# Model Selection, Evaluation, Diagnosis

INFO-4604, Applied Machine Learning

University of Colorado Boulder

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# Today

How do you estimate how well your classifier will perform?

- Pipeline for model **evaluation**
- Introduction to important **metrics**

How do you tune a model and select the best *hyperparameters*?

- Approaches to **model selection**

# Evaluation

In homework, you've seen that:

- training data is usually separate from **test data**
- training accuracy is often much higher than test accuracy
  - Training accuracy is what your classifier is optimizing for (plus regularization), but not a good indicator of how it will perform

# Evaluation

Distinction between:

- **in-sample** data
  - The data that is available when building your model
  - “Training” data in machine learning terminology
- **out-of-sample** data
  - Data that was not seen during training
  - Also called **held-out data** or a **holdout set**
  - Useful to see what your classifier will do on data it hasn’t seen before
  - Usually assumed to be from the same distribution as in-sample data

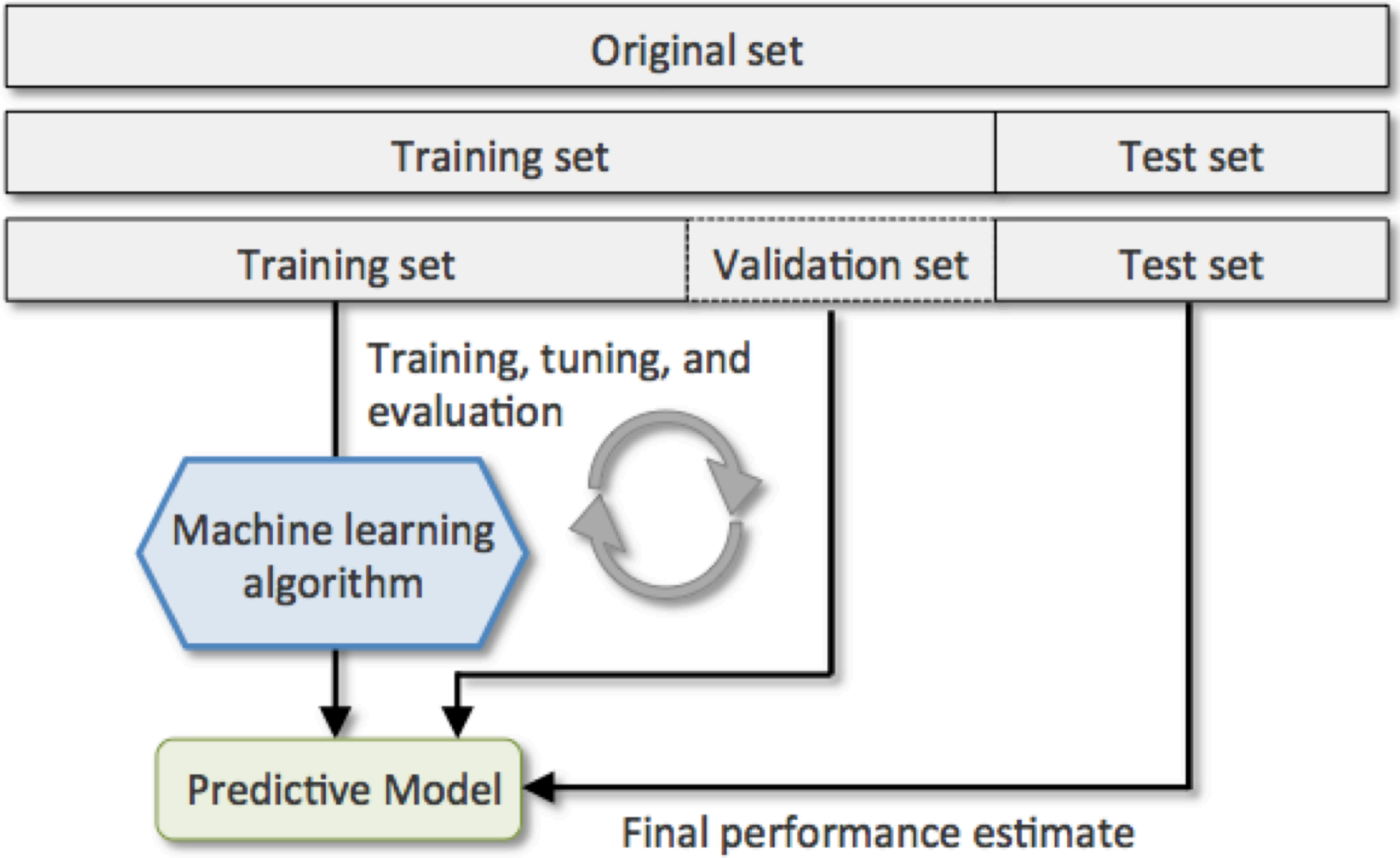
# Evaluation

Ideally, you should be “blind” to the test data until you are ready to evaluate your final model

Often you need to evaluate a model repeatedly (e.g., you’re trying to pick the best regularization strength, and you want to see how different values affect the performance)

- If you keep using the same test data, you risk overfitting to the test set
- Should use a different set, still held-out from training data, but different from test set
- We’ll revisit this later in the lecture

# Evaluation


Original set
Training set
Test set
Training set
Validation set
Test set
Training, tuning, and evaluation
Machine learning algorithm
Predictive Model
Final performance estimate

# Held-Out Data

Typically you set aside a random sample of your labeled data to use for testing

- A lot of ML datasets you download will already be split into training vs test, so that people use the same splits in different experiments

How much data to set aside for testing? Tradeoff:

- Smaller test set: less reliable performance estimate
- Smaller training set: less data for training, probably worse classifier (might underestimate performance)

# Held-Out Data

A common approach to getting held-out estimates is **k-fold cross validation**

General idea:

- split your data into *k* partitions (“folds”)
