Variable Selection

Consider: Y= XB+ E. E ~ Naco, 6ºIn) where

Y= 12°. B= 12° (unknown). X= M°1. ((X)=P.

Mo: (0 Ipn) $\beta = 0$ is test for whether all the variables influence Y (lata). $\beta = c \beta_0 \beta_1 - \beta_{p-1}$) $X = (J_n \ X_1 - \cdots \ X_{pn})$. β_0 is fixed.

Mo: $\beta_i = 0$ is test for single one.

(1) Consequence of Selection:

but retain the accuracy of estimation at the same time.

Suppose $X_2 \in M^{n \times 2}$. $P_2 \in \mathcal{R}^2$. $X = (X_2 \times x_2)$. $B = \begin{pmatrix} \beta_2 \\ \beta_2 \end{pmatrix}$. rewrite the model in:

Y = X2 82 + Xt Bt + E

Choose 2-1 unriables X2 from P-1 variables

X then generate a alternative model:

 $Y = X_2 \beta_2 + \Sigma. \quad \text{Correspond} : M.: LO It) \beta = 0 \quad (\Lambda = (0.It))$ $R = \sum_{k=1}^{\infty} \frac{(\Lambda^{k} \beta_{k})^{T} (\Lambda^{T} (X^{T} X)^{T} \Lambda^{T} \beta_{k})^{T} (\Lambda^{T} \beta_{k})^{T} (\Lambda^{T} X^{T} X)^{T} \Lambda^{T} \beta_{k}}{t \, \text{mst}} \geq F_{\alpha}(t, n-t)$

MSE

Where
$$D = (X_{t}^{T}(I - P_{x_{t}}) X_{t})^{T}$$
. $P_{x_{t}} = X_{t} (X_{t}^{T} X_{t})^{T} X_{t}^{T}$

$$P_{t} : \begin{pmatrix} I_{t} & 0 \\ -X_{t}^{T} X_{t} (X_{t}^{T} X_{t})^{T} & I_{t} \end{pmatrix} X^{T} X \begin{pmatrix} I_{t} & -(X_{t}^{T} X_{t})^{T} X_{t}^{T} X_{t} \\ 0 & I_{t} \end{pmatrix}$$

$$= \begin{pmatrix} X_{t}^{T} X_{t} & 0 \\ 0 & D^{T} \end{pmatrix} \cdot D_{t} D_{t}^{T} A D A^{T} - A D$$

$$\Rightarrow (X_{t}^{T} X_{t})^{T} = \begin{pmatrix} (X_{t}^{T} X_{t})^{T} + A D A^{T} & -A D \\ -D A^{T} & D \end{pmatrix}$$

Denote: i)
$$\hat{\beta} = (\chi^T \chi)^T \chi^T \gamma$$
, $\hat{G}^2 = \frac{\gamma^T (I-m) \gamma}{n-r(\chi_1)}$, $\hat{g} = \chi^T \hat{\beta} \in \chi'$

ii) $\hat{\beta}_1 = (\chi^T_2 \chi_2)^T \chi_1^T \gamma$, $\hat{G}_2 = \frac{\gamma^T (I-m_1) \gamma}{n-r(\chi_2)}$ $\hat{\gamma} = \chi^T \hat{\beta}_2 \in \chi'$

where $\hat{\chi} = (\hat{\chi}_1 \hat{\chi}_2)$, $\hat{\gamma}$ is estimate

iii) $MSE(\hat{\theta}) = E((\hat{\theta} - \theta)(\hat{\theta} - \theta)^T)$

7hm. (Influence on estimation)

- i) $E(\vec{\beta}) = \beta$ if the full model is correct. $\beta_t = 0$ or $X_2^T X_t = 0 \iff E(\vec{P_2}) = P_2$
- ii) Varcipo Varcipo >0
- Vare \begin{aligned}
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 \begin{aligned}
 \text{Vare \beta \genumber 2 Be \beta \beta \beta \columber \beta \beta \columbe
- iv) $E(\tilde{\delta}_{2}^{2}) \Rightarrow E(\tilde{\delta}^{2}) = \tilde{\delta}^{2}$ "" holds if mote only if $\beta t = 0$.

