

Machine Learning for Official Statistics and SDGs

Regression



[LINEAR REGRESSION]

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Expressed as:

$$y = \beta_0 + x' \beta + \varepsilon \quad E(\varepsilon|x) = 0$$

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with possibly many regressors x_j

[LINEAR REGRESSION: CENTERING VARIABLES]

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- ▶ β_0 is the mean of y **if all x_j are equal to zero**

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- ▶ Centering the variables has no effect on the coefficients

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Except: α_0 is the mean of y **if all x_j are equal their mean**

[LINEAR REGRESSION: SCALING]

We can also scale each variable by its own standard deviation to obtain

$$y = \alpha_0 + \gamma_1 \tilde{x}_1 + \dots + \gamma_k \tilde{x}_k + \varepsilon \quad E(\varepsilon|x) = 0$$

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- ▶ Now γ_j is the *ceteris paribus* marginal effect of \tilde{x}_j on y .
↪ when \tilde{x}_j increases by one standard deviation, y increases by γ_j units
- ▶ The goal is to have variables and coefficients that are comparable

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[LINEAR REGRESSION: EXAMPLE]

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► Example on a regression model with few variables

	Est.	S.E.	t val.	p
(Intercept)	4.390	0.136	32.204	0.000
Trans	-0.002	0.001	-1.603	0.110
HighTrans	0.013	0.003	3.945	0.000
Checks	0.008	0.005	1.534	0.126
Years	0.096	0.008	11.579	0.000

Initial regression with original values

[LINEAR REGRESSION: EXAMPLE]

► Example on a regression model with few variables

	Est.	S.E.	t val.	p
(Intercept)	5.927	0.039	150.243	0.000
Trans	-0.002	0.001	-1.603	0.110
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Regression with centred variables

[LINEAR REGRESSION: EXAMPLE]

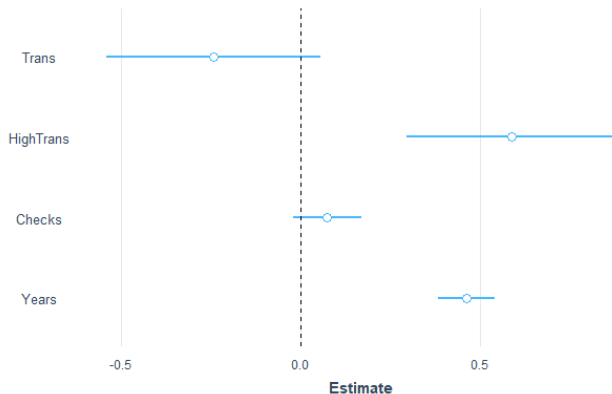
► Example on a regression model with few variables

	Est.	S.E.	t val.	p
(Intercept)	5.927	0.039	150.243	0.000
Trans	-0.243	0.152	-1.603	0.110
HighTrans	0.586	0.149	3.945	0.000
Checks	0.074	0.048	1.534	0.126
Years	0.462	0.040	11.579	0.000

Regression with scaled variables

[LINEAR REGRESSION: EXAMPLE]

- Example on a regression model with few variables
The goal is to have *comparable* effects (same range)



Visual regression with scaled variables

[PROBLEMS IN LINEAR REGRESSION]

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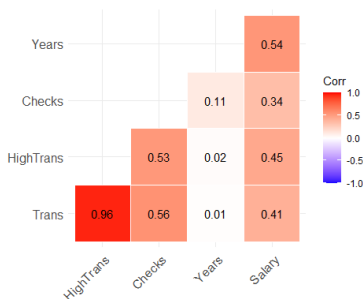
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- ↪ Correlation plot

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↪ Correlation plot



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- ▶ Measure of multi-collinearity between variables
- ▶ Measure how much the variance of the coefficient of x_j is inflated due to the presence of other regressors.
- ▶ VIF for x_j is calculated by running a regression of x_j on all other regressors, computing the R_j^2 and use the formula:

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$$VIF_j = \frac{1}{1 - R_j^2}$$

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$VIF_j = 1$ indicates no collinearity; a $VIF \geq 10$ is considered as large and problematic

