Sliced Inverse Regression For Dimension Reduction (Ker-Chau Li)

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On the Agenda

Regression Analysis

- Study the relationship of a response y and its covariates x
- Use the information of x to explain y (Forward Rregression)

Curse of Dimensionality and Dimension Reduction

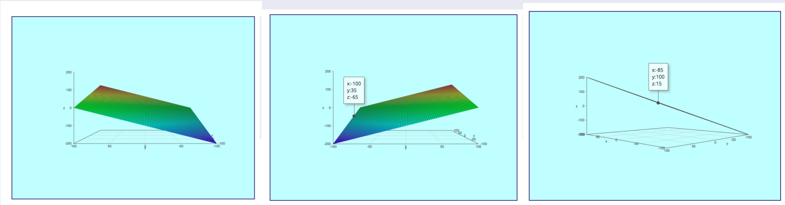
- When the dimension of x gets higher, observations are far away from each other
- Standard methods probably will break down due to the sparseness of data
- One solustion is reducing the demension of x

A toy example

Simulation settings

$$y = x_1 + x_2$$

What will be the best direction to visualize data?



On the Agenda

Model structure

Model Settings

$$Y = f(X, \epsilon) = f(\beta_1 X, \ldots, \beta_k X, \epsilon)$$

x is explanatory variable, column vectors on $\mathcal{R}^p$,
$\beta' s$ are unknown row vectors,
ϵ is independent of X,
f is an arbitrary unknown function on $\mathcal{R}^{k+1}$

- $(\beta_1 X, \ldots, \beta_k X)'$ is the projection of the $X \in \mathcal{R}^p$ into $\mathcal{R}^K$, $K << p$
- Lower dimension projection of X contains most of the information

The space spaned by $\beta' s$

Effective dimension-reduction

1. Effective dimension-reduction direction (e.d.r)
   - A Linear combination of $\beta' s$
2. A Linear space $\mathcal{B}$:
   - Spanned by $\beta' s$ ($Span(\beta)$) $\Leftrightarrow$ All the possible linear combination of $\beta' s$

- Since f is arbitrary, f and $\beta' s$ are not Estimable
- Only the $\mathcal{B}$ can be identified
- Inverse Regression is one of the methods of estimating the Effective dimension-reduction space ($\mathcal{B}$)

On the Agenda

Inverse Regression

Inverse Regression

- Regress x against of y
- Use the information of y to explain x (Inverse Regression)
- From one p-dimension problem to p One-dimension regression problems

Inverse Regression Curve

Inverse Regression Curve

$$E(X|Y) \in \mathcal{R}^p$$

Centered Inverse Regression Curve

$$E(X|Y) - E(X)$$

- $E[E(X|Y)] = E(X)$ is the center
- With certain conditions, the centered inverse curve is related with the e.d.r.!

Conditions

Condition 1.1

Conditional Independence

$$y = f(\beta_1 X, \ldots, \beta_k X, \epsilon) \Leftrightarrow (Y \perp\!\!\!\perp X) | \beta_1 X, \ldots, \beta_k X$$

Condition 3.1

Linear Condition

For any b in $\mathcal{R}^p$,

$$E(bX | \beta_1 X = \beta_1 x, \ldots, \beta_k X = \beta_k x) = c_0 + c_1 \beta_1 x, \ldots, c_k \beta_k x$$

Centered Inverse Regression Curve and e.d.r

Theorem 3.1

Under the previous Conditions,

$$E(x|y) - E(x) \subset Span(\beta_k \Sigma_{xx}), k = 1, \ldots, K$$

The centered inverse regression curve is contained in the linear subsapce spanned by $\beta_k \Sigma_{xx}$

