Big Data Dimension Reduction using PCA

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November 29, 2017

Challenge of Big Data

1. Memory Barrier
   - The size of data is too large to load into memory
   - More specifically, n is way more large than p
2. The computation time
   - It could be very time consuming if only use single core or cluster

Solution

1. Sufficient statistics
   - PCA regression only uses sufficient statistics
   - Sufficient statistics can be calculated by scanning the data row-by-row
2. Parallel computation
   - Multiple threads
   - Map-Reduced structure

Basic idea of PCA

Singular Value Decomposition

$$X_s = UDV^T \quad \text{,where} \quad x_{ij,s} = \frac{x_{ij} - \bar{x}}{s_j}$$

$U = (u_1, \ldots, u_r)$ is a n by r orthogonal matrix

$D = diag(d_1, \ldots, d_r)$ is a r by r diagonal matrix

$V = (v_1, \ldots, v_r)$ is a p by r orthogonal matrix

Basic idea of PCA

Principle Component and Loading

$$X_s = \underbrace{\begin{bmatrix} d_1 u_1 \dots d_r u_r \end{bmatrix}}_{\text{PCs}} \underbrace{\begin{bmatrix} {v_1}^T \\ \vdots \\ {v_r}^T \end{bmatrix}}_{\text{Loading}}$$

- $PC_j = d_j \mathbf{u_j} = X\mathbf{v_j}$ is the jth principle component
- The sample variance of PC_j is d_j^2/n

Basic idea of PCA

Reduced matrix $X_{s,k}$

$$X_{s,k} = \sum_{j=1}^{k} d_j \boldsymbol{u_j} \boldsymbol{v_k} = U_k D_k V_k^T, \quad \text{Its Variation} \quad \sum_{j=1}^{k} d_j^2/n.$$

Its proportion of the total variation is

$$\lambda_k = \frac{\sum_{j=1}^{k} d_j^2}{\sum_{j=1}^{r} d_j^2}$$

- If a small k such that $\lambda_k \approx 1$, we can use $U_k D_k$ in the follow up analysis

Follow-up analysis

The PCA approach is applied to a linear regression

Model

$$y = \mathbb{1}_n \alpha_s + U_k D_K \beta_{s,k} + \epsilon_{s,k},$$

Where $\epsilon_{s,k} \sim N(0, \sigma^2_{s,k} \boldsymbol{I}_n)$

LSE and their variance

$$\hat{\alpha}_s = \bar{Y}, \quad \hat{\beta}_{s,k} = D_k^{-1} U_k^T y \quad \textcolor{red}{(\textit{PCs are Orthogonal})}$$

$$\mathbb{V}(\hat{\sigma}^2_{s,k}) = [y^T \underbrace{(\mathbb{I}_n - \mathbb{J}_n/n - U_k U_k^T)}_{\mathbb{I}_n - P_k} y]/(n-k)$$

Sufficient Statistics

Factorization Theorem

$$f(x_1, x_2, ..., x_n; \theta) = \phi\left[u(x_1, ..., x_n); \theta\right] h(x_1, ..., x_n)$$

- $u(x_1, ..., x_n)$ is the sufficient statistics for θ
- If θ is a vector, then $u(x_1, ..., x_n)$, the Joint Sufficient Statistics, will be also a vector.

Sufficient Statistics

model

$$y = \mathbb{1}_n\alpha + X\beta + \epsilon,\ \ \epsilon \sim N(0, \sigma^2 \boldsymbol{I}_n)$$

Log-Likelihood function

$$\log\{f(y|x,\alpha,\beta,\sigma)\} = \frac{n}{2}\log 2\pi - \frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(c_{yy} - 2\alpha c_y + 2c_{xy}\beta + n\alpha^2 + 2\alpha c_x^T\beta + \beta^T C_{xx}\beta)$$

- Define: $\mathcal{C}(y, X) = (c_0, c_{yy}, c_y, \boldsymbol{c}_{xy}, \boldsymbol{c}_x, C_{xx})$
- Note that $\ell(\alpha, \beta, \sigma)$ only depends on $\mathcal{C}(y, X)$

