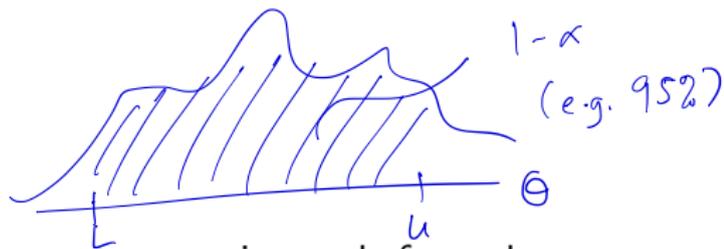
# Using the posterior

The posterior can be used in many ways to estimate the parameters. For example, you might compute:

- ▶ The mean
- ▶ The median
- ▶ The mode
- ▶ etc.

Depending on context, these are all potentially useful ways to estimate model parameters from a posterior.

## Using the posterior



In the same way, it is possible to construct intervals from the posterior. These are called *credible* intervals (in contrast to “confidence” intervals in frequentist inference).

Given a posterior distribution on a parameter  $\theta$ , a  $1 - \alpha$  credible interval  $[L, U]$  is an interval such that:

$$\mathbb{P}(L \leq \theta \leq U | \mathbf{Y}) \geq 1 - \alpha.$$

Note that here, in contrast to frequentist confidence intervals, the endpoints  $L$  and  $U$  are *fixed* and the parameter  $\theta$  is *random*!

## Using the posterior

More generally, because the posterior is a full distribution on the parameters, it is possible to make all sorts of probabilistic statements about their values, for example:

- ▶ “I am 95% sure that the true parameter is bigger than 0.5.”
- ▶ “There is a 50% chance that  $\theta_1$  is larger than  $\theta_2$ .”
- ▶ etc.

In Bayesian inference, you should not limit yourself to just point estimates and intervals; visualization of the posterior distribution is often quite valuable and yields significant insight.

## Example: Biased coin flipping

Recall that with a  $\text{Beta}(a, b)$  prior on  $q$ , the posterior (with  $k$  heads and  $n - k$  tails) is  $\text{Beta}(a + k, b + n - k)$ .

The mode of this distribution is  $\hat{q} = \frac{a+k-1}{a+b+n-2}$ .

Recall that the MLE is  $k/n$ , and the mode of the  $\text{Beta}(a, b)$  prior is  $(a - 1)/(a + b - 2)$ . So in this case we can also write:

$$\text{posterior mode} = c_n \text{MLE} + (1 - c_n)(\text{prior mode}),$$

where:

$$c_n = \frac{n}{a + b + n - 2}.$$

## Bayesian estimation and the MLE

The preceding example suggests a close connection between Bayesian estimation and the MLE. This is easier to see by recalling that:

$$\text{posterior} \propto \text{likelihood} \times \text{prior}.$$

So if the prior is *flat* (i.e., uniform), then the parameter estimate that maximizes the posterior (the mode, also called the *maximum a posteriori* estimate or *MAP*) is the same as the maximum likelihood estimate.

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In general:

- ▶ Uniform priors may not make sense (because, e.g., the parameter space is unbounded).
- ▶ A non-uniform prior will make the MAP estimate different from the MLE.

## Example: Normal data

Suppose that  $Y_1, \dots, Y_n$  are i.i.d.  $\mathcal{N}(\mu, 1)$ . Suppose a prior on  $\mu$  is that  $\mu \sim \mathcal{N}(a, b^2)$ . Then it can be shown that the posterior for  $\mu$  is  $\mathcal{N}(\hat{a}, \hat{b}^2)$ , where:

$$\begin{aligned}\hat{a} &= c_n \bar{Y} + (1 - c_n)a; \\ \hat{b}^2 &= \frac{1}{n + 1/b^2}; \\ c_n &= \frac{n}{n + 1/b^2}.\end{aligned}$$

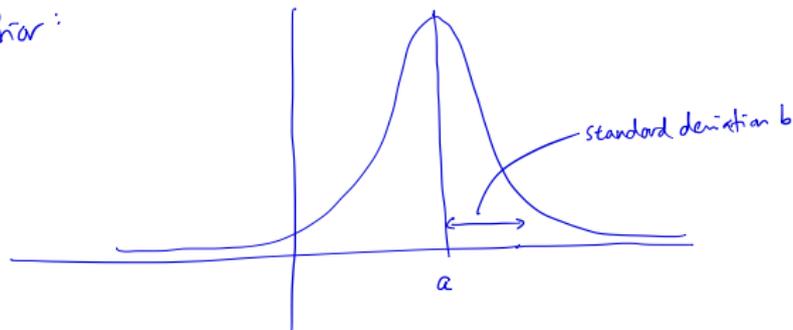
So the MAP estimate is  $\hat{a}$ ; and a 95% credible interval for  $\mu$  is  $[\hat{a} - 1.96\hat{b}, \hat{a} + 1.96\hat{b}]$ .

