Variable Selection and Regularization

Christoph Kern

Mannheim Machine Learning Modules

c.kern@uni-mannheim.de

February 6 and 7, 2018

Outline

Introduction

Selecting Features for Prediction

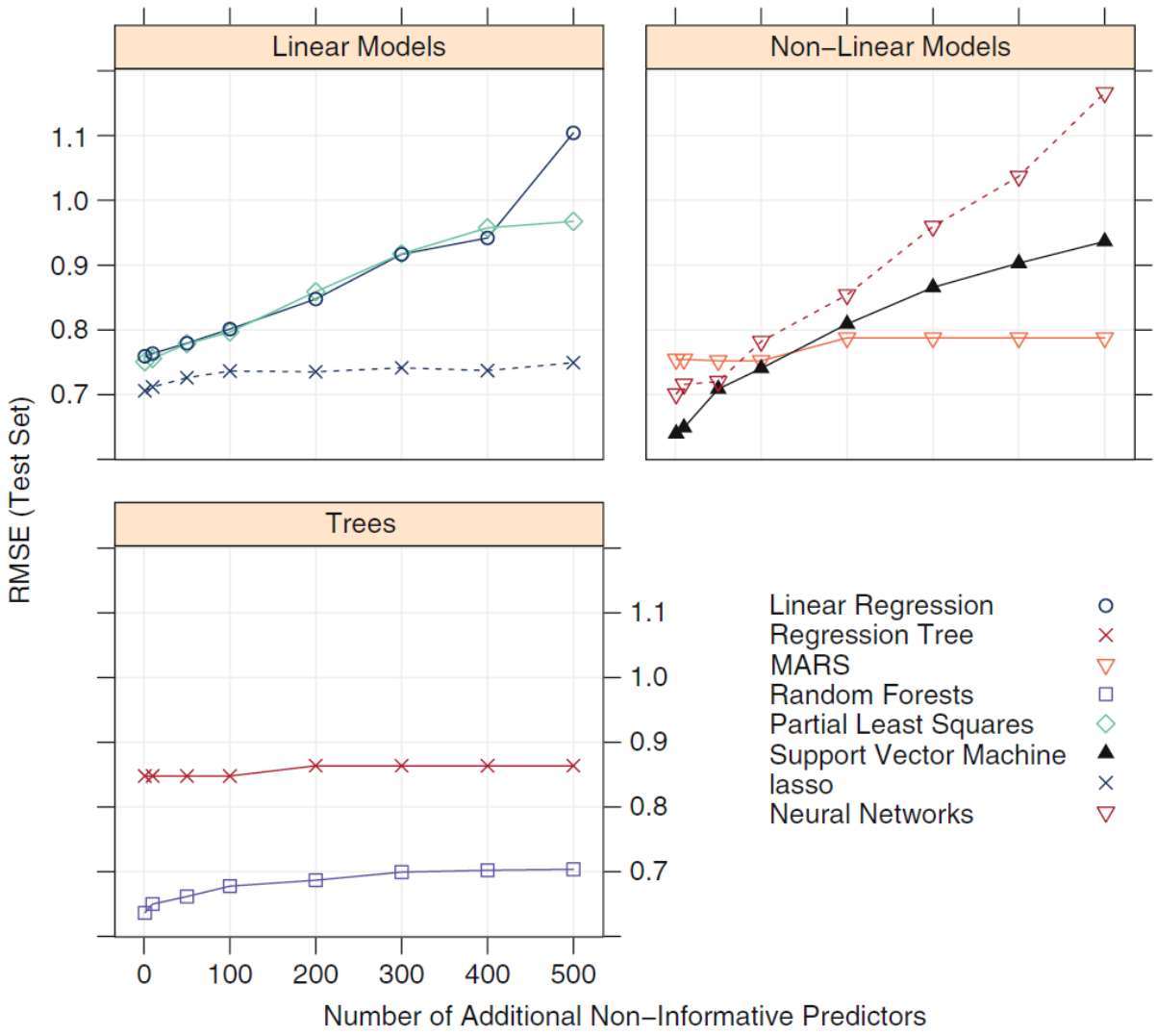
- Prediction problems might involve data with many potential features (and less domain knowledge)
  - Contrasts causal inference perspective / testing hypotheses
  - Relates to building parsimonious models (e.g. with respect to AIC, BIC)
- Interest in developing sparse models to improve:
  - Model interpretability
  - Prediction accuracy
    - Performance in a new **test set** given estimation in **training data**