Centered Inverse Regression Curve and e.d.r

Corollary 3.1

$$z = \Sigma_{xx}^{-1/2}[x - E(x)]$$

x is the standardized

$$f(\beta_1 x, \ldots, \beta_k x, \epsilon) \Rightarrow f(\eta_1 z, \ldots, \eta_k z, \epsilon) \Rightarrow \beta_k = \eta_k \Sigma_{xx}^{-1/2}$$

$$E(z|y) - E(z) \subset Span(\eta_k), k = 1, \ldots, K$$

An Important consequence

Covariance matrix is the key

- The Covariance matrix $Cov(E(z|y))$ is degenerated in any direction which is orthogonal to $\eta' s$
- $\eta_k' s$ $(k = 1, \ldots, K)$ associated with largest K eigenvalues of $Cov(E(z|y))$

How to estimate the $Cov(E(z|y))$

That leads to Sliced Inverse Regression Method

On the Agenda

Slice Inverse Regression Method

Y_1	$\mathbf{x}_1(=(x_{11}, x_{12}, \cdots, x_{1p})')$
Y_2	$\mathbf{x}_2(=(x_{21}, x_{22}, \cdots, x_{2p})')$
Y_3	$\mathbf{x}_3(=(x_{31}, x_{32}, \cdots, x_{3p})')$
Y_4	$\mathbf{x}_4(=(x_{41}, x_{42}, \cdots, x_{4p})')$
Y_5	....
.	....
.	....
.	....
Y_n	$\mathbf{x}_n(=(x_{n1}, x_{n2}, \cdots, x_{np})')$

Original data

$Y_{(1)}$	$\mathbf{x}_{(1)}(=(x_{(1)1}, x_{(1)2}, \cdots, x_{(1)p})')$
$Y_{(2)}$	$\mathbf{x}_{(2)}(=(x_{(2)1}, x_{(2)2}, \cdots, x_{(2)p})')$
$Y_{(3)}$	$\mathbf{x}_{(3)}(=(x_{(3)1}, x_{(3)2}, \cdots, x_{(3)p})')$
$Y_{(4)}$	$\mathbf{x}_{(4)}(=(x_{(4)1}, x_{(4)2}, \cdots, x_{(4)p})')$
$Y_{(5)}$	....
.	....
.	....
.	....
$Y_{(n)}$	$\mathbf{x}_{(n)}(=(x_{(n)1}, x_{(n)2}, \cdots, x_{(n)p})')$

Sorted and sliced by y

$\bar{Y}_1$	$\bar{\mathbf{x}}_1(=(\bar{x}_{11}, \bar{x}_{12}, \cdots, \bar{x}_{1p})')$
$\bar{Y}_2$	$\bar{\mathbf{x}}_2(=(\bar{x}_{21}, \bar{x}_{22}, \cdots, \bar{x}_{2p})')$
.	....
.	....
.	....
$\bar{Y}_H$	$\bar{\mathbf{x}}_H(=(\bar{x}_{H1}, x_{H2}, \cdots, x_{Hp})')$

Slice means of standardized data

$$\hat{V} = n^{-1} \sum_{h=1}^{H} n_h \bar{x}_h \bar{x}_h^T$$

Estimated Covariance matrix

Conduct PCA on $\hat{V}$
Find the first Kth eigenvectors $\hat{\eta}$

$$\hat{\beta}_k = \hat{\eta}_k \Sigma_{xx}^{-1/2}$$

Sliced Inverse Regression Method with detials

1. Standardize x
   - $z_i = \Sigma_{xx}^{-1/2}(x_i - \bar{x})(i = 1, \ldots, n)$
2. Divide the range of y into H slices, $I_1, \ldots, I_H$
   - $\hat{p}_h = (1/n)\sum_{i=1}^{n}(I_{y_i \in I_h})$
3. Calculate the sample mean for each slice
   - $\hat{m}_h = (1/n\hat{p}_h)\sum_{y_i \in I_h} z_i$
4. Conduct a Principal Component Analysis on the estimated Covariance matrix
   - $\hat{V} = \sum_{h=1}^{H} \hat{p}_h \hat{m}_h \hat{m}_h'$
5. Select the K largest eigenvectors (row vectors)
   - $\hat{\eta}_k(k = 1, ..., K)$
6. Transform the eigenvectors back to original scale
   - $\hat{\beta}_k = \hat{\eta}_k \hat{\Sigma}_{xx}^{-1/2}$