- Rmk: i) means by isn't a unbinsed estimator
 generally
 - ii) means if we used the reduced model but the origin model is time. then variance of estimator will reduce.
 - iii) means the Variables Bt Liscarded exactly effects the estimation. Since Bt com't be estimated and have large Variance (Varib) to 3 Bt Bt.). Delete Bt can reduce Variance.
 - iv) means on isn't unbinsed estimator for o'

 if the origin model is true.
 - $\frac{Pf: i)}{E(\vec{\beta})} = (x^{T}x)^{T}x^{T}x^{\beta} = \vec{\beta}.$ $\frac{E(\vec{\beta})}{E(\vec{\beta})} = (x^{T}x_{0})^{T}x^{T}x^{\beta} = \vec{\beta}.$ $\frac{E(\vec{\beta})}{E(\vec{\beta})} = (x^{T}x_{0})^{T}x^{T}x^{\beta} = (x^{T}x_{0})^{T}x^{T}x^{T}x^{\gamma}x^{\gamma} = \beta_{2} + A\beta_{2}$ $= \beta_{2} + (x^{T}x_{0})^{T}x^{T}x^{\gamma}x^{\gamma} + \beta_{3} = \beta_{2} + A\beta_{4}$
 - (ii) $V_{AP}(\vec{\beta}) = (x^T X)^{-1} X^T V_{PP}(Y) X (X^T X)^{-1}$ $= \delta^{-1} (X^T X)^{-1} = \delta^{-1} \left((X_2^T X_2)^T + ADA^T - AD \right)$ $= \rho A^T D$
 - $VARC\widehat{\beta}_{2} = \delta^{*}((X_{1}^{*}X_{2})^{*} + ADA^{*})$ $With Varc \widehat{\beta}_{2}) = \delta^{*}((X_{2}^{*}X_{2})^{*} + ADA^{*})$ $\Rightarrow VARC\widehat{\beta}_{2} VARC\widehat{\beta}_{2}) = \delta^{*}ADA^{*} \geq 0$

 $MSE(\vec{\beta}_{1}) = V_{AV}(\vec{\beta}_{2}) + CE(\vec{\beta}_{2}) - \beta_{1}I(E(\vec{\beta}_{1}) - \beta_{1})^{T}$ $= V_{AV}(\vec{\beta}_{2}) + A\beta_{1}\beta_{1}^{T}A^{T}$ $= V_{AV}(\vec{\beta}_{2}) + A\beta_{1}\beta_{1}^{T}A^{T}$ $= V_{AV}(\vec{\beta}_{2}) + ASE(\vec{\beta}_{2}) = A(\delta^{2}D - \beta_{1}\beta_{1}^{T})A^{T}$ $= V_{AV}(\vec{\beta}_{2}) = \frac{1}{n-r(X_{1})} E(\vec{\gamma}^{2}) + \frac{1}{n-r(X_{2})} E(\vec{\gamma}^{2}) + \frac{1}{n-r(X_{2})} E(\vec{\gamma}^{2}) + \frac{1}{n-r(X_{2})} E(\vec{\gamma}^{2})$ $= \frac{1}{n-r(X_{2})} tr(CI-m_{2})(\delta^{2}I + \chi \rho \beta_{1}^{T}\chi^{2}))$ $= \sigma^{2} + \frac{1}{n-r(X_{2})} \beta_{1}^{T}\chi^{2}(I-m_{2})\chi \beta$ $= \sigma^{2} + \frac{1}{n-r(X_{2})} \beta_{1}^{T}\chi^{2}(I-m_{2})\chi \beta_{1}$

7hm. (Influence on estimate)

- i) $E(\hat{\eta}) = x^{T}\beta$ if the origin model is true $\beta_{t} = 0 \iff E(\hat{\eta}) = x^{T}\beta$
 - ii) Varen xt B) > Varen xt Bi)
 - iii) Vare B)+ B+B+ = 0 = Varen x B) = Ecn-x Boj

Rmk: It means if origin model is true.

then Fr isn't unbiased. But its MSE

will reduce if Varifit > pt pt. i.e. its

variance is large.

 $E(\hat{\eta}) = \chi^{T} E(\hat{\beta}) = \chi^{T} \beta.$ $E(\hat{\eta}_{2}) = \chi^{T}_{1}(\beta_{1} + \beta_{2} + \beta_{3} + \lambda_{1}^{T} \beta_{2} + \lambda_{1}^{T} \beta_{2}$

iii) $E(\eta - \chi_{2}^{T} \vec{\beta}_{1})^{2} = V_{NY}(\eta - \chi_{1}^{T} \vec{\beta}_{1}) + E^{2}(\eta - \chi_{2}^{T} \vec{\beta}_{2})$ $= V_{NY}(\eta - \chi_{1}^{T} \vec{\beta}_{1}) + C(\chi^{T} \beta - \chi_{1}^{T} (\beta_{2} + \beta_{2} + \beta_{2}))^{T}$ $= V_{NY}(\eta - \chi_{1}^{T} \vec{\beta}_{1}) + (A^{T}\chi_{1} - \chi_{2})^{T}\beta_{2}\beta_{1}^{T}(A^{T}\chi_{2} - \chi_{2})$

