

Group Project 2 & 3

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Introduction

- ▶ **Group project 2:** optimization algorithms on a breast cancer diagnosis dataset
- ▶ **Group project 3:** bootstrapping on developing classification model

Breast Cancer Data

- ▶ **Variable Selection:** reduce multicollinearity based on both correlation coefficient and eigenvalue of correlation matrix
- ▶ 18 variables remain

Logistic Model with Newton-Raphson

Logistic Regression:

y : the vector of n response random variable

X : the $n \times p$ design matrix (X_i denote the i th row)

β : the $p \times 1$ coefficient

- The logistic regression model:

$$\log\left(\frac{\eta}{1 - \eta}\right) = X\beta$$

- The likelihood function:

$$L(\beta; X, y) = \prod_{i=1}^n \left\{ \left(\frac{\exp(X_i\beta)}{1 + \exp(X_i\beta)} \right)^{y_i} \left(\frac{1}{1 + \exp(X_i\beta)} \right)^{1-y_i} \right\}$$

- ▶ The log likelihood:

$$l(\beta) = \sum_{i=1}^n \{y_i(X_i\beta) - \log(1 + \exp(X_i\beta))\}$$

- ▶ The gradient:

$$\nabla l(\beta) = X^T(y - p)$$

where $p = \frac{\exp(X\beta)}{1 + \exp(X\beta)}$

- ▶ The Hessian:

$$\nabla^2 l(\beta) = -X^T W X$$

where $W = \text{diag}(p_i(1 - p_i)), i = 1, \dots, n$. The Hessian is negative definite.

Newton-Raphson

Update coefficients

$$\beta_{i+1} = \beta_i - [\nabla^2 l(\beta_i)]^{-1} \nabla l(\beta_i)$$

Step-halving

$$\beta_{i+1}(\gamma) = \beta_i - \gamma [\nabla^2 l(\beta_i)]^{-1} \nabla l(\beta_i)$$

- ▶ Set $\gamma = 1$
- ▶ If $f(\theta_{i+1}(1)) \geq f(\theta_i)$, then set $\theta_{i+1} = \theta_{i+1}(1)$
- ▶ If $f(\theta_{i+1}(1)) \leq f(\theta_i)$, search for a value $\gamma \in (0, 1)$ for which $f(\theta_{i+1}(\gamma)) \geq f(\theta_i)$, set $\theta_{i+1} = \theta_{i+1}(\gamma)$

Newton-Raphson: gradient decent

For Newton's method with a large p , the computational burden in calculating the inverse of the Hessian Matrix $[\nabla^2 f(\beta_i)]^{-1}$ increases quickly with p . One can update

$$\beta_{i+1} = \beta_i + H_i \nabla f(\beta_i)$$

where $H_i = (X^T X)^{-1}$ for every i . This is easy to compute, but could be slow in convergence.

The steps are:

- ▶ get the objective (loglik,grad,Hess) function
- ▶ use the principle of newton raphson to update the estimate, if the step size too large, step-halving step
- ▶ stop searching until the convergences of the estimates.

Logistic-LASSO Model with Pathwise Coordinate Descent

- ▶ Applied coordinate-wise descent with weighted update:

$$\tilde{\beta}_j^{lasso}(\lambda) \leftarrow \frac{S(\sum_{i=1}^n \omega_i x_{i,j} (y_i - \tilde{y}_i^{(-j)}), \lambda)}{\sum_{i=1}^n \omega_i x_{i,j}^2}$$

where $\tilde{y}_i^{(-j)} = \sum_{k \neq j} x_{i,k} \tilde{\beta}_k$ and $S(\hat{\beta}, \lambda) = \text{sign}(\hat{\beta})(|\hat{\beta}| - \lambda)_+$

- ▶ In the context of logistic regression, we are aiming to maximize the penalized log likelihood:

$$\max_{\beta \in \mathbb{R}^{p+1}} \frac{1}{n} \sum_{i=1}^n \{y_i (X_i \beta) - \log(1 + \exp(X_i \beta))\} - \lambda \sum_{j=0}^p |\beta_j|$$

for some $\lambda \geq 0$

Estimation Path

Cross validation for LASSO

Model Comparison

Conclusion

Down Syndrome Data