Computer Science

CSC380: Principles of Data Science

Linear Models 3

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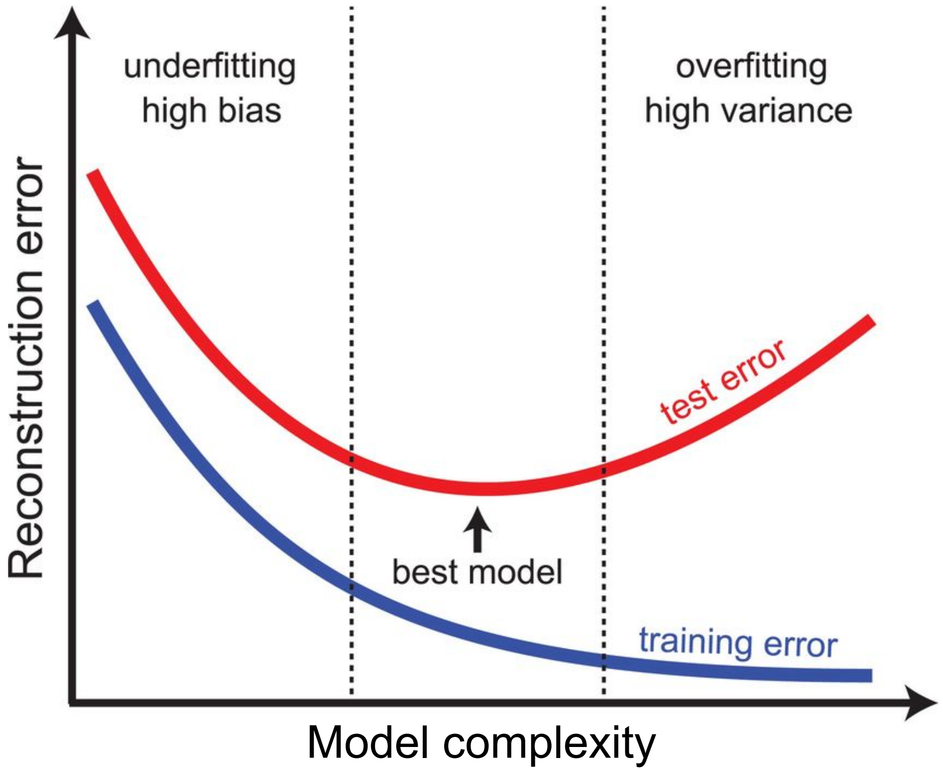
Bias-Variance Tradeoff



Regularized Least Squares

Ordinary least-squares (OLS) estimation (no regularizer),

$$w^{\mathrm{OLS}} = \arg\min_w \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2$$

L2 norm: $\|w\| = \sqrt{\sum_{d=1}^{D} w_d^2}$

L1 norm: $\|w\|_1 = \sum_{d=1}^{D} |w_d|$

L2-regularized Least-Squares (Ridge)

$$w^{\mathrm{L2}} = \arg\min_w \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2 + \lambda \|w\|^2$$

Convention: Just saying 'RLS' means L2-RLS

L2 Regularized Least Squares (RLS) solution:

$$w^{\mathrm{L2}} = (\mathbf{X}^T \mathbf{X} + \lambda I)^{-1} \mathbf{X}^T \mathbf{y}$$

Constrained Optimization Viewpoint

(Theorem) If

$$w^{\mathrm{L2}} = \arg\min_w \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2 + \lambda \|w\|^2$$

then there exists a function $\delta(\lambda)$ s.t.

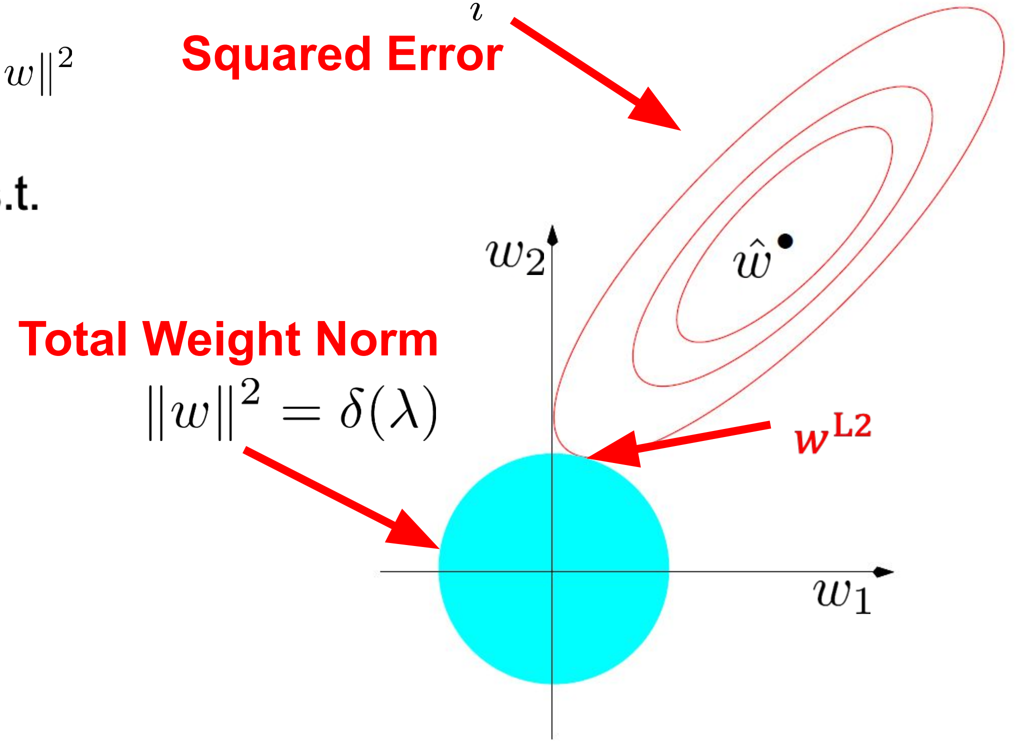
$$w^{\mathrm{L2}} = \arg\min_w \textstyle\sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2$$
$$\text{subject to} \quad \|w\|^2 \le \delta(\lambda)$$

$$\hat{w} = \arg\min_w \sum_i (y^{(i)} - w^T x^{(i)})^2$$

Squared Error

Total Weight Norm

$$\|w\|^2 = \delta(\lambda)$$



[Source: Hastie et al. (2001)]

