STA242 Report: HyperCube

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- Bitbucket SSH: `git@bitbucket.org:taeyen/sta242_15_project.git`

Report

What we did

We built a package as an implementation of the Hypercube Estimator introduced by (Beran 2014). Hypercube estimator can be applied in various cases for fitting linear models. Due to time constraints, we only implemented some of the important cases.

We implemented the Hypercube Estimator with S3 classes and methods. We built a "formula" interface for the Hypercube Estimator, which is similar to other linear model fitting functions in R. Along with the classes and methods, we wrote helps files with Roxygen2. We also wrote vignettes with Rmarkdown. With the help files and vignettes, users can self-learn how to use the package. We also included some data sets used in (Beran 2014) so that users can try out the examples easily. We wrote some tests with testthat.

Further Works

Due to time constraint, we have only implement some parts of the paper (Beran 2014): Penalized weighted least square and Shrinkage on ANOVA submodels. In future, we may also implement more parts, for example polynomial submodel fits, projection matrices from eigen-decomposition of matrix, Stein multiple shrinkage, etc.

One of the greatest challenge in implementing the Hypercube estimator is the design of the classes and methods. Although the mathematics of Hypercube Estimator is simple, the unification of different applications of Hypercube Estimator is not obvious. We admit that the current design is not perfect. The information stored in the objects is not compact, wasting some memory. Many codes have not been not optimized. Also, the user inferface with the "formula" class is not simple enough. The output of the fitted model is not informative enough. If time allows, we should improve the design of the classes and methods, and optimize some of the codes. More

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Appendix

Vignette: `vignette("introduction", package="HyperCube")`

Introduction

The R package HyperCube is an implementation of the Hypercube Estimator introduced by (Beran 2014). Hypercube estimator is a richer class of regularized estimators of linear model, which extends penalized least squares estimators with quadratic penalties. The R package HyperCube lets users Hypercube Estimators to fit linear model.

In the following sections, we first briefly introduce the theoretical background of Hypercube Estimator. Then we demonstrate how to use the R package HyperCube to produce the examples given in (Beran 2014).

Theoretical background

Motivation

Given a data set (y, X) where y is the $n \times 1$ vector of observations, X is a given $n \times p$ design matrix of rank $p \leq n$, we fit the linear model:

$$y = X\beta + \epsilon.$$

with the components of ϵ are independent $\sim (0, \sigma^2)$, and finite fourth moment.

Let $\eta = \mathrm{E}(y) = X\beta$.

The least squares estimator of η is $\hat{\eta}_{LS} = X(X'X)^{-1}X'y$. However, $\hat{\eta}_{LS}$ usually overfits. If the error vector ϵ is Gaussian and $p \geq 3$, then $\hat{\eta}$ is an inadmissible estimator of η under the quadratic risk function $R(\hat{\eta}) = E|\hat{\eta} - \eta|^2$. In other words, the least square estimator of η does not minimized the risk.

We would like to find an estimator $\hat{\eta}$ so that the risk $\mathrm{E}|\hat{\eta} - \eta|^2$ is minimized. We may sacrifice the unbiasedness (least square estimator) to obtain a risk-minimizing estimator of $\hat{\eta}$. It is the so-call bias-variance trade-off. The Hypercube estimator is a class of $\hat{\eta}$ which performs much better than least square estimator in term of minimizing the risk.

Definition of the Hypercube Estimator

Define the hypercube estimator of η to be

$$\hat{\eta}_{\mathrm{H}}(V) = A(V)y \quad \text{with} \quad A(V) = XV(VX'XV + I_p - V^2)^{-1}VX'$$

where V is a symmetric matrix with all eigenvalues $\in [0, 1]$ and A(V) is called the operator. We can compute the V so that the risk $\mathrm{E}|\hat{\eta}_{\mathrm{H}}(V) - \eta|^2$ is minimized. Thus, we obtain an estimator which is better than the least square estimator.

Let $\eta = \mathrm{E}(y) = X\beta$. We would like to find an Hypercube Estimator $\hat{\eta}$,

$$\hat{\eta}_{\mathrm{H}}(V) = XV(VX'XV + I_p - V^2)^{-1}VX'y$$

where V is a symmetric matrix with all eigenvalues $\in [0, 1]$. (That's why it is named Hypercube Estimator.)

