Assignment Project Exam Help

Linear Regression

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MAST90083 Computational Statistics and Data Mining

Dr Karim Seghouane

School of Mathematics & Statistics
The University of Melbourne

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Outline

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Statistical Models

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- What is the simplest mathematical model that describes the relationship between two variables ?
- Straight line

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- Statistical models are fitted for a variety of reasons:
- Explanation and prediction: Uncover causes by studying the relationship between an interested variable (the response) and a set of variables called the explanatory variables& use the model for prediction

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- Examine and test scientific hypotheses

Linear Models

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- Linear models have a long history in statistics, but even in today's computer era they are still important and widely used in supervised learning.

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- They are simple and provide a picture of how the inputs affect the output
- For prediction purposes they can sometimes outperform fancier nonlinear models, particularly in small sample cases, low signal-to-noise ratio or sparse data

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- We will study some of the key questions associated with the linear regression model

Linear regression

Given a vector of input variables $\mathbf{x} = (x_1, \ldots, x_p)^\top \in \mathbb{R}^p$ and a response variable $y \in \mathbb{R}$

$$y \approx f(\mathbf{x})$$

where

$$f(\mathbf{x}) = \beta_0 + \sum_{i=1}^{p} \beta_i x_i = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p$$

- The linear model assumes that the dependence of y on $x_1, x_2, \ldots, x_p$ is linear. Or, it can be well approximated by the linear relationships.
- Although it may seem overly simplistic, linear regression is extremely useful both conceptually and practically.
- The β_j's are the unknown parameters that need to be determined.

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Parameter Estimation

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- We have at our disposal a set of training data $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$ from which to estimate the parameters $\boldsymbol{\beta}$

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- The most popular method is least squares where β is obtained by minimizing the residual sum of squares

$$\mathrm{RSS}(\beta) = \sum_{i=1}^{N} (y_i - f(x_i))^2 = \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

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- **What is the statistical interpretation ?**

Statistical Interpretation

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- From a statistical point of view, this represents the maximum likelihood estimation of $\boldsymbol{\beta}$ assuming

$$y_i = \mathbf{x}_i^\top \boldsymbol{\beta} + \epsilon_i \quad i = 1, \dots, N$$

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- and $\epsilon_1, \dots, \epsilon_N$ are independent random samples from $\mathcal{N}(0, \sigma^2)$, $\sigma > 0$ an unknown parameter so that $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_N)$
- Taking X as the $N \times (p+1)$ matrix with each row an input vector and 1 in the first position and $\mathbf{y}$ an $N \times 1$ vector of responses: $E(\mathbf{y}) = X\boldsymbol{\beta}$ and $\mathrm{Cov}(\mathbf{y}) = \sigma^2 \mathbf{I}_N$, so that

$$\mathbf{y} \sim \mathcal{N}\left(X\boldsymbol{\beta}, \sigma^2 \mathbf{I}_N\right)$$

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Note 1

Matrix Form

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- The residual sum of square takes the matrix form

$$\mathrm{RSS}(\beta) = (\mathbf{y} - X\beta)^\top (\mathbf{y} - X\beta)$$

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- Assuming that X has full column rank or $X^\top X$ is positive definite gives a unique solution

$$\hat{\beta} = \left(X^\top X\right)^{-1} X^\top \mathbf{y}$$

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- and the fitted values at the training inputs are (Note 2)

$$\hat{\mathbf{y}} = X\hat{\beta} = X\left(X^\top X\right)^{-1} X^\top \mathbf{y} = H\mathbf{y}$$

Geometric Interpretation

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- The hat matrix H is square and satisfies: $H^2 = H$ and $H^\top = H$ (Note 3)
- H is the orthogonal projector onto $V = Sp(X)$ (column space of X or the subspace of $\mathcal{R}^N$ spanned by the column vectors of X)

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- and $\hat{\mathbf{y}}$ is the orthogonal projection of $\mathbf{y}$ onto $Sp(X)$
- The residual vector $\mathbf{y} - \hat{\mathbf{y}}$ is orthogonal to this subspace

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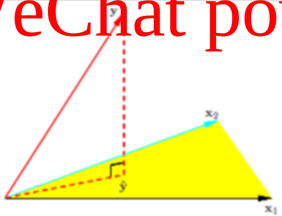

Statistical Properties

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- Assuming the model $\mathbf{y} \sim \mathcal{N}\left(X\beta, \sigma^2 \mathbf{I}_N\right)$ gives

$$\hat{\beta} \sim \mathcal{N}\left(\beta, \sigma^2 \left(X^\top X\right)^{-1}\right)$$

or

$$\hat{\mathbf{y}} \sim \mathcal{N}\left(X\beta, \sigma^2 H\right)$$

- where σ^2 is estimated by

$$\hat{\sigma}^2 = \frac{1}{N-p-1}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 = \frac{1}{N-p-1}(\mathbf{y} - \hat{\mathbf{y}})^\top (\mathbf{y} - \hat{\mathbf{y}})$$

- and $(N-p-1)\hat{\sigma}^2 \sim \sigma^2 \chi^2_{N-p-1}$
- Furthermore $\hat{\sigma}^2$ and $\hat{\beta}$ are statistically independent. (**Why** ?)

