Probabilistic models

Bayesian Methods

Tal Linzen

Slides based on Lecture 08a from David Rosenberg's course materials (https://github.com/davidrosenberg/mlcourse) and Marylou Gabrié's materials

CDS, NYU

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- 2 Bayesian Statistics: Introduction
- 3 Bayesian Decision Theory

Interim summary

- 5 Recap: Conditional Probability Models
- 6 Bayesian Conditional Probability Models
- Gaussian Regression Example
- (8) Gaussian Regression: Closed form

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Parametric Family of Densities

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- where $p(y \mid \theta)$ is a density on a sample space \mathcal{Y} , and
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- where $p(y \mid \theta)$ is a density on a **sample space** \mathcal{Y} , and
- θ is a **parameter** in a [finite dimensional] **parameter space** Θ .
- This is the common starting point for a treatment of classical or Bayesian statistics.
- In this lecture, whenever we say "density", we could replace it with "mass function." (and replace integrals with sums).

Frequentist or "Classical" Statistics

• We're still working with a parametric family of densities:

 $\{p(y \mid \theta) \mid \theta \in \Theta\}.$

• Assume that $p(y \mid \theta)$ governs the world we are observing, for some $\theta \in \Theta$.

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- If we knew the right $\theta\in\Theta,$ there would be no need for statistics.
- But instead of θ , we have data \mathcal{D} : y_1, \ldots, y_n sampled i.i.d. from $p(y \mid \theta)$.
- Statistics is about how to get by with ${\mathcal D}$ in place of $\theta.$

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- Maximum likelihood estimators are consistent and efficient under reasonable conditions.

Example of Point Estimation: Coin Flipping

• Parametric family of mass functions:

 $p(\mathsf{Heads} \mid \theta) = \theta,$

for $\theta \in \Theta = (0, 1)$.

- Data $\mathcal{D} = (H, H, T, T, T, T, T, H, \dots, T)$, assumed i.i.d. flips.
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$$L_{\mathcal{D}}(\theta) = \boldsymbol{\rho}(\mathcal{D} \mid \theta) = \theta^{n_h} (1 - \theta)^{n_t}$$

• As usual, it is easier to maximize the log-likelihood function:

$$\begin{split} \hat{\theta}_{\mathsf{MLE}} &= \operatorname*{arg\,max}_{\theta \in \Theta} \log \mathcal{L}_{\mathcal{D}}(\theta) \\ &= \operatorname{arg\,max}_{\theta \in \Theta} [n_h \log \theta + n_t \log(1 - \theta)] \end{split}$$

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2 A **prior distribution** $p(\theta)$ on parameter space Θ .

• Putting the pieces together, we get a joint density on θ and $\mathcal{D}:$

 $\boldsymbol{p}(\mathcal{D},\boldsymbol{\theta}) = \boldsymbol{p}(\mathcal{D} \mid \boldsymbol{\theta})\boldsymbol{p}(\boldsymbol{\theta}).$

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- The posterior represents the rationally updated belief about θ , after seeing \mathcal{D} .

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- $\bullet\,$ Then both sides are densities on Θ and we can write

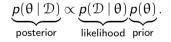
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 \bullet Where \propto means we've dropped factors that are independent of $\theta.$

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for $\theta \in \Theta = (0, 1)$.

- We need a prior distribution $p(\theta)$ on $\Theta = (0, 1)$.
- One convenient choice would be a distribution from the Beta family

• Prior:

$$\begin{array}{ll} \theta & \sim & \mathsf{Beta}(\alpha,\beta) \\ \rho(\theta) & \propto & \theta^{\alpha-1} \left(1\!-\!\theta\right)^{\beta-1} \end{array}$$

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Figure by Horas based on the work of Krishnavedala (Own work) [Public domain], via Wikimedia Commons http://commons.wikimedia.org/wiki/File:Beta_distribution_pdf.svg.

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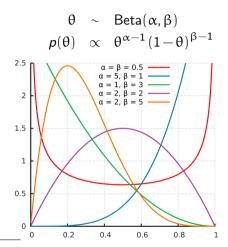


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• Mode of Beta distribution:

$$\arg\max_{\theta} p(\theta) = \frac{h-1}{h+t-2}$$

for h, t > 1.