Penalized Least Squares Estimator

Let W be any $p \times p$ positive semidefinite matrix, and the associated penalized least squared (PLS) estimators of η

$$\hat{\eta}_{\text{PLS}} = X\hat{\beta}_{\text{PLS}}$$

where

$$\hat{\beta}_{\text{PLS}} = \text{argmin}_{\beta}[|y - X\beta|^2 + \beta' W\beta] = (X'X + W)^{-1}X'y$$

The mapping from $\hat{\beta}_{\text{PLS}}(W)$ to $\hat{\beta}_{\text{PLS}}(W)$ is one-to-one. The matrix $V = (I_P + W)^{-\frac{1}{2}}$ is symmetric with all eigenvalues in $(0, 1]$.

$$\hat{\eta}_{\text{PLS}}(W) = \hat{\eta}_H((I_P + W)^{-\frac{1}{2}})$$

Minimizing the estimated risk over V

The normalized quadratic risk is

$$R(\hat{\eta}_H, \eta, \sigma^2) = p^{-1}E|\hat{\eta}_H(V) - \eta|^2 = p^{-1}tr[\sigma^2 A^2(V) + (I_n - A(V))^2\eta\eta']|.$$

The risk depends on the unknown parameters η and σ^2. We consider the normalized estimated risk

$$\hat{R_H}(V) = p^{-1}[|y - A(V)y|^2 + \{2tr(A(V)) - n\}\hat{\sigma}^2]$$

where $\hat{\sigma}^2$ is an unbiased estimator of σ^2.

The goal of the Hypercube Estimator is to choose V for the Hyercube Estimator to obtain $\hat{\eta}$ with smaller estimated risk.

Demonstration of Examples

Example 1

It is the Example 1 in (Beran 2014).

In the Canadian earnings data considered by (Ullah 1985), we consider a linear model on log(incomes) versus ages.

A model for the data is

$$y = Cm + e$$

Here y is $n \times 1$ vector of observation, m is the $p \times 1$ vector of mean, C is the $n \times p$ data-incidence matrix with elements 0 or 1. The is a special case of linear model in which $X = C, \text{and} \beta = m$

Consider the $(g - 1) \times g$ difference matrix $\Delta(g) = \{\delta_{u,w}\}$ in which $\delta_{u,u} = 1, \delta_{u,u+1} = -1$ for every u and all other entries are zero.

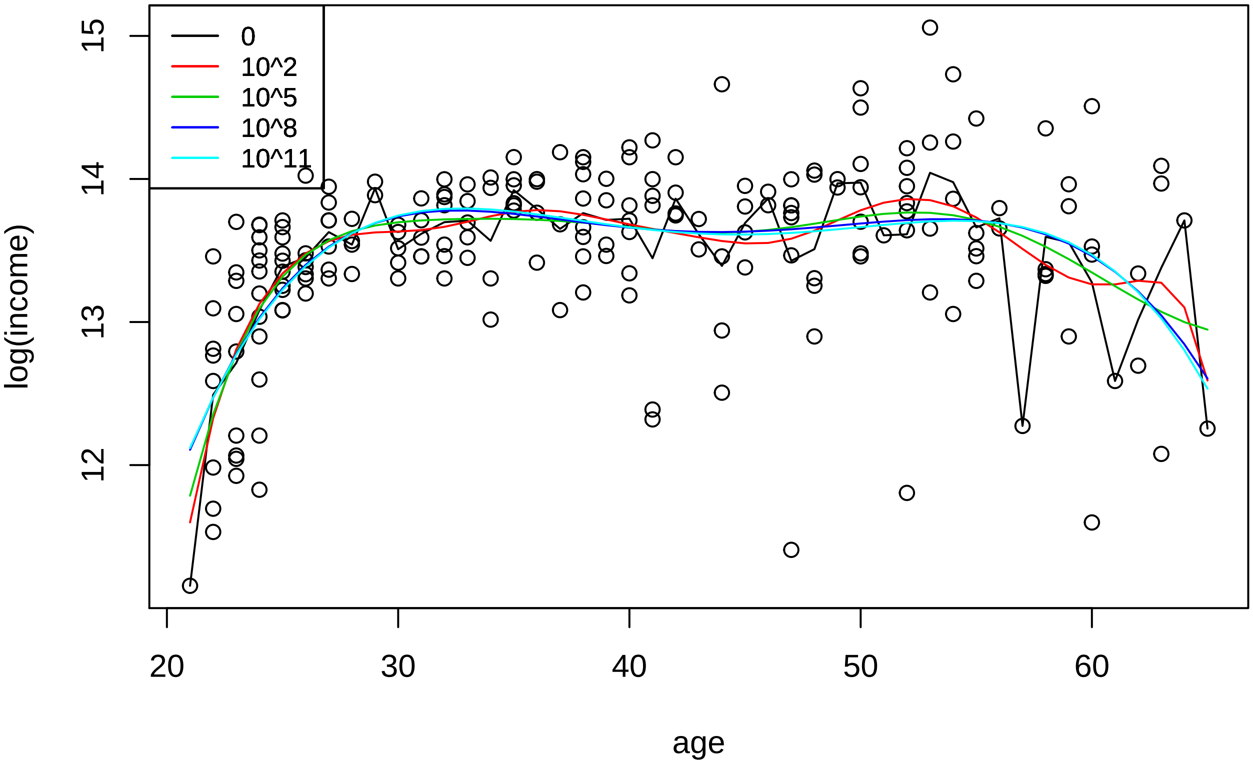
Here, define $D_5 = \Delta(p - 4)\Delta(p - 3)\Delta(p - 2)\Delta(p - 1)\Delta(p)$ with $p = 45$