Assessing the Accuracy of the coefficient estimates

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- Approximate confidence set for the parameter vector β

$$C_{\beta} = \{\beta | \left(\hat{\beta} - \beta\right)^{\top} X^{\top} X \left(\hat{\beta} - \beta\right) \leq \hat{\sigma}^2 \chi^{(1-\alpha)}_{p+1}\}$$

- Test the null hypothesis of $H_0 : \beta_j = 0$ vs. $H_1 : \beta_j \neq 0$ using

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$$z_j = \frac{\hat{\beta}_j}{\hat{\sigma}\sqrt{v_j}}$$

- and v_j is the jth diagonal element of $(X^{\top} X)^{-1}$. Under H_0, z_j is t_{N-p-1}.

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- Testing for a group of variables, H_0 : smaller model is correct

$$F = \frac{(RSS_0 - RSS_1)/(p_1 - p_0)}{RSS_1/(N - p_1 - 1)} \sim F_{p_1 - p_0, N - p_1 - 1}$$

Note 4

Gauss-Markov Theorem

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- LSE of β have the smallest variance among all linear unbiased estimates
- Assuming the estimation of $\theta = \mathbf{a}^\top \beta$, then its LSE is

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$$\hat{\theta} = \mathbf{a}^\top \hat{\beta} = \mathbf{a}^\top \left(X^\top X\right)^{-1} X^\top \mathbf{y} = \mathbf{c}_0^\top \mathbf{y}$$

- Then $E\left(\mathbf{a}^\top \hat{\beta}\right) = \mathbf{a}^\top \beta$ is unbiased and

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$$\mathrm{Var}\left(\hat{\theta}\right) \leq \mathrm{Var}\left(\mathbf{c}^\top \mathbf{y}\right)$$

- for any other linear estimator $\tilde{\theta} = \mathbf{c}^\top \mathbf{y}$

Reducing the MSE

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- The LSE has the smallest MSE of all linear estimators with no bias.
- Biased estimator can generate smaller MSE

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- Shrinking a set of coefficients to zero may result in a biased estimate
- MSE is related to the prediction accuracy of a new response $y_0 = f(x_0) + \epsilon_0$ at input x_0

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$$E\left[y_0 - \tilde{f}(x_0)\right]^2 = \sigma^2 + E\left[x_0^\top \tilde{\beta} - f(x_0)\right]^2 = \sigma^2 + MSE\left[\tilde{f}(x_0)\right]$$

Note 5

Assessing the Overall Accuracy of the Model

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- Quantify *how well the model fits the observations*
- Two quantities are used: the residual standard error (RSE) which measures the lack of fit

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$$RSE = \sqrt{\frac{\mathrm{RSS}\left(\hat{\beta}\right)}{N-p-1}} = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{N-p-1}}$$

- R^2 Statistics

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$$R^2 = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}}$$

- measure the amount of variability $\left(\mathrm{TSS} = \sum (y_i - \bar{y})^2\right)$ removed by the model

Other Considerations in the Regression Model

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- Correlation of the error terms
- Interactions or collinearity
- Categorical predictors and their interpretation (two or more categories).
- Non-linear effects of predictors
- Outliers and high-leverage points
- Multiple outputs

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Correlation of the error terms

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- Use generalized LS

$$\mathrm{RSS}(\beta) = (\mathbf{y} - X\beta)^\top \Sigma^{-1} (\mathbf{y} - X\beta)$$

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- Similar to assuming

$$\mathbf{y} \sim \mathcal{N}(X\beta, \Sigma)$$

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- Still least square but using a different metric matrix Σ instead of $\mathbf{I}$

Note 6

Interactions or collinearity

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- Variables closely related to one another which leads to linear dependence or collinearity among the columns of X.
- It is difficult to separate the individual effects of collinear variables on the response.

