GENERAL ASSEMBLY

MODEL VALIDATION (TRAIN/TEST SPLIT AND CROSS VALIDATION)

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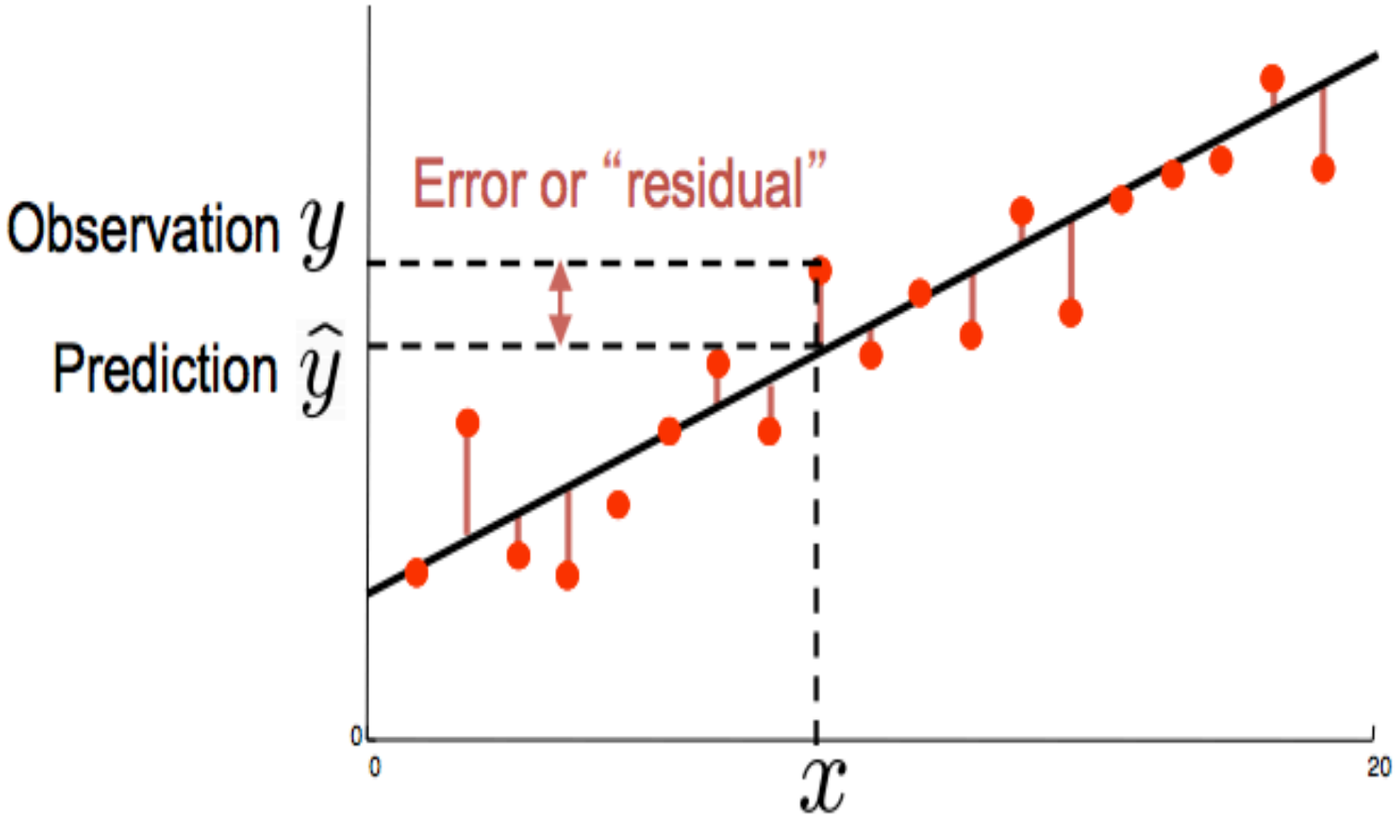
AGENDA

- Review: Modeling
- Training, Validating, Testing
- Cross Validation
- Three-way Train/Test Split
- Coding Implementation

