Bayesian Learning

Lecture 5 - Large sample approximations. Classification.



Department of Statistics Stockholm University











Lecture overview

- Classification
- Normal approximation of posterior
- Logistic regression demo in R

Bayesian classification

- Classification: output is a discrete label.
 - ▶ Binary (0-1). Spam/Ham.
 - ▶ Multi-class. (c = 1, 2, ..., C). Brand choice.
- Bayesian classification

$$\operatorname*{argmax}_{c \in \mathcal{C}} p(c|\mathbf{x})$$

where $\mathbf{x} = (x_1, ..., x_p)^{\top}$ is a covariate/feature vector.

- **Discriminative models** model $p(c|\mathbf{x})$ directly.
 - Examples: logistic regression, support vector machines.
- **Generative models** Use Bayes' theorem

$$p(c|\mathbf{x}) \propto p(\mathbf{x}|c)p(c)$$

with class-conditional distribution $p(\mathbf{x}|c)$ and prior p(c).

Examples: discriminant analysis, naive Bayes.

Classification with logistic regression

- Response is assumed to be binary (y = 0 or 1).
- Example: Spam/Ham. Covariates: \$-symbols, etc.
- Logistic regression

$$\Pr(y_i = 1 \mid \mathbf{x}_i) = \frac{\exp(\mathbf{x}_i^{\top} \boldsymbol{\beta})}{1 + \exp(\mathbf{x}_i^{\top} \boldsymbol{\beta})}.$$

Likelihood

$$p(\mathbf{y}|\mathbf{X},\boldsymbol{\beta}) = \prod_{i=1}^{n} \frac{[\exp(\mathbf{x}_{i}^{\top}\boldsymbol{\beta})]^{y_{i}}}{1 + \exp(\mathbf{x}_{i}^{\top}\boldsymbol{\beta})}.$$

- Prior $\beta \sim N(0, \tau^2 I)$. Posterior is non-standard (demo later).
- Alternative: Probit regression

$$Pr(y_i = 1 | \boldsymbol{x}_i) = \Phi(\boldsymbol{x}_i^{\top} \boldsymbol{\beta})$$

Multi-class (c = 1, 2, ..., C) logistic regression

$$\Pr(y_i = c \mid \mathbf{x}_i) = \frac{\exp(\mathbf{x}_i^{\top} \boldsymbol{\beta}_c)}{\sum_{k=1}^{C} \exp(\mathbf{x}_i^{\top} \boldsymbol{\beta}_k)}$$

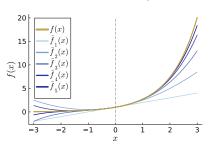
Taylor approximation

Taylor approximation of the function f(x) around x = a

$$f(x) \approx f(a) + \sum_{k=0}^{K} \frac{f^{(k)}(a)}{k!} (x - a)^{k}$$

■ Taylor approximation of $f(x) = \exp(x)$

$$\exp(x) \approx \sum_{k=0}^{K} \frac{x^k}{k!}$$



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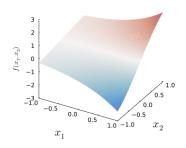
Multi-dimensional Taylor approximation

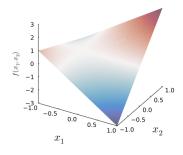
Multi-dimensional Taylor approximation of f(x)

$$f(\mathbf{x}) \approx f(\mathbf{a}) + \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} (\mathbf{x} - \mathbf{a}) + \frac{1}{2} (\mathbf{x} - \mathbf{a})^{\top} \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} (\mathbf{x} - \mathbf{a}) + \dots$$

$$f(x_1, x_2) = \exp(x_1)\sin(x_2)$$

Taylor 2nd order





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Likelihood asymptotics

Taylor expansion of log-likelihood around the MLE $\theta = \hat{\theta}$:

$$\ln p(\mathbf{x}|\theta) = \ln p(\mathbf{x}|\hat{\theta}) + \frac{\partial \ln p(\mathbf{x}|\theta)}{\partial \theta}|_{\theta = \hat{\theta}} (\theta - \hat{\theta})$$
$$+ \frac{1}{2!} \frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta^2}|_{\theta = \hat{\theta}} (\theta - \hat{\theta})^2 + \dots$$