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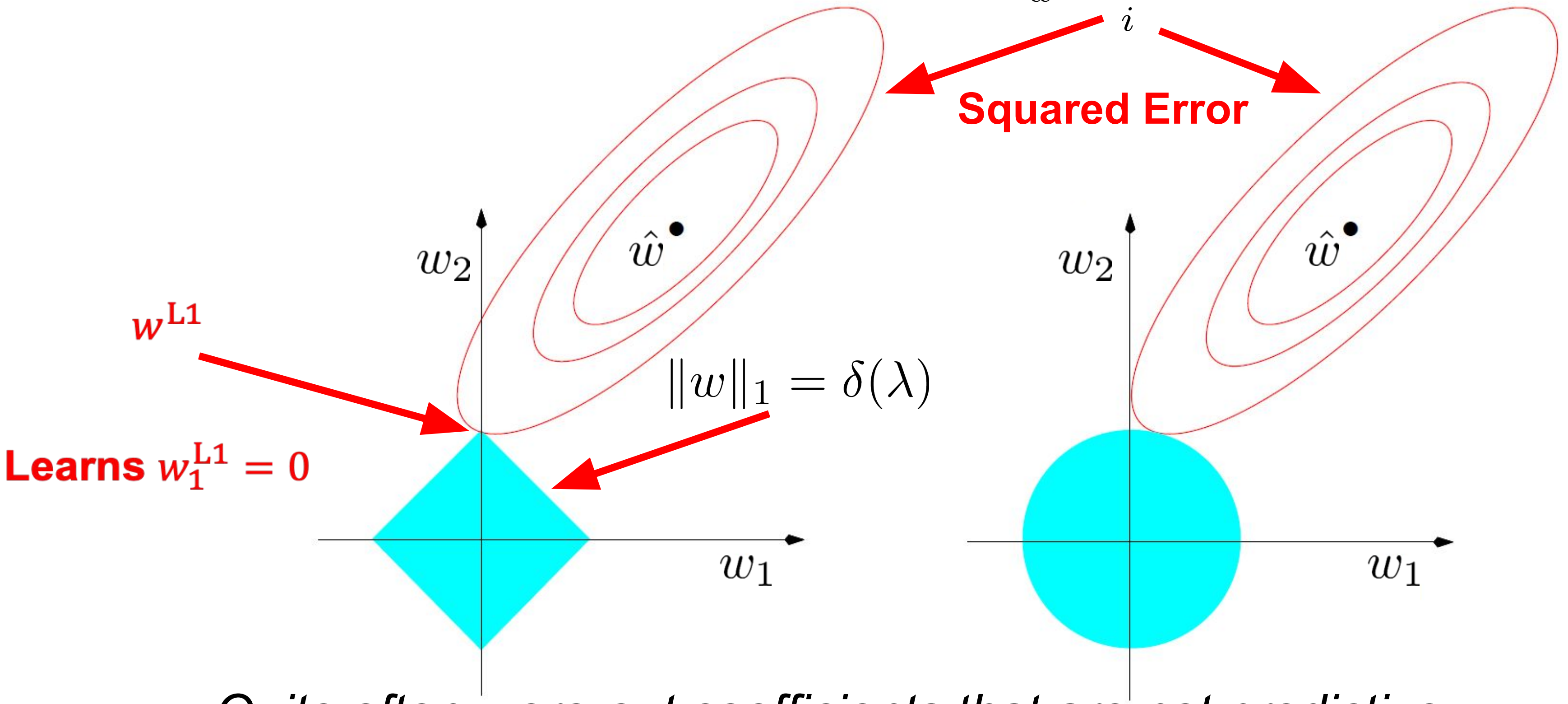
L1-regularized Least-Squares (LASSO)

$$w^{\text{L2}} = \arg\min_w \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2 + \lambda \|w\|_1$$