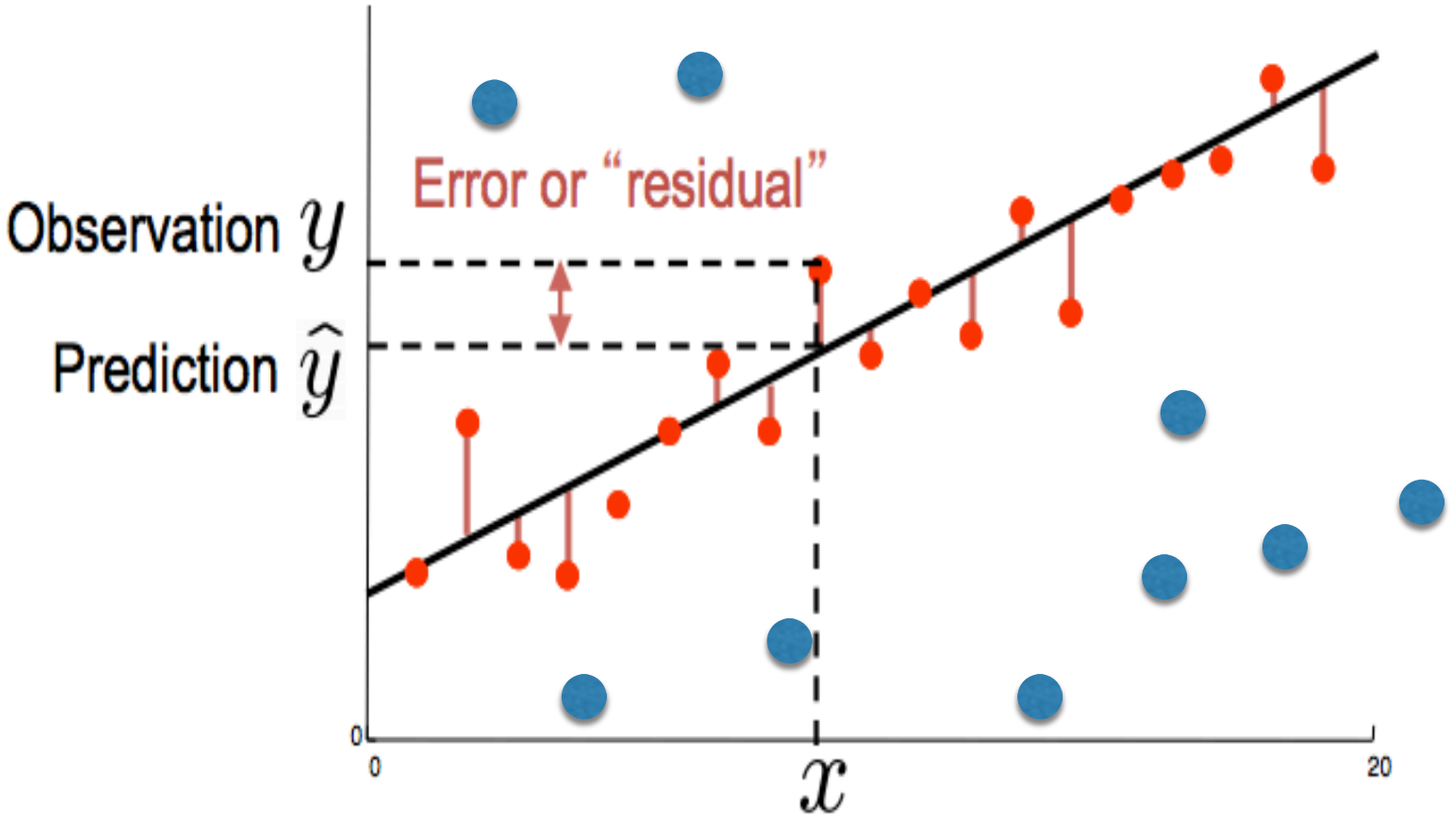
MODELING REVIEW

- Imagine we have EVERY point possible in the universe
- How would we model our data?



