

数据科学导论第十五次课

Motivation

- airline data.
 - $n = 120$ million, $p = 29$.
 - Each observation corresponds to a piece of flight information within the United States.
 - The data occupies about 12G of space on the hard disk.
- Census income data set.
 - $n = 48,842$.
 - want to conduct a classification analysis using residents' information such as age, work class, education and etc to predict whether the residents are high income residents, i.e., those with annual income more than \$50K, or not.

Statistical analysis challenge for Big Data

- Extraordinary size of data.
- Limited computation resource.
- **Data reduction**: The focus is on reducing the size of n .
- Selecting a subdata suitable for limited computing resource.
- Tradeoffs Between Computational Costs and Statistical Efficiency.

- 1 Subsampling for linear model
- 2 Subsampling for Logistic model

Big Data Linear Regression

- Linear model:

$$\mathbf{y} = \beta_0 \mathbf{1} + \mathbf{Z}\beta_1 + \epsilon = \mathbf{X}^\top \beta + \epsilon,$$

where \mathbf{Z} is an $n \times p$ matrix, $\mathbf{X} = [\mathbf{1}, \mathbf{Z}]$, y_i 's are uncorrelated given \mathbf{Z} , and $\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$.

- OLS (Ordinary Least Squares):

$$\hat{\beta}_{OLS} = \arg \min_{\beta \in \mathbb{R}^p} \|\mathbf{y} - \mathbf{X}\beta\|^2 = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Computational Cost

- Inference under linear regression has a computational complexity of $O(np^2)$, which can be problematic for large n .
- Wisely chosen subdata can be used so that useful conclusions can be obtained with limited computational resources.
- If subdata size is k , the overall computational complexity is $O(kp^2 + ?)$, where ? depends on the computational complexity of the algorithm for selecting the subdata.

- Assign each data point (\mathbf{x}_i, y_i) a proper sampling probability π_i , $\sum_{i=1}^n \pi_i = 1$, and sample $k (k \ll n)$ data points with replacement according to $\boldsymbol{\pi} = (\pi_1, \dots, \pi_n)$, and do statistical inference using the subdata.
- How to define π_i so that the data points that really affect the result have a greater probability of being collected?
- How to analyze the k data points to get an estimator close enough to the estimator based on the full data?

Sampling strategies

- Uniform sampling (UNIF): $\pi_i = 1/n$.
- Leverage-based sampling (LEV): $\pi_i = h_{ii} / \sum_{i=1}^n h_{ii}$ where h_{ii} is the leverage score of the i^{th} data point.
- Information-Based Optimal Subdata Selecion (IBOSS).

Leverage-based Subsampling

- $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$, $\mathbf{H} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$.
- $h_{ii} = \mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i$. Generally, the greater the leverage score, the more important the data point is.
- $0 \leq h_{ii} \leq 1$: First, note that \mathbf{H} is an idempotent matrix satisfying $\mathbf{H} = \mathbf{H}^2$, then $h_{ii} = h_{ii}^2 + \sum_{j \neq i} h_{ij}^2 \Rightarrow h_{ii} > h_{ii}^2$.
- Define the i^{th} regression residual $e_i = y_i - \hat{y}_i$, we have $\text{Var}(e_i) = (1 - h_{ii})\sigma^2$. In other words, the greater the score, the closer \hat{y}_i will be to the y_i .

How to analyze the subdata?

- Use these k data points directly for linear regression.
- Reweight these k data points.

- sampling matrix $\mathbf{S}_{k \times n}^\top$:
 - $\mathbf{S}^\top = (\mathbf{e}_1, \dots, \mathbf{e}_k)^\top$ where $\mathbf{e}_j \in \mathbb{R}^n$ be a unit vector with the j^{th} element being 1 and 0 otherwise.
 - if the r^{th} data unit (or observation) in the original data set is chosen in the i^{th} random trial, then the i^{th} row of \mathbf{S}^\top equals \mathbf{e}_r ;
 - The subsample: $(\mathbf{X}^*, \mathbf{y}^*) = (\mathbf{S}^\top \mathbf{X}, \mathbf{S}^\top \mathbf{y})$.
- rescaling (reweighting) matrix \mathbf{D} :
 - an $k \times k$ diagonal matrix whose i^{th} diagonal element equals $1/\sqrt{k\pi_r}$ if the r^{th} data point is chosen in the i^{th} random trial.
 - every diagonal element of \mathbf{D} equals $\sqrt{n/k}$ for uniform sampling.