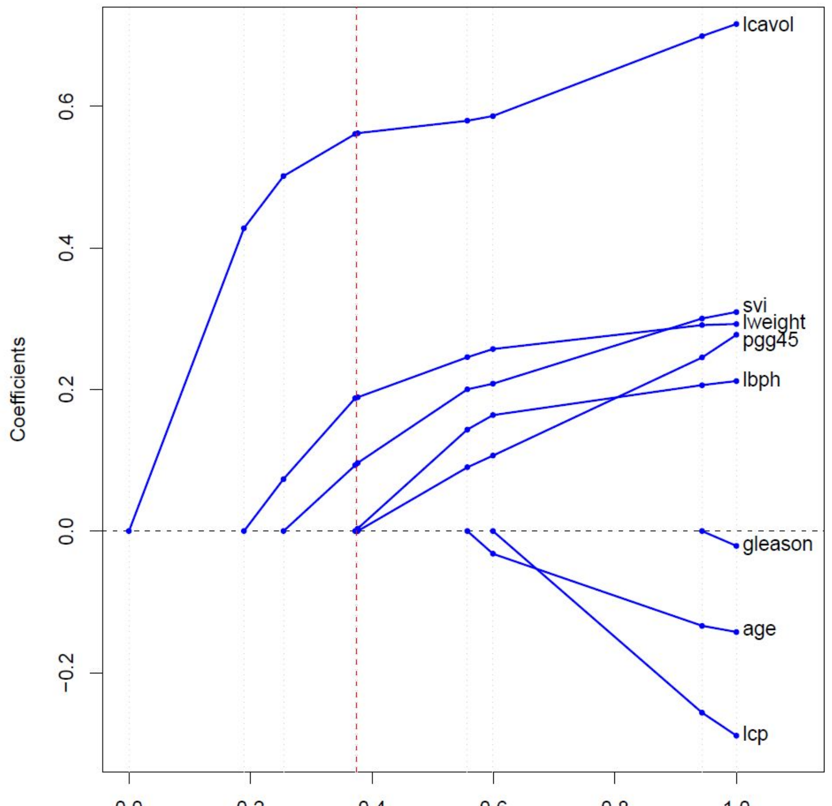
L1 vs L2

$$\hat{w} = \arg\min_w \sum_i (y^{(i)} - w^T x^{(i)})^2$$



Quite often, zero-out coefficients that are not predictive…

Feature Weight Profiles



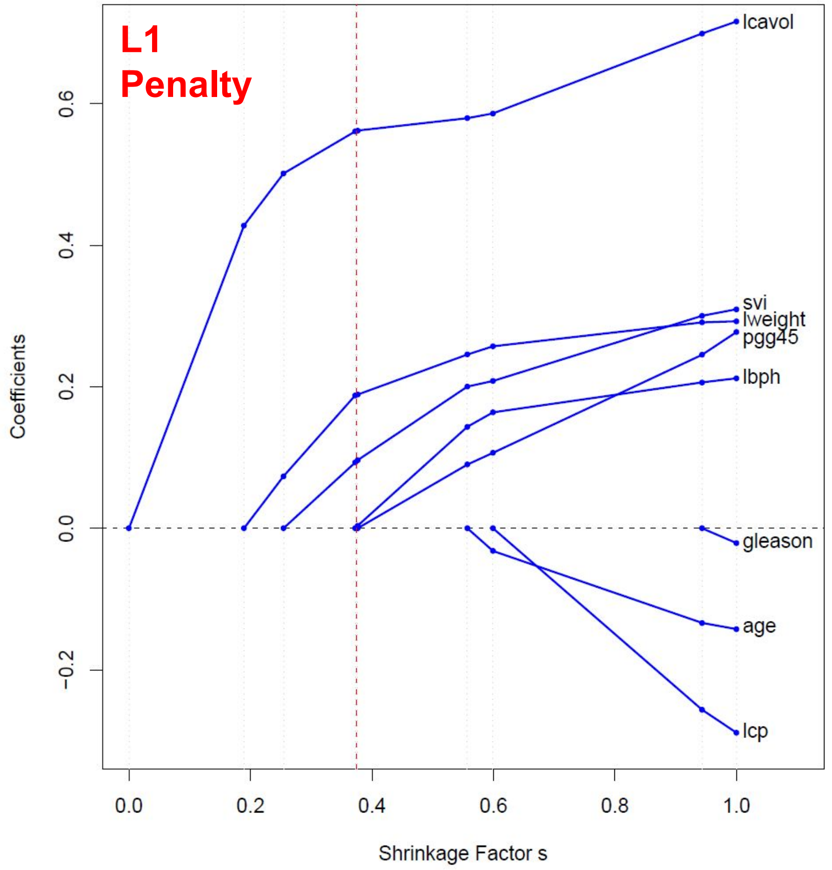
Shrinkage Factor s $(\propto 1/\lambda)$

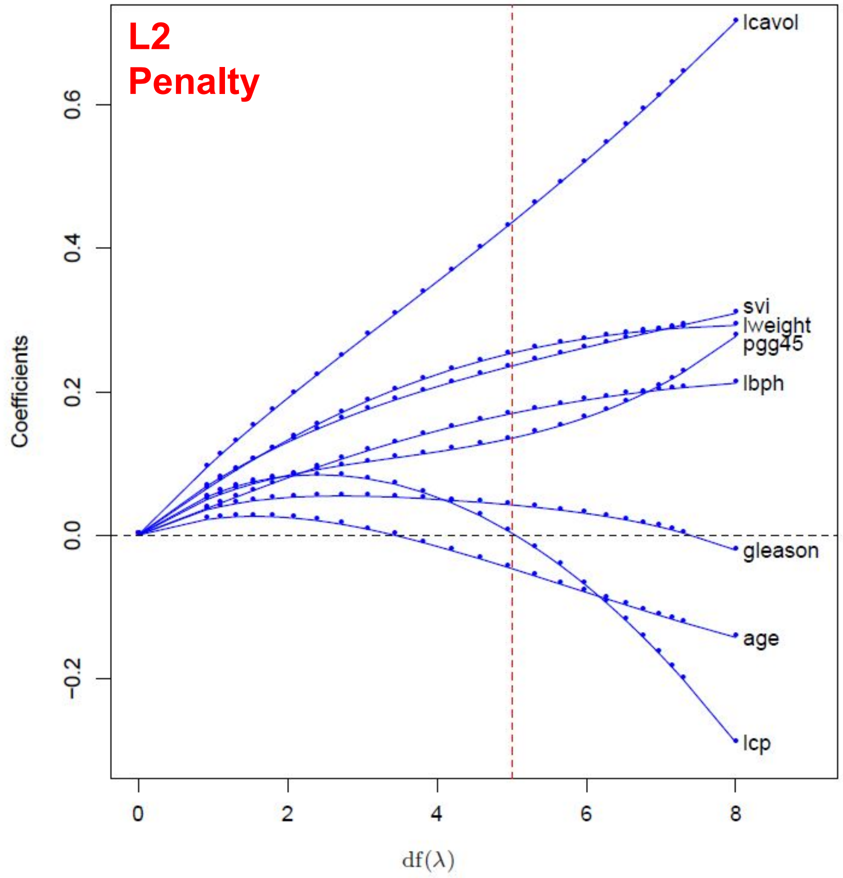
Varying regularization parameter adjusts *shrinkage factor*

For moderate regularization strength weights for many features go to zero

- Induces *feature sparsity*
- Ideal for high-dimensional settings since it reduced variance from having too many features!
- Gracefully handles D>m case, for D features and m training data

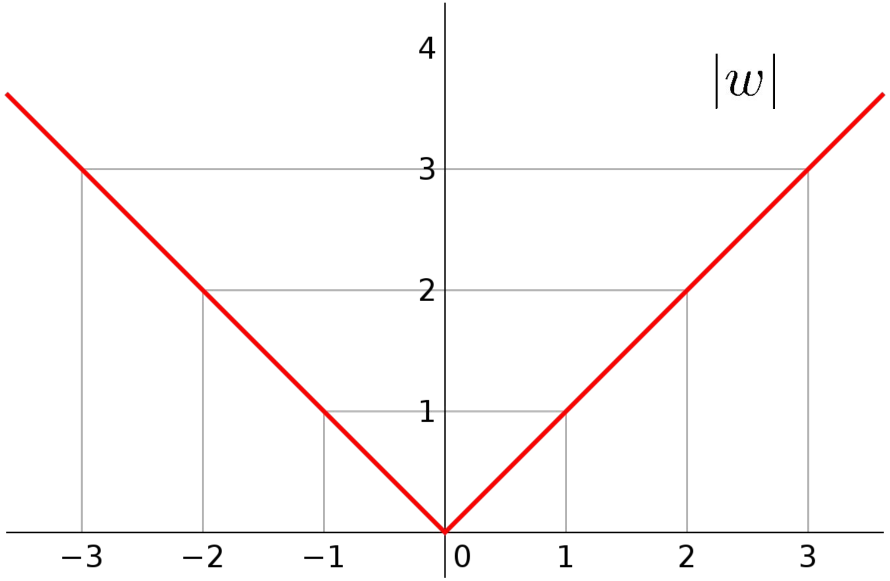
Feature Weight Profiles





Learning L1 Regularized Least-Squares

$$w^{\mathrm{L2}} = \arg\min_w \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2 + \lambda \|w\|_1$$