On the Agenda

Simulation 1

Simulation settings

$$y = x_1 + x_2 + x_3 + x_4 + 0x_5 + \epsilon$$

- $n = 100, \ p = 5$
- Only one component $\beta = (1, 1, 1, 1, 0)$
- Normalized target $\beta^* = (0.5, 0.5, 0.5, 0.5, 0)$
- The number of slice $H = (5, 10, 20)$

Simulation 1 results

Table 1. Mean and Standard Deviation of $\hat{\beta}_1$ = (*
the linear model (6.1), n = 100; the Target is (.5

H	$\hat{\beta}_{11}$	$\hat{\beta}_{12}$	$\hat{\beta}_{13}$	$\hat{\beta}$
5	.505	.498	.494	.4
	(.052)	(.049)	(.056)	(.0
10	.502	.500	.492	.4
	(.046)	(.045)	(.055)	(.0
20	.500	.502	.497	.4
	(.048)	(.046)	(.053)	(.0

*Numbers in parentheses represent standard deviations.

Simulation 2

Simulation settings

$$y = x_1(x_1 + x_2 + 1) + \sigma \cdot \epsilon$$
$$y = \frac{x_1}{0.5 + (x_2 + 1.5)^2} + \sigma \cdot \epsilon$$

- $n = 400, \ p = 10$
- $\sigma = (0.5, \ 1)$
- The number of slice $H = (5, 10, 20)$
- Two components $\beta_1 = (1, 0, 0, \ldots, 0), \ \beta_2 = (0, 1, 0, \ldots, 0)$

Evaluate the effectiveness of estimated e.d.r direction

Criterion of one direction

$$R^2(\hat{b}) = \max_{\beta \in \mathcal{B}} \frac{(\hat{b}\Sigma_{xx}\beta')^2}{\hat{b}\Sigma_{xx}\hat{b}' \cdot \beta\Sigma_{xx}\beta'}$$

Squared correlation coefficient between the bx and $\beta_1 x, \ldots, \beta_k x$

Invariant under affine transformation of x

Criterion of the subspace $\mathcal{B}$

$$R^2(\hat{\mathcal{B}}) = \frac{\sum_{k=1}^{K} R^2(\hat{b}_k)}{K}$$

Simulation 2 results

Table 2. Mean and Standard Deviation of $R^2(\hat{\beta}_1)$ a
Quadratic Model (6.2), $p = 10$, $n =$

	$\sigma = 0.5$		σ
H	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$	$R^2(\hat{\beta}_1)$
5	.91	.75	.88
	(.05)	(.15)	(.07)
10	.92	.80	.89
	(.04)	(.13)	(.08)
20	.93	.77	.88
	(.04)	(.15)	(.08)

Simulation 3 results

Table 3. *Mean and Standard Deviation of $R^2(\hat{\beta}_1)$ ar*
Rational Function Model (6.3), $p = 10$, n

	$\sigma = 0.5$		σ
H	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$	$R^2(\hat{\beta}_1)$
5	.96	.83	.89
	(.02)	(.08)	(.06)
10	.96	.88	.90
	(.02)	(.06)	(.06)
20	.96	.89	.90
	(.02)	(.06)	(.06)

Graphics

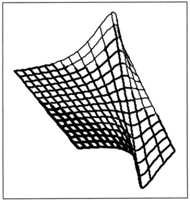


Figure 2: Response surface of simulation 3

How to visualize the data?

Directions found by SIR

Thank you

Reference

Li, Ker-Chau. 1991. “Sliced Inverse Regression for Dimension Reduction.”