- use all but one for training, use the last fold for testing
- Repeat *k* times, so each fold gets used for testing once

This will give you *k* different held-out performance estimates

- Can then average them to get final result

# Held-Out Data


Illustration of 10-fold cross-validation

# Held-Out Data

How to choose *k*?

- Generally, larger is better, but limited by efficiency
- Most common values: 5 or 10
- Smaller *k* means less training data used, so your estimate may be an underestimate

When *k* is the number of instances, this is called

**leave-one-out** cross-validation

- Useful with small datasets, when you want to use as much training data as possible

# Held-Out Data

Benefits of obtaining multiple held-out estimates:

- More robust final estimate; less sensitive to the particular test split that you choose
- Multiple estimates also gives you the variance of the estimates; can be used to construct confidence intervals (but not doing this in this class)

# Other Considerations

When splitting into train vs test partitions, keep in mind the unit of analysis

Some examples:

- If you are making predictions about people (e.g., guessing someone's age based on their search queries), probably shouldn't have data from the same person in both train and test
  - Split on people rather than individual instances (queries)
- If time is a factor in your data, probably want test sets to be from later time periods than training sets
  - Don't use the future to predict the past

# Other Considerations

If there are errors in your annotations, then there will be errors in your estimates of performance

- Example: your classifier predicts “positive” sentiment but it was labeled “neutral”
- If the label actually should have been (or at least could have been) positive, then your classifier will be falsely penalized

This is another reason why it’s important to understand the quality of the annotations in order to correctly understand the quality of a model

# Other Considerations

If your test performance seems “suspiciously” good, trust your suspicions

- Make sure you aren’t accidentally including any training information in the test set
- More on debugging next time

General takeaway:

- Make sure the test conditions are as similar as possible to the actual prediction environment
- Don’t trick yourself into thinking your model works better than it does

# Evaluation Metrics

How do we measure performance?

What *metrics* should be used?

