Cross validation

Jeffrey Leek, Assistant Professor of Biostatistics
Johns Hopkins Bloomberg School of Public Health

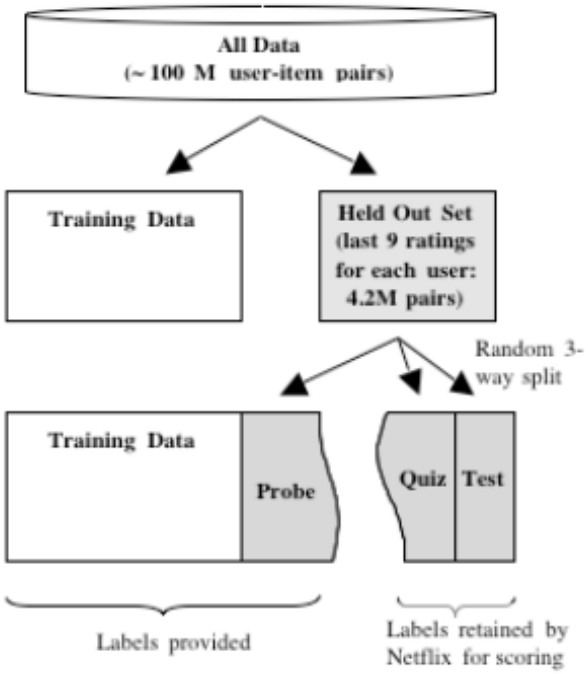
Key ideas

- Sub-sampling the training data
- Avoiding overfitting
- Making predictions generalizable

Steps in building a prediction

1. Find the right data
2. Define your error rate
3. Split data into:
   - Training
   - Testing
   - Validation (optional)
4. On the training set pick features
5. On the training set pick prediction function
6. On the training set cross-validate
7. If no validation - apply 1x to test set
8. If validation - apply to test set and refine
9. If validation - apply 1x to validation