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• Posterior density:

 $p(\theta \mid \mathcal{D}) \propto p(\theta)p(\mathcal{D} \mid \theta)$

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• Posterior density:

$$\begin{array}{ll} \rho(\theta \mid \mathcal{D}) & \propto & \rho(\theta) \rho(\mathcal{D} \mid \theta) \\ & \propto & \theta^{h-1} \left(1 - \theta\right)^{t-1} \times \theta^{n_h} \left(1 - \theta\right)^{n_h} \end{array}$$

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• Interpretation:

- Prior initializes our counts with *h* heads and *t* tails.
- Posterior increments counts by observed n_h and n_t .

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A family of distributions π is conjugate to parametric model *P* if for any prior in π , the posterior is always in π .

• The beta family is conjugate to the coin-flipping (i.e. Bernoulli) model.

Coin Flipping: Concrete Example

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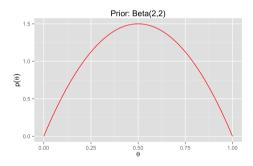
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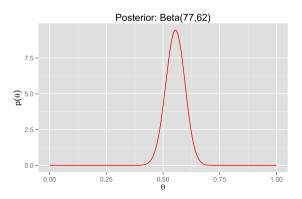


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- Heads: 75 Tails: 60 • $\hat{\theta}_{MLE} = \frac{75}{75+60} \approx 0.556$
- Posterior distribution: $\theta \mid D \sim \text{Beta}(77, 62)$:



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- Common options:
 - posterior mean $\hat{\boldsymbol{\theta}} = \mathbb{E}\left[\boldsymbol{\theta} \mid \mathcal{D}\right]$
 - maximum a posteriori (MAP) estimate $\hat{\theta} = \operatorname{arg max}_{\theta} p(\theta \mid D)$
 - Note: this is the mode of the posterior distribution

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- Select a point estimate using **Bayesian decision theory**:
 - Choose a loss function.
 - Find action minimizing expected risk w.r.t. posterior

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- A Bayes action a^* is an action that minimizes posterior risk:

$$r(a^*) = \min_{a \in \mathcal{A}} r(a)$$

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- Find action $\hat{\theta} \in \Theta$ that minimizes the $% \hat{\theta} \in \Theta$ posterior risk:

$$r(\hat{\theta}) = \mathbb{E}\left[\ell(\hat{\theta}, \theta) \mid \mathcal{D}\right]$$

- General Setup:
 - Data \mathcal{D} generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
 - We want to produce a **point estimate** for $\theta.$
- Choose:
 - **Prior** $p(\theta)$ on $\Theta = R$.
 - Loss $\ell(\hat{\theta}, \theta)$
- Find action $\hat{\theta} \in \Theta$ that minimizes the $% \hat{\theta} \in \Theta$ posterior risk:

$$r(\hat{\theta}) = \mathbb{E}\left[\ell(\hat{\theta}, \theta) \mid \mathcal{D}\right]$$
$$= \int \ell(\hat{\theta}, \theta) \rho(\theta \mid \mathcal{D}) d\theta$$

Important Cases

• Squared Loss :
$$\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \Rightarrow$$
 posterior mean

• Zero-one Loss:
$$\ell(\theta, \hat{\theta}) = 1(\theta \neq \hat{\theta}) \implies \text{posterior mode}$$

• Absolute Loss :
$$\ell(\hat{\theta}, \theta) = \left| \theta - \hat{\theta} \right| \Rightarrow$$
 posterior median

 \bullet Find action $\hat{\theta}\in\Theta$ that minimizes posterior risk

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• The Bayes action for square loss is the posterior mean.

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 - For decision making, we need a loss function.

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- This is the common starting point for either classical or Bayesian regression.

Classical treatment: Likelihood Function

- **Data:** $D = (y_1, ..., y_n)$
- $\bullet\,$ The probability density for our data ${\mathcal D}$ is

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• For fixed \mathcal{D} , the function $\theta \mapsto p(\mathcal{D} \mid x, \theta)$ is the likelihood function:

$$L_{\mathcal{D}}(\theta) = \boldsymbol{p}(\mathcal{D} \mid \boldsymbol{x}, \theta),$$

where $x = (x_1, ..., x_n)$.

• The maximum likelihood estimator (MLE) for θ in the family $\{p(y \mid x, \theta) \mid \theta \in \Theta\}$ is

$$\hat{\theta}_{\mathsf{MLE}} = \underset{\substack{\theta \in \Theta}}{\operatorname{arg\,max}} L_{\mathcal{D}}(\theta).$$

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• The corresponding prediction function is

$$\hat{f}(x) = p(y \mid x, \hat{\theta}_{\mathsf{MLE}}).$$

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• A prior distribution $p(\theta)$ on $\theta \in \Theta$.