 $\Rightarrow V_{\alpha r i} \gamma - \chi^{\tau} \hat{\beta}) - \mathcal{E}_{i} \gamma - \chi_{i}^{\tau} \hat{\beta}_{i})^{\tau} =$ $\sigma^{2} (A^{7} \chi_{i} - \chi_{t})^{7} (\sigma^{2} D - \beta_{t} \beta_{t}^{2}) (A^{7} \chi_{i}^{2} - \chi_{t}^{2}) \geq 0$ $\text{With } V_{\alpha r i} \hat{\beta})_{t} - \beta_{t} \beta_{t}^{T} = \sigma^{2} D - \beta_{t} \beta_{t}^{T}.$

PMK: Back to the hypothesis testing: Replace para.

in $\delta^*D - \beta t \beta \tilde{t} \stackrel{?}{?} 0$ with estimator, then, $\hat{\delta}^*D - \hat{\beta} t \hat{\beta} \tilde{t} \stackrel{?}{?} 0 \iff \hat{\beta} \tilde{t} \stackrel{?}{D}^{-1} \hat{\beta} t / t \hat{\sigma}^* \approx \frac{1}{t}$ i.e. if $\frac{1}{t} = F_{r}(t, n-p)$, then we accept

Mo: $\beta t = 0$. [Let $A = D^{-1} \hat{\beta} t$. Prove: $\hat{\delta}^* I \stackrel{?}{?} a A^* I$ $\Rightarrow \hat{\delta}^* \stackrel{?}{?} a^* I$. it's easy to see)

(2) Principlus:

If we have p variables to be selected.

Then there re 2°-1 possible regression equation

Denote: i) SST = YTY, SSE = YCI-M)Y SSE2 = YTCI-M2)Y.

> ii) $R^2 = 1 - \frac{55E}{55T}$ $R_2^2 = 1 - \frac{55E_2}{55T}$ Rmk: 42 = p. $SSE = 5SE_2$ $R^2 > R_3$

O For fitting the model:

i) Minimize the mean of SSE_2 :

i.e. find $2 \cdot \tilde{\sigma}_2^* = \min_{r} \frac{SSE_r}{n-r}$

Rmk: SSE2 f as 2 v. n-2 f as 2 v

if [xi], effects of Significantly

then SSE2 v fast as 2 f.

if not. then SSE2 v slowly as 2 f

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\frac{1}{n-2} f as 2 f \tau is penalty of increase

of number of variables.

ii) Maximize $R_{1}^{+} =: 1 - \frac{SSE_{1}/n-2}{SST/n-1} = 1 - CI-R_{1}^{+})\frac{n-1}{n-2}$ $R_{1}^{+} =: 1 - \frac{SSE_{1}/n-2}{SST/n-1} = 1 - CI-R_{1}^{+})\frac{n-1}{n-2}$ $R_{2}^{+} =: 1 - \frac{SSE_{1}/n-2}{SST/n-1} = 1 - CI-R_{1}^{+})\frac{n-1}{n-2}$

We call Ri adjustment complex duision coefficient.

1) Minimize the Estimator of JJt:

$$JJ_{t} = \stackrel{\sim}{\mathcal{I}} V_{AI}(Y_{i} - \chi_{i2}^{7} \overline{\beta}_{2}) = \stackrel{\sim}{\mathcal{I}}_{i1}^{2} (1 + \chi_{i2}^{7} (\chi_{i2}^{7} \chi_{i1}) \sigma^{2}$$

$$Note that RMS = n\sigma^{2} + tr((\chi_{i1}^{7} \chi_{i1})^{7} \stackrel{\sim}{\mathcal{I}} (\chi_{i2}^{7} \chi_{i2}) \sigma^{2})$$

$$= (n+1) \sigma^{2}$$

Replace or by its estimator or.

ii) Minimize S2 = 62 / (n-9-1)

