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

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January 11, 2018

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- Inverse Regression
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- Simulation

# On the Agenda

- Introduction

Sliced Inverse Regression Method

# Regression Analysis

- Study the relationship of a response y and its covariates x
- Use the information of x to explain y
- Parametric model
  - Linear Regression model
- Nonparametric model
  - Local smoothing (kNN)

- 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

Introduction

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A Model for dimension reduction

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### A Model for dimension reduction

### **Model Settings**

$$y = f(\beta_1 X, \dots, \beta_k X, \epsilon)$$

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

- $(\beta_1 x, \dots, \beta_k x)'$  is the projection of the  $x \in \mathbb{R}^p$  into  $\mathbb{R}^K$ , K << p
- Captures all we need to know about y

### A Model for dimension reduction

#### Effective dimension-reduction

- Effective dimension-reduction direction (e.d.r)
  - A Linear combination of β's
- $\bigcirc$  A Linear space  $\mathcal{B}$ :
  - Spanned by  $\beta's$  (Span( $\beta$ ))  $\Leftrightarrow$  All the possible linear combination of  $\beta's$
  - Since f is arbitrary, 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**

Sliced Inverse Regression Method

# Inverse Regression

### Inverse Regression

- Regress x against of y
- Use the information of y to explain x
- 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.!

Introduction

# Conditions

#### Condition 1.1

Conditional Independence

$$y = f(\beta_1 x, \dots, \beta_k x, \epsilon) \Leftrightarrow (y \perp\!\!\!\perp x) | \beta x$$

#### Condition 3.1

Linear Condition

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

$$E(b\mathbf{x}|\beta_1\mathbf{x}=\beta_1x,\ldots,\beta_k\mathbf{x}=\beta_kx)=c_0+c_1\beta_1x,\ldots,c_k\beta_kx$$

# Centered Inverse Regression Curve and e.d.r

#### Theorem 3.1

Under the previous Conditions,

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

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

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

x is the standardized

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

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

# 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, ..., 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

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Original data

Sorted and sliced by y

Slice means of standardized data

$$\hat{V} = n^{-1} \sum_{i=1}^{H} n_h \bar{x}_h \bar{x}_h^T \qquad \qquad \text{Conduct PCA on } \hat{V} \\ \hat{\beta}_k = \hat{\eta}_k \Sigma_{xx}^{-1/2}$$

Estimated Covariance matrix

# Sliced Inverse Regression Method with detials

Standardize x

• 
$$z_i = \sum_{xx}^{-1/2} (x_i - \bar{x})(i = 1, ..., n)$$

2 Divide the range of y into H slices,  $I_1, \ldots, I_H$ 

• 
$$\hat{p}_h = (1/n) \sum_{i=1}^n (I_{y_i \in I_h})$$

Calculate the sample mean for each slice

$$\bullet \hat{m}_h = (1/n\hat{p}_h) \sum_{y_i \in I_h} z_i$$

Conduct a Principal Component Analysis on the estimated Covariance matrix

• 
$$\hat{V} = \sum_{h=1}^{H} \hat{p}_h \hat{m}_h \hat{m}'_h$$

Select the K largest eigenvectors (row vectors)

• 
$$\hat{\eta}_k(k = 1, ..., K)$$

- Transform the eigenvectors back to original scale
  - $\hat{\beta}_k = \hat{\eta}_k \hat{\Sigma}_{xx}^{-1/2}$

Simulation

# On the Agenda

A Model for dimension reduction

- Simulation

### 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  $\hat{\beta}_1 = (\hat{\beta}_{11}, ..., \hat{\beta}_{15})$  for the linear model (6.1), n = 100; the Target is (.5, .5, .5, .5, 0)

Н	β <sub>11</sub>	$\hat{eta}_{12}$	$\hat{eta}_{13}$	$\hat{eta}_{14}$	$\hat{eta}_{15}$
5	.505	.498	.494	.488	.002
	(.052)	(.049)	(.056)	(.056)	(.066)
10	.502 (.046)	.500 (.045)	.492 (.055)	.491 (.049)	.001
20	.500	.502	.497	.487	003
	(.048)	(.046)	(.053)	(.054)	(.060)

<sup>\*</sup>Numbers in parentheses represent standard deviations.

- Repeat the simulation 100 times to generate the empirical distribution of  $\hat{\beta}'s$
- $\beta$  and  $\hat{\beta}$  are standardized

## Simulation 2

### Simulation settings

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

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

#### 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  $\beta_1 x, \dots, \beta_k x$ Invariant under affine transformation of x

#### Criterion of the subspace $\mathcal{B}$

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

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## Simulation 2 results

A Model for dimension reduction

Table 2. Mean and Standard Deviation of  $R^2(\hat{\beta}_1)$  and  $R^2(\hat{\beta}_2)$  for the Quadratic Model (6.2), p = 10, n = 400

	$\sigma = 0.5$		$\sigma = 1$	
н	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$	$R^2(\hat{\beta}_1)$	R²(β̂₂)
5	.91	.75	.88	.52
	(.05)	(.15)	(.07)	(.21) .55
10	.92	.80	.89	.55
	(.04)	(.13)	(80.)	(.24)
20	(.04) .93	(.13) .77	.88	(.24) .49
	(.04)	(.15)	(80.)	(.26)

 Repeat the simulation 100 times to generate the empirical distribution of  $\beta's$ 

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Table 3. Mean and Standard Deviation of  $R^2(\hat{\beta}_1)$  and  $R^2(\hat{\beta}_2)$  for the Rational Function Model (6.3), p = 10, n = 400

	$\sigma = 0.5$		$\sigma = 1$	
н	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$
5	.96	.83	.89	.51
	(.02)	(80.)	(.06) .90	(.23) .56
10	(.02) .96	.88	.90	.56
		(.06)	(.06)	(.23)
20	(.02) .96	.89	.90	(.23) .53
	(.02)	(.06)	(.06)	(.24)

Repeat the simulation 100 times to generate the empirical distribution of  $\beta's$ 

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Figure 2: Response surface of simulation 3

#### How to visualize the data?

Directions found by SIR

# Thank you

SIR

# Reference

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