- Higher order terms (...) negligible in large samples.
- From the definition of the MLE:

$$\frac{\partial \ln p(\mathbf{x}|\theta)}{\partial \theta}|_{\theta = \hat{\theta}} = 0$$

So, in large samples

$$p(\mathbf{x}|\theta) \approx p(\mathbf{x}|\hat{\theta}) \exp\left(-\frac{1}{2}J_{\mathbf{x}}(\hat{\theta})(\theta - \hat{\theta})^{2}\right)$$

Observed information

$$J_{\mathbf{x}}(\hat{\theta}) = -\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta^2}|_{\theta = \hat{\theta}}$$

Likelihood asymptotics

 $J_{\mathbf{x}}(\hat{\theta})$ varies from sample to sample. Fisher information

$$I(\theta) = \mathbb{E}_{\mathbf{x}|\theta} \left(J_{\mathbf{x}}(\hat{\theta}) \right)$$

■ Multiparameter observed information matrix

$$J_{\mathbf{x}}(\hat{\boldsymbol{\theta}}) = -\frac{\partial^2 \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T}|_{\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}}$$

Example: $\boldsymbol{\theta} = (\theta_1, \theta_2)^{\top}$

$$\frac{\partial^2 \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^{\top}} = \begin{pmatrix} \frac{\partial^2 \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \theta_1^2} & \frac{\partial^2 \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \theta_1 \partial \theta_2} \\ \frac{\partial^2 \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \theta_1 \partial \theta_2} & \frac{\partial^2 \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \theta_2^2} \end{pmatrix}.$$

Posterior asymptotics

We can do the same Taylor approximation on log posterior

$$\log p(\boldsymbol{\theta}|\mathbf{x}) = \log p(\mathbf{x}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}) - \log p(\boldsymbol{x})$$

Approximate normal posterior in large samples

$$\boldsymbol{\theta} | \mathbf{x} \overset{\mathrm{approx}}{\sim} \boldsymbol{N} \left[\tilde{\boldsymbol{\theta}}, \textit{J}_{\mathbf{x}}^{-1}(\tilde{\boldsymbol{\theta}}) \right]$$

- $ilde{oldsymbol{ heta}} = rg \max oldsymbol{p}(oldsymbol{ heta}|\mathbf{x})$ is the posterior mode and
- $\mathbf{J}_{\mathbf{x}}^{-1}(\tilde{\boldsymbol{\theta}})$ is now with respect to posterior $\log p(\boldsymbol{\theta}|\mathbf{x})$.
- Likelihood will dominate the prior in large samples so
 - ightharpoons $\tilde{oldsymbol{ heta}} pprox \hat{oldsymbol{ heta}}$
 - $> J_{\mathbf{x}}^{-1}(\tilde{\boldsymbol{ heta}})$ will be close to the observed information.
- Important: sufficient with proportional form

$$\log p(\theta|\mathbf{x}) = \log p(\mathbf{x}|\theta) + \log p(\theta)$$

Large sample asymptotics

Normal posterior approximation

The posterior can in large samples be approximated by

$$\boldsymbol{\theta} | \mathbf{y} \stackrel{\text{a}}{\sim} N \Big(\tilde{\boldsymbol{\theta}}, J_{\boldsymbol{\theta}, \mathbf{y}}^{-1}(\tilde{\boldsymbol{\theta}}) \Big)$$

where $\tilde{\theta}$ is the posterior mode and

$$J_{\tilde{\boldsymbol{\theta}},\mathbf{y}} = -\frac{\partial^2 \ln p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^{\top}}|_{\boldsymbol{\theta} = \tilde{\boldsymbol{\theta}}}$$

is the $d \times d$ observed information matrix at $\tilde{\theta}$.

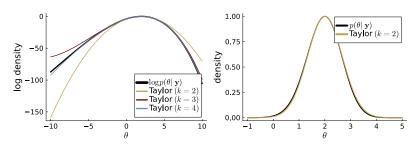
Normal approximation example

Posterior

$$\rho(\theta|\mathbf{y}) \propto \exp\left(-\exp(\theta/\kappa_0)(\theta-\bar{\mathbf{y}})^2\right)$$

where κ_0 is a prior hyperparameter and \bar{y} is the sample mean.