[SOLUTIONS TO MULTI-COLLINEARITY]

2 solutions to multi-collinearity:

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2 solutions to multi-collinearity:

- ▶ Create new variables from the ones that are collinear
↪ using *e.g.* Principal Components Analysis
- ▶ Remove some variables

[USING *VIF* TO REMOVE COLLINEARITY]

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Computing VIFs for all x_j s

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Computing VIFs for all x_j s

	Est.	S.E.	t val.	p	VIF
(Intercept)	5.93	0.04	150.24	0.00	NA
Trans	-0.24	0.15	-1.60	0.11	14.71
HighTrans	0.59	0.15	3.94	0.00	14.15
Checks	0.07	0.05	1.53	0.13	1.47
Years	0.46	0.04	11.58	0.00	1.02

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	Est.	S.E.	t val.	p	VIF
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- *Trans* has the highest VIF

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	Est.	S.E.	t val.	p	VIF
(Intercept)	5.93	0.04	149.79	0.00	NA
HighTrans	0.36	0.05	7.69	0.00	1.40
Checks	0.06	0.05	1.24	0.22	1.41
Years	0.46	0.04	11.63	0.00	1.02

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- ▶ does not change the fit of the model
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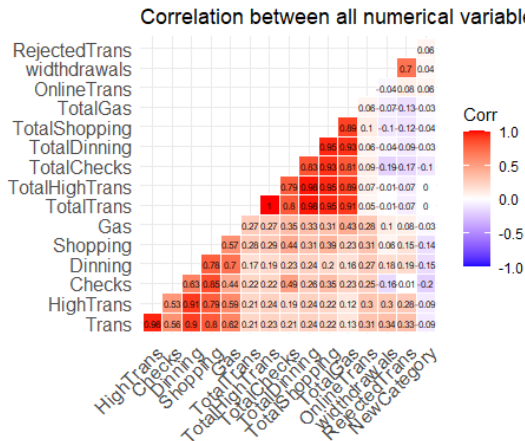
- ▶ does not change the fit of the model
- ▶ does not change the coefficients of the uncorrelated regressors
- ▶ reduces all the *VIFs*

[REAL LIFE EXAMPLE]

In real life, one may have many variables

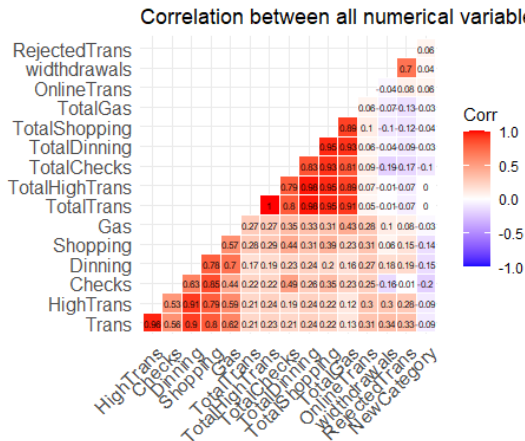
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↪ Automatic selection of regressors

[AUTOMATIC SELECTION OF REGRESSORS]

Classic (but still alive) methods based on the variations of RSS

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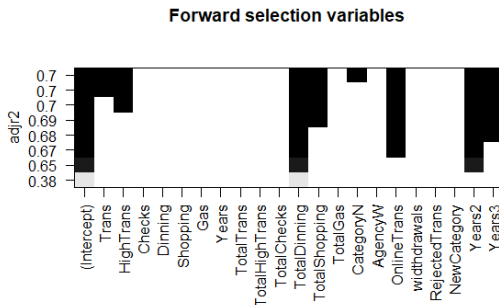
- ▶ The optimal number of regressors is unknown!
- ↪ *The number of possible combinations with k regressors is 2^k*
- ▶ Compute the optimal nb of regressors before testing which regressors to include with Cross Validation

[APPLICATION ON AN EXAMPLE]

To reduce the computational burden we restrict our choice to 8 variables in the final regression.