Study design

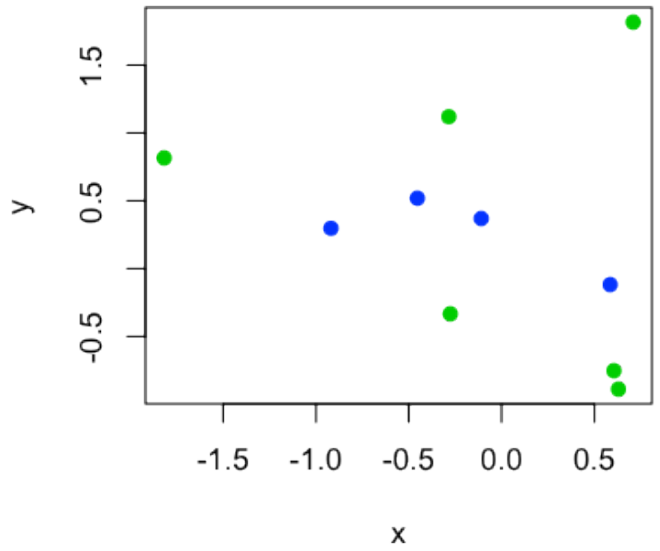


http://www2.research.att.com/~volinsky/papers/ASAStatComp.pdf

4/14

Overfitting

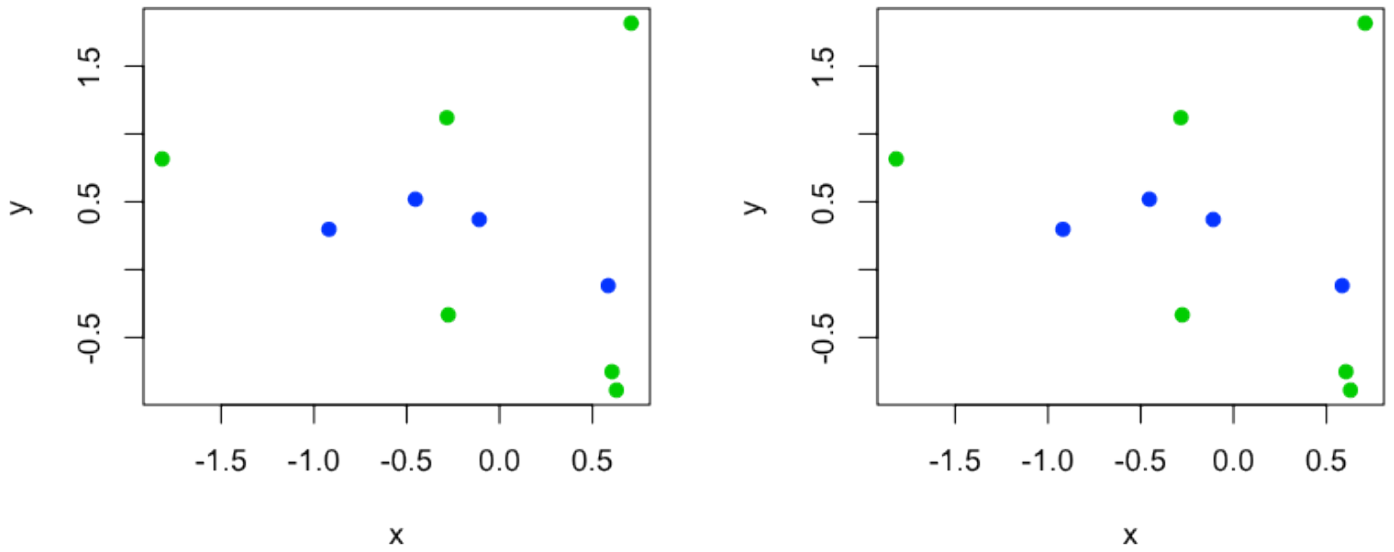
```
set.seed(12345)
x <- rnorm(10); y <- rnorm(10); z <- rbinom(10,size=1,prob=0.5)
plot(x,y,pch=19,col=(z+3))
```



Classifier

If -0.2 < y < 0.6 call blue, otherwise green

```
par(mfrow=c(1,2))
zhat <- (-0.2 < y) & (y < 0.6)
plot(x,y,pch=19,col=(z+3)); plot(x,y,pch=19,col=(zhat+3))
```



6/14

New data

If -0.2 < y < 0.6 call blue, otherwise green

```
set.seed(1233)
xnew <- rnorm(10); ynew <- rnorm(10); znew <- rbinom(10,size=1,prob=0.5)
par(mfrow=c(1,2)); zhatnew <- (-0.2 < ynew) & (ynew < 0.6)
plot(xnew,ynew,pch=19,col=(z+3)); plot(xnew,ynew,pch=19,col=(zhatnew+3))
```

Key idea

1. Accuracy on the training set (resubstitution accuracy) is optimistic
2. A better estimate comes from an independent set (test set accuracy)
3. But we can't use the test set when building the model or it becomes part of the training set
4. So we estimate the test set accuracy with the training set.

Cross-validation

Approach:

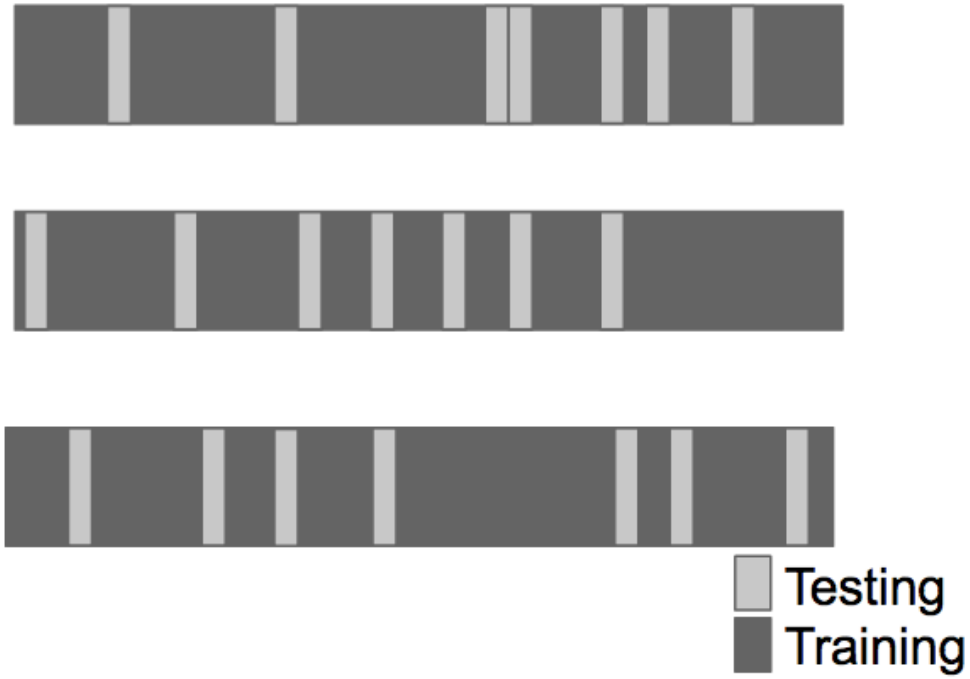
1. Use the training set
2. Split it into training/test sets
3. Build a model on the training set
4. Evaluate on the test set
5. Repeat and average the estimated errors

