ST451 - Lent term
Bayesian Machine Learning

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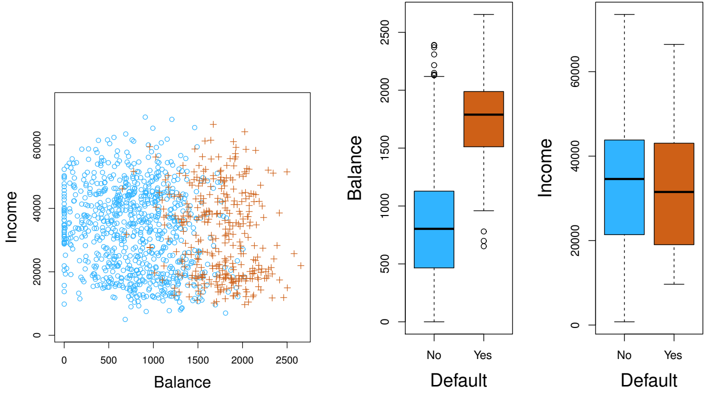
Linear Models for Classification

Summary of last lecture

- Bayesian Linear regression: derivation of posterior when both β and σ^2 are unknown.
- Bayesian multi-parameter models, focus on the marginal posterior $\pi(\beta|y, X, \sigma^2)$
- Bayesian model choice: Bayes factor, Jeffreys Lindley paradox and unit information priors.
- Implementation: Explicit formulae for the posterior mean, Monte Carlo for credible intervals and prediction, ‘candidate property’ for marginal likelihood calculation.

Motivating Example

'Default' dataset consist of three variables: annual income, credit card balance and whether or not the person has defaulted in his/her credit card.



The aim is to build a model to predict whether a person will default based on annual income and monthly credit card balance.

Classification

Generally we will assume that have a number of covariates or features (denoted by X) as well as the response y which is now a categorical variable taking values $c_1, \ldots, c_K$.

Usually we will assume that $k = 2$ (binary classification) but also consider $k > 2$ multiple classes

Existing approaches can be split into two categories:

1. Generative models: specify $\pi(X|c_k)$, so that we can *generate* X, assign prior probabilities on each c_k and use Bayes theorem to obtain $\pi(c_k|X)$. e.g. linear and quadratic discriminant analysis.
2. Discriminative models: specify the model (likelihood) $\pi(c_k|X)$ and perform statistical inference and prediction as in linear regression. e.g. logistic and probit regression

Outline

Outline

Logistic regression

Model for (y_i, X_i):

$$
\begin{aligned}
y_i &= \text{Bernoulli}\big(\pi(c_k|X_i)\big) \\
\pi(c_k|X_i) &= \sigma\big(X_i\beta\big) \;\text{ or else }\; \log\left(\frac{\pi(c_k|X_i)}{1-\pi(c_k|X_i)}\right) = X_i\beta
\end{aligned}
$$

Interpretation of coefficients:

- X consists of of either dummy or continuous variables.
- A dummy variable Z is an indicator of a category - say A. Its β coefficient reflects the log-odds ratio between A and A^c.

$$
\log\left(\frac{\frac{p(y_i=1|X=1)}{1-p(y_i=1|X=1)}}{\frac{p(y_i=1|X=0)}{1-p(y_i=1|X=0)}}\right)
$$

- The coefficient of a continuous variable X_c reflects the log odds ratio for a unit change in X_c.

Logistic regression

Check your understanding on the following output.

	Coefficient	Std. error	Z-statistic	P-value
Intercept	−10.6513	0.3612	−29.5	<0.0001
balance	0.0055	0.0002	24.9	<0.0001

	Coefficient	Std. error	Z-statistic	P-value
Intercept	−3.5041	0.0707	−49.55	<0.0001
student[Yes]	0.4049	0.1150	3.52	0.0004

	Coefficient	Std. error	Z-statistic	P-value
Intercept	−10.8690	0.4923	−22.08	<0.0001
balance	0.0057	0.0002	24.74	<0.0001
income	0.0030	0.0082	0.37	0.7115
student[Yes]	−0.6468	0.2362	−2.74	0.0062

Note that the coefficient of 'student' is positive in table 2 and negative in table 3. How can we interpret this?