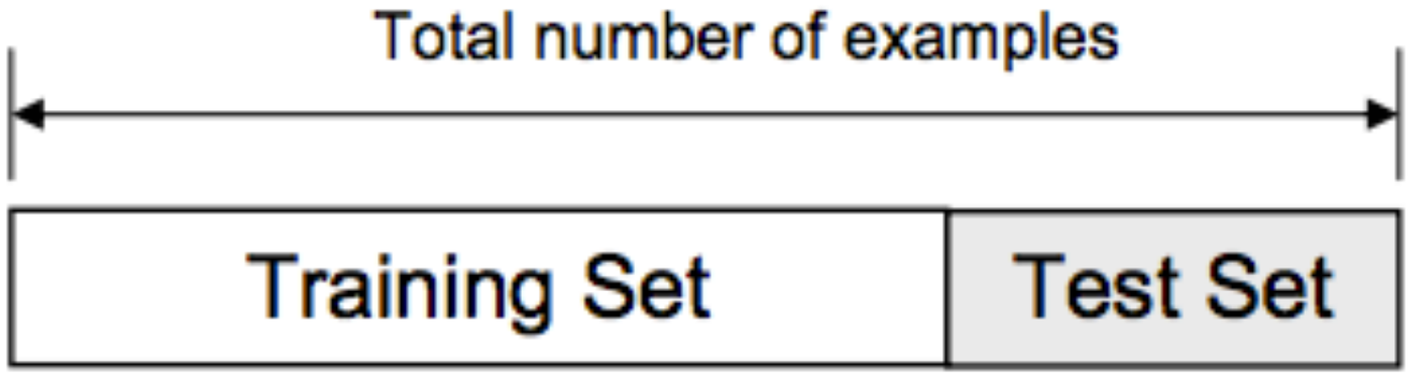
MODELING REVIEW

- Imagine we DO NOT have every point possible in the universe
- How would we model our data?
- Any possible solutions?



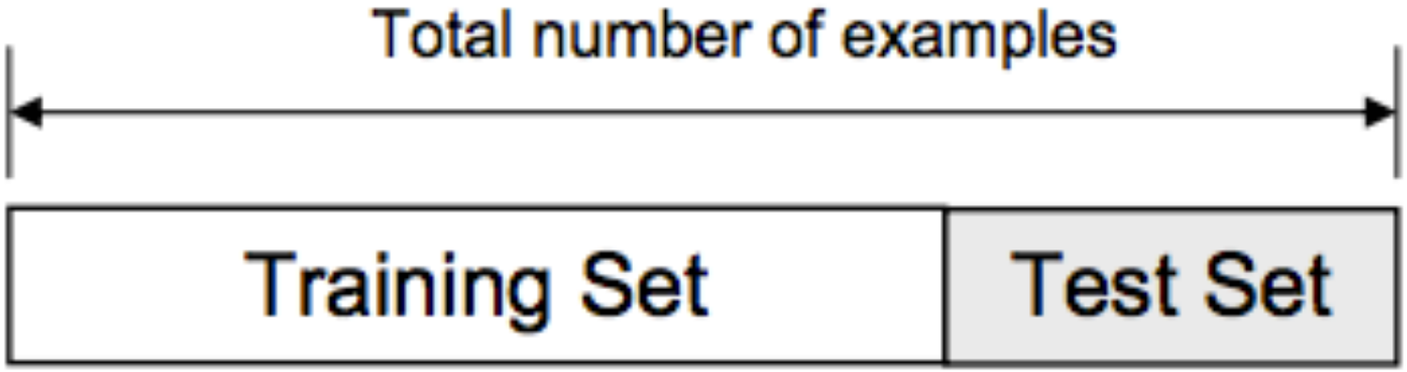
SPLITTING OUR DATA: TRAINING SET, TESTING SET

- THE HOLDOUT METHOD: Train/Test Split
- **Training Set**: Used to train the classifier
- **Testing Set:** Used to estimate the error rate of the trained classifier
- **Advantages?**
- **Disadvantages?**



SPLITTING OUR DATA: TRAINING SET, TESTING SET

- THE HOLDOUT METHOD: Train/Test Split
- **Training Set**: Used to train the classifier
- **Testing Set:** Used to estimate the error rate of the trained classifier
- **Advantages?** Fast! Simple! Computationally inexpensive!
- **Disadvantages?** Eliminating data! Imperfect splits!