Let $W(v) = vD_5' D_5$, for every $v \geq 0$

$$\hat{m_{\text{PLS}}}(W(\nu)) = \text{argmin}[|y - Cm|^2 + \nu|D_5 m|^2] = (C'C + W(\nu))^{-1}C'y$$

We use Hypercube estimator to obtain fits to the Canadian earnings data for various values of penalty weight ν.

```r
library(HyperCube)

# The package includes the data set canadian.earnings.
# The age is considered as factor in the data set.
canadian.earnings$age <- factor(canadian.earnings$age)

# Plot the data
plot(as.numeric(as.character(canadian.earnings$age)), canadian.earnings$log.income,
     xlab = "age", ylab = "log(income)")

# The number of ages in the data set, p, in Example 1 in Beran (2014).
p <- length(unique(canadian.earnings[,1]))

# D_5 as in equation (3.10) in Beran (2014)
D <- diffMatrix(p, 5)

# The parametor nu in equation (3.11) in Beran (2014)
nu <- c(0, 10^c(2,5,8,11))

# Plotting Hypercube Estimator fits for varying nu
lcolor <- 1:5
for(k in 1:5) {

  # The matrix W in equation (3.11) in Beran (2014)
  W <- nu[k] * t(D) %*% D

  # Convert W to V, as described in (1.6) in Beran (2014)
  V <- plsW2V(W)

  # Hyperpercube Estimator Fit
  hcmod <- hypercube( log.income ~ age -1, data=canadian.earnings, V)

  # Plot the fits
  lines(as.numeric(levels(canadian.earnings$age)),
        hcmod$coefficients, col = lcolor[k])
  legend("topleft", cex = 0.8,
         legend = c("0", "10^2", "10^5", "10^8", "10^11"),
         lty = rep(1,5), col=1:5)
}
```



Example 2

It is the Example 2 in (Beran 2014).

We consider the rat litter data treated by (Scheffé 1959). Each response recorded is the average weight-gain of a rat litter when the infants in the litter are nursed by a rat foster-mother. Factor 1, with four levels, is the genotype of the foster-mother. Factor 2, with the same levels, is the genotype of the infant litter.

Two-way ANOVA considers competing least squares fits to the rat litter data. Let $u_r = (1/2, 1/2, 1/2, 1/2)'$ for $r = 1, 2$. Set $J_r = u_r u_r'$ and $H_r = I_4 - J - R$. The standard ANOVA projections are

$$P_1 = J_2 \otimes J_1, \qquad P_2 = J_2 \otimes H_1, \qquad P_3 = H_2 \otimes J_1, \qquad P_4 = H_2 \otimes H_1.$$

The $\{P_k\}$ are symmetric, idempotent, mutually orthogonal matrices such that $\sum_{k=1}^{4} P_k = I$. Let $d = (d_1, d_2, d_3, d_4) \in [0, 1]^4$ and $V(d) = d_1 V_1 + d_2 V_2 + d_3 V_3 + d_4 V_4$. We want to minimize the risk $\hat{\eta}_H(V(d))$ over $d \in [0, 1]^4$.

```
library(HyperCube)

# The package includes the data set litter.
# The formula specifying the two-way layout is "weight ~ mother:infant -1".
# hypercubeOptimization computes the optimal d
hcmodopt <- hypercubeOptimization( weight ~ mother:infant -1, data = litter)

# The optimal d
# Same result as stated in Example 2 in Beran (2014)
hcmodopt$projcoef
```

```
## [1] 0.9971043 0.6931901 0.0000000 0.4150027
```

```r
# Compare the estimated risk
summary(hcmodopt$est)
```

```
## Call:
## hypercube.formula(formula = formula, data = data, V = V)
##
## The estimated risk of hypercube estimation: 16.1214335561813
## The estimated risk of least square estimation:  54.2403666666667
```

References

Beran, Rudolf. 2014. "Hypercube Estimators: Penalized Least Squares, Submodel Selection, and Numerical Stability." *Computational Statistics & Data Analysis* 71. Elsevier: 654–66.

Scheffé, H. 1959. "The Analysis of Variance. a Wiley Publication in Mathematical Statistics." Wiley.

Ullah, Aman. 1985. "Specification Analysis of Econometric Models." *Journal of Quantitative Economics* 1: 187–209.