Logistic regression - maximum likelihood

The likelihood, log-likelihood, gradient and Hessian can be written as

$$
\begin{aligned}
f(y|X,\beta) &= \prod_i \left\{\sigma(X_i\beta)^{y_i}\left[1-\sigma(X_i\beta)\right]^{1-y_i}\right\}. \\
\ell(\beta) &= \sum_i \left\{y_i \log\left(\sigma(X_i\beta)\right) + (1-y_i)\log\left(1-\sigma(X_i\beta)\right)\right\}, \\
\nabla_\beta \ell(\beta) &= \sum_i \left\{\frac{y_1 \nabla_\beta \sigma(X_i\beta)\left(1-\sigma(X_i\beta)\right) - (1-y_i)\nabla_\beta\sigma(X_i\beta)\sigma(X_i\beta)}{\sigma(X_i\beta)\left(1-\sigma(X_i\beta)\right)}\right\} \\
&\quad \text{using } \nabla_x \sigma(x) = \sigma\left(1-\sigma(x)\right) \text{ gives} \\
&= \sum_i y_i\left(1-\sigma(X_i\beta)\right)X_i^T - (1-y_i)\sigma(X_i\beta)X_i^T \\
&= \sum_i \left(\sigma(X_i\beta)-y_i\right)X_i^T = X^T\left(\sigma(X\beta)-y\right) \\
H(\beta) &= \sum_i \sigma(X_i\beta)\left(1-\sigma(X_i\beta)\right)X_i^T X_i = X^T S X,
\end{aligned}
$$

where S is a diagonal matrix with entries $\sigma(X\beta)\left(1-\sigma(X_i\beta)\right)$

Logistic regression - maximum likelihood

- There is no closed form solution but the Newton-Raphson maximisation algorithm can be used given $\nabla_\beta \ell(\beta)$ and H_β.
$$\beta_{\text{new}} = \beta_{\text{old}} - H(\beta_{\text{old}})^{-1} \; \nabla_\beta \ell(\beta)\big|_{\beta=\beta_{\text{old}}}.$$
- Use of normal CDF as a function instead of the sigmoid provides the probit regression.
- There is no conjugate prior for β so the posterior is not available in closed form.

Outline

Laplace approximation / Bayesian CLT

- Given data $y = (y_1, \ldots, y_n)$ denote the likelihood $f(y|\theta)$.

- The prior $\pi(\theta)$ could be improper but we assume that the posterior is proper and that its mode exists.

- Let $\pi^*(\theta|x) = f(x|\theta)\pi(\theta)$ and denote the posterior mode θ_M, which is (under regularity conditions) a solution of
$$\nabla_\theta \log \pi^*(\theta_M|x) = 0, \quad \text{for all} \quad i = 1, \ldots, p.$$
Also, let $H(\theta)$ be the Hessian matrix.

- Then as $n \to \infty$
$$\pi(\theta|x) \to N\left(\theta_M, H^{-1}(\theta_M)\right)$$

Proof: Similar to that of the asymptotic distribution of MLEs.

Bayesian CLT - Example 1: Binomial

- Let y be an observation from a Binomial(n, θ) and $\pi(\theta) \propto 1$.
- The mode can be found as $\theta_M = y/n$.
- The Hessian is equal to
$$H(\theta) = \frac{y}{\theta^2} + \frac{n-y}{(1-\theta)^2}$$
- Then as $n \to \infty$
$$\pi(\theta|y) \to N\left(\frac{y}{n}, \frac{\frac{y}{n}(1-\frac{y}{n})}{n}\right)$$

Bayesian Logistic Regression - Laplace approximation

- Let's return to the logistic regression model. Assign the Normal prior on β with mean β_0 and covariance Σ_0.