$\rightarrow$ Remove non-informative variables to improve effectiveness

Is feature selection necessary?

- Regression models
  - Run into problems in high dimensions (large p, small n)
    - $p \approx n$: Overfitting and poor prediction performance
    - $p > n$: OLS can not be estimated
- Tree-based models
  - Involve build-in feature selection
  - Less affected by irrelevant features
- Support vector machines, neural networks
  - Negatively affected by irrelevant features

Figure: Consequences of non-informative predictors



Kuhn & Johnson (2013)

Feature selection methods

- Wrapper
  - Search algorithms that add and/or remove predictors to optimize performance
  - e.g. forward, backward, and best subset selection
- Filter
  - Test individual predictors outside of the predictive model
  - e.g. t-tests, r, χ^2
- ℓ_1 **Regularization**

Stepwise Variable Selection

Algorithm 1: Classical forward selection

```
Set p-value threshold τ;
Initialize empty model;
repeat
    for each predictor not in the model do
        Add the predictor to the current model;
        Estimate the statistical significance of the new term;
    end
    if the smallest p is less than τ then
        Include the corresponding predictor in the model;
    end
until no significant predictor remains outside the model;
```

There are a number of **serious** problems here!

- Multiple testing issue
- Objective function does not focus on prediction accuracy
- Prone to performance evaluation bias

Adjusting stepwise selection approaches

- Usage of performance measures instead of p-values
- Implement feature selection in a **proper resampling setting**

$\rightarrow$ Feature selection needs to be interweaved in the model-building process

Algorithm 2: Forward selection with resampling

```
Set the number of resampling iterations;
Set the number of features p;
Initialize empty model;
for each resampling iteration do
    Partition data into training and hold-out set;
    for k = 0, ..., p − 1 do
        Consider all p − k models that add an additional predictor to the current
         model;
        Choose the best among these models in terms of loss in the training data;
    end
end
Determine the best model over all hold-out sets;
```

Regularization

Penalized regression models

- (Even) regression models can be over-parameterized (large p, small n)
- Shrinkage / Regularization methods
  - Consider model complexity in the estimation process by...
  - ...shrinking regression coefficients towards zero

$\rightarrow$ Ridge regression & Lasso

OLS regression

$$\hat{\beta}_{OLS} = \underset{\beta}{\text{argmin}} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 \right\}$$

$\rightarrow$ Minimizes ("only") RSS

Ridge regression

$$\hat{\beta}_{ridge} = \underset{\beta}{\text{argmin}} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}$$

$$= RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

$\rightarrow$ Introduces a **shrinkage penalty**: Fit - complexity trade-off

OLS regression

$$\hat{\beta}_{OLS} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 \right\}$$

$\rightarrow$ Minimizes ("only") RSS

Ridge regression

$$\begin{aligned} \hat{\beta}_{ridge} &= \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\} \\ &= RSS + \lambda \sum_{j=1}^{p} \beta_j^2 \end{aligned}$$

$\rightarrow$ Introduces a **shrinkage penalty**: Fit - complexity trade-off

Comparing OLS and Ridge regression

$$RSS = (\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta)$$

$$RSS(\lambda) = (\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta) + \lambda\beta'\beta$$

$$\hat{\beta}_{OLS} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

$$\hat{\beta}_{ridge} = (\mathbf{X}'\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}'\mathbf{y}$$

As a result...

