Resampling

Practical Machine Learning (with R)

UC Berkeley

MODEL PERFORMANCE

Model Performance (thus far)

- Determine performance metric:
  - **RMSE (regression)**
  - **Accuracy (classification)**
- Fit Model
- Calculate statistic (“metric”) on Data

“*training*” or “*apparent*” performance will:

- over-fit to training data
- predict very well, unbelievably well
- Not generalize to *new data.*

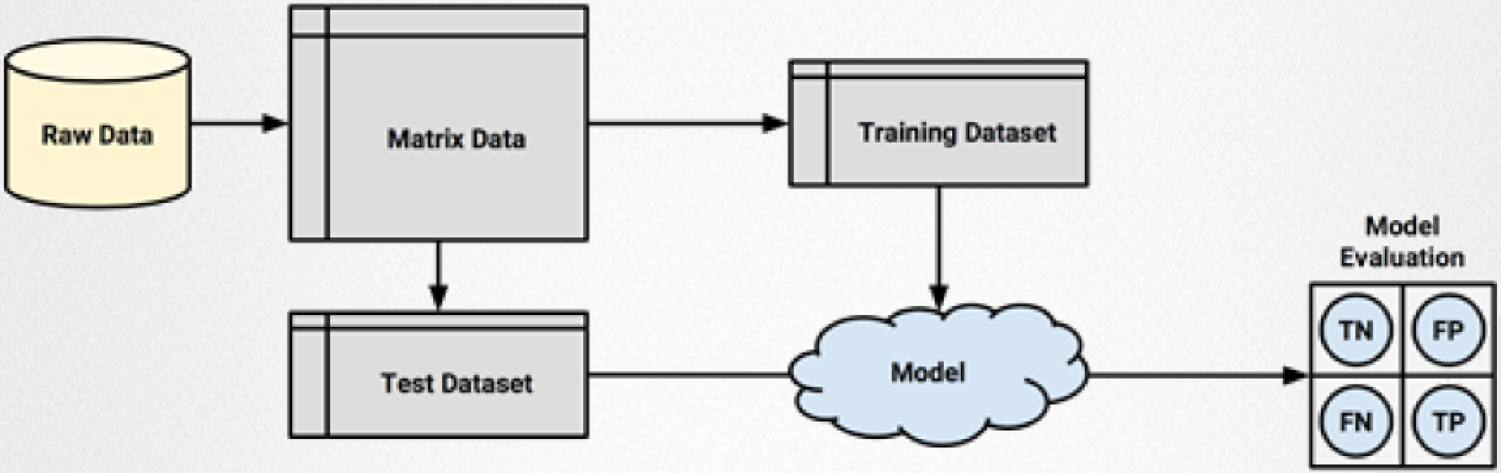
Cardinal Rule

DO NOT ESTIMATE PERFORMANCE ON YOUR TRAINING DATA

→ Need technique for unbiased estimate for calculating performance

1: Hold Out Method

- Partition data into train and test sets



- What are the partition ratios?
  - Large N: doesn’t matter
  - Small N: Need to provide sufficient

IS THERE A BETTER WAY?

Measurements and Statistics

Measurement

Quantification of a phenomena

Deterministic

≠

Stochastic

Statistic

measurement of a *stochastic* phenomena

Examples:

- `mean(x)   <- x is generated by a stochastic process`
- `sd(x)`

EXERCISE: CALCULATE `sd( mean(x) )`

Statistics

- “True” value unknown → uncertainty
- Uncertainty can be measured
  - Variance
  - Standard deviation
  - Confidence Interval
  - …