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$$\operatorname{Var}\left(\hat{\beta}\right) = \sigma^2 \left(X^\top X\right)^{-1}$$

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- Collinearity has considerable effect on the precision of $\hat{\beta} \mapsto$ large variances, wide confidence interval and low power of the tests
- It is important to identify and address potential collinearity problems

Detection of collinearity

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- Look at the correlation matrix of the variables to detect pair of highly correlated variables
- Collinearity between three or more variables compute *variance inflation factor VIF* for each variable

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$$\mathrm{VIF}\left(\hat{\beta}_j\right) = \frac{1}{1 - R_j^2}$$

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- Geometrically $1 - R_j^2$ measures how close x_j is to the subspace spanned by X_{-j}

$$\mathrm{Var}\left(\hat{\beta}_j\right) = \frac{\sigma^2}{1 - R_j^2} \leq \lambda_{max}\lambda_{min}^{-1} = \kappa\left(X\right)^2$$

- Examine the eigenvalues and eigenvectors **Note 7**

Categorical predictors

- Also referred as categorical or discrete predictors or variables.
- Prediction task is called regression for quantitative output and classification for qualitative outputs
- Qualitative variables are represented by numerical codes

$$x_i = \begin{cases} 1 & \text{if the } ith \text{ experiment is a success} \\ 0 & \text{if the } ith \text{ experiment is a failure} \end{cases}$$

- This results in the model

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if the } ith \text{ exp. is a success} \\ \beta_0 + \epsilon_i & \text{if the } ith \text{ exp. is a failure} \end{cases}$$

Note 8

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Non-linear effects of predictors

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- The linear model assumes a linear relationship between the response and predictors
- The true relationship between the response and the predictors may be non-linear
- Polynomial regression is simple way to extend linear models to accommodate non-linear relationships
- In this case non-linearity is obtained by considering transformed versions of the predictors
- The parameters can be estimated using standard linear regression methods.

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Note 9

Outliers

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- Different reasons can lead to outliers. Example: incorrect recording of an observation
- The residual as an estimate of the error can be used to identify outliers by examination for extreme values

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- Better use the studentized residuals

$$E[\mathbf{e}] = E\left[\left(I_p - H\right)\mathbf{y}\right] = \left(I_p - H\right)\delta$$

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- If the diagonal of H is not close to 1 (small) then $\mathbf{e}$ reflects the presence of outliers.

Note 10

High-leverage points

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- Observations with high leverage have an unusual value for x_i
- Difficult to identify when there are multiple predictors
- To quantify an observation's leverage use the leverage statistic

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$$h_i = \frac{1}{N} + (N-1)^{-1}(\mathbf{x}_i - \bar{\mathbf{x}})\mathbf{S}^{-1}(\mathbf{x}_i - \bar{\mathbf{x}})$$

- $\mathbf{S}$ is the ample covariance matrix, $\mathbf{x}_i$ the ith row of X and $\bar{\mathbf{x}}$ the average row

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- The leverage statistic $\frac{1}{n} \leq h_i \leq 1$ and the average is $(p+1)/n$.
- If an observation has h_i greatly exceeds $(p+1)/n$, then we may suspect that the corresponding point has high leverage.

Note 11

Multiple outputs

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- Multiple outputs $y_1, \dots, y_K$ need to be predicted from $x_1, \dots, x_p$ where a linear model is assumed for each output

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$$\mathbf{y}_k = \beta_{0k} + \sum_{j=1}^{p} \mathbf{x}_j \beta_{jk} + \epsilon_k = f_k(X) + \epsilon_k$$

- In matrix notation $\mathbf{Y} = \mathbf{XB} + \mathbf{E}$ where $\mathbf{Y}$ is $N \times K$, $\mathbf{X}$ is $N \times (p+1)$, $\mathbf{B}$ is $(p+1) \times K$ (matrix of parameters) and $\mathbf{E}$ is $N \times K$ matrix of errors.

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$$RSS(\mathbf{B}) = \sum_{k=1}^{K} \sum_{i=1}^{N} (y_{ik} - f_k(x_i))^2 = \mathrm{tr}\left[(\mathbf{Y} - \mathbf{XB})^\top (\mathbf{Y} - \mathbf{XB})\right]$$

Multiple outputs

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- The least squares estimates have exactly the same form

$$\hat{\mathbf{B}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y}$$

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- In case of correlated errors $\epsilon \sim \mathcal{N}(0, \Sigma)$ the multivariate criterion becomes

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$$RSS(\mathbf{B}) = \sum_{i=1}^{N} \left(y_i - f\left(x_i\right)\right)^\top \Sigma^{-1} \left(y_i - f\left(x_i\right)\right)$$

Note 11

Why ?