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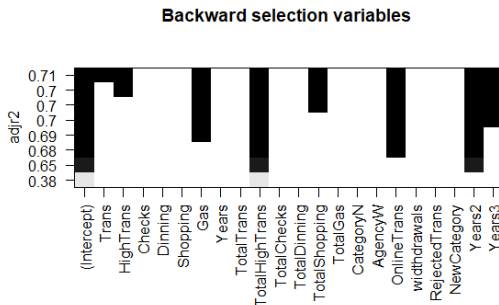
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Visual representation of variables used (Forward)

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Visual representation of variables used (Backward)

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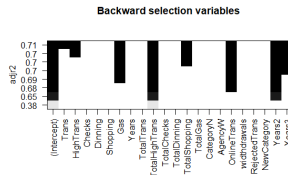
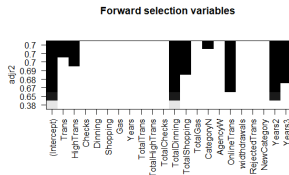
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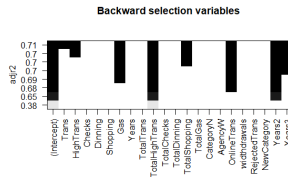
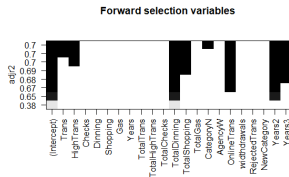
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- *Great Need for Criteria*

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↪ *Mean Squared Error of Prediction* or MSEP:

$$MSEP = n^{-1}E\|y_{new} - X_p\hat{\beta}_p\|^2$$

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The MSEP can be decomposed to help define criterions:

$$\begin{aligned}MSEP &= n^{-1}E\|y_{new} - X_p\hat{\beta}_p\|^2 \\&= n^{-1}\left\{E\|y_{new} - X\beta\|^2 + E\|X\beta - X_p\hat{\beta}_p\|^2\right\} \\&= (1 + (p + 1)/n)\sigma^2 + (1/n)\beta'X'M_pX\beta\end{aligned}$$

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- ▶ Akaike Information Criterion (**AIC**) $\propto C_p$ for linear regression
- ▶ Bayesian Information Criterion (**BIC**):

$$BIC \propto \frac{RSS_p}{n} + \frac{(p+1) \log n}{n} \frac{RSS_k}{n-k-1}$$

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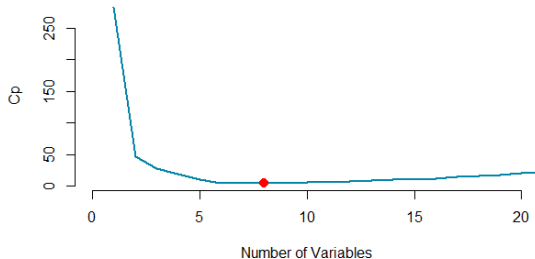
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[APPLICATION ON THE EXAMPLE]

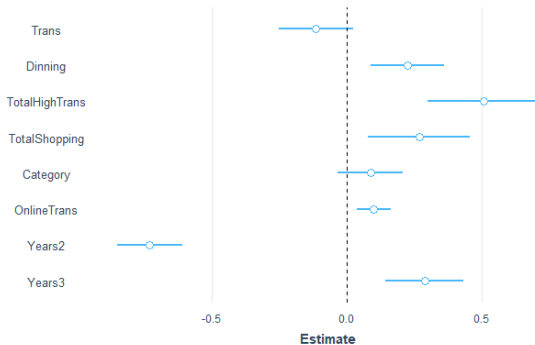
[APPLICATION ON THE EXAMPLE]

Selection using Mallows's C_p (\rightarrow 8 variables)