- OLS regression needs $\mathbf{X}$ to be of full column rank
- Ridge regression (still) allows matrix inversion due to $\lambda\mathbf{I}$

Other penalties are possible

Ridge regression

- Penalty on ℓ_2 norm of $\boldsymbol{\beta}$
- $\|\boldsymbol{\beta}\|_2 = \sqrt{\sum_{j=1}^{p} \beta_j^2}$

Lasso (Least Absolute Shrinkage and Selection Operator)

$$\hat{\beta}_{lasso} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}$$

- Penalty on ℓ_1 norm of β
- $\|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|$

Other penalties are possible

Ridge regression

- Penalty on ℓ_2 norm of $\boldsymbol{\beta}$
- $\|\boldsymbol{\beta}\|_2 = \sqrt{\sum_{j=1}^{p} \beta_j^2}$

Lasso (Least Absolute Shrinkage and Selection Operator)

$$\hat{\boldsymbol{\beta}}_{lasso} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}$$

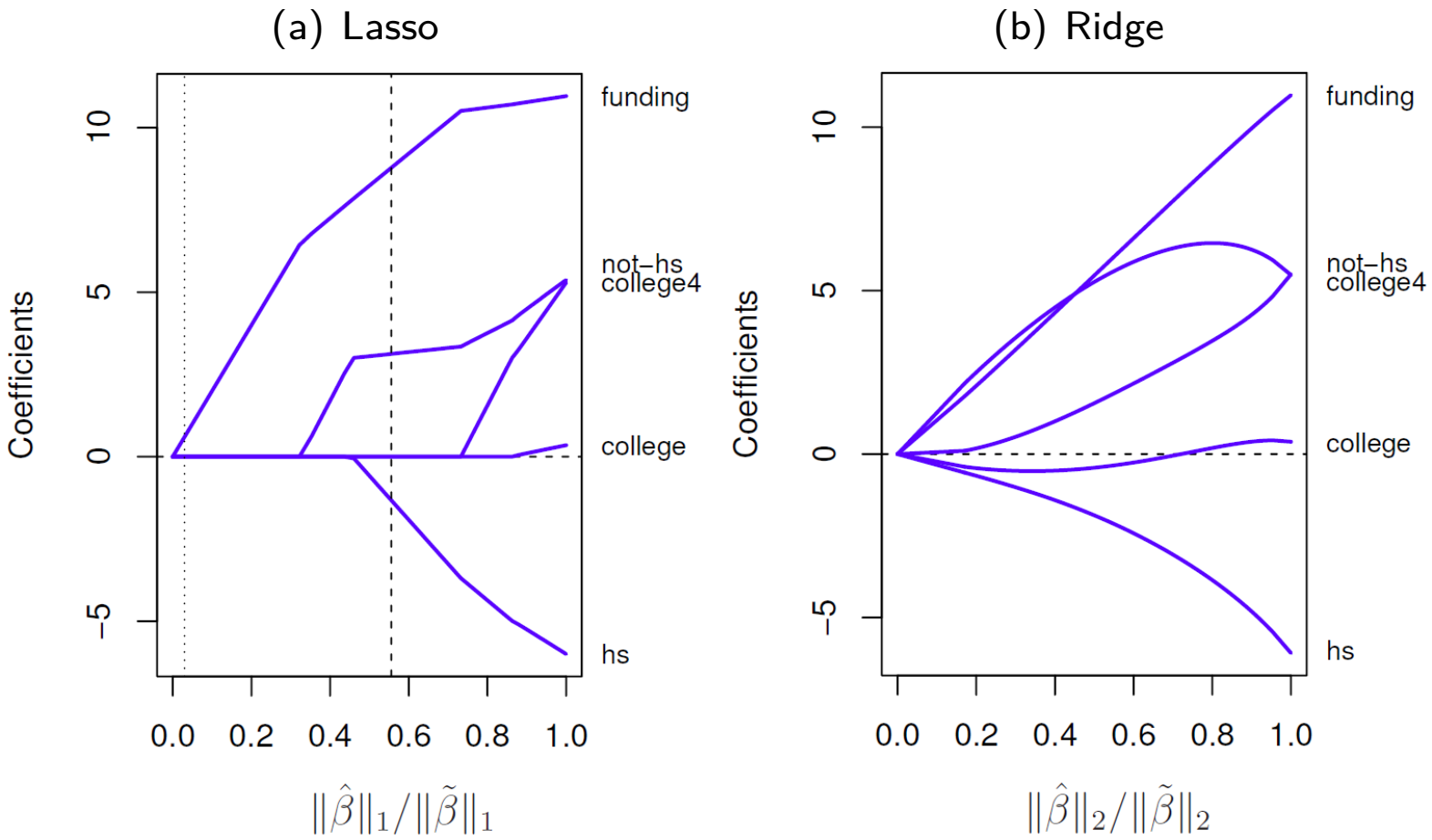
- Penalty on ℓ_1 norm of $\boldsymbol{\beta}$
- $\|\boldsymbol{\beta}\|_1 = \sum_{j=1}^{p} |\beta_j|$