THERE MUST BE ANOTHER WAY!

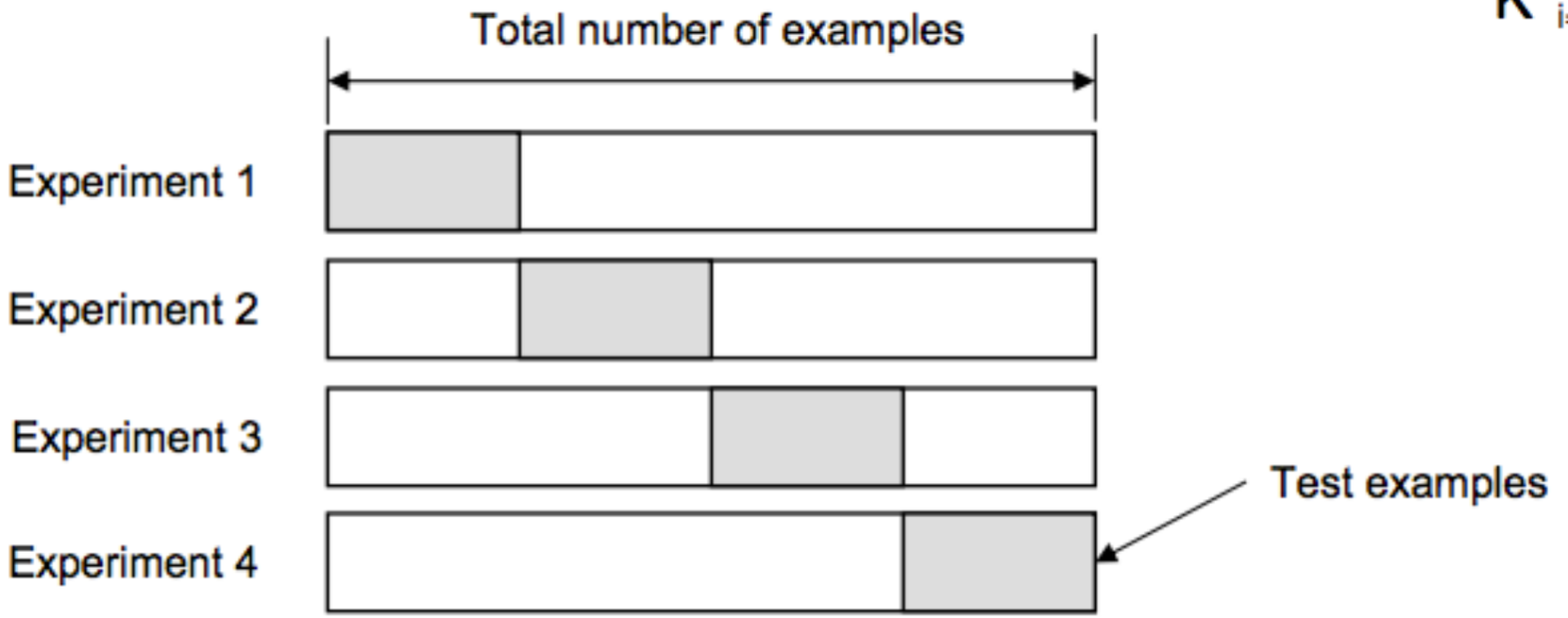
- **How can we use the maximum amount of our data points while still ensuring model integrity?**

- Toss out answers – your answers are valuable parts of being an inquisitive data scientist wanting to test your assumptions

K-FOLDS CROSS VALIDATION

- Split our data into a number of different pieces (folds)
- Train using k-1 folds for training and a different fold for testing
- Average our model against EACH of those iterations
- Choose our model and TEST it against the final fold

