Methodology: Assessment and Cross-Validation

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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**: 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 selection**: compare prediction error of many models to select the best one

Two goals

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

Model selection: compare prediction error of many models to select the best one

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

Data-Generating Mechanism

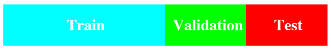
- Assumption: training data representative of future unseen data
- Formally, training examples and future test examples drawn *independently* from same probability distribtuion $\mathcal{P}$

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

- 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

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 → more accurate classifier
- More test data → 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?

Fancier methods:

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

Warning: There is no single agreed-upon methodology that is always best. Methods are applied somewhat flexibly. It’s best to understand the *principles* so you can judge what is (or is not) appropriate.