Increasing the penalty on model complexity

- $\lambda = 0$
  - Models are equivalent to OLS
- $\lambda \to \infty$
  - Ridge regression ($RSS + \lambda \sum \beta_j^2$)
    - Coefficients are shrunken towards zero
    - Shrinks coefficients of correlated predictors towards each other
  - Lasso ($RSS + \lambda \sum |\beta_j|$)
    - Coefficients are eventually shrunken exactly to zero (i.e. performs **variable selection**)
    - Erratic paths for correlated predictors

$\to$ The penalty λ is a tuning parameter

Figure: Coefficient paths



Efron & Hastie (2016)

A compromise between ridge and lasso

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ \frac{1}{2} \sum_{i=1}^{n} (y_i - \beta_0 - x_i'\beta)^2 + \lambda \left[\tfrac{1}{2}(1-\alpha)\|\beta\|_2^2 + \alpha\|\beta\|_1 \right] \right\}$$

Elastic net

- Introduces a mixing parameter $\alpha \in [0, 1]$
  - $\alpha = 0$: Ridge regression
  - $\alpha = 1$: Lasso
- α is an additional tuning parameter

Standardization

- Contribution to penalty term dependent on scale
- Ridge and Lasso typically applied with standardized features

Group lasso

- Standard lasso considers predictors independently
- Group lasso in- or excludes groups of variables together

Categorical outcomes

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ -\frac{1}{n}\mathcal{L}(\beta_0, \beta; \mathbf{y}, \mathbf{X}) + \lambda \|\beta\|_1 \right\}$$

- Shrinkage can be applied with binary and multinomial outcomes...
- ...by introducing a penalty in the likelihood function

Tuning and Cross-Validation

Lasso regression modeling process

1. Choose a series of λ values
2. Estimate a sequence of penalized regression models
   - Since we are interested in the best prediction model for new data...
   - ...this sequence is estimated in a Cross-Validation loop
3. Choose the best λ based on step 2
4. Re-fit model with chosen λ on full training data

$\rightarrow$ Data is split into training and validation set(s) for **model tuning**

