MATH 637: Mathematical Techniques in Data Science
Model selection

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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.
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2. Ridge regression (ℓ_2 penalty)
    - Regularized solution.
    - Estimator exists and is stable, even when $n < p$.
    - Easy to compute (add multiple of identity to $X^T X$).
    - Coefficients not set to zero (no model selection).

Comparison of regression methods seen so far (cont.)

3. 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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   - Can be computationally intensive (e.g. best subset can only be computed for small p)
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4. Lasso (ℓ_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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- An *optimal* parameter needs to be chosen in a principled way.
- **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 $\to$ $j$-th test error.
    end for
    Compute average test errors for parameter $\lambda_i$.
end for
Pick parameter with smallest average error.
```

K-fold CV

More precisely,

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

1	2	3	4	5
Train	Train	Validation	Train	Train

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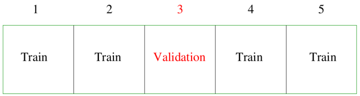

- Let $L(y, \hat{y})$ be a *loss function*. For example, $L(y, \hat{y}) = \|y - \hat{y}\|_2^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2$.

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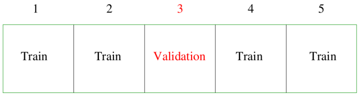

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- Let $f_\lambda^{-k}(\mathbf{x})$ be the model fitted on all, but the k-th fold.

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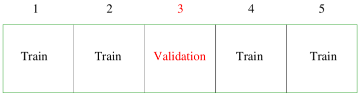

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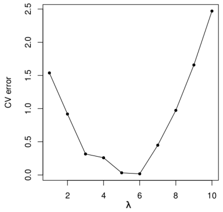
- Let

$$CV(\lambda) := \frac{1}{n}\sum_{k=1}^{n}\sum_{i \in F_k} L(y_i, f_\lambda^{-i}(\mathbf{x}_i))$$



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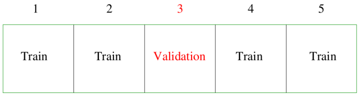

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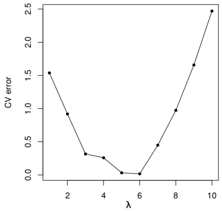


- Pick λ among a *relevant* set of parameters

$$\hat{\lambda} = \operatorname*{argmin}_{\lambda \in \{\lambda_1, \dots, \lambda_m\}} CV(\lambda)$$

Python

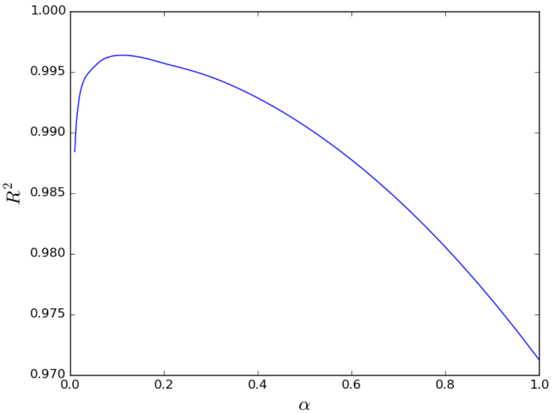
Scikit-learn has nice general methods for splitting data.

```
from sklearn.model_selection import train_test_split
import numpy as np
from sklearn.linear_model import Lasso

# Generate random data
n = 100
p = 5

X = np.random.randn(n,p)
epsilon = np.random.randn(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.model_selection import KFold
kf = KFold(n_splits=10)
for train, test in kf.split(X):
        print("Train %s \n Test %s" % (train, test))
```

Python: Implementing CV

```
import numpy as np
from sklearn.linear_model import Lasso
from sklearn.model_selection import KFold

# Generate random data
n = 100
p = 100

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
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_splits=10)

for i in range(N):
   clf = Lasso(alphas[i])
   for j, (train, test) in enumerate(kf.split(X)):
      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 α to *maximize* the R^2.

Exercise: Implement 10-fold CV for Ridge regression. Plot CV error.

LassoCV

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

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

# Generate random data
n = 100
p = 100

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)
```

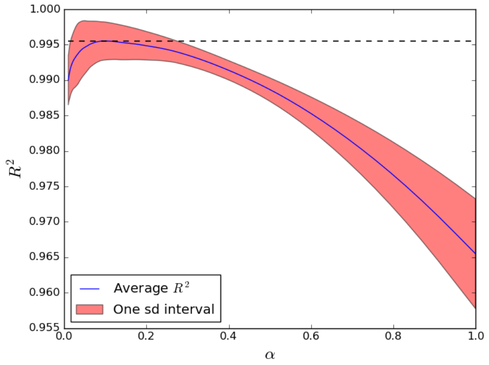
Remark: safer to examine CV curve.

One SD rule

For each parameter, one can also naturally report the standard deviation of the error acroos the different folds.

```
# 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, s
  cores_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).

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Two related, but different goals:

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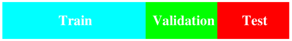
- When *enough* data is available, it is better to separate the data into three parts: train/validate, and test.



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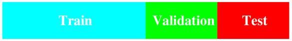

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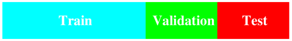

- Typically: 50% train, 25% validate, 25% test.
- Test data is "kept in a vault", i.e., not used for fitting or choosing the model.
- Other methods (e.g. AIC, BIC, etc.) can be used when working with very little data.