■ Taylor expansion of log posterior



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Example: gamma posterior

Poisson model: $\theta|y_1,...,y_n \sim \text{Gamma}(\alpha + \sum_{i=1}^n y_i, \beta + n)$

$$\log p(\theta|y_1,...,y_n) \propto (\alpha + \sum_{i=1}^n y_i - 1) \log \theta - \theta(\beta + n)$$

First derivative of log density

$$\frac{\partial \ln p(\theta|\mathbf{y})}{\partial \theta} = \frac{\alpha + \sum_{i=1}^{n} y_i - 1}{\theta} - (\beta + n)$$
$$\tilde{\theta} = \frac{\alpha + \sum_{i=1}^{n} y_i - 1}{\beta + n}$$

lacksquare Second derivative at mode $ilde{ heta}$

$$\frac{\partial^2 \ln p(\theta|\mathbf{y})}{\partial \theta^2}\Big|_{\theta=\tilde{\theta}} = -\frac{\alpha + \sum_{i=1}^n y_i - 1}{\left(\frac{\alpha + \sum_{i=1}^n y_i - 1}{\beta + n}\right)^2} = -\frac{(\beta + n)^2}{\alpha + \sum_{i=1}^n y_i - 1}$$

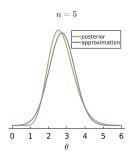
Normal approximation

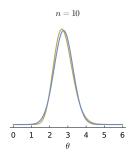
$$N\left[\frac{\alpha + \sum_{i=1}^{n} y_i - 1}{\beta + n}, \frac{\alpha + \sum_{i=1}^{n} y_i - 1}{(\beta + n)^2}\right]$$

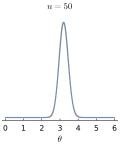
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Example: gamma posterior for eBay bidders data







Normal approximation of posterior

- $\qquad \qquad \blacksquare \; \theta | \mathbf{y} \overset{\mathrm{approx}}{\sim} \; \mathcal{N} \left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta}) \right] \; \text{works also when} \; \theta \; \text{is a vector}.$
- How to compute $\tilde{\boldsymbol{\theta}}$ and $J_{\mathbf{y}}(\tilde{\boldsymbol{\theta}})$?
- Standard optimization routines may be used. (optim.r).
 - ▶ Input: expression proportional to $\log p(\theta|\mathbf{y})$. Initial values.
 - **Output**: $\log p(\tilde{\boldsymbol{\theta}}|\mathbf{y})$, $\tilde{\boldsymbol{\theta}}$ and Hessian matrix $(-J_{\mathbf{y}}(\tilde{\boldsymbol{\theta}}))$.
- Automatic differentation efficient derivatives on computer.
- Re-parametrization may improve normal approximation. [Don't forget the Jacobian!]
 - ▶ If $\theta \ge 0$ use $\phi = \log(\theta)$.
 - $\qquad \qquad \mathbf{If} \ 0 \leq \theta \leq 1 \text{, use } \phi = \ln[\theta/(1-\theta)].$
- Heavy tailed approximation: $\theta | \mathbf{y} \overset{\text{approx}}{\sim} t_v \left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\boldsymbol{\theta}}) \right]$ for suitable degrees of freedom v.

Reparametrization - Gamma posterior

- Poisson model. Reparameterize to $\phi = \log(\theta)$.
- Change-of-variables formula from a basic probability course

$$\log p(\phi|y_1,...,y_n) \propto (\alpha + \sum_{i=1}^n y_i - 1)\phi - \exp(\phi)(\beta + n) + \phi$$

 \blacksquare Taking first and second derivatives and evaluating at $\tilde{\phi}$ gives

$$\tilde{\phi} = \log\left(\frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n}\right) \text{ and } \frac{\partial^2 \ln p(\phi|y)}{\partial \phi^2}|_{\phi = \tilde{\phi}} = \alpha + \sum_{i=1}^{n} y_i$$

So, the normal approximation for $p(\phi|y_1,...y_n)$ is

$$\phi = \log(\theta) \sim N \left[\log \left(\frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n} \right), \frac{1}{\alpha + \sum_{i=1}^{n} y_i} \right]$$

which means that $p(\theta|y_1,...y_n)$ is log-normal:

$$\theta | \mathbf{y} \sim LN \left[\log \left(\frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n} \right), \frac{1}{\alpha + \sum_{i=1}^{n} y_i} \right]$$