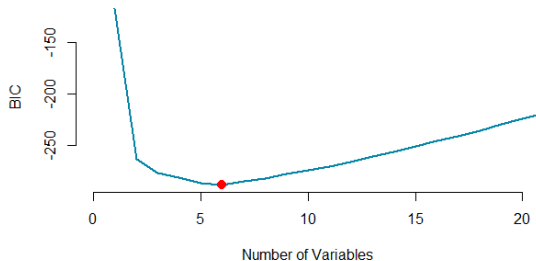
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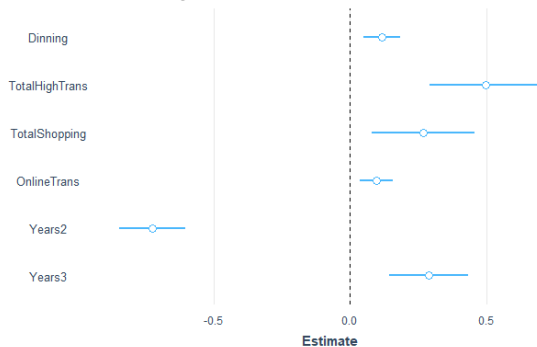
[APPLICATION ON THE EXAMPLE]

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Selection using BIC (→ 6 variables)

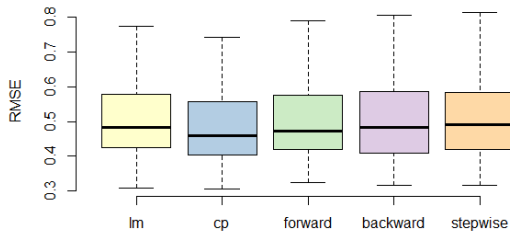


[CROSS VALIDATION]

Now we can use cross Validation on all models

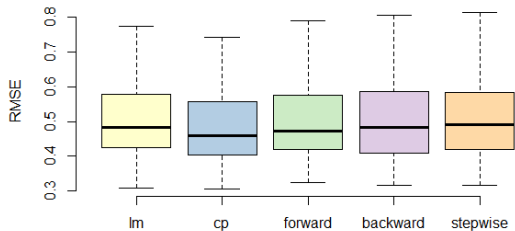
[CROSS VALIDATION]

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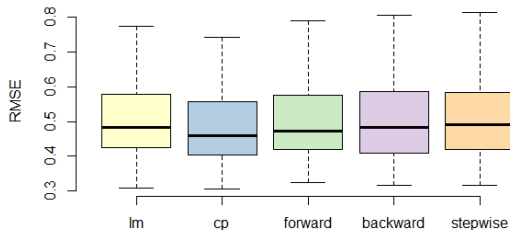
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- The model selected with C_p is doing the best job

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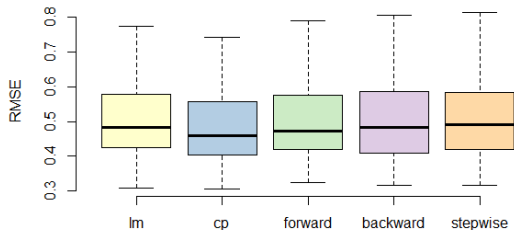
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[CROSS VALIDATION]

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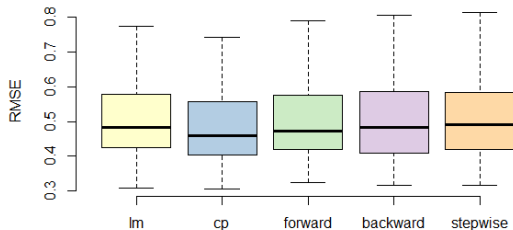
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When using CV with stepwise selection different p-models are selected for each K-fold

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- ▶ The model selected with C_p is doing the best job
- ↳ **Technical issue:**
When using CV with stepwise selection different p-models are selected for each K-fold
- ▶ Modern methods are available...

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[QUIZ TIME]

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wrap-up
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[QUIZ TIME]

[TAKEAWAYS]

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- ▶ Other (modern) methods exist

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wrap-up
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[PENALIZATION METHODS]

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[PENALIZATION METHODS]

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NB: If $\lambda = 0$ the regression is just the classic OLS estimator

[PENALIZATION METHODS: RIDGE REGRESSION]

Ridge regression is the solution of:

$$\min_{\beta} \frac{1}{2n} \sum_{i=1}^n (y_i - \beta_0 - x'_i \beta)^2 + \lambda \frac{\|\beta\|^2}{2}$$

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- ↪ When there is collinearity, $X'X$ cannot be inverted, while if $\lambda > 0$ the matrix $(X'X + \lambda I)$ is invertible

[RIDGE REGRESSION IN PRACTICE]

How to choose λ ?