It's from: Consider 1 = B. + = Bi Xji + Ej = Fo+ IBi (Xji - Xj) + Ej i.e. Y = PAXB + (I-PA)XB + E. CCENTIALiZAtion) Pa = JaJa/n $\hat{Y} = P_n \hat{Y} + (Z - P_n) \hat{X} \hat{\beta} = (X^T (Z - P_n) \hat{X})^T \hat{X}^T (Z - P_n) \hat{Y}$ \Rightarrow estimate $\hat{\eta} = \hat{\eta} + (x - \hat{x})^{T} \hat{\beta}$. $V_{AFG}(\hat{\eta} - \hat{\eta}) = (\frac{n\tau_{1}}{n} + (x - \hat{x})^{T} \hat{s}(x - \hat{x})) \hat{s}^{T}$ where S = XT(I-Pn) X = I(X,-X) (X, X) X from X. (X) - Non. I) Note that not 1 (x-x) 5'(x-x) ~ F(2-1. N-2-1) => EUVALLA-9 (X.x)) = n+1 1-1 (IN - IXX IXX) . Set St = 02

Consider to minimize
$$J_{\rho} = \frac{1}{\sigma^{2}} \sum_{i} (\vec{q}_{i} - E_{i} Y_{i})^{2}$$

$$= \frac{1}{\sigma^{2}} \sum_{i} (X_{i}^{2} \vec{p}_{i} - X_{i}^{2} \vec{p}_{i})^{2}, \quad 7ndn \text{ it } (X_{pertion}^{2})^{2}$$

$$= \sum_{i} \sum_{i} (X_{i}^{2} X_{i}^{2})^{2} \times i_{1} + \frac{1}{\sigma^{2}} \sum_{i} (X_{i}^{2} \vec{p}_{i} - X_{i}^{2} \vec{p}_{i})^{2}$$

$$= \sum_{i} X_{i} (X_{i}^{2} X_{i}^{2})^{2} \times i_{1} + \frac{1}{\sigma^{2}} \sum_{i} (X_{i}^{2} (\vec{p}_{i} + A \vec{p}_{i}) - X_{i}^{2} \vec{p}_{i})^{2}$$

$$= 2 + \frac{1}{\sigma^{2}} \sum_{i} (X_{i}^{2} X_{i}^{2} - X_{i}^{2} \vec{p}_{i})^{2}$$

$$= 2 + \frac{1}{\sigma^{2}} \sum_{i} (X_{i}^{2} X_{i}^{2} - X_{i}^{2} \vec{p}_{i})^{2} + \frac{1}{\sigma^{2}} \sum_{i} (X_{i}^{2} - X_{i}^$$

16p-21 is Small.

IV) Minimize PRESS:

Denote:
$$Y^{(-i)} = \begin{pmatrix} \gamma' \\ n_{i+1} \\ n_{i+1} \end{pmatrix}$$
 $X^{(-i)} = \begin{pmatrix} \chi_{i}^{\top} \\ \chi_{i+1}^{\top} \\ \chi_{i}^{\top} \end{pmatrix}$ Cremove ith component)

Lasiler Y (-1) = X (-1) B + I

Def: PRESS =
$$\sum_{i=1}^{n} (\hat{\ell}^{(i)})^{-1}$$
, prediction of Sum of square of error.

Penote: hii = Xi (XTX) Xi (ith lingual element of X (XTX) XT)

To intentite PRESS:

$$\hat{Z}^{(i)} = \eta_i - \chi_i^T (X^{(i)}^T X^{(i)})^{-1} (X^{(i)}^T Y^{(i)})$$

$$= \eta_i - \chi_i^T (X^T X - \chi_i \chi_i^T)^{-1} (X^T Y - \chi_i \eta_i)$$

$$(\chi^{T}\chi - \chi_{i}\chi_{i}^{T})^{-1} = (\chi^{T}\chi)^{-1} + \frac{(\chi^{T}\chi)^{T}\chi_{i}\chi_{i}^{T}(\chi^{T}\chi)^{-1}}{1 - hii}$$
(and to check)

$$\widehat{\mathcal{Z}}^{(-1)} = \widehat{\mathcal{Z}}_i + hii \gamma_i - \frac{hii \, \chi_i^* \widehat{\beta}}{1 - hii} + \frac{hii \, \eta_i}{1 - hii} \, \widehat{\mathcal{Z}}_i = \eta_i - \chi_i^* \widehat{\beta}$$

$$= \frac{\hat{\mathcal{L}}i}{1-kii}$$

RMK: For PRESS2 =
$$\frac{\tilde{\Sigma}}{|\tilde{\Sigma}|} \left(\tilde{\Sigma}_{2}^{(i)} \right)^{2}$$
. We have:
$$\tilde{Z}_{2}^{(i)} = \frac{\hat{Z}_{12}}{1-hiir} \cdot hiir is i^{th} \text{ linguous element}$$
of $M_{2} = \chi_{2} (\chi_{1}^{2} \chi_{2})^{2} \chi_{2}$

3 By MLE:

i) AIC: (Aknike information Criteria)

If In Noo. o'In). Then: In LCB. 0° (Y) = - = Inczzó) - = (Y-xp) (Y-xp) In Lmax = In LCLXTX) XTY, SSE) = -= ln (==) - = ln (SSE) -=

Def: AIC = -2 log Log(X) +2p. P= limt.