Normal approximation of posterior

- Even if the posterior of θ is approx normal, **interesting** functions of $g(\theta)$ may not be (e.g. predictions).
- But approximate posterior of $g(\theta)$ can be obtained by simulating from $N\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$.
- Posterior of Gini coefficient
 - ▶ Model: $x_1, ..., x_n | \mu, \sigma^2 \sim LN(\mu, \sigma^2)$.
 - ▶ Let $\phi = \log(\sigma^2)$. And $\theta = (\mu, \phi)$.
 - Joint posterior $p(\mu, \phi)$ may be approximately normal: $\theta | \mathbf{y} \overset{\mathrm{approx}}{\sim} \mathcal{N} \left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta}) \right]$.
 - $\qquad \qquad \mathsf{Simulate} \ \boldsymbol{\theta}^{(1)},...,\boldsymbol{\theta}^{(N)} \ \mathsf{from} \ \mathit{N} \left[\tilde{\boldsymbol{\theta}}, \mathit{J}_{\mathtt{y}}^{-1}(\tilde{\boldsymbol{\theta}}) \right].$
 - $\qquad \qquad \textbf{Compute } \sigma^{(1)},...,\sigma^{(\textit{N})}.$
 - ▶ Compute $G^{(i)} = 2\Phi\left(\sigma^{(i)}/\sqrt{2}\right)$ for i = 1, ..., N.

Bayesian logistic regression

Logistic regression

$$\Pr(y_i = 1 \mid \mathbf{x}_i) = \frac{\exp(\mathbf{x}_i^{\top} \boldsymbol{\beta})}{1 + \exp(\mathbf{x}_i^{\top} \boldsymbol{\beta})}.$$

Odds

$$Odds(\mathbf{x}) \equiv \frac{\Pr(y = 1 | \mathbf{x})}{\Pr(y = 0 | \mathbf{x})} = \exp(\mathbf{x}^{\top} \boldsymbol{\beta}).$$

Odds ratio

$$OR_j = \frac{Odds(x_1, \dots, x_j + 1, \dots, x_p)}{Odds(x_1, \dots, x_j, \dots, x_p)} = \exp(\beta_j)$$

Likelihood

$$p(\mathbf{y}|\mathbf{X},\boldsymbol{\beta}) = \prod_{i=1}^{n} \frac{[\exp(\mathbf{x}_{i}^{\top}\boldsymbol{\beta})]^{y_{i}}}{1 + \exp(\mathbf{x}_{i}^{\top}\boldsymbol{\beta})}.$$

Normal approximation:

$$\boldsymbol{\beta}|\boldsymbol{y} \sim \textit{N}\left(\tilde{\boldsymbol{\beta}},\textit{J}_{\boldsymbol{y}}^{-1}(\tilde{\boldsymbol{\beta}})\right).$$

Logistic regression - who survived the Titanic?

Prior

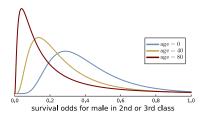
$$oldsymbol{eta} \sim \mathcal{N}(oldsymbol{\mu}, oldsymbol{\Omega})$$

with

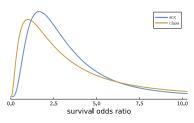
$$\mu = (-1, -1/80, 1, 1)^{\top}$$

$$\boldsymbol{\mu} = \begin{pmatrix} -1, -1/80, 1, 1 \end{pmatrix}^{\top}$$
 $\boldsymbol{\Omega} = \begin{pmatrix} 0.25 & 0 & 0 & 0 \\ 0 & 1/(80^2) & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

age



sex and class

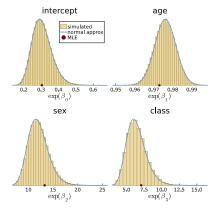


Logistic regression - who survived the Titanic?

Normal posterior approximation

$$oldsymbol{eta} | oldsymbol{y} \sim oldsymbol{\mathcal{N}} \left(ilde{oldsymbol{eta}}, J_{oldsymbol{y}}^{-1}(ilde{oldsymbol{eta}})
ight).$$

- Means that the posterior of each β_i is univariate normal.
- Marginal posterior for each $\exp(\beta_j)$ is LogNormal.



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Logistic regression - who survived the Titanic?

Comparison with non-informative prior $\beta \sim N(\mathbf{0}, 10^2 I_p)$.