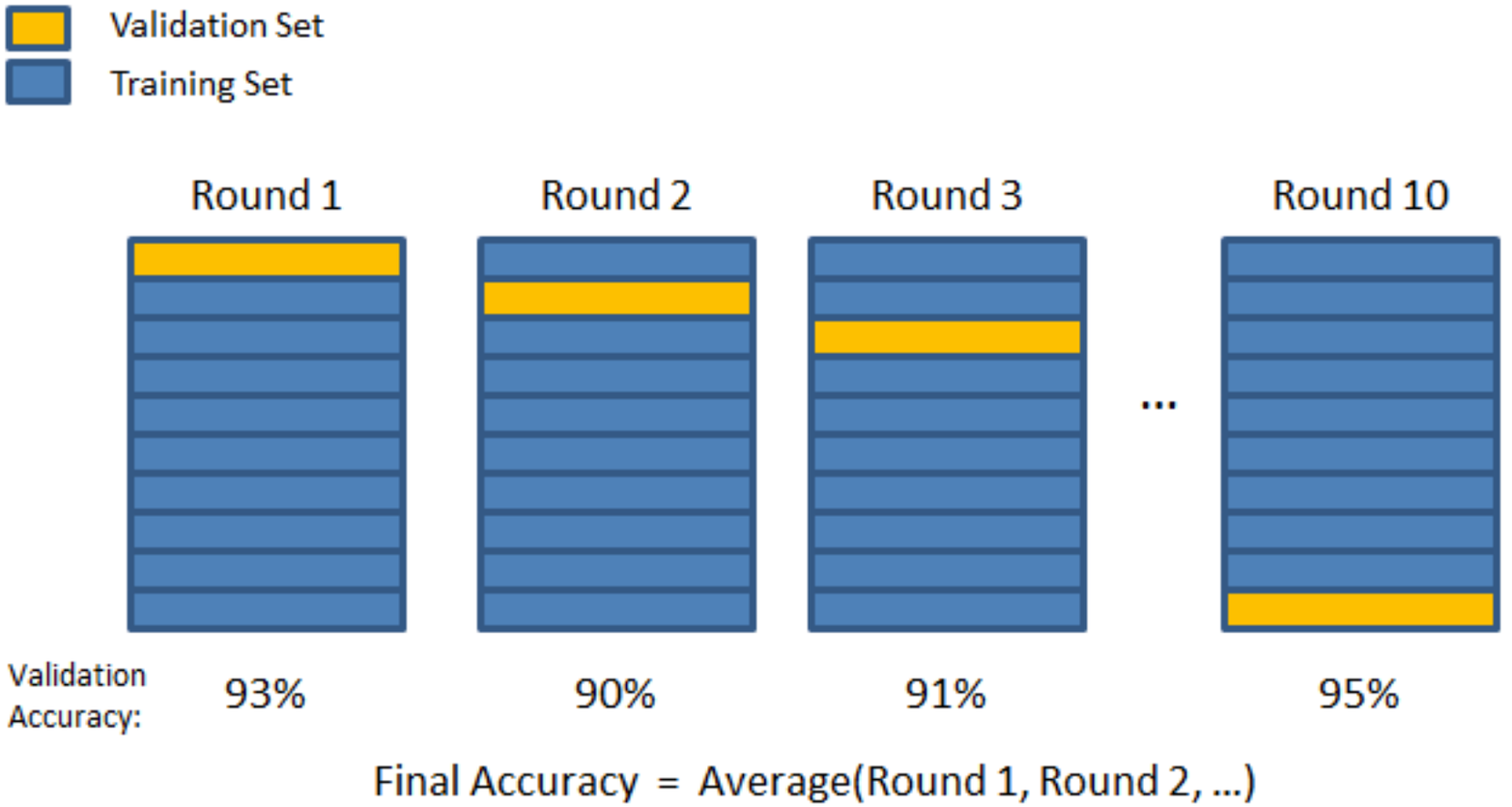
$$E = \frac{1}{K}\sum_{i=1}^{K} E_i$$



HOW MANY FOLDS ARE IN A K-FOLDS MODEL?