- Repeated measurements decrease the uncertainty

RESAMPLING

Kuhn benefits of resampling

- Selection of optimal tuning parameter(s) “With so many choices how do we

- Unbiased estimate of model performance

Resampling Strategies

- Repeated Holdouts
- K-Fold Cross Validation
- Bootstrap

Repeated Holdout

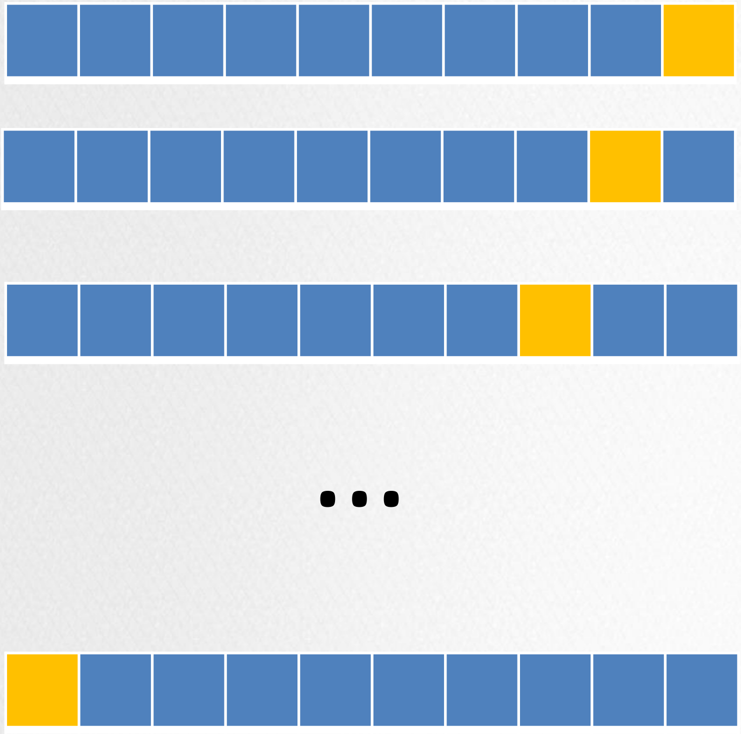
AKA Monte Carlo Splitting

- Split data 75%-25%
  - Fit Model
  - Calculate Performance Metric
  - Repeat with Different Split(K-times)

- Calculate Metric

$$Metric = AVG_i(metric)$$

10-Fold Cross Validation



LOOCV : K→n

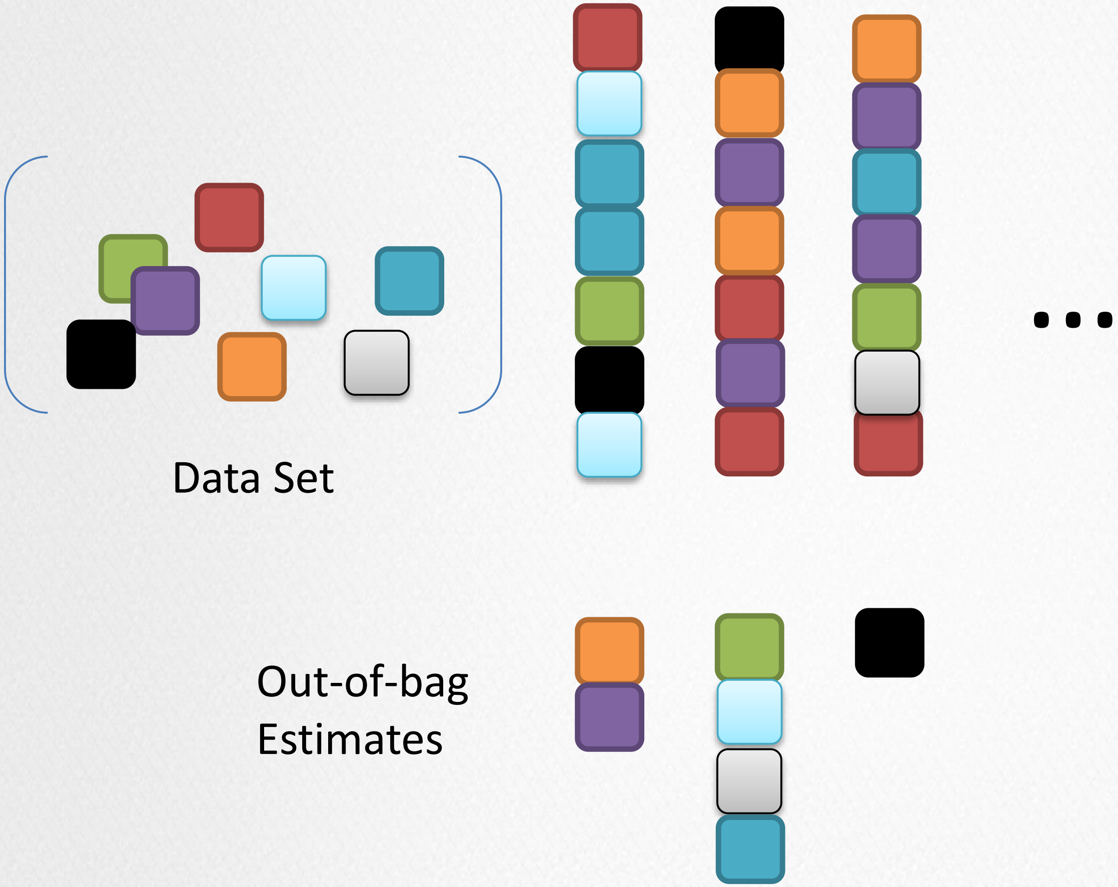
- Split the data set into 10 equal sized samples.
- Leave one sample out (fold)
  - Fit the model
  - calculate the metric on the fold
  - Repeat choosing another sample until done
- Calculate Metric

