Comparison of regression methods seen so far

1. **Ordinary least squares (OLS)**
   - Minimizes sum of squares.
   - Best linear unbiased estimator.
   - Solution not unique when \( n < p \).
   - Estimate unstable when the predictors are collinear.
   - Generally does not lead to best prediction error. Bias-variance trade-off.
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2. Ridge regression ($\ell_2$ penalty)
   - Regularized solution.
   - Estimator exists and is stable, even when $n < p$.
   - Easy to compute (add multiple of identity to $X^TX$).
   - Coefficients not set to zero (no model selection).
Subset selection methods (best subset, stepwise and stagewise approaches)

- Generally leads to a favorable bias-variance trade-off.
- Model selection. Leads to models that are easier to interpret and work with.
- Can be computationally intensive (e.g. best subset can only be computed for small $p$)
- Some of the approaches are greedy/less-rigorous.
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4 Lasso ($\ell_1$ penalty)
   - Shrinks and sets to zero the coefficients (shrinkage + model selection).
   - Generally leads to a favorable bias-variance trade-off.
   - Model selection. Leads to models that are easier to interpret and work with.
   - Can be efficiently computed.
   - Supporting theory. Active area of research.
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Cross-validation is a popular approach for rigorously choosing parameters. *K*-fold cross-validation: Split data into *K* equal (or almost equal) parts/folds at random. For each parameter $\lambda_i$ do for $j = 1, \ldots, K$ do

- Fit model on data with fold *j* removed.
- Test model on remaining fold $\rightarrow j$-th test error.

end for

Compute average test errors for parameter $\lambda_i$.

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Pick parameter with smallest average error.
Choosing parameters: cross-validation

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**K-fold cross-validation:**

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  end for
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Pick parameter with smallest average error.
More precisely,

- Split data into \( K \) folds \( F_1, \ldots, F_K \).

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- Let $L(y, \hat{y})$ be a *loss function*. For example,

$$L(y, \hat{y}) = \|y - \hat{y}\|_2^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2.$$
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$$CV(\lambda) := \frac{1}{n} \sum_{k=1}^{n} \sum_{i \in F_k} L(y_i, f_{\lambda}^{-i}(x_i))$$
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\]

- Pick \( \lambda \) among a relevant set of parameters

\[
\hat{\lambda} = \arg\min_{\lambda \in \{\lambda_1, \ldots, \lambda_m\}} CV(\lambda)
\]
Scikit-learn has nice general methods for splitting data.

```python
from sklearn.cross_validation import train_test_split
import numpy as np

# Generate random data
n = 100
p = 5

X = np.random.randn(n,p)
epsilon = np.random.randn(n) # Not (n,1)
beta = np.random.rand(p)
y = X.dot(beta) + epsilon

# Train-test split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25)

print X_train.shape
print X_test.shape
print y_train.shape
print y_test.shape

# K-fold CV
from sklearn.cross_validation import KFold
kf = KFold(100, n_folds=10)
for train, test in kf:
    print("%s %s" % (train, test))
```
import numpy as np
from sklearn.linear_model import Lasso
from sklearn.cross_validation import KFold

# Generate random data
n = 100
p = 100
X = np.random.randn(n,p)
epsilon = np.random.randn(n)
beta = np.zeros((p,1))
beta[0:8] = 10*np.random.rand(8,1)
y = X.dot(beta) + epsilon

K = 10  # K-fold CV
alphas = np.exp(np.linspace(np.log(0.01),np.log(1),100))
N = len(alphas)  # Number of lasso parameters
scores = np.zeros((N,K))
kf = KFold(n, n_folds=K)

for i in range(N):
    clf = Lasso(alphas[i])
    for j, (train, test) in enumerate(kf):
        X_train, X_test, y_train, y_test =
            X[train], X[test], y[train], y[test]
        clf.fit(X_train, y_train)
        scores[i,j] = clf.score(X_test, y_test)  # Returns $R^2$

# Compute average CV score for each parameter
scores_avg = scores.mean(axis=1)
Implementing CV

Note: Here we want to choose $\alpha$ to maximize the $R^2$.

Scikit-learn sometimes has automatic methods for performing cross-validation.

```python
import numpy as np
from sklearn.linear_model import LassoCV
import matplotlib.pyplot as plt

# Generate random data
n = 100
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X = np.random.randn(n,p)
epsilon = np.random.randn(n,1)
beta = np.zeros((p,1))
beta[0:8] = 10*np.random.rand(8,1)
y = X.dot(beta) + epsilon
K = 10  # K-fold CV
y = y.reshape(n) # LassoCV doesn't work if y is (n x 1)
clf = LassoCV(n_alphas = 100, cv = K)
clf.fit(X,y)

Remark: safer to examine CV curve.
```
For each parameter, one can also naturally report the standard deviation of the error across the different folds.

```python
# Compute average CV score for each parameter
scores_avg = scores.mean(axis=1)
scores_std = scores.std(axis=1)

plt.plot(alphas, scores_avg,'-b')
plt.fill_between(alphas, scores_avg-scores_std, scores_avg+scores_std, facecolor='r', alpha=0.5)
plt.legend([r'Average $R^2$', r'One sd interval'], loc = 'lower left')
plt.plot(alphas, np.ones((len(alphas),1))*scores_avg.max(),'--k', linewidth=1.2)
plt.xlabel(r'$\alpha$', fontsize=18)
plt.ylabel(r'$R^2$', fontsize = 18)
plt.show()
```
One sd rule (cont.)

- Provides an idea of the error made when estimating the $R^2$.
- Can pick a lasso parameter for which the maximum $R^2$ is within a one standard deviation interval of the actual value.
- Useful technique to select a model that is more sparse in a principled way (when necessary).
Two related, but different goals:

- **Model selection**: estimating the performance of different models in order to choose the “best” one.

- **Model assessment**: having chosen a final model, estimating its prediction error (generalization error) on new data.

  Generally speaking, the CV error provides a good estimate of the prediction error.

  When enough data is available, it is better to separate the data into three parts: train/validate, and test.

  Typically:
  - 50% train,
  - 25% validate,
  - 25% test.

  Test data is kept in a vault, i.e., not used for fitting or choosing the model.

  Other methods (e.g. AIC, BIC, etc.) can be used when working with very little data.
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  ![Train Validation Test](image)

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