More about $\mathcal{C}(y, X)$

Elements of $\mathcal{C}(y, X)$

$$c_0 = n, \; c_{yy} = \sum_{i=1}^{n} Y_i^2, \; c_y = \sum_{i=1}^{n} Y_i,$$
$$c_{xy} = \sum_{i=1}^{n} Y_i x_i, \; c_x = \sum_{i=1}^{n} x_i, \; C_{xx} = \sum_{i=1}^{n} x_i x_i^T$$

- Notice that $\mathcal{C}(y, X)$ is the Joint sufficient statistics for (α, β, σ)
- All terms are in the summation format, so it can be calculated by reading the data row-by-row

Computation of $\mathcal{C}(y, X)$

Algorithm 1 Computation of $\mathcal{C}(\mathbf{y}, \mathbf{X})$ Based on A Single Processor

Input: row-by-row of the data
Output: $\mathcal{C}(\mathbf{y}, \mathbf{X})$

1: **procedure** ALGORITHM FOR $(c_0, c_{yy}, c_y, \mathbf{c}_{xy}, \mathbf{c}_x, \mathbf{C}_{xx})$
2: Let c_0, c_{yy}, c_y, $\mathbf{c}_{xy}$, $\mathbf{c}_x$, and $\mathbf{C}_{xx}$ be values, vectors, and matrix, respectively, all equal to zero
3: **for** the ith row of the data **do** update $c_0 = c_0 + 1$, $c_{yy} = s_{yy} + Y_i^2$, $c_y = c_y + Y_i$, $\mathbf{c}_{xy} = \mathbf{c}_{xy} + Y_i\mathbf{x}_i$, $\mathbf{c}_x = \mathbf{c}_x + \mathbf{x}_i$, and $\mathbf{C}_{xx} = \mathbf{C}_{xx} + \mathbf{x}_i\mathbf{x}_i^T$ until the last row is scanned
4: **end for**
5: Output
6: **end procedure**

- $\mathcal{O}((p+1)^2)$ memory size
- $\mathcal{O}(n(p+1)^2)$ floating operations

Sufficient Statistics based on X_s

Statistics affected by standardization

$$C_{s,xx} = X_s^T X_s, \quad c_{s,xy} = X_s^T y, \quad c_{s,x} = \mathbb{1}_n^T X_s / n$$

- It can be proved that, those statistics can be computed directly from $\mathcal{C}(y, X)$

Key step

$$c_{s,k,xy} = V_k^T c_{s,xy} = V_k^T VDU^T y = D_k U_k^T y \;\Rightarrow\; U_k^T y = D_k^{-1} c_{s,k,xy}$$

Back to PCA regression

$$X_s = UDV^T$$

Since n is large, it's not available to calculate U. However, we can only use V and D to get the estimated coefficients and variance.

PCA regression based on sufficient statistics

1. D, V can be calculated by $C_{s,xx} = X_s^T X_s = VD^2 V^T$
2. $U_k^T y = D_k^{-1} c_{s,k,xy}$, so $\hat{\beta}_{s,k} = D_k^{-2} c_{s,k,xy}$
3. $\mathbb{V}(\hat{\sigma}_{s,k}^2) = [c_{yy} - c_{yy}/n - c_{s,k,xy}^T D_k^{-2} c_{s,k,xy}]/(n-k)$

Parallel Computation with Distributed Systems

Algorithm 2 Computation of $C(\mathbf{y}, \mathbf{X})$ in MapReduce

Input: row-by-row of individual sub-data sets
Output: $C(\mathbf{y}, \mathbf{X})$

1: **procedure** PARALLEL COMPUTATION BASED ON (17)
2: **Map tasks:** compute $C(\mathbf{y}_i, \mathbf{X}_i)$ using Step 3 of Algorithm 1 for $i = 1, \cdots, K$ individually
3: **Reduce task:** let $C(\mathbf{y}, \mathbf{X}) = \sum_{i=1}^{K} C(\mathbf{y}_i, \mathbf{X}_i)$
4: Output
5: **end procedure**

Thank you

Reference

Tonglin Zhang, Baijian Yang. 2016. "Big Data Dimension Reduction Using Pca."