# Evaluation Metrics

So far, we have mostly talked about **accuracy** in this class

- The number of correctly classified instances divided by the total number of instances

**Error** is the complement of accuracy

- Accuracy = 1 – Error
- Error = 1 – Accuracy

# Evaluation Metrics

Accuracy/error give an overall summary of model performance, though sometimes hard to interpret

Example: fraud detection in bank transactions

- 99.9% of instances are legitimate
- A classifier that never predicts fraud would have an accuracy of 99.9%
- Need a better way to understand performance

# Evaluation Metrics

Some metrics measure performance with respect to a particular class

With respect to a class *c*, we define a prediction as:

- True positive: the label is c and the classifier predicted c
- False positive: the label is not c but the classifier predicted c
- True negative: the label is not c and the classifier did not predict c
- False negative: the label is c but the classifier did not predict c

# Evaluation Metrics

Two different types of errors:

- False positive (“type I” error)
- False negative (“type II” error)

Usually there is a tradeoff between these two

- Can optimize for one at the expense of the other
- Which one to favor? Depends on task

# Evaluation Metrics

**Precision** is the percentage of instances predicted to be positive that were actually positive

$$PRE = \frac{TP}{TP + FP}$$

Fraud example:

- Low precision means you are classifying legitimate transactions as fraudulent

# Evaluation Metrics

**Recall** is the percentage of positive instances that were predicted to be positive

$$REC = TPR = \frac{TP}{P} = \frac{TP}{FN + TP}$$

Fraud example:

- Low recall means there are fraudulent transactions that you aren't detecting

# Evaluation Metrics

Similar to optimizing for false positives vs false negatives, there is usually a tradeoff between prediction and recall

- Can increase one at the expense of the other
- One might be more important than the other, or they might be equally important; depends on task

Fraud example:

- If a human is reviewing the transactions flagged as fraudulent, probably optimize for recall
- If the classifications are taken as-is (no human review), probably optimize for precision

# Evaluation Metrics

Can modify prediction rule to adjust tradeoff

- Increased prediction threshold (i.e., score or probability of an instance belonging to a class) → increased precision
  - Fewer instances will be predicted positive
  - But the ones that are classified positive are more likely to be classified correctly (more confidence classifier)
- Decreased threshold → increased recall
  - More instances will get classified as positive (the bar has been lowered)
  - But this will make your classifications less accurate, lower precision

# Evaluation Metrics

The **F1 score** is an average of precision and recall

- Used as a summary of performance, still with respect to a particular class *c*
- Defined using *harmonic* mean, affected more by lower number
  - Both numbers have to be high for F1 to be high
  - F1 is therefore useful when both are important

$$F1 = 2\frac{PRE \times REC}{PRE + REC}$$

# Evaluation Metrics

Precision/recall/F1 are specific to one class

- How to summarize for all classes?

Two different ways of averaging:

- A **macro** average just averages the individually calculated scores of each class
  - Weights each *class* equally $$PRE_{macro} = \frac{PRE_1 + \cdots + PRE_k}{k}$$
- A **micro** average calculates the metric by first pooling all instances of each class
  - Weights each *instance* equally $$PRE_{micro} = \frac{TP_1 + \cdots + TP_k}{TP_1 + \cdots + TP_k + FP_1 + \cdots + FP_k}$$

# Evaluation Metrics

Which metrics to use?

- Accuracy easier to understand/communicate than precision/recall/F1, but harder to interpret correctly
- Precision/recall/F1 generally more informative
  - If you have a small number of classes, just show P/R/F for all classes
  - If you have a large number of classes, then probably should do macro/micro averaging
- F1 better if precision/recall both important, but sometimes you might highlight one over the other

# Evaluation Metrics

It is often a good idea to contextualize your results by comparing to a *baseline* level of performance

- A “dummy” baseline, like always outputting the majority class, can be useful to understand if your data is imbalanced (like in fraud example)
- A simple, “default” classifier for your task, like using standard 1-gram features for text, can help you understand if your modifications resulted in an improvement

# Model Selection

Evaluation can help you choose (or *select*) between competing models

- Which classification algorithm to use?
- Best preprocessing steps?
- Best feature set?
- Best hyperparameters?