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- *The least squares estimates is in most cases not satisfied when a large number of potential explanatory variables are available*
- *Improving prediction accuracy:* LSE often has low bias but large variance, sacrifice a little bit of bias to reduce the variance of the predicted values and improve overall prediction accuracy
- *Interpretation:* Do all the predictors help to explain $\mathbf{y}$? determine a smaller subset with strongest effects and sacrifices the small details

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Linear Model Selection and Regularization

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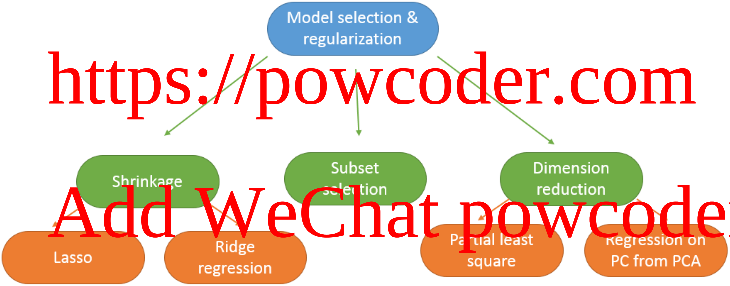

Deciding on the Important Variables

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Subset selection

- **All subsets** or **best subsets** regression (examine all potential combinations)
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- **Forward selection** - begin with intercept and iteratively add one variable.
- **Backward selection** - begin with the full model and iteratively remove one variable.
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- **What is best for cases where $p > n$?**

Best Subset

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- Retain a subset of predictor and eliminate the rest
- LSE is used to obtain the coefficients of the retained variables
- For each $k \in \{0, 1, 2, \ldots, p\}$ find the subset k that gives the smallest residual
- The choice of k is obtained using a criterion and involves a tradeoff between bias & variance
- Different criteria $\leftarrow$ minimizes an estimate of the expected prediction error

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Infeasible for large p

Note 12

Forward Selection

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- Sequential addition of predictors $\rightarrow$ forward stepwise selection
- Starts with the intercept and sequentially add the predictor that most improve the fit

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- Add predictor producing the largest value of

$$F = \frac{\mathrm{RSS}\left(\hat{\boldsymbol{\beta}}_i\right) - \mathrm{RSS}\left(\hat{\boldsymbol{\beta}}_{i+1}\right)}{\mathrm{RSS}\left(\hat{\boldsymbol{\beta}}_{i+1}\right) / (N-k-2)}$$

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- Use 90th or 95th percentile of $F_{1,N-k-2}$ as F_e

Note 14

Backward Elimination

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- Start with the full model and sequentially remove predictors
- Use F_d to choose the predictor to delete (smallest value of F)
- Stop when each predictor in the model produces $F > F_d$
- Can be used only when $N > p$

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$F_d \simeq F_e$

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Note 15

Alternative: Shrinkage Methods

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- Subset selection produces produce an interpretable model with possible lower prediction error than the full model
- The selection is discrete $\rightarrow$ often exhibits high variance
- Shrinkage methods are continuous and don't suffer as much from high variability
- We fit a model containing all p predictors using a technique that **constrains** or **regularizes** the coefficient estimates, or equivalently, that shrinks the coefficient estimates towards zero.
- Shrinking the coefficient estimates can significantly reduce their variance (not immediately obvious).

Ridge Regression

- Recall that the least squares fitting procedure estimates $\beta_0, \beta_1, \ldots, \beta_p$ using the values that minimize

$$\text{RSS} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2.$$

- In contrast, the ridge regression coefficient estimates $\hat{\beta}^R$ are the values that minimize

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2 = \text{RSS} + \lambda\sum_{j=1}^{p}\beta_j^2,$$

where $\lambda \geq 0$ is a *tuning parameter*, to be determined separately.

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Ridge Regression

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$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}\beta_j^2=\mathrm{RSS}+\underbrace{\lambda\sum_{j=1}^{p}\beta_j^2}_{\text{The shrinkage penalty.}}$$

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The tuning parameter.

- It serves to control the relative impact of the penalty on the regression coefficient estimates.
- Selecting a good value for λ is critical.
- cross-validation is used for this.

The shrinkage penalty.

- It is small when $\beta_1, \beta_2, \ldots, \beta_p$ are close to zero.
- So it has the effect of *shrinking* the estimates of β_j towards zero.