Note that for large  $n$ ,  $\hat{a} \approx \bar{Y}$ , and  $\hat{b} \approx 1/\sqrt{n} = \text{SE}$ , the frequentist standard error of the MLE.

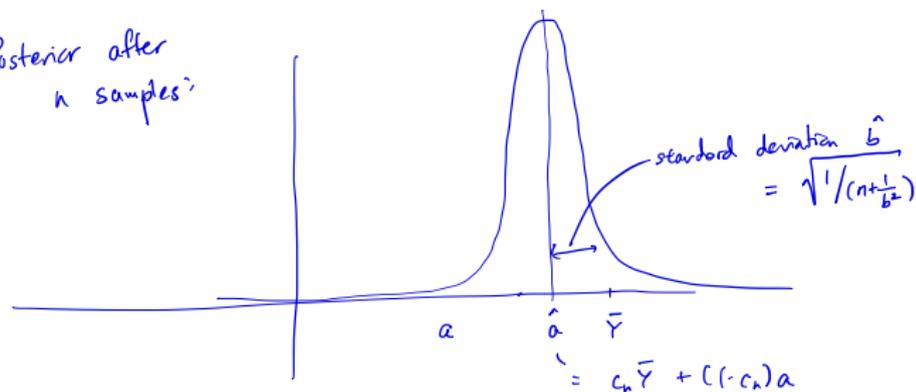
# Example: Normal data

A picture:

Prior:



Posterior after  
 $n$  samples:



# Maximum likelihood and Bayesian inference

The preceding observations are more general.

If the prior is “reasonable” then the posterior is *asymptotically normal*, with mean that is the MLE  $\hat{\theta}_{\text{MLE}}$ , and variance that is  $\hat{S\hat{E}}^2$ , where  $\hat{S\hat{E}}$  is the standard error of the MLE.

So for example:

- ▶ In large samples, the posterior mean (or mode) and the MLE are approximately the same.
- ▶ In large samples, the  $1 - \alpha$  normal (frequentist) confidence interval is the same as the  $1 - \alpha$  (Bayesian) credible interval.

# Computation

Even simple Bayesian inference problems can rapidly become computationally intractable: computing the posterior is often not straightforward.

The last few decades have seen a revolution in computational methods for Bayesian statistics, headlined by *Markov chain Monte Carlo* (MCMC) techniques for estimating the posterior.

Though not perfect, these advances mean that you don't need to consider computational advantages when choosing one approach over another.

## When do Bayesian methods work well?

Bayesian methods work well, quite simply, when *prior information matters*.

An example with biased coin flipping: if a perfectly normal coin is flipped 10 times, with 8 heads, what is your guess of the bias?

- ▶ A frequentist would say 0.8.
- ▶ A Bayesian would likely use a prior that is very strongly peaked around 0.5, so the new evidence from just ten flips would not change her belief very much.

## When do Bayesian methods work poorly?

Analogously, Bayesian methods work poorly when the prior is poorly chosen.

For example, suppose you try out a new promotion on a collection of potential customers.

Previous promotions may have failed spectacularly, leading you to be pessimistic as a Bayesian.

However, as a consequence, you will be more unlikely to detect an objectively successful experiment.

# Combining methods

A good frequentist estimation procedure:

- ▶ Uses only the data for inferences
- ▶ Provides guarantees on how the procedure will perform, if repeatedly used

A good Bayesian estimation procedure:

- ▶ Leverages available prior information effectively
- ▶ Combines prior information and the data into a single distribution (the posterior)
- ▶ Ensures the choice of estimate is “optimal” given the posterior (e.g., maximum *a posteriori* estimation)

# Combining methods

It is often valuable to:

- ▶ Ask that Bayesian methods have good frequentist properties
- ▶ Ask that estimates computed by frequentist methods “make sense” given prior understanding

Having both approaches in your toolkit is useful for this reason.