Cross-Validation with the Lasso

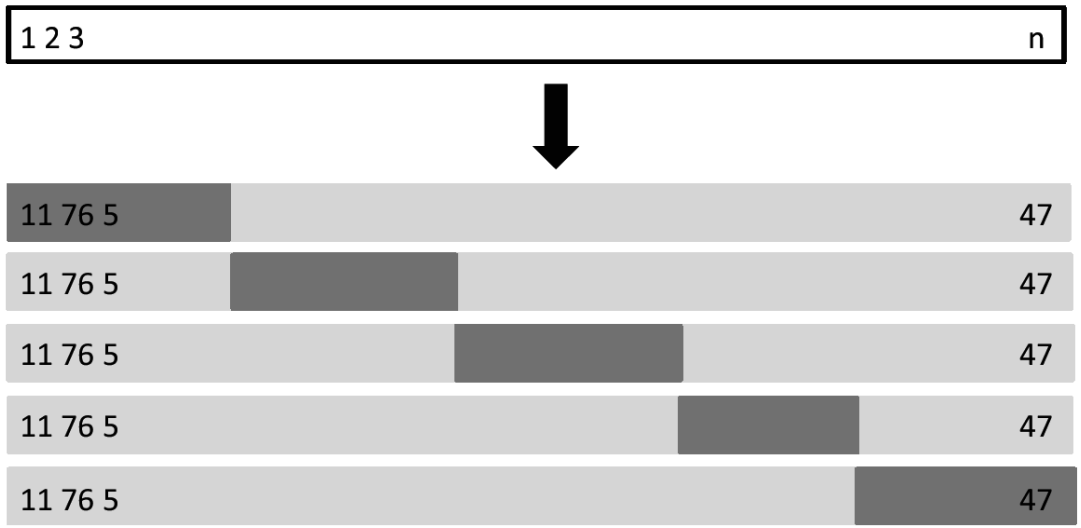
1. Split the data into k sets at random
2. Fit a sequence of regularized models using $k-1$ parts of the data
3. Estimate model performances on the holdout set
4. Repeat step 2 & 3 k times

Cross-validated errors (κ indicates data partitions)

$$CV(\hat{f}_\lambda) = \frac{1}{n}\sum_{i=1}^{n} L(y_i, \hat{f}_\lambda^{-\kappa(i)}(x_i))$$

with $L(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$ for regression problems.

Figure: 5-Fold Cross-Validation with training set and validation set (example)



James et al. (2013)

Cross-Validation done wrong

- **Never** separate feature selection and CV
  - CV *after* selection on full data *biases* performance measures
  - Hold-out samples are no longer independent test sets
- Include feature selection within the CV loop
- Unsupervised screening on full data is valid

Figure: Correlations of y with unrelated x's with incorrect and correct CV

Hastie et al. (2009)

Summary

- Beware of pitfalls when applying (stepwise) variable selection
- Ridge, lasso and elastic net penalize complexity
  - Can be used to fit sparse and stable models
  - Typically applied in large p, small n situations
  - Utilize Cross-Validation for parameter tuning
- Statistical inference after feature selection?
  - Selection needs to be taken into account (Taylor & Tibshirani 2015)!

Software Resources

Resources for R

- Stepwise selection e.g. available in `leaps` and `klaR` package
- Standard package for ridge regression, lasso and elastic net: `glmnet`
- Group lasso penalization implemented in `grpreg` and `gglasso`
- Tools for post-selection inference: `selectiveInference`

References

Efron, B. and Hastie, T. (2016). Sparse Modeling and the Lasso. In Efron, B. and Hastie, T. (Eds.), *Computer Age Statistical Inference: Algorithms, Evidence and Data Science* (pp. 298–324). New York, NY: Cambridge University Press

Hastie, T., Tibshirani, R., Friedman, J. (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. New York, NY: Springer.

Hastie, T., Tibshirani, R., Wainwright, M. (2015). *Statistical Learning with Sparsity: The Lasso and Generalizations*. Boca Raton, FL: Chapman & Hall/CRC.

James, G., Witten, D., Hastie, T., Tibshirani, R. (2013). *An Introduction to Statistical Learning*. New York, NY: Springer.

Kuhn, M., Johnson, K. (2013). *Applied Predictive Modeling*. New York, NY: Springer.

Taylor, J. and Tibshirani, R. (2015). Statistical Learning and Selective Inference. *Proceedings of the National Academy of Sciences, 112*(25), 7629–7634.