Used for:

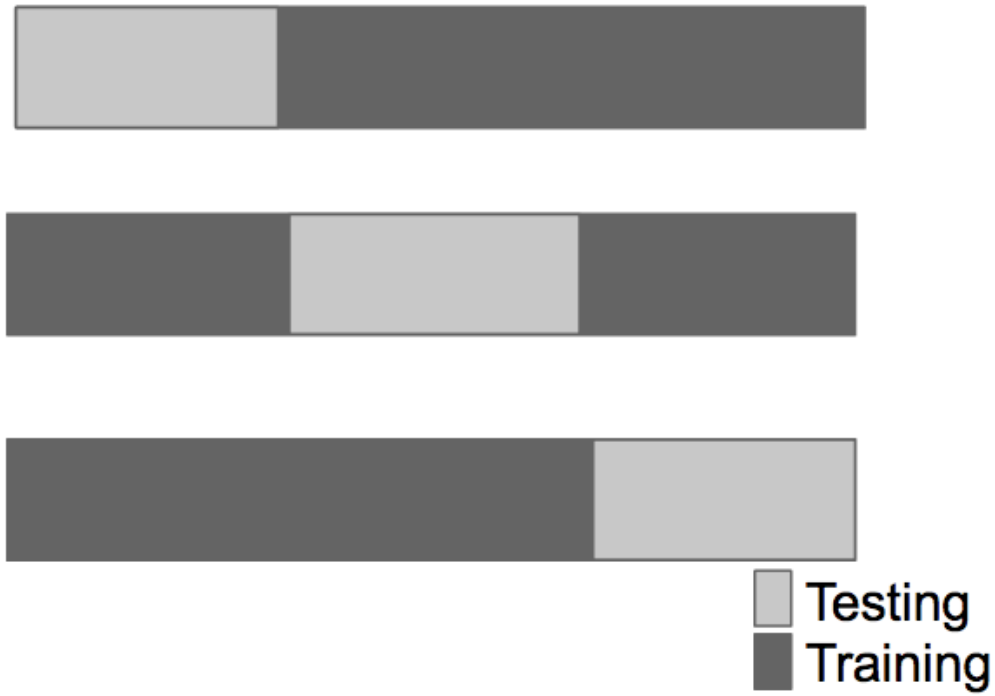
1. Picking variables to include in a model
2. Picking the type of prediction function to use
3. Picking the parameters in the prediction function
4. Comparing different predictors