Usually these are all decided *empirically* based on testing different possibilities on your data

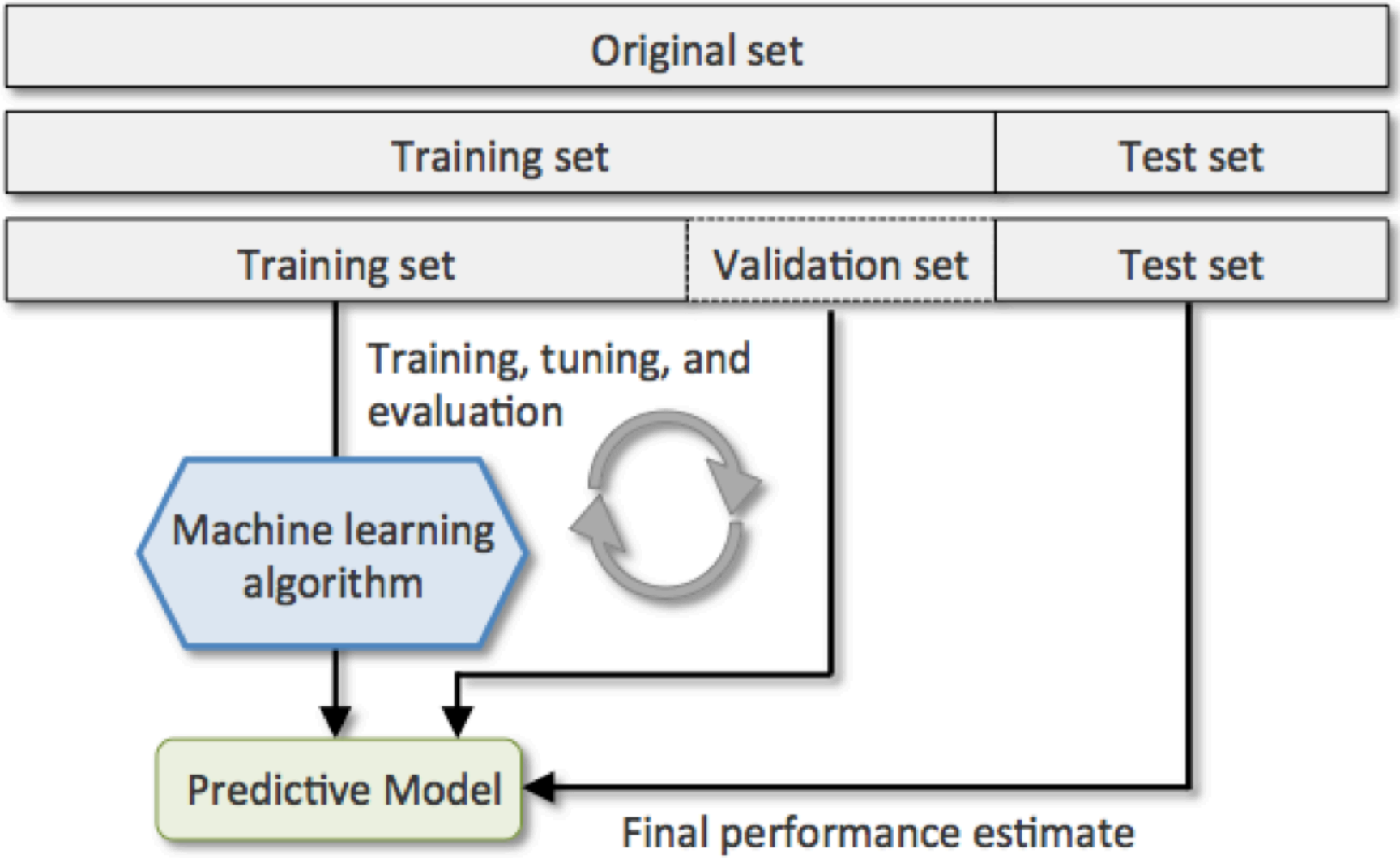
# Model Selection

Selecting your model to get optimal test performance is risky

- What works best for the particular test set might not actually be the best in general
- Overfitting to the test data

**Validation** (or **development**) data refers to data that is held-out for measuring performance, but is separate from the final test set