## Choosing the prior

# Where did the prior come from?

There are two schools of thought on the prior:

- ▶ *Subjective* Bayesian
  - ▶ The prior is a summary of our subjective beliefs about the data.
  - ▶ E.g., in the coin flipping example: the prior for  $q$  should be strongly peaked around  $1/2$ .

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Objective Bayesian inference was a response to the basic criticism that subjectivity should not enter into scientific conclusions. (Worth considering whether this is appropriate in a business context...)

## Objectivism: Flat priors

A *flat* prior is a uniform prior on the parameter:  $f(\theta)$  is constant.

As noted this doesn't make sense when  $\theta$  can be unbounded...or does it?

## Example: Normal data

Suppose again that  $Y_1, \dots, Y_n$  are i.i.d.  $\mathcal{N}(\mu, 1)$ , but that now we use a “prior”  $f(\mu) \equiv 1$ .

Of course this prior is not a probability distribution, but it turns out that we can still formally carry out the calculation of a posterior, as follows:

- ▶ The product of the *likelihood* and the *prior* is just the likelihood.
- ▶ If we can *normalize* the likelihood to be a probability distribution over  $\mu$ , then this will be a well-defined posterior.

Note that in this case the posterior is just a scaled version of likelihood, so the MAP estimate (posterior mode) is *exactly the same* as the MLE!

## Improper priors

This example is one where the flat prior is *improper*: it is not a probability distribution on its own, but yields a well-defined posterior.

Flat priors are sometimes held up as evidence of why Bayesian estimates are at least as informative as frequentist estimates, since at worst by using a flat prior we can recover maximum likelihood estimation.

Another way to interpret this is as a form of *conservatism*: The most conservative thing to do is to assume you have no knowledge, except what is in the data; this is what the flat prior is meant to encode.

## Jeffreys' priors [\*]

But flat priors can also lead to some unusual behavior. For example, suppose we place a flat prior on  $\mu$ . What is our prior on, e.g.,  $\mu^3$ ? It is not flat:

$$f(\mu^3) = \frac{f(\mu)}{3\mu^2} = \frac{1}{3\mu^2}.$$

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The problem is that flat priors are not *invariant* to transformations of the parameter.

Jeffreys showed that a reasonable uninformative prior that is also transformation invariant is obtained by setting  $f(\theta)$  to the inverse of the Fisher information at  $\theta$ ; see [AoS], Section 11.6.

# Applications

# Bayesian linear regression

Assume a linear normal model  $Y_i = \vec{X}_i \boldsymbol{\beta} + \varepsilon_i$ , where the  $\varepsilon_i$  are  $\mathcal{N}(0, \sigma^2)$ .

In Bayesian linear regression, we also put a prior distribution on  $\boldsymbol{\beta}$ .

Here we look at two examples of this approach.

## Bayesian linear regression: Normal prior

Suppose that the prior distribution on the coefficients  $\beta$  is:

$$\beta \sim \mathcal{N}\left(\mathbf{0}, \frac{1}{\lambda\sigma^2}\mathbf{I}\right).$$

In other words: the higher  $\lambda$  is, the higher the prior “belief” that  $\beta$  is close to zero.<sup>2</sup>

For this prior, the MAP estimator is the same as the *ridge regression* solution.

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<sup>2</sup>Note that this is a “partial” Bayesian solution, since  $\sigma^2$  is assumed known. In practice an estimate of  $\sigma^2$  is used.

## Bayesian linear regression: Laplace prior

Now suppose instead that the prior is that all the  $\beta_j$  are independent, each with density:

$$f(\beta) = \left( \frac{\lambda}{2\sigma} \right) \exp \left( -\frac{\lambda|\beta|}{\sigma} \right).$$

This is called the *Laplace* distribution; it is symmetric around zero, and more strongly peaked as  $\lambda$  grows.<sup>3</sup>

With this prior, the MAP estimator is the same as the *lasso* solution.

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<sup>3</sup>Note that this is again a solution that assumes  $\sigma^2$  is known. In practice an estimate of  $\sigma^2$  is used.

# Bayesian model selection

The BIC (Bayesian information criterion) is obtained from a Bayesian view of model selection.

Basic idea:

- ▶ Imagine there is a prior over possible models.

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- ▶ We would want to choose the model that has the highest posterior probability.
- ▶ In large samples, the effect of this prior becomes small relative to the effect of the data, so asymptotically BIC estimates the posterior probability of a model by (essentially) ignoring the effect of the prior.
- ▶ Choosing the model that maximizes BIC is like choosing the model that has the highest posterior probability in this sense.