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Ridge Regression

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$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda \underbrace{\sum_{j=1}^{p}\beta_j^2}_{\text{The shrinkage penalty.}}$$

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Accuracy $\leftrightarrow$ Complexity

Ridge Regression

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- Ridge regression shrinks the regression coefficients by constraining their size

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- This is the approach used in neural networks where it is known as weight decay
- The larger the value of λ, the greater the amount of shrinkage
- β_0 is left out of the penalty term

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Note 16

Ridge Regression

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- Because we have now the addition of the penalty term, the ridge regression coefficient estimates can change substantially when multiplying a given predictor by a constant!

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- It is best to apply ridge regression after *standardizing the predictors*, using the formula

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$$\tilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_{ij})^2}}$$

Ridge Regression

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$$\mathrm{RSS}(\lambda) = (\mathbf{y} - X\beta)^\top (\mathbf{y} - X\beta) + \lambda\beta^\top\beta$$

$$\hat{\beta}^{ridge} = \left(X^\top X + \lambda \mathbf{I}\right)^{-1} X^\top \mathbf{y}$$

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- The ridge solution is a linear function of $\mathbf{y}$
- Avoid singularity when $X^\top X$ is not full by adding a positive constant to the diagonal of $X^\top X$.
- For orthogonal predictor $\hat{\beta}^{ridge} = \gamma\hat{\beta}$ where $0 \leq \gamma \leq 1$
- The effective degrees of freedom of the ridge regression fit is

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$$\mathbf{df}(\lambda) = \mathrm{tr}\left(X[X^\top X + \lambda \mathbf{I}]^{-1} X^\top\right)$$

Note 17

Ridge regression - credit data example

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balance ∼
age, *cards*, *education*, *income*, *limit*, *rating*, *gender*, *student*, *status*, *ethnicity*

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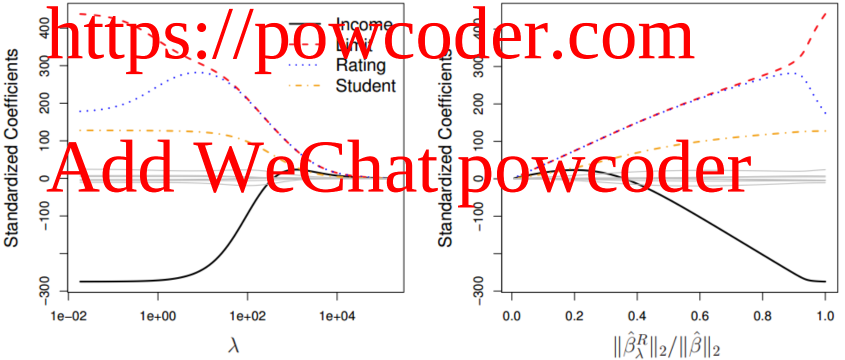

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Ridge regression vs. LS

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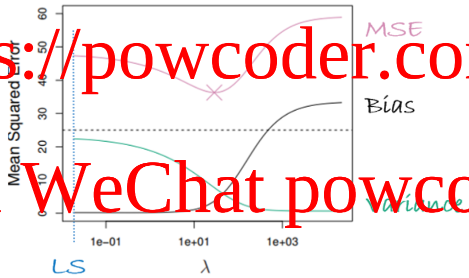
- Shrinkage methods can reduce the variance of the estimate $\hat{f}(x)$

  $\lambda \uparrow$ -> # of (influential) variables $\downarrow$

  -> Variance $\downarrow$ & Bias $\uparrow$



- Ridge regression (& Lasso) improves on LS!
- The MSE is reduced
- The variance is much smaller at the expense of a small increase in bias.

Lasso

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- **Ridge regression** disadvantage: includes all p predictors (some of them with minor influence)

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- **Lasso**, in contrast, select subset.
- The lasso coefficients, $\hat{\beta}^L_\lambda$, minimize the quantity

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$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = \mathrm{RSS} + \lambda\sum_{j=1}^{p}|\beta_j|$$

The Variable Selection Property of the Lasso

Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero?

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One can show that the lasso and ridge regression coefficient estimates solve the problems

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$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s$$

and

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$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s,$$

respectively.

Some Remarks on Lasso

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- Making s sufficiently small will cause some of the coefficients to be exactly zero $\to$ continuous subset selection
- If $s = \sum_{i=1}^{p} \|\hat{\beta}_j^{ls}\|$, then the lasso estimates are the $\hat{\beta}_j^{ls}$'s.
- s should be adaptively chosen to minimize an estimate of expected prediction error.