K-FOLDS CROSS VALIDATION

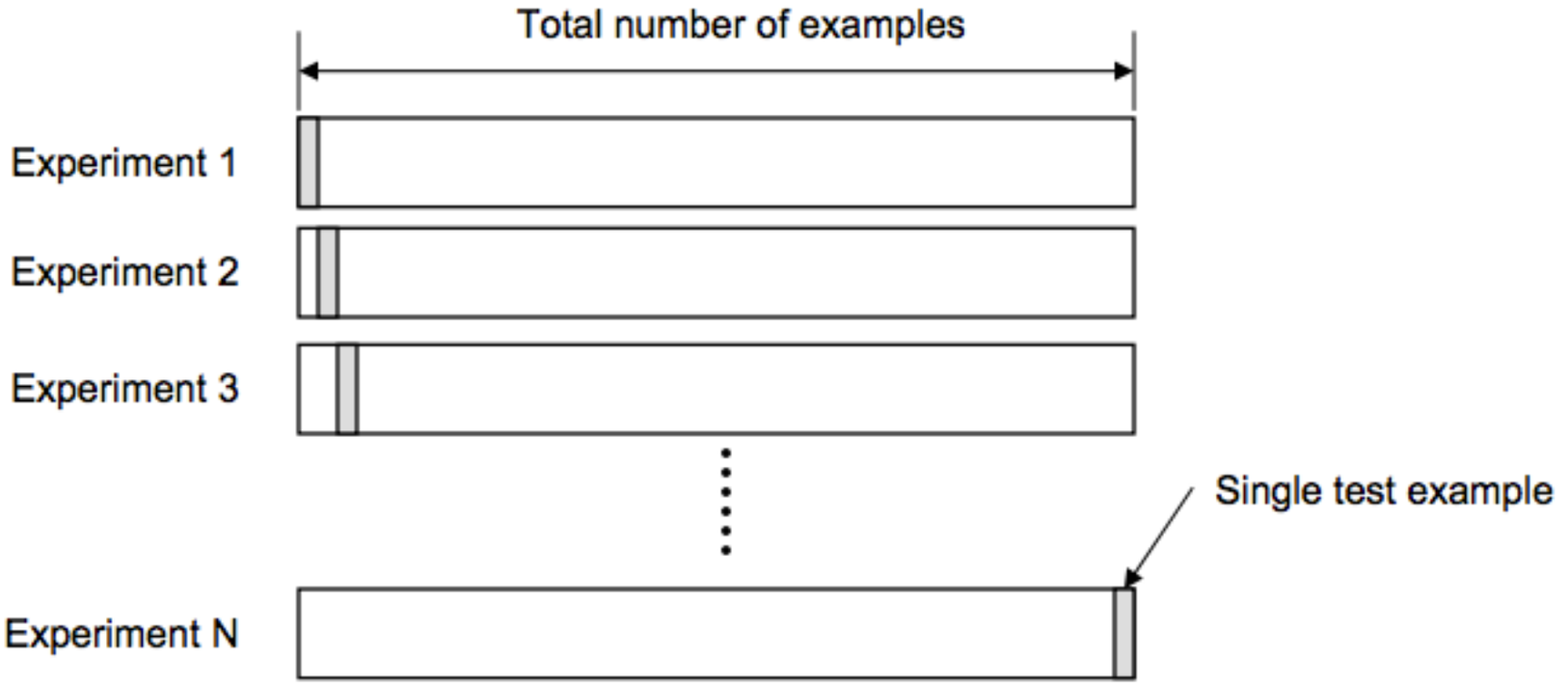
- K=10
- Round 1: Check 9 training sets against one validation set. . . Round 2. . .



LEAVE ONE OUT CROSS VALIDATION (LOOCV)

- K-folds is taken to the logical extreme: K = N
- For a dataset of N examples, perform N experiments
- Average our model against EACH of those iterations
- Choose our model and TEST it against the final fold

