# STAT 339 <br> Bayesian Inference IV 

December 3rd, 2021

Colin Reimer Dawson

## Outline

The Predictive Distribution

Model Selection and Bayesian Occam's Razor

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## Model Selection and Bayesian Occam's Razor

## Inference vs Prediction

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- If our goal is understanding that process, this is an end in itself
- However, many of our ML models are designed to to make predictions about some $\mathbf{y}_{\text {new }}$.
- When using optimization methods such MLE, we get a single value $\hat{\theta}$ and can then predict using $p\left(\mathbf{y}_{\text {new }} \mid \hat{\theta}\right)$
- With Bayesian inference, however, we get a distribution, $p\left(\theta \mid \mathbf{y}_{\text {train }}\right)$, not a single value.
- How do we use this to make predictions?


## Option 1: Distribution to Point Estimate

- One option: Find $\hat{\theta}$, a point estimate of $\theta$ from the posterior (e.g., the mean, or mode) and use $p\left(\mathbf{y}_{\text {new }} \mid \hat{\theta}\right)$ for prediction


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- One option: Find $\hat{\theta}$, a point estimate of $\theta$ from the posterior (e.g., the mean, or mode) and use $p\left(\mathbf{y}_{\text {new }} \mid \hat{\theta}\right)$ for prediction
- However, this discards our uncertainty, and one of the main points of a Bayesian approach is principled handling of uncertainty


## Option 2: Posterior Predictive Distribution

A more "fully Bayesian" solution: Compute the posterior predictive distribution:

$$
\begin{aligned}
p\left(\mathbf{y}_{\text {new }} \mid \mathbf{y}_{\text {train }}\right) & =\int p\left(\mathbf{y}_{\text {new }}, \theta \mid \mathbf{y}_{\text {train }}\right) d \theta \\
& =\int p\left(\mathbf{y}_{\text {new }} \mid \theta, \mathbf{y}_{\text {train }}\right) p\left(\theta \mid \mathbf{y}_{\text {train }}\right) d \theta
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$$

If $\mathbf{y}_{\text {new }}$ and $\mathbf{y}_{\text {train }}$ are conditionally independent given $\theta$, this simplifies to

$$
p\left(\mathbf{y}_{\text {new }} \mid \mathbf{y}_{\text {train }}\right)=\int p\left(\mathbf{y}_{\text {new }} \mid \theta\right) p\left(\theta \mid \mathbf{y}_{\text {train }}\right) d \theta
$$

which is expressed in terms of the data-generating model (likelihood) and the posterior. In fact, it is equivalent to

$$
\mathbb{E}\left[p\left(\mathbf{y}_{\text {new }} \mid \theta\right) \mid \mathbf{y}_{\text {train }}\right]
$$

## Example: Beta-Bernoulli Model

- Suppose we have data-generating model and prior

$$
\begin{gathered}
y_{1}, \ldots y_{N} \stackrel{i . i . d .}{\sim} \operatorname{Bernoulli}(\mu) \\
\mu \sim \operatorname{Unif}(0,1)
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- MLE: $\hat{\mu}=p\left(y_{\text {new }}=1 \mid \hat{\mu}\right)=\frac{12}{40}=0.30$.


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- MLE: $\hat{\mu}=p\left(y_{\text {new }}=1 \mid \hat{\mu}\right)=\frac{12}{40}=0.30$.
- Posterior mean: $\mathbb{E}\left[\mu \mid \mathbf{y}_{\text {new }}\right]=\frac{12+1}{40+2}=0.31$


## Beta-Bernoulli: Predictive Distribution

Alternatively, calculating the predictive probability directly:

$$
p\left(y_{\text {new }}=1 \mid \mathbf{y}_{\text {train }}\right)=\int_{0}^{1} p\left(y_{\text {new }}=1 \mid \mu\right) p\left(\mu \mid \mathbf{y}_{\text {train }}\right) d \mu
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In this case, the predictive probability of interest is just the posterior mean (this will not always be true, however).