[RIDGE REGRESSION IN PRACTICE]

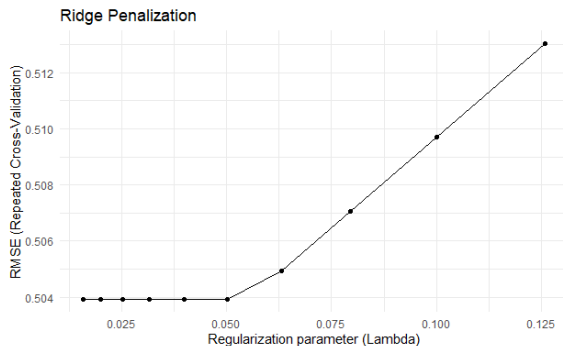
How to choose λ ?

- ▶ We compute the (CV-averaged) *RMSE* for many values of λ

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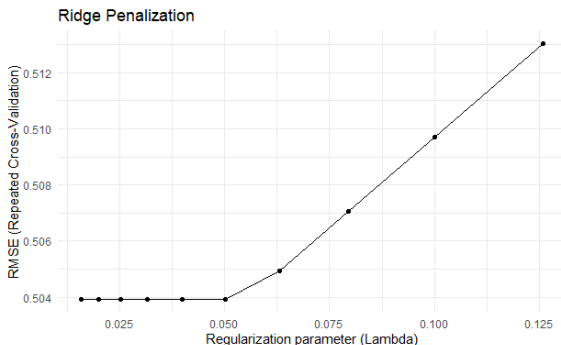
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Remark: λ is typically small, and we usually select it on the log scale.

[RIDGE REGRESSION IN PRACTICE]

Ridge regression with optimal λ^*

[RIDGE REGRESSION IN PRACTICE]

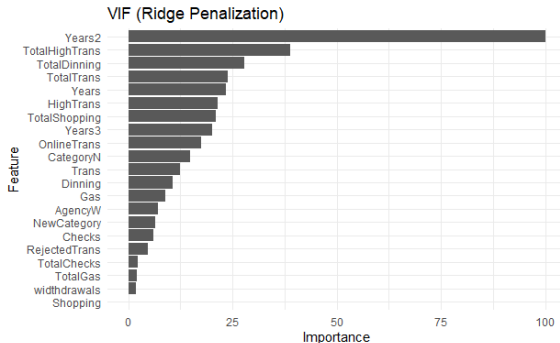
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[PENALIZATION METHODS: LASSO]

LASSO or *Least Absolute Shrinkage and Selection Operator*, is another common penalization method, is the solution of:

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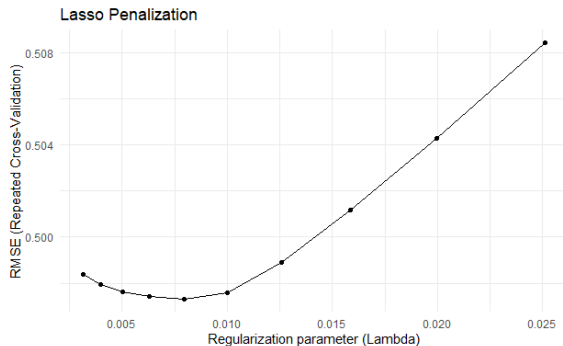
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[LASSO IN PRACTICE]

We compute the (CV-averaged) *RMSE* for many values of λ

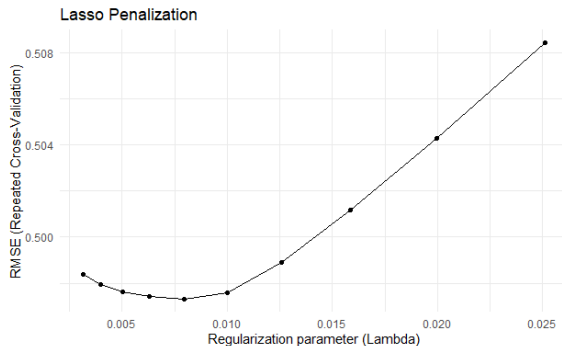
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Regression with optimal λ^* for LASSO