Not differentiable…

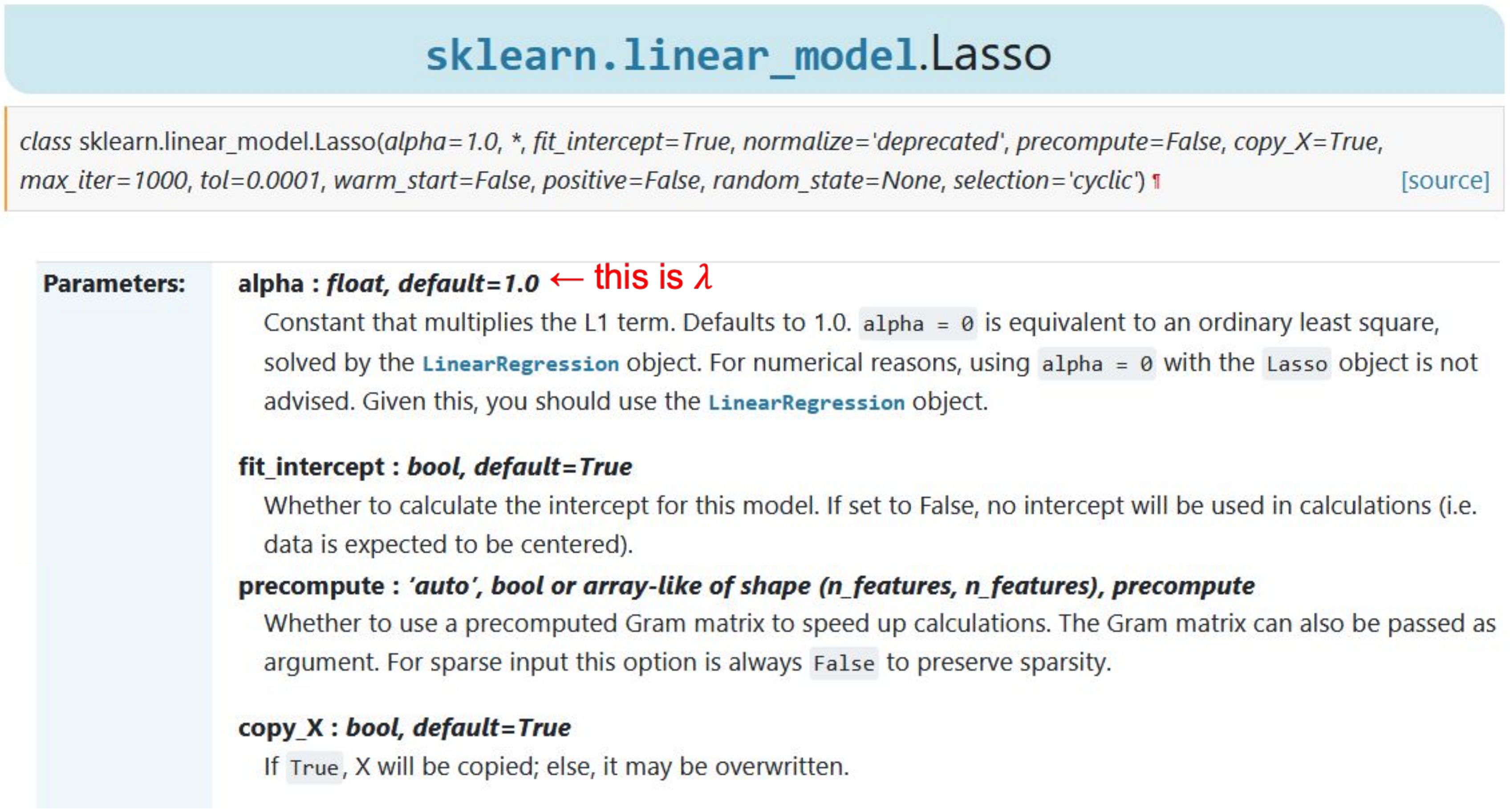
$$\frac{d}{dx}|x|$$

…doesn't exist at x=0

Can't set derivatives to zero as in the L2 case!

Learning L1 Regularized Least-Squares

- **Not differentiable**, no closed-form solution. => Need to use iterative methods
- But it is **convex**!
  - Global minimum can be found!
  - Efficient optimization algorithms exist
- *Least Angle Regression* (LAR) computes full solution path for a range of values λ



sklearn.linear_model.Lasso

class sklearn.linear_model.Lasso(*alpha=1.0*, ***, *fit_intercept=True*, *normalize='deprecated'*, *precompute=False*, *copy_X=True*, *max_iter=1000*, *tol=0.0001*, *warm_start=False*, *positive=False*, *random_state=None*, *selection='cyclic'*) ¶ [source]

Parameters:

alpha : *float, default=1.0* ← this is λ

Constant that multiplies the L1 term. Defaults to 1.0. `alpha = 0` is equivalent to an ordinary least square, solved by the `LinearRegression` object. For numerical reasons, using `alpha = 0` with the `Lasso` object is not advised. Given this, you should use the `LinearRegression` object.

fit_intercept : *bool, default=True*

Whether to calculate the intercept for this model. If set to False, no intercept will be used in calculations (i.e. data is expected to be centered).

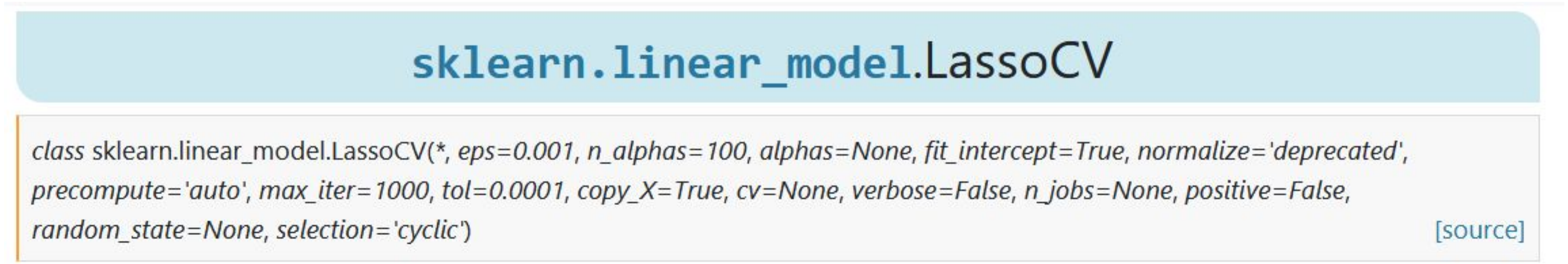
precompute : *'auto', bool or array-like of shape (n_features, n_features), precompute*

Whether to use a precomputed Gram matrix to speed up calculations. The Gram matrix can also be passed as argument. For sparse input this option is always `False` to preserve sparsity.

copy_X : *bool, default=True*

If `True`, X will be copied; else, it may be overwritten.