# Model Selection

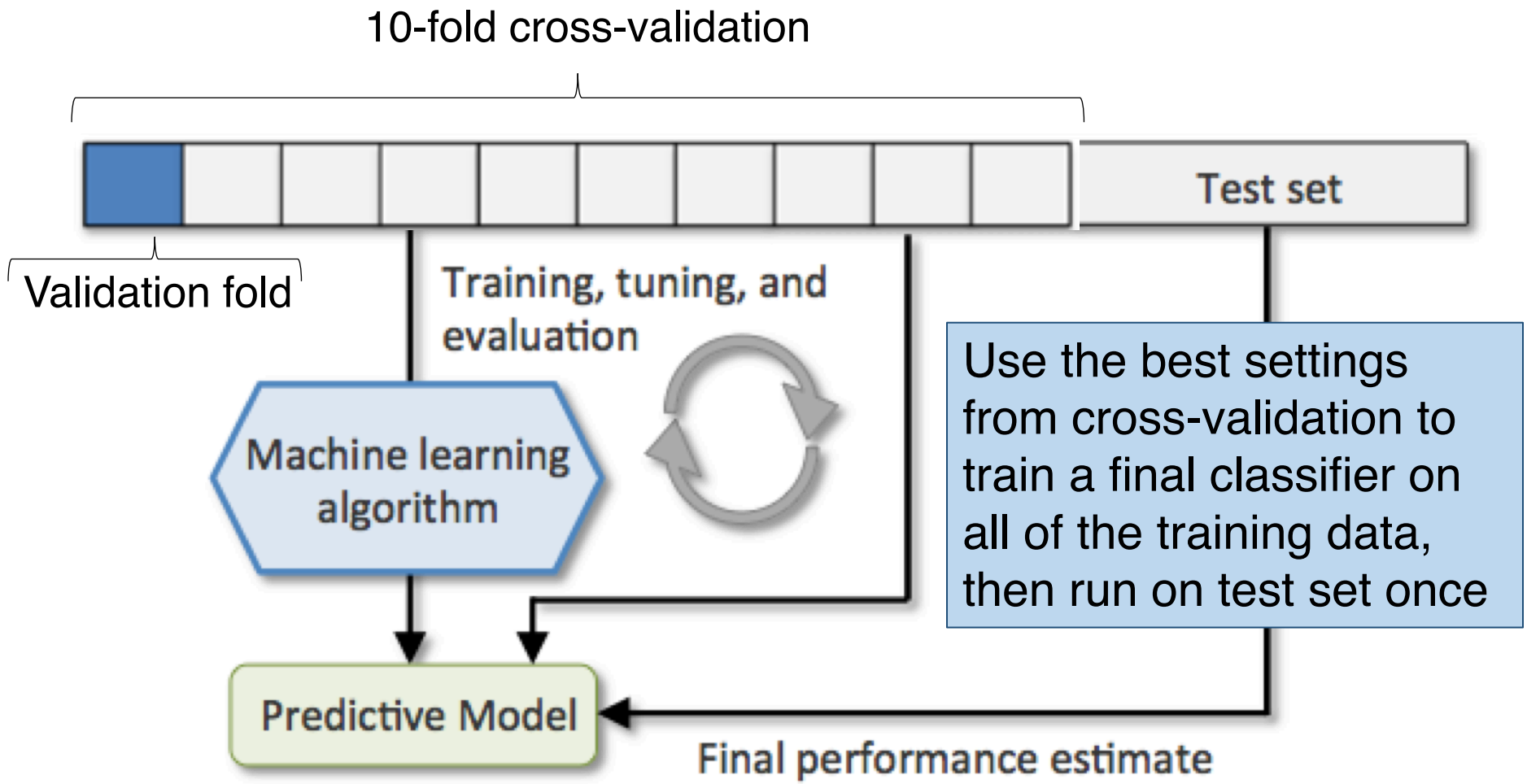


# Model Selection

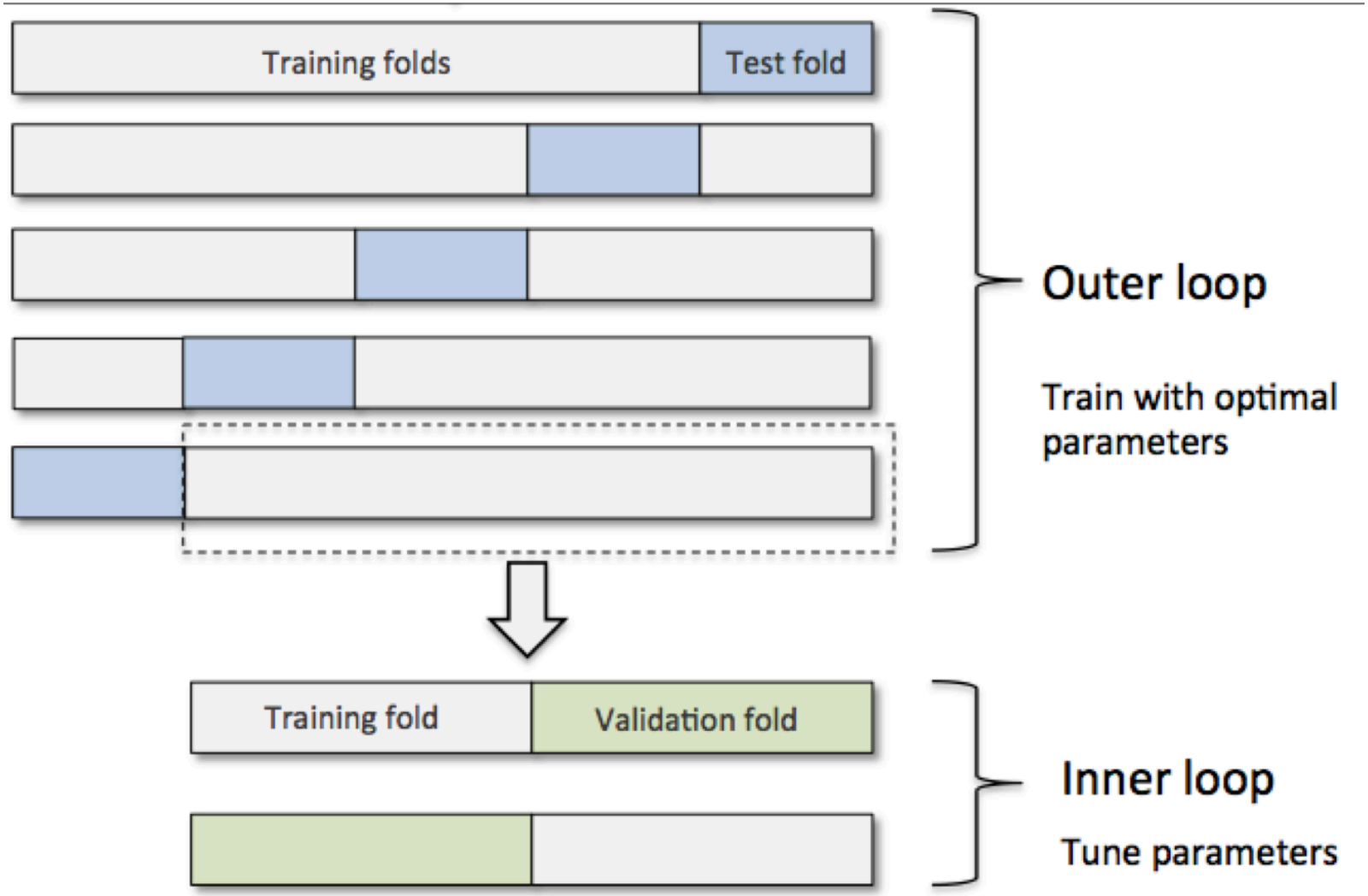
How to select validation data? Cross-validation often used, in one of two ways:

- Use cross-validation for model selection, then evaluate on a single held-out test set after tuning
- Use nested cross-validation, where a fold is used for testing and a different fold is used for validation (and all other folds used for training, as usual)

# Model Selection



# Model Selection



# Model Selection

Nested cross-validation may have different optimal settings in each iteration

- Useful for estimating what the test performance would be after doing model selection on a validation set
- Still need to choose final settings – usually with (non-nested) cross-validation one final time on the entire data

# Model Selection

What settings should you test? Lots of possibilities.