=> AICe = nlm 55 Ee + 21 in this case Find 2 to minimize AIC2

ii) BIC C Bagesian information criteria) BICZ = nln SSE2 + 27 lnn

(3) Selection:

By above we have three Common criteria:

- i) rhjrsp criterin: max Ri
- ii) Cp criteria = min C+ = min (55 E2 +22-n)
- iii) AIC: min mln55E2 + 22

O Global Selection:

Chark 2°-1 possible regression models for optimal q. But it's low efficient when p is large.

E.g. choose $A(k) = I \chi_{ii} - \chi_{ik} = I \chi_{ij}$.

Calculate Criterion on A(k).

O Stepwise methol:

i) Test for Significant:

Consider $Mo^2 \beta_1 = \beta_2 = \cdots = \beta_p = 0$ i.e. test

whether $ZXiS_1^2$ influences y a lot.

Denote: $SST = Y^T (J - P_n^T) Y$. Aft = n-1. $SSR = Y^T (M - P_n^T) Y$. Afk = P $SSE = Y^T (J - M) Y$. Afk = n-P-1

=> SST = SSR + SSE. SSE inAspt with SSR

F = \frac{\sigma_{\sigma}PP}{\sigma_{\sigma}\left[\rho_{\color-p-1}\right]} \sigma_{\sigma}P(P, n-P-1). under Mo.

we obtain p-value: P=P(F(p,n-p-1)>F)consider Ho: Bio=0 i.e. test the influence of individual variable.

Denote RSS (-in) is RSS on IXXB kt in.

Pio = RSS - RSS (-in) = \hat{B}_{in} / Lii. (t) approve it later)

Where lii is the ith linguous element of $L^{-1} = (X^{T}(I - P_{in}^{T})X)^{-1}$.

Fi. = F(1. n-p-1) value Mo

kmk: sst = ssE + ssk = ssE (-i) + ssk(-i) => Pi= Qc-i.) - Q

Establish p regressional equations with one variable. Then calculate each p-value (F-F11.n-25)

- ⇒ Choose the Unrimble with Smallest P-value

 and introduce it into equation. (Denote X.)
- => Establish p-1 regression equations w.r.t

 [(X.Xi)]; Chook the pair with smallest p-value.
- -) Repeat the process untill we obtain the target number of variables.

RME: The later introduction of variables may reduce the significant of former variables.

iii) Bachward Selection:

Put all the variables into the equations

- =) Calculate Fi. discard the max one.
- => Put p-1 variables line equations. then
 repeat the process before.

Rmk: It needs a lot computations.

iv) Stepwise Selection:

Step one: Niscard Variable. Suppose We have introduced Exikless.

Calculate Pik = SSRzijss=1 - SSRzijsj*k. if Xo is the variable corresponds min Pix. ther test : Fo = Po SSE/(n-1-1) P=P1 F(1.n-1-1)>Fol Bo=1) if P ? 9 out. => lisened X. P < Your => Consider to introduce other variables introduce new unlimbles. Suppose we have I Xjk sk=1 out of the equation. Pik = SSRII; Si Ulius - SSRII; si. it

Step two:

Xjo is the Variable correspond max fix

Fjo = Pio Mo Fc1. n-r-2)

SSELIJS (UZjk) / (n-r-2)

P = P & F & 1. n- (-2) > Fi, | M.) . M. = Bio = 0.

if p< Kost = introlace Xj. into equation P? Year > Selection is over.

Pf of (x): { a = Y'(I - x(x'x)'x') Y X = (X, X;) (aci) = YTCI- X. (x. x.) X.) Y $(x^{T}x)^{-1} = \begin{pmatrix} (x^{T}x_{1})^{-1} + AD^{-1}A^{T} & -AD^{-1} \\ -D^{-1}A^{T} & D^{-1} \end{pmatrix}$

> A = (x, x,) x, x; D = x; (I - P ((x)) x; = 1/411 > P: = YT (ATXT - XT) TDT (ATXT - XT) Y Bi = (0 I) (XTX) XTY = (-ATX] + X!)Y/0 ⇒ Pi indept with Q. as well.