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The Variable Selection Property of the Lasso

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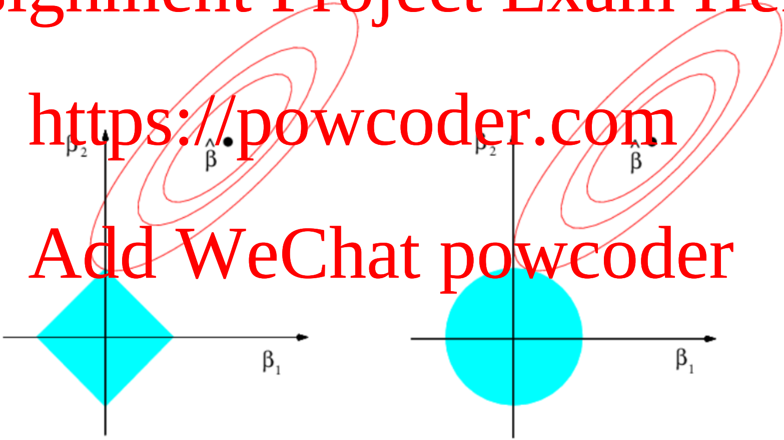
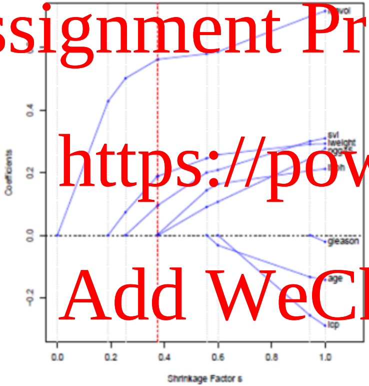


Profile of Lasso Coefficients



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- Profiles of lasso coefficients as the tuning parameter t is varied. The coefficients are plotted versus $t = s/\sum_{i=1}^{p} \|\hat{\beta}_j^{ls}\|$

Dimension Reduction Methods

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- When there is a large number of predictors, often correlated, we can select what variables (dimensions) to use.
- But, why not transform the predictors (to a lower dimension) and then fit the least squares model using the transformed variables.

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- We will refer to these techniques as **dimension reduction** methods.

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- Use a small linear combinations $\mathbf{z}_m$, $m = 1, ..., M$ of $\mathbf{x}_j$
- The methods differ in how the linear combinations are obtained

Principal Components Regression

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- The linear combinations $\mathbf{z}_m$ are the principal components
  $\mathbf{z}_m = X\mathbf{v}_m$

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$$\max_{\substack{\|\boldsymbol{\alpha}\|=1 \\ \mathbf{v}_\ell^\top \mathbf{S}\boldsymbol{\alpha}=0, \quad \ell=1,\dots,m-1}} \mathrm{Var}(X\boldsymbol{\alpha})$$

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- $\mathbf{v}_\ell^\top \mathbf{S}\alpha = 0$ ensure $\mathbf{z}_m = X\mathbf{v}_m$ is uncorrelated with all previous linear combinations $\mathbf{z}_\ell = X\mathbf{v}_\ell$, $\ell = 1, \dots, m-1$
- $\mathbf{y}$ is regressed on $\mathbf{z}_1, \dots, \mathbf{z}_M$ for $M \le p$

Principal Components Regression

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- Since $\mathbf{z}_m$ are othrogonal, this regression is just a sum of univariate regressions

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$$\hat{\mathbf{y}}^{pcr} = \bar{\mathbf{y}} + \sum_{m=1}^{M} \hat{\theta}_m \mathbf{z}_m$$

$$\hat{\theta}_m = < \mathbf{z}_m, \mathbf{y} > / < \mathbf{z}_m, \mathbf{z}_m >$$

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$$\hat{\beta}^{pcr} = \sum_{m=1}^{M} \hat{\theta}_m \mathbf{v}_m$$

- if $M = p$, $\hat{\mathbf{y}}^{pcr} = \hat{\mathbf{y}}^{LS}$ since the columns of $Z = UD$ span the column space of X
- PCR discards the $p - M$ smallest eigenvalue components.

Principal Components Regression

- Let $Z_1, Z_2, \ldots, Z_M$ represent $M < p$ *linear combinations* of our original p predictors. That is,

$$Z_m = \sum_{j=1}^{p} \phi_{mj} X_j \qquad (1)$$

for some constants $\phi_{m1}, \ldots, \phi_{mp}$.

- We can then fit the linear regression model,

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \epsilon_i, \quad i = 1, \ldots, n, \qquad (2)$$

using ordinary least squares.

