Supervised Learning

Feature selection

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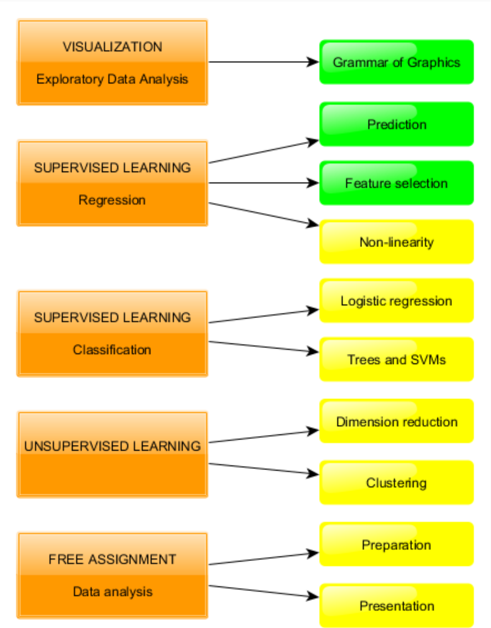
Program


VISUALIZATION
Exploratory Data Analysis
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Classification
Logistic regression
Trees and SVMs
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Content

1. Filter methods
2. Wrapper methods
3. Embedded methods
4. Dimension reduction

What's feature selection?

Bias-variance trade-off

- more model complexity reduces bias (good)
- less model complexity reduces variance (good)

Previous example with single feature and polynomial models.

But what if we have lots of features?

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p + \epsilon$$

Flexible model

- Like a kid in candy store with credit card
- It does not stop buying coefficients until the store is sold out!

How do we educate this child?

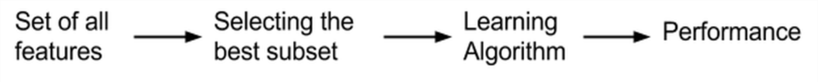
Main classes

1. **Filter methods** (subset selection)
    - select features and train the model
2. **Wrapper methods** (subset selection)
    - train the model on various subsets of features
3. **Embedded methods** (shrinkage, regularization)
    - train the model with penalties on magnitude of coefficients
4. **Dimension reduction** (unsupervised)
    - reduce coefficients by merging similar candies into a single one

Filter methods

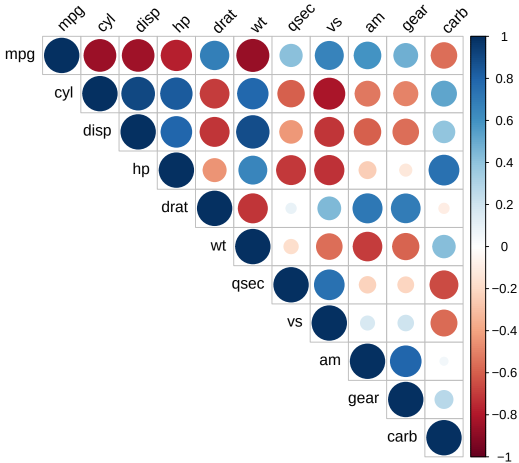
Preselection of features

- you can only buy coefficients you like best
- e.g. predictors with minimum correlation $|r_{y,x}|$



Correlation feature selection

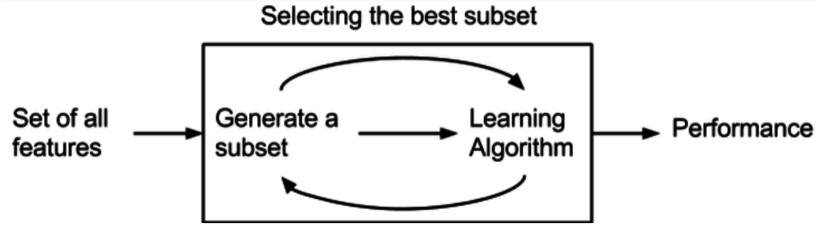
Select features x_j for which $|r_{mpg,x_j}| > r_{min}$



Wrapper methods

Selection best predictors

- you can only buy a limited number of coefficients
- e.g. the best k predictors



Best subset selection

Algorithm

1. For $k = 1, 2, \ldots, p$, fit all $\binom{p}{k}$ models
2. Use cross-validation to determine the MSE
3. Select the model with the smallest cross-validated MSE

Pros and cons

- Finds the best model
- Need to fit 2^p, which for $p = 20$ is little over one million

Alternatives: forward stepwise selection

Algorithm forward

1. Start with the null model and add predictor one-at-a-time
2. At each step, select the predictor yields the best fit
3. Select the model with the smallest cross-validated MSE

Pros and cons

- No guarantee to find the best model
- Fit only $1 + p(p+1)/2$ models, which for $p = 20$ is 211

Alternatives

Backward stepwise selection

- as forward, but the other way around
- starts with full model, and remove variable one-at-a-time

Hybrid stepwise selection

- combination of forward and backward,
- at each step predictors can be entered or removed

Stepwise in R

Backward

```
main_lm <- lm(outcome ~ ., data)
step(main_lm, scope = outcome ~ 1, direction="both")
```

Forward

```
null_lm <- lm(outcome ~ ., data)
step(null_lm, scope = outcome ~ ., direction="both")
```