- $$\tilde{\beta}_W = \arg \min_{\beta \in \mathbb{R}^p} \|DS^\top \mathbf{y} - DS^\top X\beta\|^2 = (X^\top SD^2S^\top X)^{-1}X^\top SD^2S^\top \mathbf{y}.$$

- $$W = SD^2S^\top, \quad \hat{\beta} = (X^\top WX)^{-1}X^\top W\mathbf{y}.$$

Random sampling approach

- Uniform Sampling Estimator (UNIF): uniform subsampling and weighted LS estimation.
- Basic Leveraging Estimator (LEV): exact leverage-based sampling and weighted LS estimation,
- Shrinkage Leveraging Estimator (SLEV): shrinkage leverage-based sampling and weighted LS estimation: $\pi_i = \alpha \pi_i^{Lev} + (1 - \alpha) \pi_i^{Unif}$, $\alpha \in (0, 1)$.
- Unweighted Leveraging Estimator (LEVUNW): leverage-based sampling and unweighted LS estimation.

Information-based subsampling

- How to preserve the majority information contained in the full data ?

Fisher information

首先我们看一下 Fisher Information 的定义：

假设你观察到 i.i.d 的数据 X_1, X_2, \dots, X_n 服从一个概率分布 $f(X; \theta)$, θ 是你的目标参数 (for simplicity, 这里 θ 是个标量, 且不考虑 nuisance parameter), 那么你的似然函数 (likelihood) 就是：

$$L(\mathbf{X}; \theta) = \prod_{i=1}^n f(X_i; \theta)$$

为了解得 Maximum Likelihood Estimate (MLE), 我们要让 log likelihood 的一阶导数得 0, 然后解这个方程, 得到 $\hat{\theta}_{MLE}$

这个 log likelihood 的一阶导数也叫, Score function :

$$S(\mathbf{X}; \theta) = \sum_{i=1}^n \frac{\partial \log f(X_i; \theta)}{\partial \theta}$$

那么 Fisher Information, 用 $I(\theta)$ 表示, 的定义就是这个 Score function 的二阶矩 (second moment) $I(\theta) = E[S(X; \theta)^2]$ 。

一般情况下 (under specific regularity conditions) 可以很容易地证明,

$E[S(\mathbf{X}; \theta)] = 0$, 从而得到：

$$I(\theta) = E[S(X; \theta)^2] - E[S(X; \theta)]^2 = \text{Var}[S(X; \theta)]$$

于是得到了 **Fisher Information** 的第一条数学意义：就是用来估计 MLE 的方程的方差。它的直观表述就是，随着收集的数据越来越多，这个方差由于是一个 Independent sum 的形式，也就变的越来越大，也就象征着得到的信息越来越多。

- Rather than sampling, we select subdata so as to maximize the Fisher information matrix.
- For linear regression, under normality and taking $\sigma^2 = 1$ for simplicity, the information matrix for β with subdata is

$$M(\delta) = \sum_{i=1}^n \delta_i x_i x_i^\top = X^\top \Delta X.$$

with δ_i an “inclusion” indicator, $\delta = (\delta_1, \dots, \delta_n)$ and $\Delta = \text{diag}\{\delta\}$.

Optimal Design of Experiments

- As in optimal design of experiments (DOE), we could maximize a function of the information matrix.
- D-optimality: Maximize the determinant of the information matrix.
- Find δ , subject to $\sum_{i=1}^n \delta_i = k$, that maximizes $\det(M(\delta))$.
- Need a computationally efficient algorithm to find, approximately, an optimal δ .