Specialized methods for cross-validation…



sklearn.linear_model.LassoCV

class sklearn.linear_model.LassoCV(**, eps=0.001, n_alphas=100, alphas=None, fit_intercept=True, normalize='deprecated', precompute='auto', max_iter=1000, tol=0.0001, copy_X=True, cv=None, verbose=False, n_jobs=None, positive=False, random_state=None, selection='cyclic'*) [source]

Tries out a range of α values and reports the best, but maintains other values of α as well.

L1 Regression Cross-Validation

Perform L1 Least Squares (LASSO) 20-fold cross-validation,

```
model = LassoCV(cv=20).fit(X, y)
```

Plot the error for range of alphas,

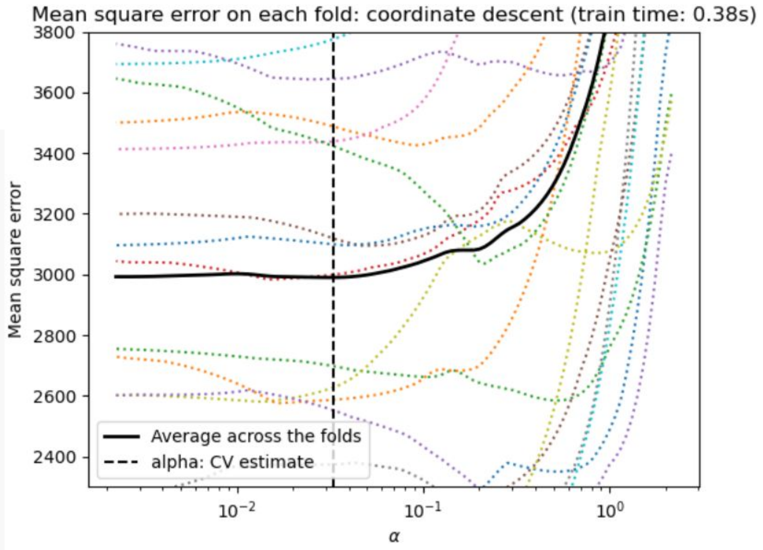
```
plt.figure()
ymin, ymax = 2300, 3800
plt.semilogx(model.alphas_ + EPSILON, model.mse_path_, ":")
plt.plot(
    model.alphas_ + EPSILON,
    model.mse_path_.mean(axis=-1),
    "k",
    label="Average across the folds",
    linewidth=2,
)
plt.axvline(
    model.alpha_ + EPSILON, linestyle="--", color="k", label="alpha: CV estimate"
)
```

all these colored dotted lines for each test fold

all alphas_

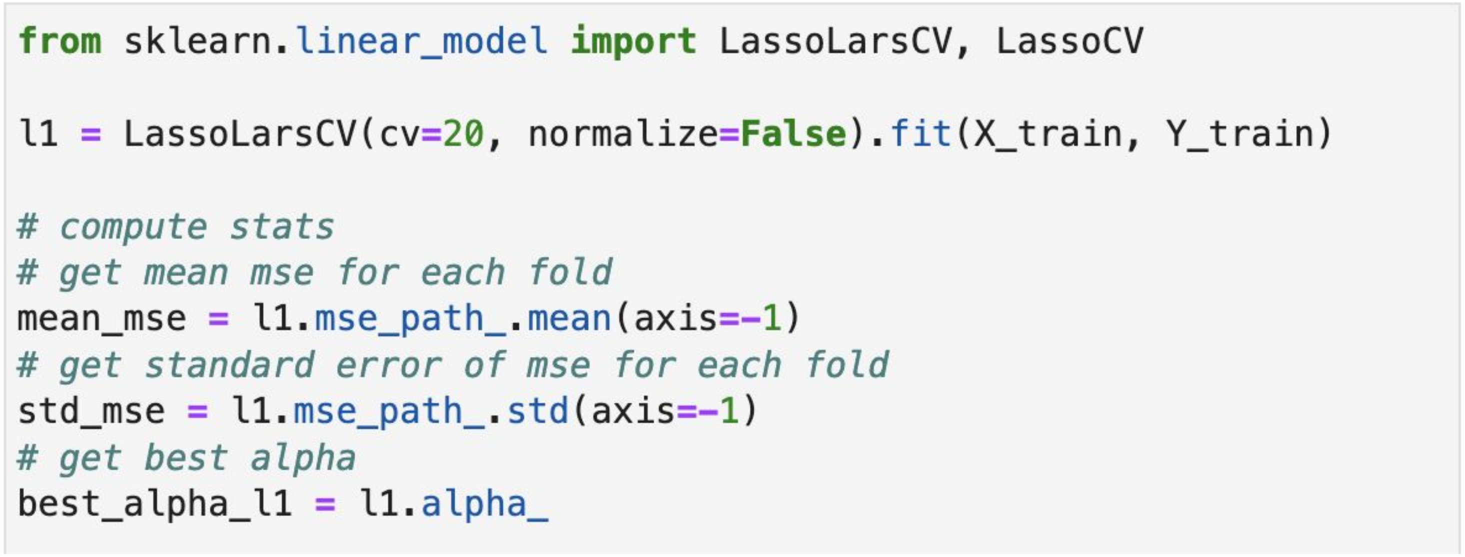
adds vertical line

the best alpha



Least Angle Regression (LAR)

If 20 fold:



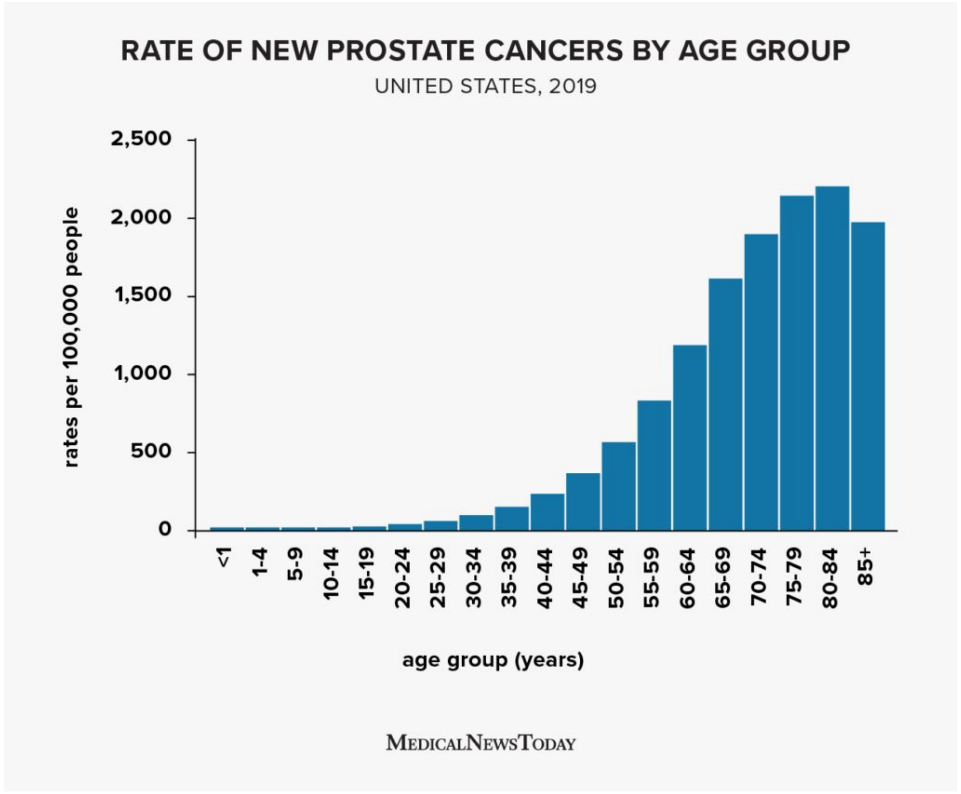
```python
from sklearn.linear_model import LassoLarsCV, LassoCV

l1 = LassoLarsCV(cv=20, normalize=False).fit(X_train, Y_train)

# compute stats
# get mean mse for each fold
mean_mse = l1.mse_path_.mean(axis=-1)
# get standard error of mse for each fold
std_mse = l1.mse_path_.std(axis=-1)
# get best alpha
best_alpha_l1 = l1.alpha_
```

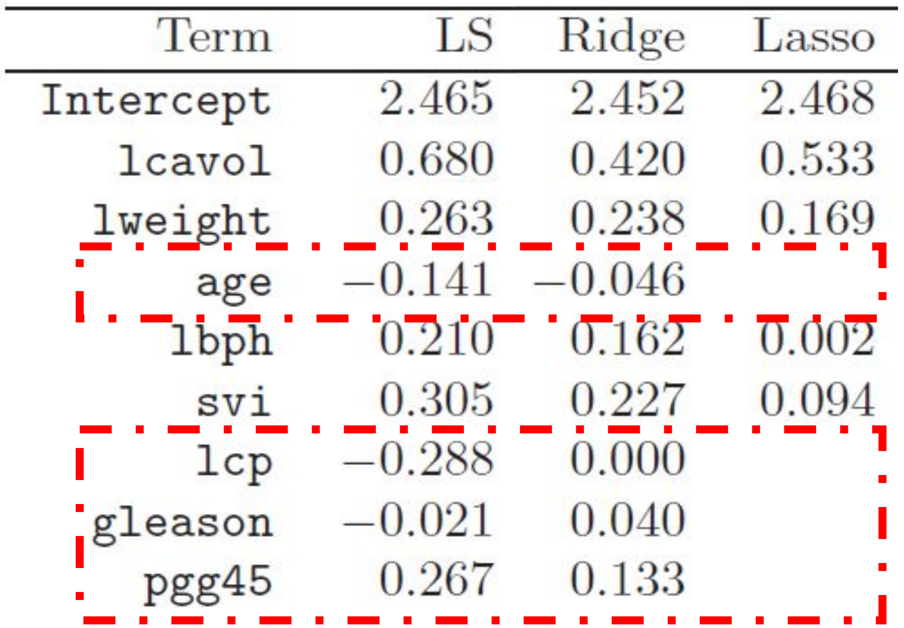
Feature Selection

Rate of Prostate Cancer



https://www.medicalnewstoday.com/articles/age-range-for-prostate-cancer

Example: Prostate Cancer Dataset



Term	LS	Ridge	Lasso
Intercept	2.465	2.452	2.468
lcavol	0.680	0.420	0.533
lweight	0.263	0.238	0.169
age	−0.141	−0.046	
lbph	0.210	0.162	0.002
svi	0.305	0.227	0.094
lcp	−0.288	0.000	
gleason	−0.021	0.040	
pgg45	0.267	0.133	

<u>Task</u>: predict logarithm of prostate specific antigen (PSA).

Best LASSO model learns to ignore several features (age, lcp, gleason, pgg45).

Wait…Is **age** really not a significant predictor of prostate cancer? What's going on here?

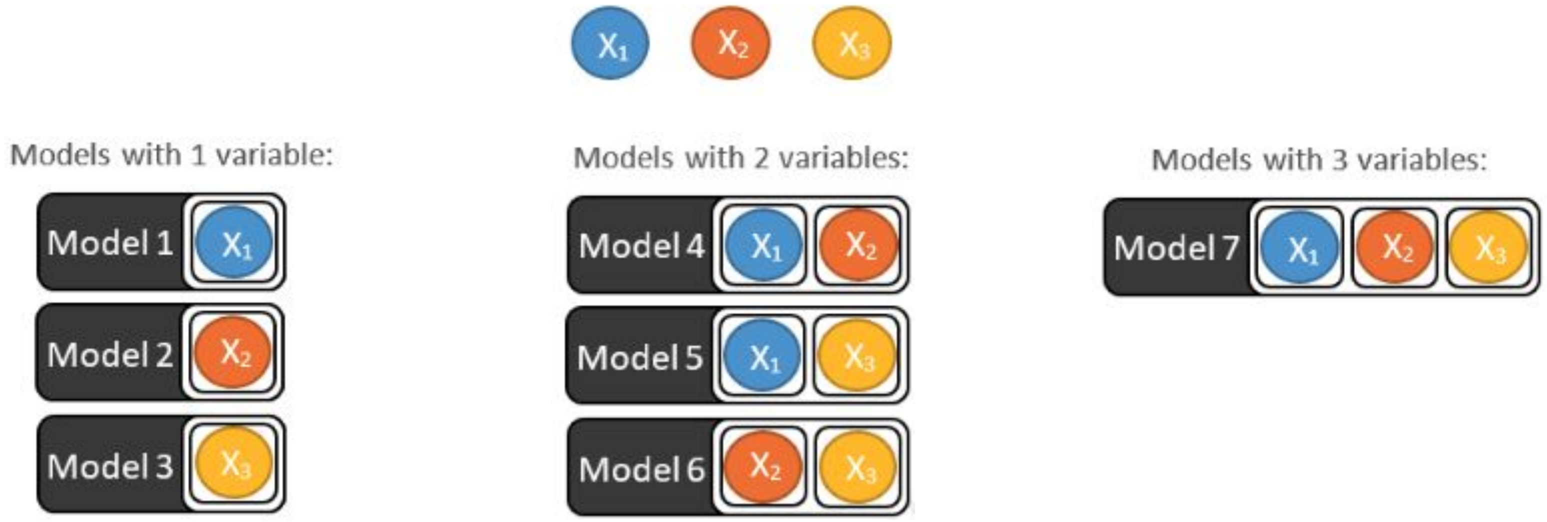
Age is highly correlated with other factors and thus *not significant* in the presence of those factors