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- A simple likelihood and prior (ignoring seasonal variation, etc.):

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- If we knew $\lambda$ we would expect $\lambda$ customers per day on average


## Gamma-Poisson: Predicting with a Point Estimate

 If we predict using $p\left(y_{\text {new }} \mid \hat{\lambda}\right)$ with$$
\hat{\lambda}_{\mathrm{MLE}}=\frac{y_{\text {train }}}{N}
$$

then

$$
\mathbb{E}\left[y_{\text {new }} \mid \hat{\lambda}\right]=\hat{\lambda}=\frac{y_{\text {train }}}{N}
$$

If instead we use

$$
\hat{\lambda}=\mathbb{E}\left[\lambda \mid y_{\text {train }}\right]=\frac{a_{\text {post }}}{b_{\text {post }}}
$$

where

$$
a_{\text {post }}=a_{0}+y_{\text {train }} \quad b_{\text {post }}=b_{0}+N
$$

then

$$
\mathbb{E}\left[y_{\text {new }} \mid \hat{\lambda}\right]=\hat{\lambda}=\frac{a_{\text {post }}}{b_{\text {post }}}=\frac{a_{0}+y_{\text {train }}}{b_{0}+N}
$$

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Alternatively, calculating the predictive distribution directly:

$$
p\left(y_{\text {new }} \mid y_{\text {train }}\right)=\int_{0}^{\infty} p\left(y_{\text {new }} \mid \lambda\right) p\left(\lambda \mid y_{\text {train }}\right) d \lambda
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& =\left(\frac{b_{\text {post }}^{a_{\text {post }}}}{\Gamma\left(a_{\text {post }}\right) y_{\text {new }}!}\right)\left(\frac{\Gamma\left(a_{\text {post }}+y_{\text {new }}\right)}{\left.\left(b_{\text {post }}+1\right)^{a_{\text {post }}+y_{\text {new }}}\right)}\right.
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& =\left(\frac{\Gamma\left(a_{\text {post }}+y_{\text {new }}\right)}{\Gamma\left(a_{\text {post }}\right) y_{\text {new }}!}\right)\left(\frac{1}{b_{\text {post }}+1}\right)^{y_{\text {new }}}\left(\frac{b_{\text {post }}}{b_{\text {post }}+1}\right)^{a_{\text {post }}}
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where $\mu:=\frac{1}{b_{\text {post }+1}}$

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where $\mu:=\frac{1}{b_{\text {post }}+1}$ Note that if $a_{0}$ (representing the number of "virtual" customers visiting in $b_{0}$ days as encoded in the prior) is an integer, then so is $a_{\text {post }}=a_{0}+y_{\text {train }}$, and we can write

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p\left(y_{\text {new }} \mid y_{\text {train }}\right)=\frac{\left(a_{\text {post }}+y_{\text {new }}-1\right)!}{\left(a_{\text {post }}-1\right)!y_{\text {new }}!} \mu^{y_{\text {new }}}(1-\mu)^{a_{\text {post }}}
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& =\binom{a_{\text {post }}+y_{\text {post }}-1}{y_{\text {new }}} \mu^{y_{\text {new }}}(1-\mu)^{a_{\text {post }}}
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This is a Negative Binomial distribution with parameters $a_{\text {post }}$ and $\mu$.

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$$
\begin{gathered}
\mathbb{E}\left[y_{\text {new }} \mid y_{\text {train }}\right]=\left(\frac{\mu}{1-\mu}\right) a_{\text {post }}=\frac{a_{\text {post }}}{b_{\text {post }}} \\
\operatorname{Var}\left[y_{\text {new }} \mid y_{\text {train }}\right]=\left(\frac{\mu}{1-\mu}\right) \frac{a_{\text {post }}}{1-\mu}=\frac{a_{\text {post }}}{b_{\text {post }}} \frac{1+b_{\text {post }}}{b_{\text {post }}}
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## Gamma-Poisson: Predictive Distribution

We have shown that, with data-generating model and prior

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y_{\text {train }} \mid & \lambda \sim \operatorname{Poisson}(N \lambda) \\
& \lambda \sim \operatorname{Gamma}\left(a_{0}, b_{0}\right)
\end{aligned}
$$

we get posterior, and posterior predictive distributions:

$$
\begin{gathered}
\lambda \mid y_{\text {train }} \sim \operatorname{Gamma}\left(a_{0}+y_{\text {train }}, b_{0}+N\right) \\
y_{\text {new }} \mid y_{\text {train }} \sim \operatorname{NegBinom}\left(a_{0}+y_{\text {train }},\left(b_{0}+N+1\right)^{-1}\right)
\end{gathered}
$$

with predictive mean and variance:

$$
\begin{aligned}
& \mathbb{E}\left[y_{\text {new }} \mid y_{\text {train }}\right]=\frac{a_{0}+y_{\text {train }}}{b_{0}+N}=\left(\frac{b_{0}}{b_{0}+N}\right) \mathbb{E}[\lambda]+\left(\frac{N}{b_{0}+N}\right) \hat{\lambda}_{M L E} \\
& \mathbb{V a r}\left[y_{\text {new }} \mid y_{\text {train }}\right]=\left(\frac{a_{0}+y_{\text {train }}}{b_{0}+N}\right)\left(1+\left(b_{0}+N\right)^{-1}\right)
\end{aligned}
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Note that as $N \rightarrow \infty$, both the predictive mean and variance converge to their values when $\lambda=\hat{\lambda}_{M L E}$.

