Probabilistic models

Bayesian Regression

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

CDS, NYU

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- A parametric family of conditional densities is a set

 $\{p(y \mid x, \theta) : \theta \in \Theta\},\$

- where $p(y | x, \theta)$ is a density on **outcome space** \mathcal{Y} for each x in **input space** \mathcal{X} , and
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- where $p(y | x, \theta)$ is a density on **outcome space** \mathcal{Y} for each x in **input space** \mathcal{X} , 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.

Likelihood Function

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

$$p(\mathcal{D} \mid x_1, \ldots, x_n, \theta) = \prod_{i=1}^n p(y_i \mid x_i, \theta).$$

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

Maximum Likelihood Estimator

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

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• We can think of this as a choice of a particular function from the hypothesis space

$$\mathcal{F} = \{ p(y \mid x, \theta) : \theta \in \Theta \}.$$

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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 $p(y | x, \theta)$.

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- $\bullet\,$ Suppose for some reason we want point estimates of $\theta.$
- We can use Bayesian decision theory to derive point estimates.
- As discussed in last video, we may want to use
 - $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}, x]$ (the posterior mean estimate)
 - $\hat{\theta} = \text{median}[\theta \mid \hat{D}, x]$
 - $\hat{\theta} = \arg \max_{\theta \in \Theta} p(\theta \mid \mathcal{D}, x)$ (the MAP estimate)
- depending on our loss function.

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- Having set our Bayesian model, how do we predict a distribution on y for input x?
- There is no selection from hypothesis space.

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- Such an average is also called a mixture distribution.
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 \bullet In frequentist approach, we choose $\hat{\theta}\in\Theta,$ and predict

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• In 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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- Each of these can be derived from p(y | x, D).

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- Prior distribution: $w = (w_0, w_1) \sim \mathcal{N}(0, \frac{1}{2}I)$

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)



Bishop's PRML Fig 3.7

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

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

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• Posterior Variance Σ_P gives us a natural uncertainty measure.

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

which is of course the ridge regression solution.

Posterior Mean and Posterior Mode (MAP)

• Let's find \hat{w}_{MAP} another way to elaborate on connection to ridge.
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- Posterior density on w for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

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• To find MAP, sufficient to minimize the negative log posterior:

$$\hat{w}_{MAP} = \operatorname*{arg\,min}_{w \in \mathbf{R}^d} [-\log p(w \mid \mathcal{D})]$$

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$$= \underset{w \in \mathbf{R}^{d}}{\operatorname{arg\,min}} \underbrace{\sum_{i=1}^{n} (y_{i} - w^{T} x_{i})^{2}}_{\operatorname{log-likelihood}} + \underbrace{\lambda \|w\|^{2}}_{\operatorname{log-prior}}$$

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• Which is the ridge regression objective.

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• For Gaussian regression, predictive distribution has closed form.

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• Model:

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 $y_i \mid x, w$ i.i.d. $\mathcal{N}(w^T x_i, \sigma^2)$

• Predictive Distribution

$$p(y_{\text{new}} | x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} | x_{\text{new}}, w) p(w | \mathcal{D}) dw.$$

• Averages over prediction for each w, weighted by posterior distribution.

• Model:

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Averages over prediction for each w, weighted by posterior distribution.
Closed form:

$$y_{\text{new}} \mid x_{\text{new}}, \mathfrak{D} \quad \sim \quad \mathfrak{N}\left(\eta_{\text{new}}, \, \sigma_{\text{new}}^2\right)$$

• Model:

$$w \sim \mathcal{N}(0, \Sigma_0)$$

 $y_i \mid x, w$ i.i.d. $\mathcal{N}(w^T x_i, \sigma^2)$

• Predictive Distribution

$$p(y_{\text{new}} | x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} | x_{\text{new}}, w) p(w | \mathcal{D}) dw.$$

Averages over prediction for each w, weighted by posterior distribution.
Closed form:

$$\begin{array}{lll} y_{\text{new}} \mid x_{\text{new}}, \mathcal{D} & \sim & \mathcal{N}\left(\eta_{\text{new}}, \, \sigma_{\text{new}}^2\right) \\ \eta_{\text{new}} & = & \mu_{\text{P}}^{\mathcal{T}} x_{\text{new}} \end{array}$$

• Model:

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Averages over prediction for each w, weighted by posterior distribution.
Closed form:

$$\begin{array}{rcl} y_{\text{new}} \mid x_{\text{new}}, \mathcal{D} & \sim & \mathcal{N}\left(\eta_{\text{new}}, \sigma_{\text{new}}^2\right) \\ \eta_{\text{new}} & = & \mu_{\text{P}}^{\mathcal{T}} x_{\text{new}} \\ \sigma_{\text{new}}^2 & = & \underbrace{x_{\text{new}}^{\mathcal{T}} \Sigma_{\text{P}} x_{\text{new}}}_{\text{from variance in } w} + \underbrace{\sigma_{\text{variance in } y}^2}_{\text{inherent variance in } y} \end{array}$$

Marylou Gabrié Slides based on Lecture 08b from

Predictive Distributions

• With predictive distributions, can give mean prediction with error bands:



Rasmussen and Williams' Gaussian Processes for Machine Learning, Fig.2.1(b)