Best-Subset Selection

The optimal strategy for p features looks at models over *all possible combinations* of features,

```
For k in 1,…,p:
  subset  = Compute all subset of k-features (p-choose-k)
  For kfeat in subset:
    model  =  Train model on kfeat features
    score  = Evaluate model using cross-validation
Choose the model with best cross-validation score
```

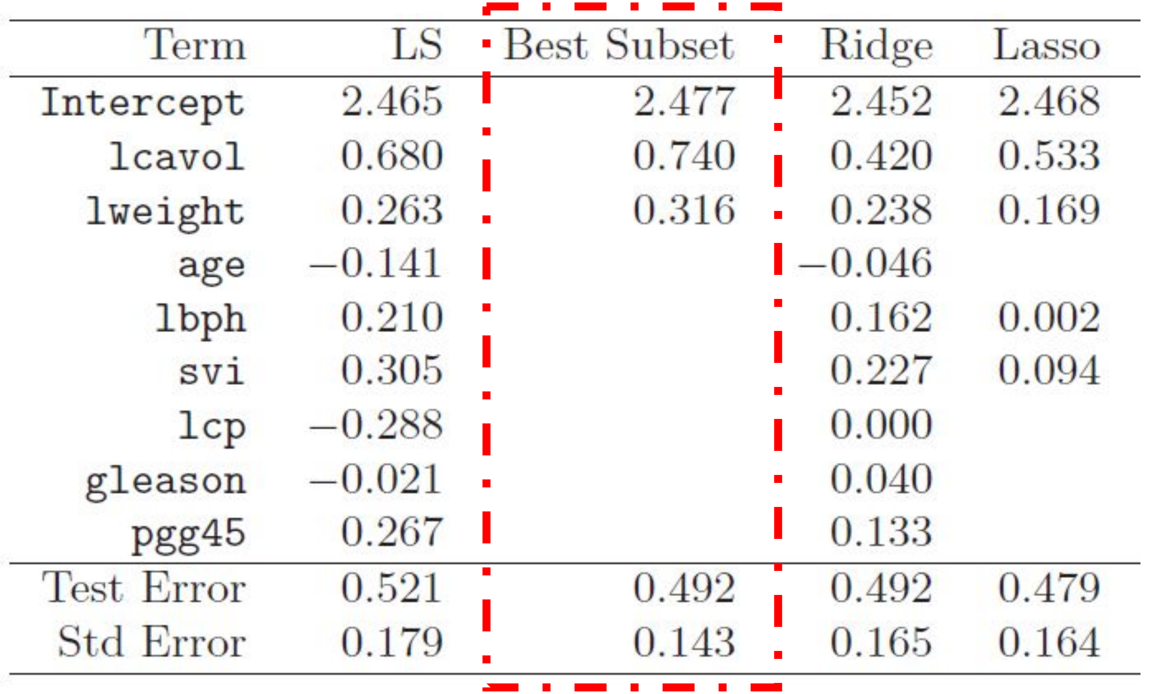
Best-Subset Selection



Feature Selection: Prostate Cancer Dataset

Best subset works well!

reasonably good test error, low standard deviation, and only based on two features!



Term	LS	Best Subset	Ridge	Lasso
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svi	0.305		0.227	0.094
lcp	−0.288		0.000	
gleason	−0.021		0.040	
pgg45	0.267		0.133	
Test Error	0.521	0.492	0.492	0.479
Std Error	0.179	0.143	0.165	0.164

[Source: Hastie et al. (2001)]

Best-Subset Selection : Prostate Cancer Dataset

Time complexity

- Data have 8 features, there are 8-choose-k subsets for each k=1,…,8 for a total of 255 models
- Using 10-fold cross-val requires 10 x 255 = 2,550 training runs!
- In general, $O(2^p)$ time complexity

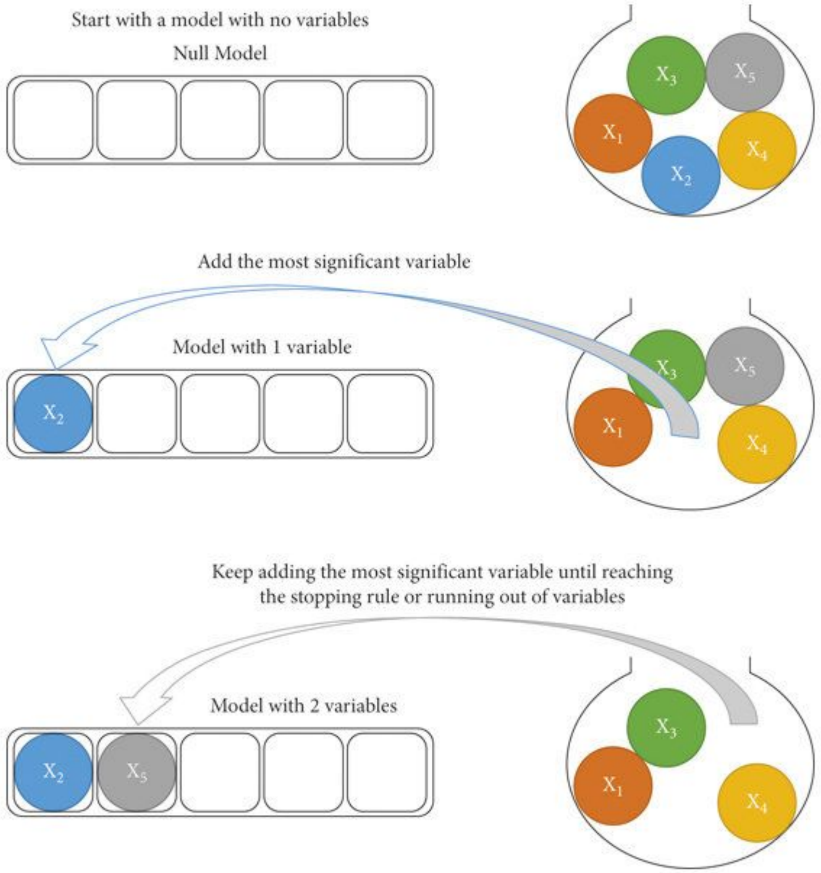
… who can afford exponential time complexity?