Different decisions/hyperparameters depend on each other; not independent

- e.g., optimal regularization strength depends on what kind of regularizer (L2 vs L1), what kind of feature selection, etc

Best to optimize *combinations* of settings, rather than optimizing individually

# Model Selection

A **grid search** is the process of evaluating every combination of settings (from a specified set of potential values) on validation data

Quickly becomes expensive… example:

- 5 regularization values
- 2 regularizer types
- 3 kernel settings
- 5 feature selection settings
- 2 preprocessing options
- = 300 combinations

# Model Selection

Might only perform a grid search on a subset of combinations initially

One option: start by searching a small number of very different values (e.g., C={0.1, 1.0, 10.0, 100.0}), then fine-tune with more values close to the optimal one

(e.g. find that C=1.0 and C=10.0 are the best of the above options, so now try C={1.0,2.0,4.0,6.0,8,0,…})

# Understanding and Diagnosis

In addition to *measuring* performance, also important to *understand* performance

Want to be able to answer:

- Why does the model make the predictions it does?
- What kinds of errors does the model make?
- What can be done to improve the model?

# Error Analysis

What kinds of mistakes does a model make?

Which classes does a classifier tend to mix up?

# Error Analysis

# Error Analysis

A **confusion matrix** (or **error matrix**) is a table that counts the number of test instances with each true label vs each predicted label.

| | | Predicted | | | |
|---|---|---|---|---|---|
| | | **Iris-setosa** | **Iris-versicolor** | **Iris-virginica** | **Σ** |
| Actual | **Iris-setosa** | 100.0 % | 0.0 % | 0.0 % | **50** |
| | **Iris-versicolor** | 0.0 % | 88.7 % | 6.4 % | **50** |
| | **Iris-virginica** | 0.0 % | 11.3 % | 93.6 % | **50** |
| | **Σ** | **50** | **53** | **47** | **150** |

From: https://docs.orange.biolab.si/3/visual-programming/widgets/evaluation/confusionmatrix.html

# Error Analysis

A **confusion matrix** (or **error matrix**) is a table that counts the number of test instances with each true label vs each predicted label.

- In binary classification, the confusion matrix is just a 2x2 table of true/false positive/negatives
- But can be generalized to multiclass settings

# Error Analysis

Just as false negatives vs false positives are two different types of errors where one may be preferable, different types of multiclass errors may have different importance

- Mistaking a deer for an antelope is not such a bad mistake
- Mistaking a deer for a cereal box would be an odd mistake

Are the mistakes acceptable? Need to look at confusions, not just a summary statistic.

# Error Analysis

Another way to understand why your classifier is behaving a certain way is to examine the parameters that are learned after training

- e.g., the decision tree structure, or the weight vector values

If features are associated with classes in a way that doesn't make sense to you, that might mean the model is not working the way you intended

- Caveat: features interact in ways that can be hard to understand, so unintuitive parameters not necessarily wrong

# Error Analysis

Another good practice: look at a sample of misclassified instances

test11.png

| | |
|---|---|
| **msft_captions** | a close up of a stuffed animal (55) |
| **msft_tags** | indoor (94) , food (87) , bread (74) , dessert (30) |

From: https://medium.freecodecamp.org/chihuahua-or-muffin-my-search-for-the-best-computer-vision-api-cbda4d6b425d

# Error Analysis

Another good practice: look at a sample of misclassified instances

- Might help you understand why the classifier is making those mistakes
- Might help you understand what kinds of instances the classifier makes mistakes on
  - Maybe they were ambiguous to begin with, so not surprising the classifier had trouble

# Error Analysis

Another good practice: look at a sample of misclassified instances

- If you have multiple models, can compare how they do on individual instances
- If your model outputs probabilities, useful to examine
  - If the correct class was the 2nd most probable, that's a better mistake than if it was the 10th most probable