$$Metric = AVG_i(metric)$$

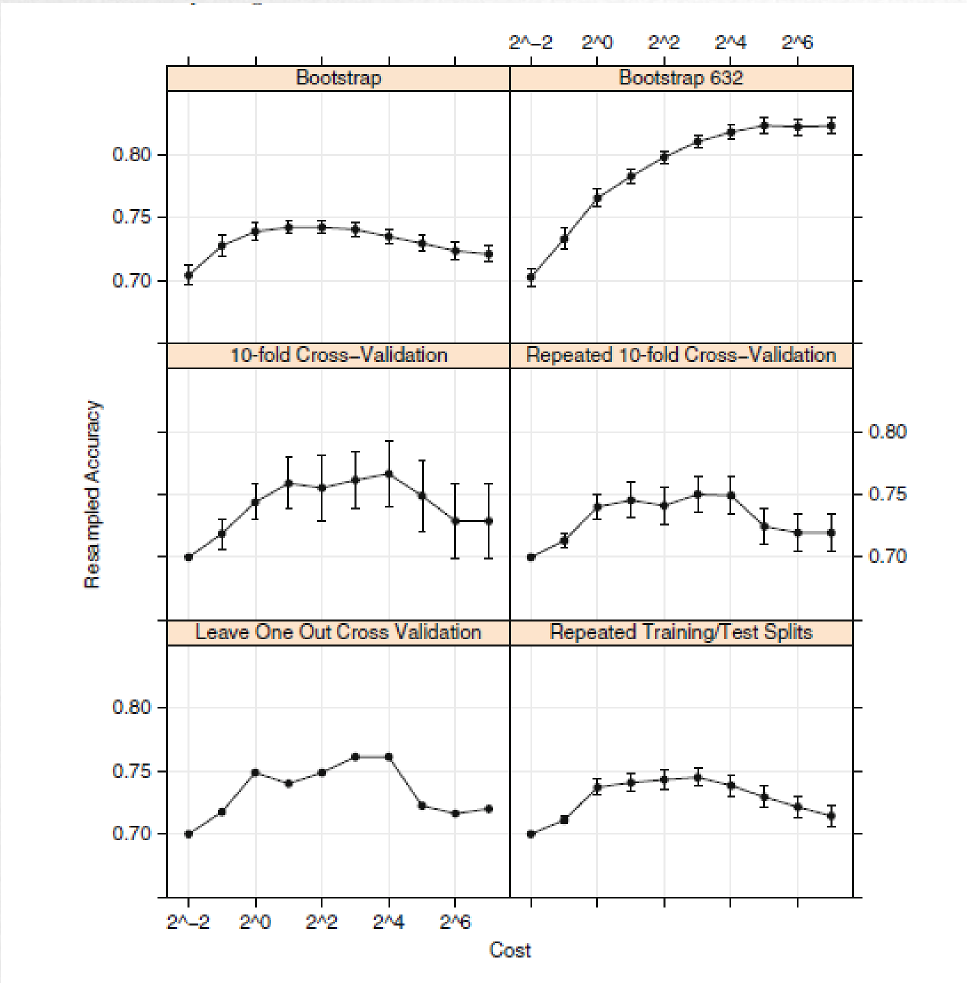
- 5 or 10-fold common

Bootstrap

- "Sampling with Replacement"



Which Is Best?



- There isn’t one.