Forward Sequential Selection

An efficient method adds the most predictive feature one-by-one

```
featSel = empty
featUnsel = All features
For iter in 1,…,p:
  For kfeat in featUnsel:
    thisFeat = featSel + kfeat
    model = Train model on thisFeat features
    score = Evaluate model using cross-validation
  featSel = featSel + best scoring feature
  featUnsel = featUnsel – best scoring feature
Choose the model with best cross-validation score
```

Forward Sequential Selection

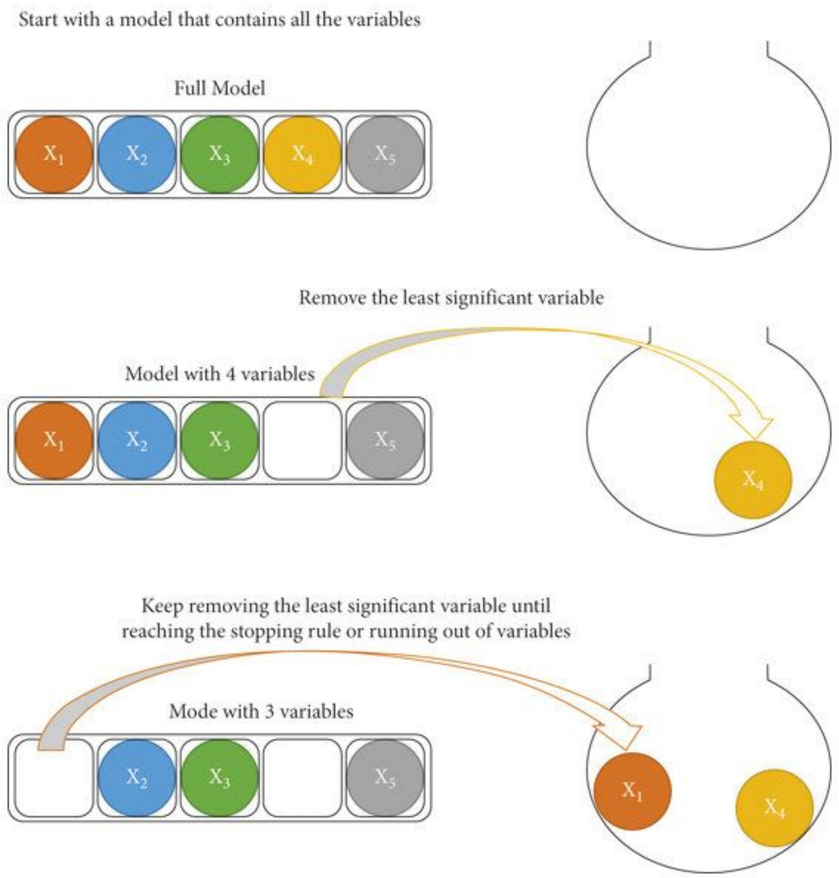

Start with a model with no variables
Null Model
X_3
X_5
X_1
X_4
X_2
Add the most significant variable
Model with 1 variable
X_2
X_3
X_5
X_1
X_4
Keep adding the most significant variable until reaching the stopping rule or running out of variables
Model with 2 variables
X_2
X_5
X_3
X_1
X_4

Backward Sequential Selection

Backwards approach starts with *all* features and removes one-by-one

```
featSel = All features
For iter in 1,…,p:
  For kfeat in featSel:
    thisFeat = featSel - kfeat
    model = Train model on thisFeat features
    score = Evaluate model using cross-validation
  featSel = featSel – **worst** scoring feature
Choose the model with best cross-validation score
```

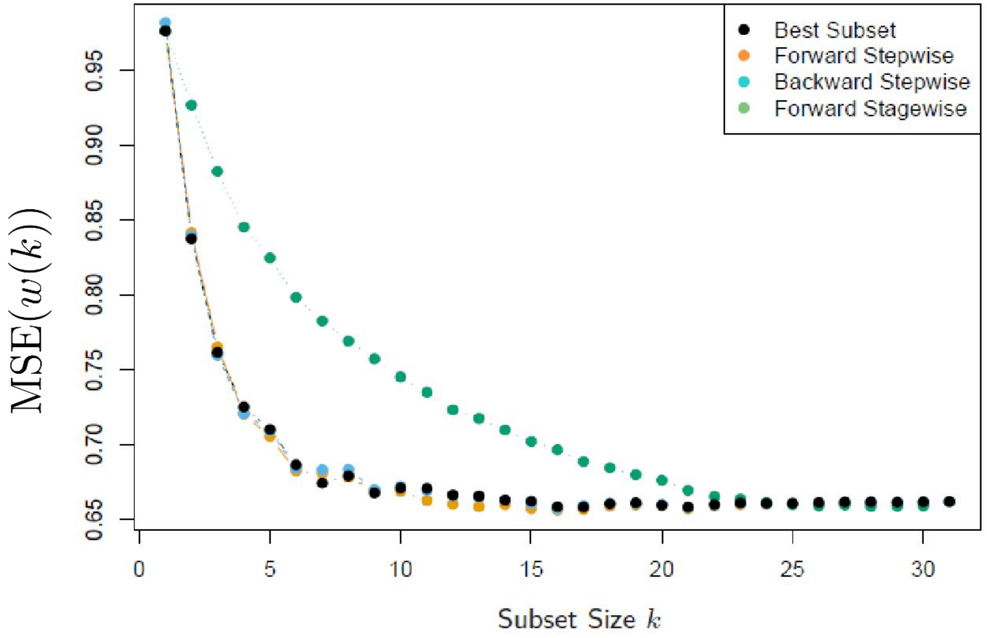
Backward Sequential Selection



Start with a model that contains all the variables
Full Model
X_1
X_2
X_3
X_4
X_5
Remove the least significant variable
Model with 4 variables
X_1
X_2
X_3
X_5
X_4
Keep removing the least significant variable until reaching the stopping rule or running out of variables
Mode with 3 variables
X_2
X_3
X_5
X_1
X_4

Comparing Feature Selection Methods

Sequential selection is greedy, but often performs well…



Example Feature selection on synthetic model with p=30 features with pairwise correlations (0.85). True feature weights are all zero except for 10 features, with weights drawn from N(0,6.25).

Sequential selection with p features takes O(p^2) time, compared to exponential time for best subset

Sequential feature selection available in Scikit-Learn under:

`feature_selection.SequentialFeatureSelector`

General Principles of Regularization

- From the loss function point of view

$$\text{Model} = \min_{\text{model}} \text{Loss}(\text{Model}, \text{Data}) + \lambda \cdot \text{Regularizer}(\text{Model})$$

Regularization Strength

Regularization Penalty

- We will see more examples of loss functions going forward.