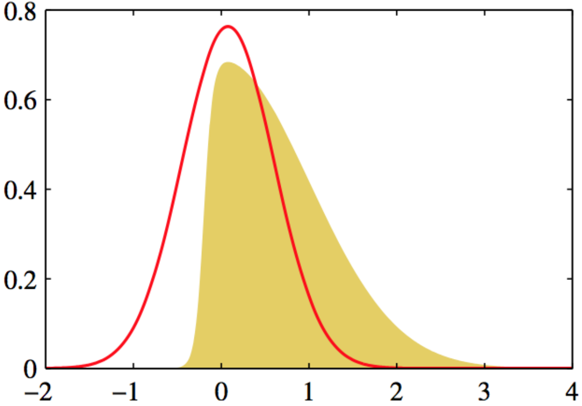
- We now need to maximise
$$\log\left(\pi(\beta|y,X)\right) = \log f(y|X,\beta) - \tfrac{1}{2}(\beta-\beta_0)^T\Sigma_0^{-1}(\beta-\beta_0)$$

- The Laplace approximation of the posterior then becomes
$$N\left[\beta_M, \left(\Sigma_0^{-1} + H(\beta_M)\right)^{-1}\right]$$

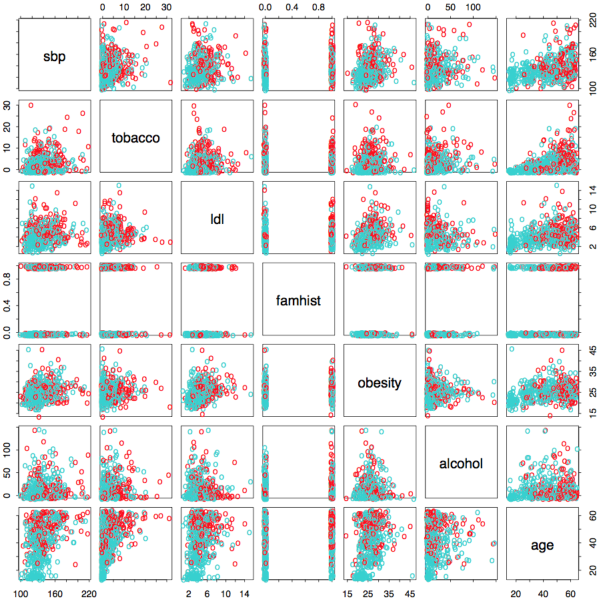
- This approximation will work well for sufficiently large n. We will say better approximations in the following weeks.

Laplace Approximation

Below is a graphical illustration of the Laplace approximation. See also Exercise 2.

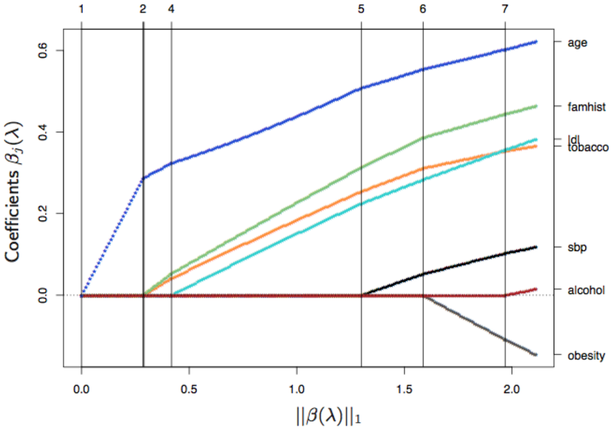


Example: South African Heart Disease Data



Laplace Approximation

As with linear regression Lasso and Ridge are special cases of the Bayesian approach by setting the corresponding priors. The Lasso results are shown below:



Model Choice

The Laplace approximation can also be viewed as Taylor expansion around β_M

$$\pi(\beta|y) \approx f(y|\beta_M)\pi(\beta_M)\exp\left(-\tfrac{1}{2}(\beta-\beta_M)^T H(\beta_m)(\beta-\beta_M)\right)$$

The model evidence / marginal likelihood $\pi(y)$ is the normalising constant of $\pi(\beta|y)$ so it may be approximated by

$$\begin{aligned}\pi(y) &\approx \int f(y|\beta_M)\pi(\beta_M)\exp\left(-\tfrac{1}{2}(\beta-\beta_M)^T H(\beta_m)(\beta-\beta_M)\right)d\beta \\ &= f(y|\beta_M)\pi(\beta_M)(2\pi)^{p/2}\left|H(\beta_M)\right|^{-1/2}\end{aligned}$$