9/14

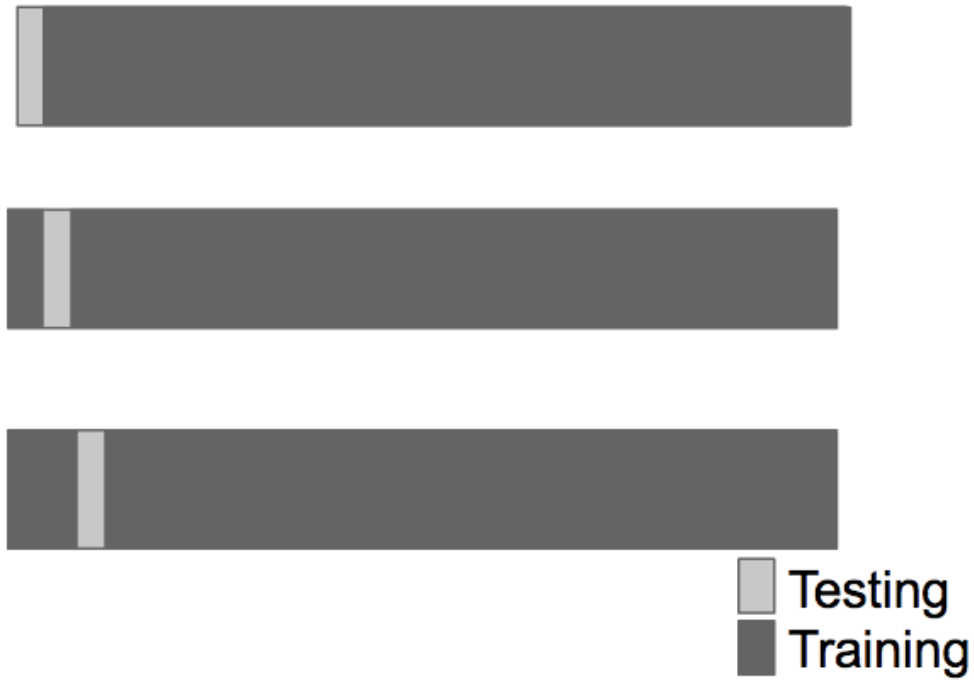
Random subsampling



K-fold



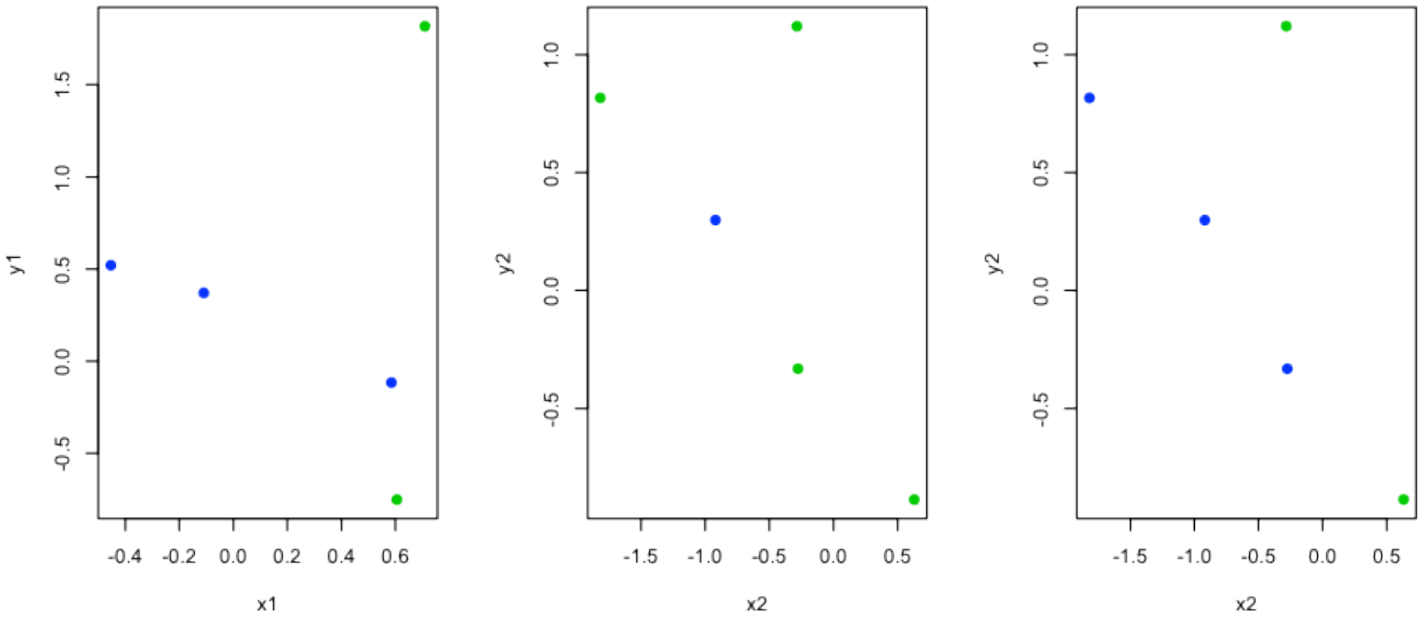
Leave one out



12/14

Example

```
y1 <- y[1:5]; x1 <- x[1:5]; z1 <- z[1:5]
y2 <- y[6:10]; x2 <- x[6:10]; z2 <- z[6:10];
zhat2 <- (y2 < 1) & (y2 > -0.5)
par(mfrow=c(1,3))
plot(x1,y1,col=(z1+3),pch=19); plot(x2,y2,col=(z2+3),pch=19); plot(x2,y2,col=(zhat2+3),pch=19)
```



13/14

Notes and further resources

- The training and test sets must come from the same popluation.
- Sampling should be designed to mimic real patterns (e.g., sampling time chunks for time series)
- Cross validation estimates have variance - it is difficult to estimate how much
- Cross validation in R
- cvTools
- boot