Methodology: Assessment and Cross-Validation

Dan Sheldon

November 18, 2014

First story

- USPS uses a classifier to distinguish 4 from 9
- Pays \$1 for every mistake
- How much money should it budget for 2015?
- **Model assessment (validation)**: estimate prediction error on future unseen data (generalization)

Second story

- USPS uses regularized logistic regression to prevent overfitting in its classifier
- What value of λ will lead to the model with the least prediction error?
- **Model comparison (selection)**: estimate prediction error for purpose of selecting the best model

Two goals

Model assessment: estimate prediction error on future unseen data (generalization)

Model comparison: estimate prediction error for purpose of selecting the best model

Two goals

Model assessment: estimate prediction error on future unseen data (generalization)

Model comparison: estimate prediction error for purpose of selecting the best model

Can't do either of these with data used to train the model

Data-Generating Mechanism

- Assumption: training data representative of future unseen data
- Formally, training examples and future test examples drawn *independently* from same probability distribtuion $\mathcal{P}$

$$(\mathbf{x}^{(i)}, y^{(i)}) \sim \mathcal{P}$$
$$(\mathbf{x}, y) \sim \mathcal{P}$$

- How to think of this
  - huge bag of input-output pairs $(\mathbf{x}, y)$ ("nature")
  - m training examples pulled out randomly
  - future data drawn also pulled out randomly
  - (picture on board)

In an Ideal World

If we are "data rich", this is what we would do:

- **Validation set**: labeled data reserved to compare models
- **Test set**: labeled data reserved to assess future performance

E.g., 50/25/25 split

In an Ideal World

If we are "data rich", this is what we would do:

- **Validation set**: labeled data reserved to compare models
- **Test set**: labeled data reserved to assess future performance

E.g., 50/25/25 split

Warning: Terminology of validation/test not always consistently used

The Dilemma: Train vs. Test Size

What if you only have 100 training examples? 50? 10?

The dilemma

- More training data $\rightarrow$ more accurate classifier
- More test data $\rightarrow$ better estimate of generalization accuracy

Cross-Validation

(Assume assessment for now... how much will USPS pay?)

Beautiful and simple solution to train/test size dilemma:

- Split data in k equal-sized "folds" (usually 2, 5, 10)
- For each fold, test on that fold while training on all others:

1	2	3	4	5
Train	Train	Validation	Train	Train

- Estimate accuracy by averaging over all folds

Example

5-fold cross-validation

	Train folds	Test folds	Accuracy
12345	2,3,4,5	1	85%
12345	1,3,4,5	2	83%
12345	1,2,4,5	3	91%
12345	1,2,3,5	4	88%
12345	1,2,3,4	5	84%

Average accuracy $= 88.2\%$

Discussion

What if you need to do both model comparison and assessment?

Discussion

What if you need to do both model comparison and assessment?

Fancier methods:

- One fold for validation (e.g. train/valid/test $= 3/1/1$)
- Nested cross-validation