Another approximation (not using priors) is offered by the Bayesian Information Criterion (BIC)

$$\log\pi(y) \approx \log f(y|\beta_M) - \tfrac{1}{2}p\log n$$

Bayesian Logistic Regression - predictive distribution

Given a new set of covariate X_n, we can forecast y_n via the predictive distribution. Based on the Laplace approximation we can write

$$\pi(y_n|X_n, y, X) \approx \int \text{Bernoulli}\big(\sigma(X\beta)\big) N\left[\beta_M, \left(\Sigma_0^{-1} + H_\beta\right)^{-1}\right] d\beta$$

The integral above cannot be computed analytically but we can sample from $\pi(y_n|X_n, y, X)$ by

1. Draw N Monte Carlo samples $\beta^i, i = 1, \ldots, N$ from $N\left[\beta_M, \left(\Sigma_0^{-1} + H_\beta\right)^{-1}\right]$
2. obtain predictive probabilities by averaging the $E[\sigma(X\beta^i)]$'s

Outline

Generative Models

The key difference with logistic regression is that we now specify a distribution for both X and y in the following way

$$\pi_\theta(y = c_k, X) = \pi_{\theta_y}(y = c_k)\pi_{\theta_x}(X|y = c_k), \quad k = 1, \dots, K.$$

The equation above is useful for training purposes. If $\theta = (\theta_x, \theta_y)$ is not treated in a Bayesian manner, we use the MLE $\hat{\theta}$.

For prediction purposes we can use Bayes theorem to forecast y_n for a new point X_n

$$\pi_{\hat{\theta}}(y_n = c_k|X_n) = \frac{\pi_{\hat{\theta}_x}(X_n|y = c_k)\pi_{\hat{\theta}_y}(y = c_k)}{\sum_{k=1}^{K} \pi_{\hat{\theta}_x}(X_n|y = c_k)\pi_{\hat{\theta}_y}(y = c_k)}, \quad k = 1, \dots, K.$$

Softmax and discriminant function

Setting $a_k(X) = \log\left[\pi_{\hat{\theta}_x}(X|c_k)\pi_{\hat{\theta}_y}(c_k)\right]$, we get the softmax function

$$\pi(c_k|X) = \frac{\exp\left(a_k(X)\right)}{\sum_{k=1}^{K}\exp\left(a_k(X)\right)}$$

which is ≈ 1 when $a_k >> a_j$ for all $k \neq j$.

In the case of two classes we the logistic sigmoid

$$\pi(c_k|X) = \frac{1}{1+\exp\left(-d(X)\right)} = \sigma\left(d(X)\right),$$

for the discriminant function $d(X)$,

$$d(X) = \log\left(\frac{\pi_{\hat{\theta}_x}(X|c_1)\pi_{\hat{\theta}_y}(c_1)}{\pi_{\hat{\theta}_x}(X|c_0)\pi_{\hat{\theta}_y}(c_0)}\right)$$

Example: Linear discriminant analysis

Assume two classes $y = 0$ or $y = 1$ and that the inputs X are $N(\mu_0, \Sigma)$ if $y = 0$ and $N(\mu_1, \Sigma)$ if $y = 1$. Also $P(y = 1) = \pi$, so $P(y = 0) = 1 - \pi$.

The likelihood for $\theta = (\pi, \mu_1, \mu_2, \Sigma)$ based $(y_i, X_i)_{i=1}^n$ can be written as

$$\pi(X, y|\theta) = \prod_{i=1}^{n} [\pi N(\mu_1, \Sigma)]^{y_i} [(1 - \pi)N(\mu_0, \Sigma)]^{1-y_i}$$

Standard techniques yield the following MLEs of θ (see exercise 1):

$$\begin{aligned}
\hat{\pi} &= \tfrac{n_1}{n}, \quad \text{where } n_1 \text{ is the number of points in class 1} \\
\hat{\mu}_1 &= \tfrac{1}{n_1} \sum_{i=1}^{n_1} y_i X_{1i} \quad \hat{\mu}_0 = \tfrac{1}{n_0} \sum_{i=1}^{n_0} (1 - y_i) X_{0i} \\
\hat{\Sigma} &= \tfrac{1}{n} \left(\sum_{i=1}^{n_1} (X_{1i} - \mu_1)(X_{1i} - \mu_1)^T + \sum_{i=1}^{n_2} ([-\mu_0)(X_{0i} - \mu_0)^T \right)
\end{aligned}$$

Notes on Linear discriminant analysis

- The parameter μ_k refers to the profile of a typical individual in class k

- We can write $\pi(y = 1|X) = \sigma(\beta X + C)$ for some $\beta = \Sigma^{-1}(\mu_1 - \mu_0)$ and a constant C, hence the discriminant function is linear.