[LASSO IN PRACTICE]

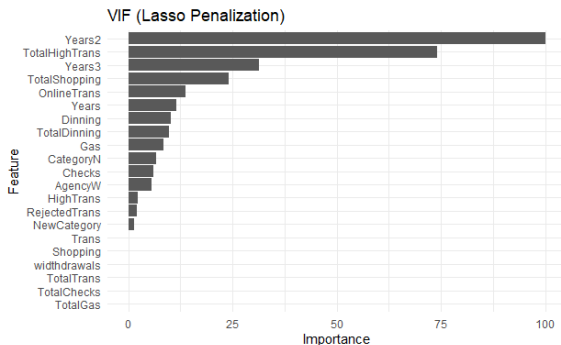
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[PENALIZATION METHODS: ELASTIC NET]

Elastic Net combines both Lasso and Ridge regression:

$$\min_{\beta} \frac{1}{2n} \sum_{i=1}^n (y_i - \beta_0 - x'_i \beta)^2 + \lambda \left((1 - \alpha) \frac{\|\beta\|^2}{2} + \alpha |\beta| \right)$$

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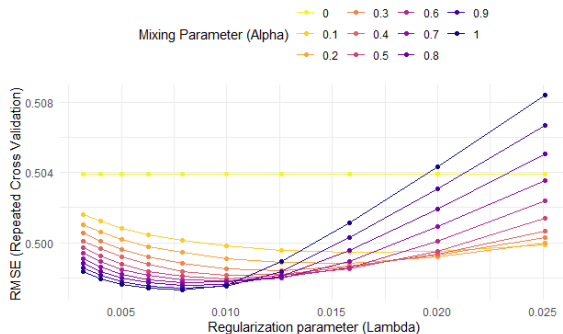
- ▶ If $\alpha = 1$ we have the Lasso estimator, if $\alpha = 0$, the Ridge regression.
- ▶ Through α we balance variable selection (Lasso) and coefficient reduction (Ridge)

[ELASTIC NET IN PRACTICE]

Compute the (CV-averaged) *RMSE* on a grid of (λ, α)

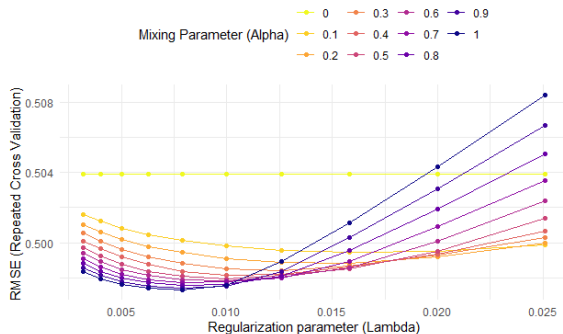
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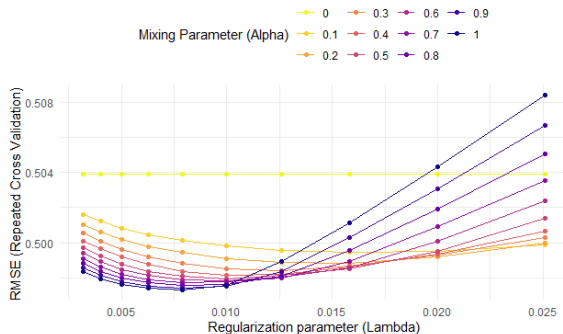
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↪ Optimal value: $\alpha^* = 1$ & $\lambda = 0.008$ ↪ Lasso estimator.

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↪ Optimal value: $\alpha^* = 1$ & $\lambda = 0.008$ ↪ Lasso estimator.

► Elastic net *encompass* both Ridge and Lasso estimators.

[ELASTIC NET IN PRACTICE]

Elastic net with optimal λ^* and α^* is LASSO since $\alpha^* = 1$!