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- \bullet Posterior represents the rationally updated beliefs after seeing $\mathcal{D}.$
- Each $\boldsymbol{\theta}$ corresponds to a prediction function,
 - i.e. the conditional distribution function $p(y | x, \theta)$.

Point Estimates of Parameter

• What if we want point estimates of θ ?

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- We can use Bayesian decision theory to derive point estimates.
- We may want to use
 - $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}, x]$ (the posterior mean estimate)
 - $\hat{\theta} = \text{median}[\theta \mid \hat{\mathcal{D}}, x]$
 - $\hat{\theta} = \operatorname{arg\,max}_{\theta \in \Theta} p(\theta \mid \mathcal{D}, x)$ (the MAP estimate)
- depending on our loss function.

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- and a prior distribution $p(\theta)$ on this set.
- Having set our Bayesian model, how do we predict a distribution on y for input x?
- We don't need to make a discrete selection from the hypothesis space: we maintain uncertainty.

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• In the Bayesian approach, we integrate out over Θ w.r.t. $p(\theta \mid D)$ and predict with

$$p(y \mid x, \mathcal{D}) = \int p(y \mid x; \theta) p(\theta \mid \mathcal{D}) d\theta$$

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What if we don't want a full distribution on y?

- Once we have a predictive distribution $p(y \mid x, \mathcal{D})$,
 - we can easily generate single point predictions.
- $x \mapsto \mathbb{E}[y \mid x, \mathcal{D}]$, to minimize expected square error.
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- $x \mapsto \arg \max_{y \in \mathcal{Y}} p(y \mid x, \mathcal{D})$, to minimize expected 0/1 loss
- Each of these can be derived from p(y | x, D).

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- Input space $\mathfrak{X} = [-1, 1]$ Output space $\mathfrak{Y} = \mathsf{R}$
- Given x, the world generates y as

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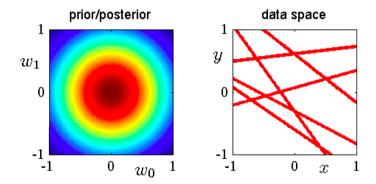
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Example in 1-Dimension: Prior Situation

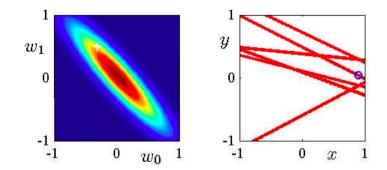
• Prior distribution: $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$ (Illustrated on left)



• On right, $y(x) = \mathbb{E}[y | x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}(0, \frac{1}{2}I)$.

Bishop's PRML Fig 3.7

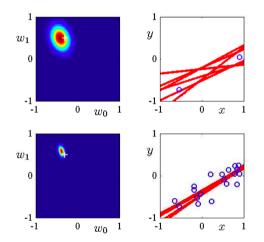
Example in 1-Dimension: 1 Observation



- On left: posterior distribution; white cross indicates true parameters
- On right:
 - blue circle indicates the training observation
 - red lines, $y(x) = \mathbb{E}[y | x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w | D)$ (posterior)

Bishop's PRML Fig 3.7

Example in 1-Dimension: 2 and 20 Observations



Bishop's PRML Fig 3.7

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$$w \mid \mathcal{D} \sim \mathcal{N}(\mu_{P}, \Sigma_{P})$$

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• Posterior Variance Σ_P gives us a natural uncertainty measure.

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• For the prior variance $\Sigma_0 = \frac{\sigma^2}{\lambda} I$, we get

$$\hat{w} = \mu_P = \left(X^T X + \lambda I\right)^{-1} X^T y,$$

• Posterior distribution is a Gaussian distribution:

$$w \mid \mathcal{D} \sim \mathcal{N}(\mu_{P}, \Sigma_{P})$$

$$\mu_{P} = (X^{T}X + \sigma^{2}\Sigma_{0}^{-1})^{-1}X^{T}y$$

$$\Sigma_{P} = (\sigma^{-2}X^{T}X + \Sigma_{0}^{-1})^{-1}$$

• If we want point estimates of w, MAP estimator and the posterior mean are given by

$$\hat{w} = \mu_P = \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y$$

• For the prior variance $\Sigma_0 = \frac{\sigma^2}{\lambda} I$, we get

$$\hat{w} = \mu_P = \left(X^T X + \lambda I\right)^{-1} X^T y,$$

which is of course the ridge regression solution.