- In case of different Σ's for each class we get a quadratic discriminant function quadrative discriminant analysis

- Fully Bayesian inference on θ can be made by assigning appropriate priors and deriving the posterior. Not pursued here.

- In case of p discrete X's (binary features) we have 2^p cases. Usually independent X's are assumed to reduce the number of cases. This is called naive Bayes.

Outline

Sensitivity, specificity and misclassification rate

To classify a new individual with X_n, we can use $\pi(y = 1|X_n)$.

Two types of error: False positives and False negatives. If equally important the optimal prediction rule classifies $y = 1$ if $\pi(y = 1|X_n) > 0.5$. Then check the misclassification/accuracy rate.

Different thresholds can also be used. Below are the in-sample confusion matrices for LDA in the'Default' dataset with threshold 0.5

		True default status		
		No	Yes	Total
Predicted	No	9,644	252	9,896
default status	Yes	23	81	104
	Total	9,667	333	10,000

Sensitivity: $81/333 = 0.24$, Specificity: $9644/9667 = 0.99$.

Sensitivity, specificity and misclassification rate (cont'd)

But if we set a lower threshold of 0.2 we get

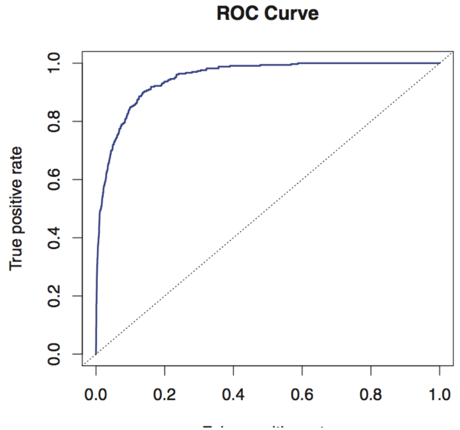
		True default status		
		No	Yes	Total
Predicted	No	9,432	138	9,570
default status	Yes	235	195	430
	Total	9,667	333	10,000

Sensitivity: $195/333 = 0.59$, Specificity: $9432/9667 = 0.97$.

So which threshold should we use when comparing models?

ROC curves

For an overall measure we can look at the area under the ROC curve (sensitivity vs 1-specificity). In this case it is 0.95 which is quite good (0.5 corresponds to random guessing).



Evaluating probabilistic forecasts - Scoring rules

- Let's say it didn't rain today. One model predicted rain with 0.99 probability and another with 0.51. Which of the two is better?
- Scoring rules are often used to evaluate probabilistic forecasts.
- Imagine a model that captures the probabilities of nature perfectly. If under a scoring rule, this model attains the optimal performance then the scoring rule is called proper. If this can only happen by this model, the rule is called strictly proper.
- Misclassification error is not even a scoring rule as it doesn't take into account these probabilities. Area under the ROC is approximately proper.

Strictly proper scoring rules

- The log score, LS$= -\log f(y|\pi)$ with $f(\cdot)$ denoting the likelihood/density, is an example of a strictly proper scoring rule.
- If it didn't rain today, for model that predicted rain with $\pi = 0.51$ it takes the value
$$LS = -\log\left[0.51^0(1-0.51)^1\right] = -\log(0.49) = 0.71$$
- For the model that predicted rain with $p = 0.99$, it takes the value
$$LS = -\log\left[0.99^0(1-0.99)^1\right] = -\log(0.01) = 4.61.$$
- Smaller values of LS are better so the model with $\pi = 0.51$ scores better.

Today's lecture - Reading

Bishop: 4.2 to 4.5.

Murphy: 4.2.1 to 4.2.4 8.1 8.2 8.3.1 8.3.3 8.3.7 and 8.4.1 to 8.4.4.