D-optimal design under approximate design theory

An upper bound for $\det M(\delta)$

Theorem (D-optimality)

For subdata of size k represented by δ ,

$$|\mathbf{M}(\delta)| \leq \frac{k^{p+1}}{4^p} \prod_{j=1}^p (z_{(n)j} - z_{(1)j})^2, \quad (3)$$

where $z_{(n)j} = \max\{z_{1j}, z_{2j}, \dots, z_{nj}\}$ and $z_{(1)j} = \min\{z_{1j}, z_{2j}, \dots, z_{nj}\}$ are the n th and first order statistics of $z_{1j}, z_{2j}, \dots, z_{nj}$. If the subdata consists of the 2^p points $(a_1, \dots, a_p)^T$ where $a_j = z_{(n)j}$ or $z_{(1)j}$, $j = 1, 2, \dots, p$, each occurring equally often, then equality holds in (3).

Algorithm 1 (Algorithm motivated by D-optimality). Suppose that $r = k/(2p)$ is an integer. Using a partition-based selection algorithm (Martínez, 2004), perform the following steps:

- (1) For z_{i1} , $1 \leq i \leq n$, include r data points with the r smallest z_{i1} values and r data points with the r largest z_{i1} values;
- (2) For $j = 2, \dots, p$, exclude data points that were previously selected, and from the remainder select r data points with the smallest z_{ij} values and r data points with the largest z_{ij} values.
- (3) Return $\hat{\beta}^D = \{(\mathbf{X}_D^*)^T \mathbf{X}_D^*\}^{-1} (\mathbf{X}_D^*)^T \mathbf{y}_D^*$ and the estimated covariance matrix $\hat{\sigma}_D^2 \{(\mathbf{X}_D^*)^T \mathbf{X}_D^*\}^{-1}$, where $\mathbf{X}_D^* = (\mathbf{1}, \mathbf{Z}_D^*)$, \mathbf{Z}_D^* is the covariate matrix of the subdata selected in the previous steps, \mathbf{y}_D^* is the response vector of the subdata and $\hat{\sigma}_D^2 = \|\mathbf{y}_D^* - \mathbf{X}_D^* \hat{\beta}^D\|^2 / (k - p - 1)$.

Algorithm for D-optimality

- To maximize $\det(M(\delta))$, we need to include points with large and small covariate values.
- For a fixed subdata size k , using a partition-based selection algorithm, for $j = 1, \dots, p$, select the $k/(2p)$ largest and smallest z_{ij} -values, and include these points in the subdata
- $\hat{\beta}^D = (X^\top \Delta X)^{-1} X^\top \Delta y$.
- Computational complexity for selection $O(np)$; Overall computational complexity $O(kp^2 + np)$, or $O(np)$ if $n > kp$.
- Can do this one covariate at a time or in parallel.

- IBOSS can be used no matter what the distribution of the covariates is.
- Let z_1, \dots, z_n be iid, and consider 3 scenarios:
 - $z_i \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
 - $z_i \sim \text{Lognormal}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
 - $z_i \sim t_\nu(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
- For all scenarios, $\text{Var}(\hat{\beta}_0^D | Z)$ is proportional to $1/k$ when $n \rightarrow \infty$.
- Elements of $\text{Var}(\hat{\beta}_1^D | Z)$ converge to 0 when $n \rightarrow \infty$ in all cases. (even though the subdata size k is fixed)
- Similar results typically do not hold for random subsampling methods.

Extension to large p

- Penalized likelihood estimators: LASSO etc.
- For linear model,

$$\hat{\beta}_{LASSO} = \arg \min_{\beta} \{ \|y - X\beta\|^2/n + \lambda \|\beta\|_1 \}.$$

- want to develop subset selection method
- D-optimality Motivated algorithm??

- 1 Subsampling for linear model
- 2 Subsampling for Logistic model

- Dependent variable is 0-1 type data.
- Sigmoid function:

$$s(x) = \frac{\exp(x)}{1 + \exp(x)}.$$

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$$P(Y_i = 1|X_i) = p_i(\beta) = \frac{\exp(X_i^\top \beta)}{1 + \exp(X_i^\top \beta)}.$$

- The joint likelihood is:

$$L(\beta) = \prod_{i=1}^n P(Y_i | X_i) = \prod_{i=1}^n p_i(\beta)^{Y_i} (1 - p_i(\beta))^{1-Y_i}$$



$$\hat{\beta}_{MLE} = \arg \max_{\beta} l(\beta) = \arg \max_{\beta} \sum_{i=1}^n [Y_i \log(p_i(\beta)) + (1 - Y_i) \log(1 - p_i(\beta))].$$