[ELASTIC NET IN PRACTICE]

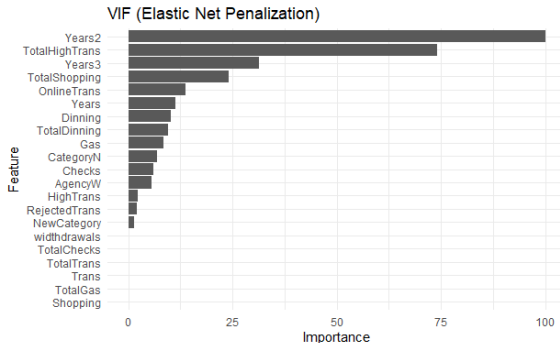
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[BEST MODEL?]

In Machine Learning, focus on prediction (RMSE)

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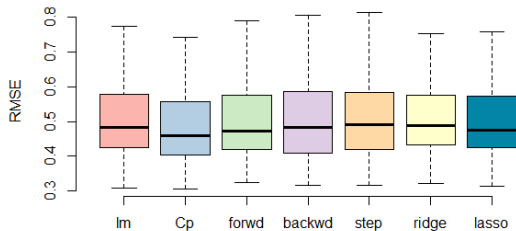
In Machine Learning, focus on prediction (RMSE)

- ▶ Cross-Validation performance (RMSE):

[BEST MODEL?]

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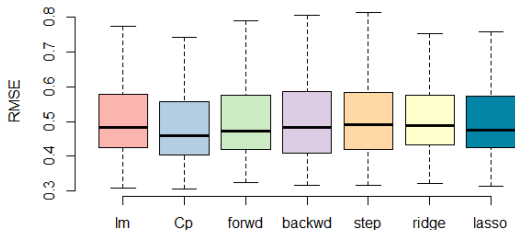
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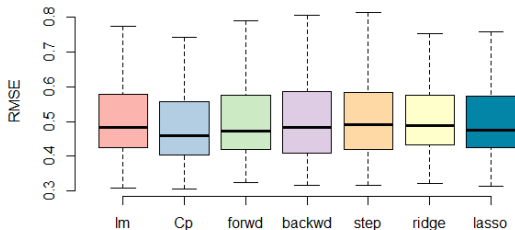


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[BEST MODEL?]

In Machine Learning, focus on prediction (RMSE)

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- LASSO is probably the best (lower RMSE)
- Model selected by Mallows's C_p (8 regressors) is almost as good!

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[QUIZ TIME]

[TAKEAWAYS]

- ▶ Penalized least-squares methods can be used with multicollinearity or with a large number of regressors.

[TAKEAWAYS]

- ▶ Penalized least-squares methods can be used with multicollinearity or with a large number of regressors.
- ▶ All solutions of a *penalized least-squares problem*

$$\min_{\beta} \frac{1}{2n} \sum_{i=1}^n (y_i - \beta_0 - x_i' \beta)^2 + \lambda \cdot J_{\alpha}(\beta_1, \dots, \beta_k)$$

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- ▶ Selection of *hyper parameters* is based on CV and RMSE

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$$\min_{\beta} \frac{1}{2n} \sum_{i=1}^n (y_i - \beta_0 - x'_i \beta)^2 + \lambda \cdot J_{\alpha}(\beta_1, \dots, \beta_k)$$

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- ▶ It is important to **center and scale** each of the x to ensure the comparability of β s
- ▶ Selection of *hyper parameters* is based on CV and RMSE
- ▶ The elastic net "encompass" both Ridge and Lasso estimators.

[TAKEAWAYS]

- ▶ Penalized least-squares methods can be used with multicollinearity or with a large number of regressors.
- ▶ All solutions of a *penalized least-squares problem*

$$\min_{\beta} \frac{1}{2n} \sum_{i=1}^n (y_i - \beta_0 - x'_i \beta)^2 + \lambda \cdot J_{\alpha}(\beta_1, \dots, \beta_k)$$

λ is a *hyperparameter*, $J_{\alpha}(\cdot)$ is the penalization function

- ▶ It is important to **center and scale** each of the x to ensure the comparability of β s
- ▶ Selection of *hyper parameters* is based on CV and RMSE
- ▶ The elastic net "encompass" both Ridge and Lasso estimators.
- ▶ Penalization methods are very popular in practice