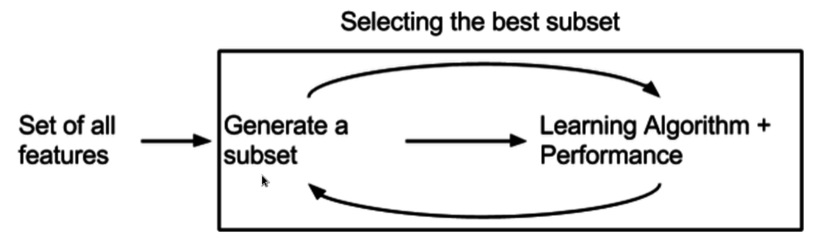
Hybrid

```
step(null_lm, scope = outcome ~ ., direction="both")
```

Embedded methods

Budgets

- You can but anything, but on a limited budget s
- Sum of absolute/squared coefficients cannot exceed s



Regularization, shrinkage, penalization

Algorithm

1. Fit the model with all p **standardized** predictors
   - ensures that size coefficient is independent of scale predictor
2. Constrain the sum of absolute/squared coefficients to budget s
3. Determine with cross-validation the optimal value for s

Lasso penalty: $\lambda \sum_{j=1}^{p} |\beta_j| < s$

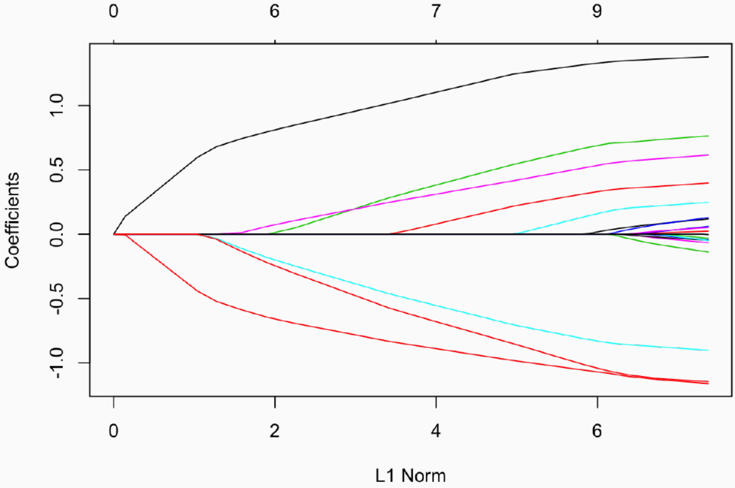
- shrinks coefficients exactly to zero

Ridge penalty: $\lambda \sum_{j=1}^{p} \beta_j^2 < s$

- shrinks coefficients, but not to zero

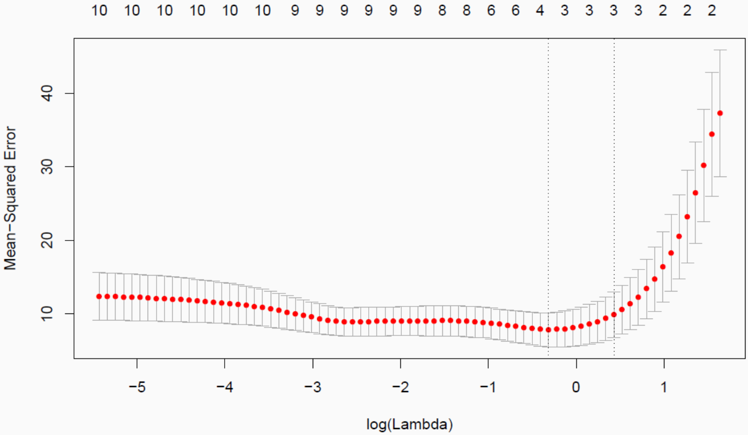
Lasso shrinkage

- As the budget (L1 norm) decreases, coefficients go to zero



Cross-validated λ

- $\log(\lambda_{min}) \approx -0.3$ (4 coefficients)
- $\log(\lambda_{optim}) \approx \log(\lambda_{min}) + 1SD \approx 0.4$ (3 coefficients)



Regularization in R

Package glmnet

```
train_ridge <- glmnet(x = as.matrix(Train[, -nr],
                      y = Train[, <nr>],          # nr = colnr outcome
                      alpha = 0)                  # alpha = 1 for lasso

plot(train_ridge, label=TRUE)                     # shrinkage plot

cv_ridge <- cv.glmnet(x, y,                       # cross validation
                      alpha=0,
                      type.measure = "mse")

plot(cv_ridge)                                     # CV plot

test_ridge <- predict(cv_ridge,
                      newx = as.matrix(Test[, -nr]))
```

Regularization with caret

```
tr <- train(x = scale(Train[, -nr]), y = Train[, nr],
      method    = "glmnet",
      metric    = "RMSE",
      tuneGrid  = expand.grid(alpha  = c(0, 1),
                              lambda = seq(1e-5, 10, length
      trControl = trainControl(method = "cv",
                               number = 5))

ggplot(tr)  # CV plot
```

Dimension reduction

PCA

Principal Components Analysis

- summarize information in p predictors in $q << p$ principal components
- principal components are orthogonal (uncorrelated)
- use PC's for prediction

More detailed discussion of PCA in unsupervied learning