- Newton iteration method:

$$\hat{\beta}^{(t+1)} = \hat{\beta}^{(t)} - \left\{ \sum_{i=1}^n w_i(\hat{\beta}^{(t)}) x_i x_i^{\top} \right\}^{-1} \frac{\partial l(\hat{\beta}^{(t)})}{\partial \beta} \text{ where.}$$

- Computation cost is $O(\zeta np^2)$, ζ is the iteration number.

Levraging type algorithm

Algorithm 1 General subsampling algorithm

- **Sampling:** Assign subsampling probabilities π_i , $i = 1, 2, \dots, n$, for all data points. Draw a random subsample of size r ($\ll n$), according to the probabilities $\{\pi_i\}_{i=1}^n$, from the full data. Denote the covariates, responses, and subsampling probabilities in the subsample as \mathbf{x}_i^* , y_i^* , and π_i^* , respectively, for $i = 1, 2, \dots, r$.
- **Estimation:** Maximize the following weighted log-likelihood function to get the estimate $\tilde{\beta}$ based on the subsample.

$$\ell^*(\beta) = \frac{1}{r} \sum_{i=1}^r \frac{1}{\pi_i^*} [y_i^* \log p_i^*(\beta) + (1 - y_i^*) \log \{1 - p_i^*(\beta)\}],$$

where $p_i^*(\beta) = \exp(\beta^T \mathbf{x}_i^*) / [1 + \exp(\beta^T \mathbf{x}_i^*)]$. Due to the convexity of $\ell^*(\beta)$, the maximization can be implemented by Newton's method, i.e., iteratively applying the following formula until $\tilde{\beta}^{(t+1)}$ and $\tilde{\beta}^{(t)}$ are close enough,

$$\tilde{\beta}^{(t+1)} = \tilde{\beta}^{(t)} - \left\{ \sum_{i=1}^r \frac{w_i^*(\tilde{\beta}^{(t)}) \mathbf{x}_i^* (\mathbf{x}_i^*)^T}{\pi_i^*} \right\}^{-1} \sum_{i=1}^r \frac{\{y_i^* - p_i^*(\tilde{\beta}^{(t)})\} \mathbf{x}_i^*}{\pi_i^*}, \quad (3)$$

where $w_i^*(\beta) = p_i^*(\beta)[1 - p_i^*(\beta)]$.

Asymptotically normal

Theorem 2. *If assumptions 1, 2, and 3 hold, then as $n \rightarrow \infty$ and $r \rightarrow \infty$, conditional on \mathcal{F}_n in probability,*

$$\mathbf{V}^{-1/2}(\tilde{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{\text{MLE}}) \longrightarrow N(0, \mathbf{I}) \quad (5)$$

in distribution, where

$$\mathbf{V} = \mathbf{M}_X^{-1} \mathbf{V}_c \mathbf{M}_X^{-1} = O_p(r^{-1}) \quad (6)$$

and

$$\mathbf{V}_c = \frac{1}{rn^2} \sum_{i=1}^n \frac{(y_i - p_i(\hat{\boldsymbol{\beta}}_{\text{MLE}}))^2 \mathbf{x}_i \mathbf{x}_i^T}{\pi_i}. \quad (7)$$

Asymptotic properties

- The subdata size is r .
- $\tilde{\beta}$ is consistent to $\hat{\beta}_{MLE}$ given the full sample and the convergence rate is $O(r^{1/2})$.
- $(\tilde{\beta} - \hat{\beta}_{MLE}) \mid \mathcal{F}_n \overset{a}{\rightsquigarrow} \mathbf{u}$ where \mathbf{u} is a normal random variable with distribution $\mathcal{N}(\mathbf{0}, \mathbf{V})$.
- Under some condition,

$$\mathbb{E} \left(\|\tilde{\beta} - \hat{\beta}_{MLE}\|^2 \mid \mathcal{F}_n \right) \text{ is close to } \mathbb{E}(\|\mathbf{u}\|^2 \mid \mathcal{F}_n).$$

- Minimize the asymptotic MSE to obtain the sampling probability.