$$E = \frac{1}{K}\sum_{i=1}^{K} E_i$$

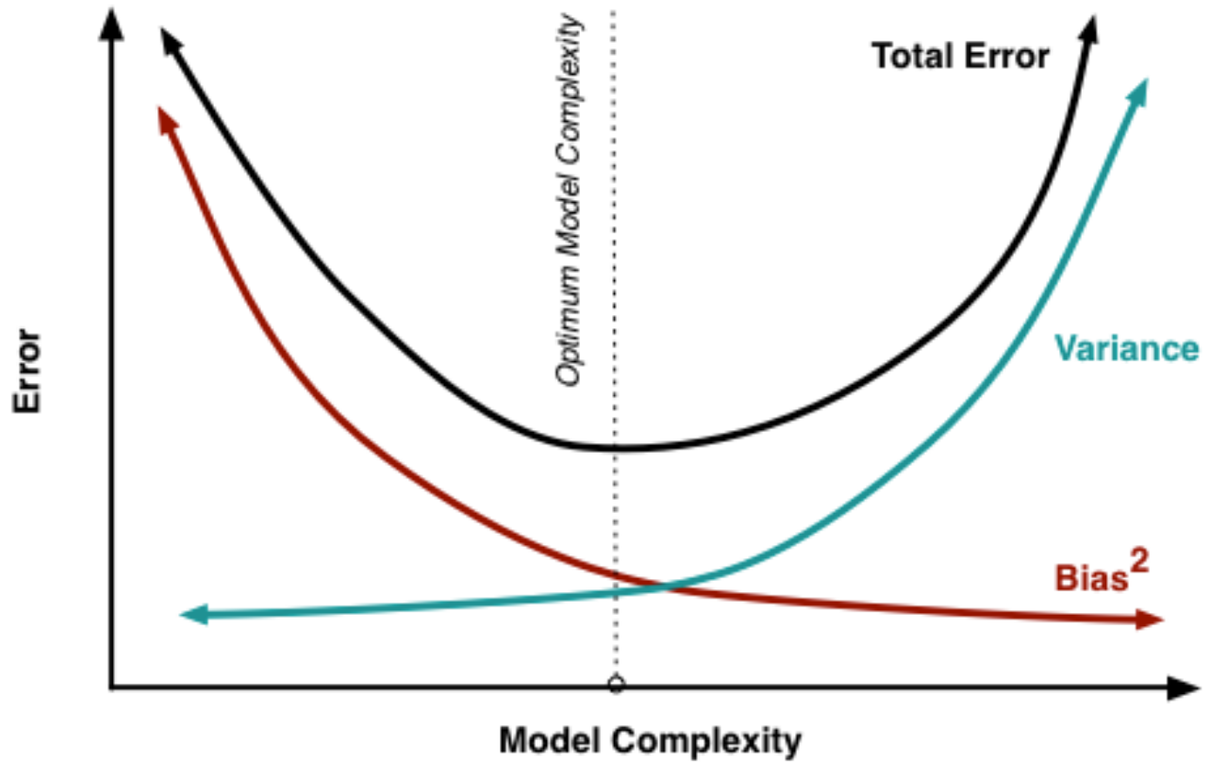


HOW MANY FOLDS SHOULD WE CHOOSE?

- A high number of folds results in what?
- A low number of folds results in what?

HOW MANY FOLDS SHOULD WE CHOOSE?

- **With a large number of folds:**
- Error due to bias is low
- Variance is quite high
- Computationally expensive
- **With a low number of folds:**
- Error due to variance is low
- The error due to bias will be large
- Computationally cheaper
- **Thus…**
- For large datasets, k=3 typically ok
- Sparse datasets, LOOCV