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Model Selection and Bayesian Occam's Razor

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p(\mathcal{M}, \theta)=p(\mathcal{M}) p(\theta \mid \mathcal{M})
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- To examine the posterior plausibility of each model class (averaging over possible $\theta$ ), we are interested in

$$
p(\mathcal{M} \mid \mathbf{y})=k_{\mathbf{y}} p(\mathbf{y} \mid \mathcal{M}) p(\mathcal{M})
$$

## Marginal Likelihood

To find $p(\mathcal{M} \mid \mathbf{y})$, we need $p(\mathcal{M})$ (which we specify as part of the prior), and $p(\mathbf{y} \mid \mathcal{M})$.

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The latter is called the marginal likelihood:

## Marginal Likelihood

The marginal likelihood for a dataset y given a model class, $\mathcal{M}$ is

$$
p\left(\mathbf{y}_{\text {train }} \mid \mathcal{M}\right)=\int p\left(\mathbf{y}_{\text {train }} \mid \theta, \mathcal{M}\right) p(\theta \mid \mathcal{M}) d \theta
$$

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- After 40 flips, we see 25 heads.
- This gives conditional posteriors:

$$
\begin{aligned}
\mu \mid \mathbf{y}, \mathcal{M}_{\mathrm{fair}} & \sim I(\mu=0.5) \\
\mu \mid \mathbf{y}, \mathcal{M}_{\text {biased }} & \sim \operatorname{Beta}(25+1,15+1)
\end{aligned}
$$

## Fair Coin: Prior and Posterior




Figure: Top: Prior on $\mu$, conditioned on the coin being fair. Bottom: Posterior on $\mu$, conditioned on the coin being fair. Note that conditioning on the coin being fair makes the data irrelevant for inferring $\mu$

## Biased Coin: Prior and Posterior




Figure: Top: Prior on $\mu$, conditioned on the coin being biased. Bottom: Posterior on $\mu$, conditioned on the coin being biased. When the coin can have any bias, the posterior concentrates mass near the observed proportion of heads

## Example: Fair or Biased Coin?

The marginal likelihood for the biased coin (average probability of 25 heads out of 40) is:

$$
p\left(y \mid \mathcal{M}_{\text {biased }}\right)=\int_{0}^{1} p\left(y \mid \mu, \mathcal{M}_{\text {biased }}\right) p\left(\mu \mid \mathcal{M}_{\text {biased }}\right) d \mu
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If the coin is fair (i.e., $\mu=0.5$ with probability 1 ), then the marginal likelihood is just

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and so the "fair coin hypothesis" yields a higher marginal likelihood than the "Bayesian alternative" with a uniform prior.

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- Thus, relative to what we believed before seeing the data, our subjective odds that the coin is biased should go down after seeing 25 heads out of 40 ! (with the "uniform" notion of what "bias" looks like)
- The ratio of marginal likelihoods, by which our "belief ratio" is scaled, is called the Bayes Factor


## Conservation of Explanatory Power



Marginal likelihood "rewards" specific predictions

Conservation of Explanatory Power


## Probabilistic Occam's Razor

Sauage Chickens
by Doug Savage


## Bayesian Occam's Razor

A "possible world" consists of a model $\mathcal{M}$, along with a (possibly trivial) parameter-setting, $\theta$

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p(\mathcal{M} \mid \mathbf{y})=\int \frac{p(\mathcal{M}, \theta) p(\mathbf{y} \mid \mathcal{M}, \theta)}{p(\mathbf{y})} d \theta d \theta
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$p(\mathbf{y} \mid \mathcal{M}, \theta) \quad$ Rewards specific predictions by $(\mathcal{M}, \theta)$

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## Other examples

- Polynomial regression: $\theta=$ coefficients $p(\theta \mid \mathcal{M})$ will be "spread thin" for "higher order" polynomials, since there are more possibilities
- Classification: $\theta=$ shapes of each class $p(\theta \mid \mathcal{M})$ will be "spread thin" for more complex shapes, since there are more possibilities


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