- Note that in model (2), the regression coefficients are given by $\theta_0, \theta_1, \ldots, \theta_M$. If the constants $\phi_{m1}, \ldots, \phi_{mp}$ are chosen wisely, then such dimension reduction approaches can often outperform OLS regression.

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Dimension Reduction Methods

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- Notice that from definition (1):

$$\sum_{m=1}^{M} \theta_m z_{im} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{mj} x_{ij} = \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{mj} x_{ij} = \sum_{j=1}^{p} \beta_j x_{ij},$$

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where

$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{mj}. \tag{3}$$

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- Hence model (2) can be thought of as a special case of the original linear regression model.
- Dimension reduction serves to constrain the estimated β_j coefficients, since now they must take the form (3).
- Can win in the bias-variance tradeoff.

Principal Components

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- Effectively, we change the orientation of the axes.
- The 1^{st} principal component is that (normalized) linear combination of the variables with the largest variance.
- The 2^{nd} principal component has the largest (remainder) variance, subject to being uncorrelated with the first.
- And so on...
- Many times we can explain most of the variation with only few principal components.
- More details in Chapter 10.2 of the book 'An introduction to statistical learning'

Principal Components

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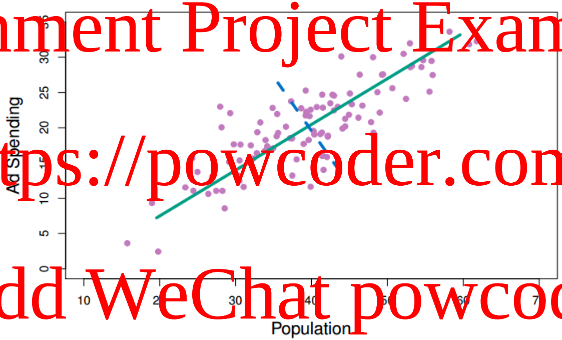

The population size (`pop`*) and ad spending (*`ad`*) for* 100 *different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.*

Principal Components

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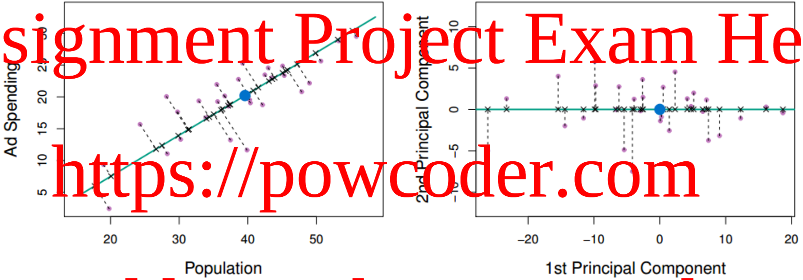

A subset of the advertising data. Left: *The first principal component, chosen to minimize the sum of the squared perpendicular distances to each point, is shown in green. These distances are represented using the black dashed line segments.* Right: *The left-hand panel has been rotated so that the first principal component lies on the x-axis.*

Principal Components Regression

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- Now we can run a regression analysis on only several principal components.
- We call it **Principal Components Regression** (**PCR**)

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- Note, these directions are identified in an *unsupervised* way, since the response Y is not used to help determine the principal component directions.

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- Consequently, PCR suffers from a potentially serious drawback: there is no guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the response.

Partial Least Squares (PLS)

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- It is a dimension reduction method, which first identifies a new set of features $Z_1, \ldots, Z_M$ that are linear combinations of the original features.

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- Then fits a linear model via OLS using these M new features.
- Up to this point very much as PCR.
- PLS identifies these new features using the response Y (*supervised way*).

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- PLS approach attempts to find directions that help explain both the response and the predictors.

Partial Least Squares (PLS)

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- Uses $\mathbf{y}$ to construct linear combinations of the inputs.
- The inputs are weighted by the strength of their univariate effect on $\mathbf{y}$

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- Regress $\mathbf{y}$ on $\mathbf{z}_m \to \hat{\theta}_m$ and orthogonalize with respect to $\mathbf{z}_m$
- Continue the process until $M < p$ directions are obtained
- PLS seeks directions that have high variance and have high correlation with the response

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$$\max_{\substack{\|\boldsymbol{\alpha}\|=1 \\ \mathbf{v}_\ell^\top \mathbf{S}\boldsymbol{\alpha}=0, \quad \ell=1,\dots,m-1}} \mathrm{Corr}^2\left(\mathbf{y}, X\boldsymbol{\alpha}\right) \mathrm{Var}\left(X\boldsymbol{\alpha}\right)$$

Partial Least Squares (PLS)