K-fold cross validation

Higher Variance
Lower Bias

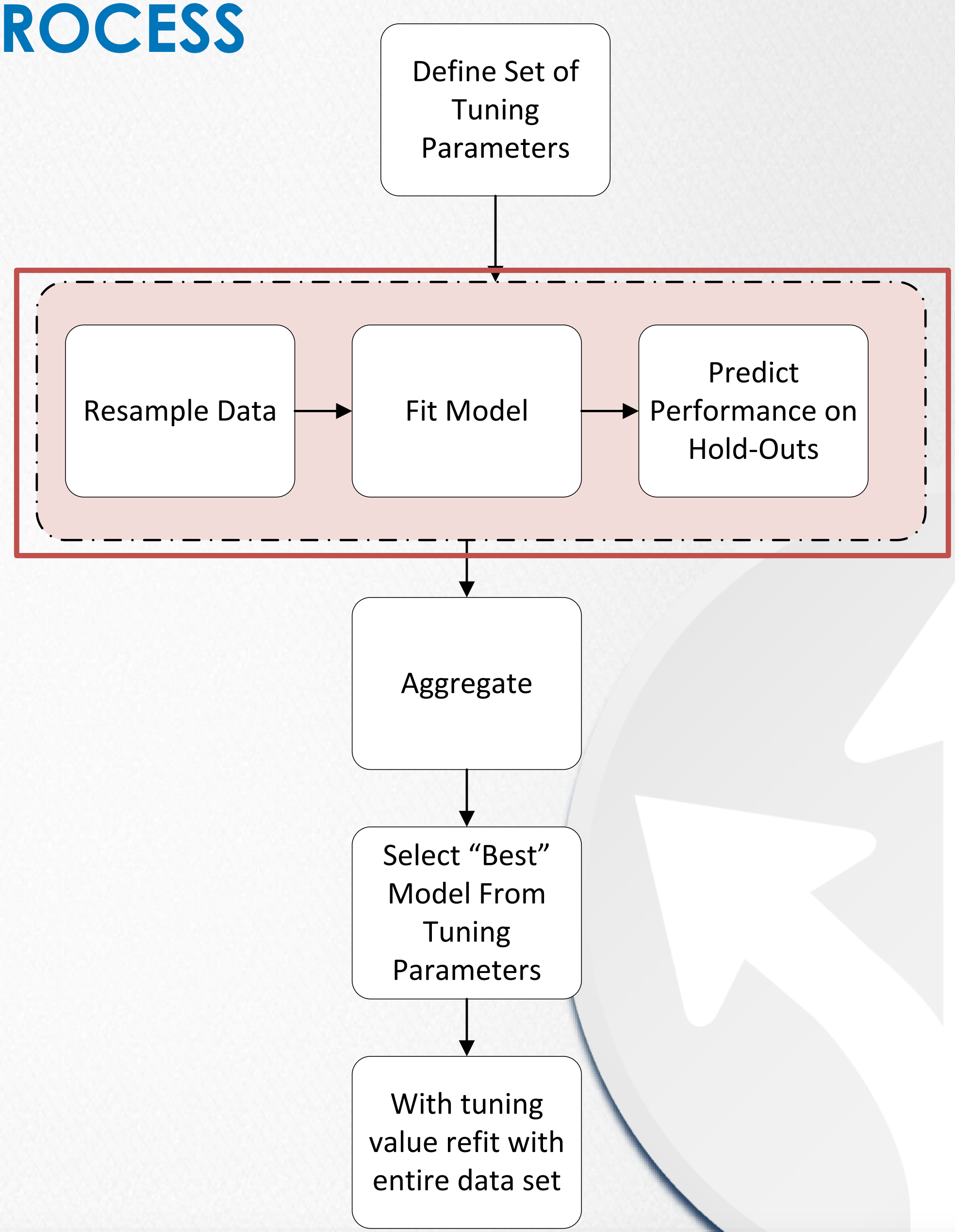
Bootstrap

Lower Variance
Higher Bias

Better to employ resampling than worry about not resampling

Kuhn's Resampling Process

Today's Focus


Define Set of Tuning Parameters
Resample Data
Fit Model
Predict Performance on Hold-Outs
Aggregate
Select "Best" Model From Tuning Parameters
With tuning value refit with entire data set

Resampling

- Best Solution (n-permitting)
  - split data into training and test data
  - and do what Kuhn says.

Why(?)

- Easy to interpret defend
- Requires data not be consumed by model
- Computationally easy
- Is generally not (by itself) the most accurate → no confidence

MODEL PERFORMANCE IS *NOT* *TRAINING* PERFORMANCE