THREE WAY DATA SPLITS

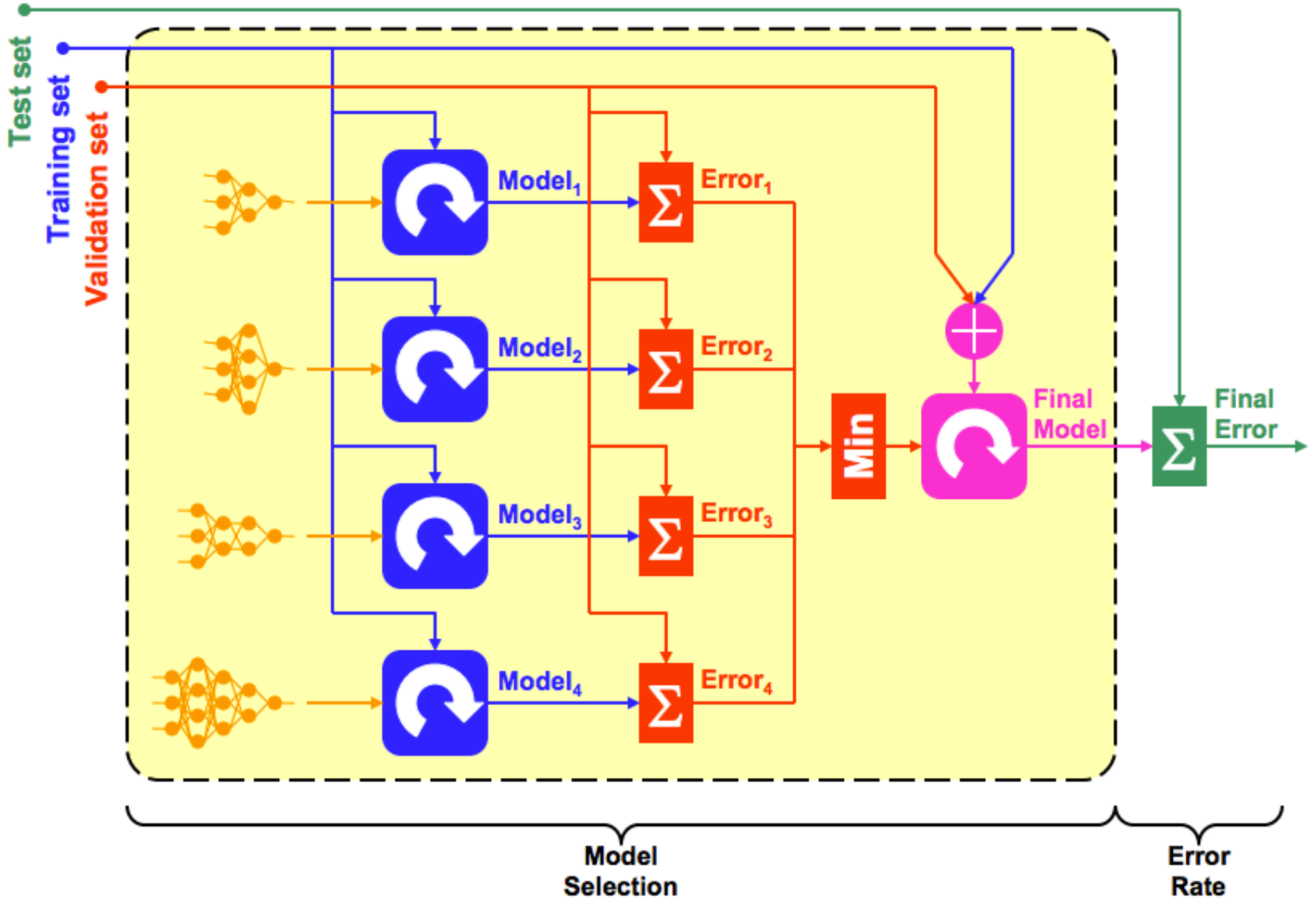
- If model selection and true error estimates are to be computed simultaneously, three disjoint data sets are best.
- **Training set:** a set of example used for learning – what parameters of the classifier
- **Validation set**: a set of examples used to tune the parameters of the classifier
- **Testing set:** a set of examples used ONLY to assess the performance of the fully-trained classifier

- **Validation and testing must be separate data sets.** Once you have the final model set, you cannot do any additional tuning after testing.

PROCEDURE

- 1. Divide data into training, validation, testing sets
- 2. Select architecture (model type) and training parameters (k)
- 3. Train the model using the training set
- 4. Evaluate the model using the training set
- 5. Repeat 2-4 selecting different architectures (models) and tuning parameters
- 6. Select the best model
- 7. Assess the model with the final testing set

PROCEDURE


Test set
Training set
Validation set
Model1
Model2
Model3
Model4
Error1
Error2
Error3
Error4
Min
Final Model
Final Error
Model Selection
Error Rate

PARTING QUESTIONS

- The demo covers a basic test/train split as well as k-fold cross-validation Check: Is 2-fold cross-validation the same as a 50:50 test/train split?

- Will two different 50:50 (or x:y) splits produce the same model score?

ADDITIONAL RESOURCES

https://www.youtube.com/watch?v= 2ij6eaaSl0&t=2m34s

http://www.win-vector.com/blog/2015/01/random-testtrain-split-is-not-always-enough/