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- The first component say $\mathbf{t} = X\boldsymbol{\alpha}_1$ maximizes

$$\boldsymbol{\alpha}_1 = \arg \max_{\|\boldsymbol{\alpha}\|=1} \operatorname{Cov}^2(\mathbf{y}, X\boldsymbol{\alpha})$$

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- Subsequent components $\mathbf{t}_2, \mathbf{t}_3, \ldots$ are chosen such that they maximizes the squared covariance to $\mathbf{y}$ and all components are mutually orthogonal
- Orthogonality is enforced by deflating the original variables X

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$$X_i = X - \mathcal{P}_{\mathbf{t}_1,\ldots,\mathbf{t}_{i-1}} X$$

- $\mathcal{P}_{\mathbf{t}_1,\ldots,\mathbf{t}_{i-1}}$ denotes the orthogonal projection onto the space spanned by $\mathbf{t}_1, \ldots, \mathbf{t}_{i-1}$
- $\hat{\mathbf{y}} = \mathcal{P}_{\mathbf{t}_1,\ldots,\mathbf{t}_m}\mathbf{y}$ instead of $\hat{\mathbf{y}} = X\hat{\beta} = X\left(X^\top X\right)^{-1} X^\top \mathbf{y}$

Illustrating the connection

The connection between these methods can be seen through the optimisation criterion they use to define projection directions

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- PCR extracts components that explain the variance of the predictor space

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$$\max_{\substack{\|\boldsymbol{\alpha}\|=1 \\ \mathbf{v}_\ell^\top \mathbf{S}\boldsymbol{\alpha}=0, \quad \ell=1,\ldots,m-1}} \mathrm{Var}\left(X\boldsymbol{\alpha}\right)$$

- PLS extracts components that have a high covariance with

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$$\max_{\substack{\|\boldsymbol{\alpha}\|=1 \\ \mathbf{v}_\ell^\top \mathbf{S}\boldsymbol{\alpha}=0, \quad \ell=1,\ldots,m-1}} \mathrm{Corr}^2\left(\mathbf{y}, X\boldsymbol{\alpha}\right)\mathrm{Var}\left(X\boldsymbol{\alpha}\right)$$

- Both method are similar in there aim to extract m components from the predictor space X

Illustrating the connection

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Both methods aims

- at expressing the solution in lower dimensional subspace $\beta = V\mathbf{z}$ where V is an $p \times m$ matrix of orthonormal columns

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- Using this basis for the subspace, an alternative approximate minimization problem is considered

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$$\min_{\beta} \|\mathbf{y} - X\beta\|_2 \approx \min_{\mathbf{z}} \|\mathbf{y} - XV\mathbf{z}\|$$

- In PCR V is directly obtained from X
- in PLS V depends on $\mathbf{y}$ in a complicated nonlinear way

Illustrating the connection

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Considering

- The singular value decomposition $X = UDV^\top$ where U is $N \times p$, $D = \mathrm{diag}(d_1, ..., d_p)$ is $p \times p$ and V is $p \times p$
- The columns of U and V are orthogonal such that $U^\top U = I_p$ and $V^\top V = I_p$

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- The least squares solution takes the form

$$\hat{\beta} = \sum_{i=1}^{p} \frac{\mathbf{u}_i^\top \mathbf{y}}{d_i} \mathbf{v}_i = \sum_{i}^{p} \beta_i$$

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- The other estimator are shrinkage estimators and can be expressed as

$$\hat{\beta} = \sum_{i}^{p} f(d_i)\beta_i$$

Multiple Outcome Shrinkage

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- When the output are not correlated $\rightarrow$ apply a univariate technique individually to each outcome or work with each column output individually
- Other approaches exploit correlations in the different responses $\rightarrow$ canonical correlation analysis

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- CCA find a sequence of linear combinations $\mathbf{X}v_m$ and $\mathbf{Y}u_m$ such that the correlations are maximized

$$\mathrm{Corr}^2\left(\mathbf{Y}u_m, \mathbf{X}v_m\right)$$

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- Reduced rank regression

$$\hat{\mathbf{B}}^{rr}(m) = \arg\min_{rank(\mathbf{B})=m} \sum_{i=1}^{N} \left(\mathbf{y}_i - \mathbf{B}\mathbf{x}_i\right)^\top \Sigma^{-1} \left(\mathbf{y}_i - \mathbf{B}\mathbf{x}_i\right)$$

Note 19

For more readings

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- Summaries on LMS.
- Chapter 3, 5 & 14.5 from 'The elements of statistical learning' book.
- Chapters 3, 6 & 10.2 from 'An introduction to statistical learning' book.

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