Theorem 3. *In Algorithm 1, if the SSP is chosen such that*

$$\pi_i^{\text{mMSE}} = \frac{|y_i - p_i(\hat{\beta}_{\text{MLE}})| \|\mathbf{M}_X^{-1} \mathbf{x}_i\|}{\sum_{j=1}^n |y_j - p_j(\hat{\beta}_{\text{MLE}})| \|\mathbf{M}_X^{-1} \mathbf{x}_j\|}, \quad i = 1, 2, \dots, n, \quad (10)$$

then the asymptotic MSE of $\tilde{\beta}$, $\text{tr}(\mathbf{V})$, attains its minimum.

Since this optimal subsampling procedure is motivated from the A-optimality criterion, it is called OSMAC.

- For two positive definite matrices \mathbf{A}_1 and \mathbf{A}_2 , $\mathbf{A}_1 \leq \mathbf{A}_2$ if and only if $\mathbf{A}_1 - \mathbf{A}_2$ is a non-negative definite matrix.
- $\mathbf{V} = \mathbf{M}_x^{-1} \mathbf{V}_c \mathbf{M}_x^{-1}$ depends on π through \mathbf{V}_c and \mathbf{M}_x does not depend on π , for given $\pi_{(1)}$ and $\pi_{(2)}$, $\mathbf{V}(\pi_{(1)}) \leq \mathbf{V}(\pi_{(2)})$ if and only if $\mathbf{V}_c(\pi_{(1)}) \leq \mathbf{V}_c(\pi_{(2)})$.
- minimize $\text{tr}(\mathbf{V}_c)$ instead of minimizing $\text{tr}(\mathbf{V})$.

Theorem 4. In Algorithm 1, if the SSP is chosen such that

$$\pi_i^{\text{mVc}} = \frac{|y_i - p_i(\hat{\beta}_{\text{MLE}})|\|\mathbf{x}_i\|}{\sum_{j=1}^n |y_j - p_j(\hat{\beta}_{\text{MLE}})|\|\mathbf{x}_j\|}, \quad i = 1, 2, \dots, n, \quad (13)$$

then $\text{tr}(\mathbf{V}_c)$, attains its minimum.

- Let $S_0 = \{i : y_i = 0\}$ and $S_1 = \{i : y_i = 1\}$, the effect of $p_i(\hat{\beta}_{\text{MLE}})$ on π_i^{mMSE} is positive for the S_0 set while the effect is negative for the S_1 set.
- The optimal subsampling approach is more likely to select data points with smaller $p_i(\hat{\beta}_{\text{MLE}})$'s when y_i 's are 1 and data points with larger $p_i(\hat{\beta}_{\text{MLE}})$'s when y_i 's are 0.
- Intuitively, it attempts to give preferences to data points that are more likely to be mis-classified.

Two-stage framework

Algorithm 2 Two-step Algorithm

- **Step 1:** Run Algorithm 1 with subsample size r_0 to obtain an estimate $\tilde{\beta}_0$, using either the uniform SSP $\pi^{\text{UNI}} = \{n^{-1}\}_{i=1}^n$ or SSP $\{\pi_i^{\text{prop}}\}_{i=1}^n$, where $\pi_i^{\text{prop}} = (2n_0)^{-1}$ if $i \in S_0$ and $\pi_i^{\text{prop}} = (2n_1)^{-1}$ if $i \in S_1$. Here, n_0 and n_1 are the numbers of elements in sets S_0 and S_1 , respectively. Replace $\hat{\beta}_{\text{MLE}}$ with $\tilde{\beta}_0$ in (10) or (13) to get an approximate optimal SSP corresponding to a chosen optimality criterion.
 - **Step 2:** Subsample with replacement for a subsample of size r with the approximate optimal SSP calculated in Step 1. Combine the samples from the two steps and obtain the estimate $\check{\beta}$ based on the total subsample of size $r_0 + r$ according to the Estimation step in Algorithm 1.
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New Subsampling Algorithm

- Can we subset data via D-optimality similar to linear model?
- Yes!

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The end!

Thank you!