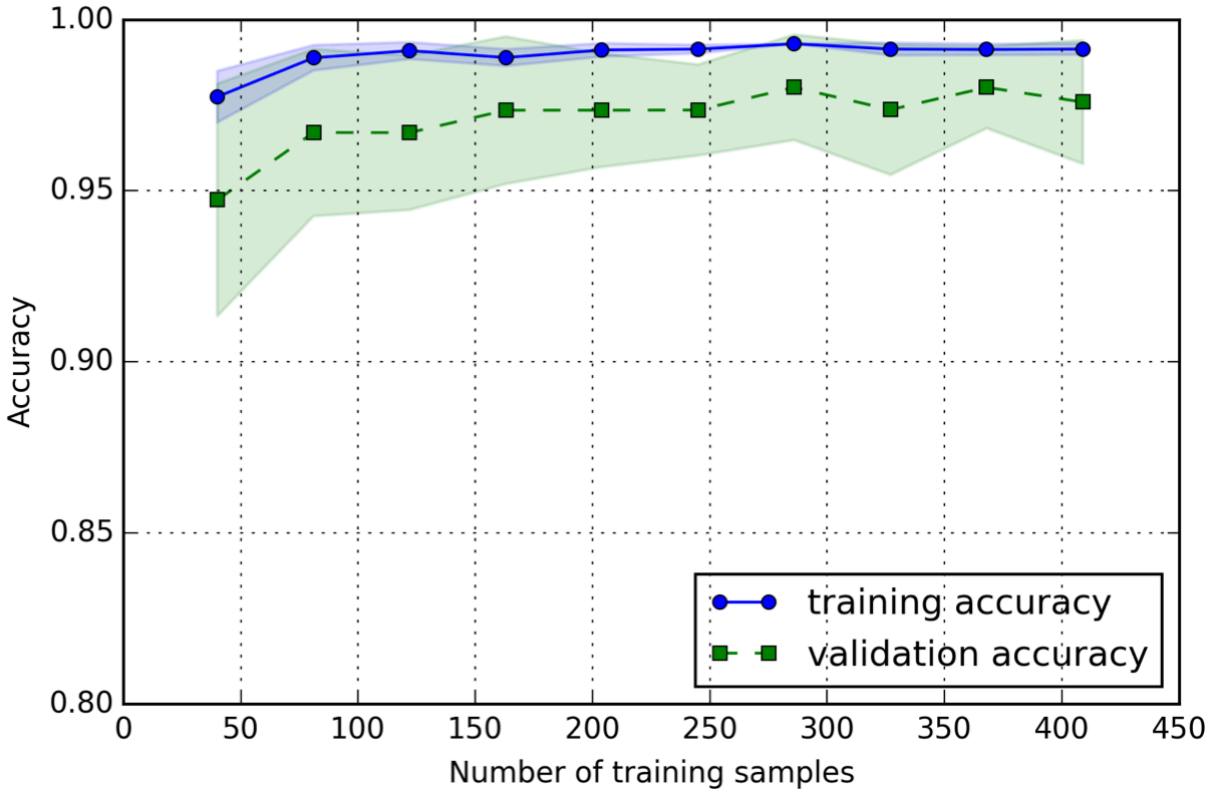
# Error Analysis

Error analysis can help inform:

- Feature engineering
  - If you observe that certain classes are more easily confused, think about creating new features that could distinguish those classes
- Feature selection
  - If you observe that certain features might be hurting performance (maybe the classifier is picking up on an association between a feature and a class that isn't meaningful), you could remove it

# Learning Curves

A **learning curve** measures the performance of a model at different amounts of training data



# Learning Curves

Primarily used to understand two things:

- How much training data is needed?
- Bias/variance tradeoff

# Learning Curves

How much training data is needed?

Usually the validation accuracy increases noticeable after an initial increase in training data, then levels off after a while

- Might still be increasing, but with diminishing returns

The learning curve can be used to predict the benefit you'll get from adding more training data

- Still increasing rapidly → get more data
- Completely flattened out → more data won't help
- Gradually increasing → need a lot more data to help

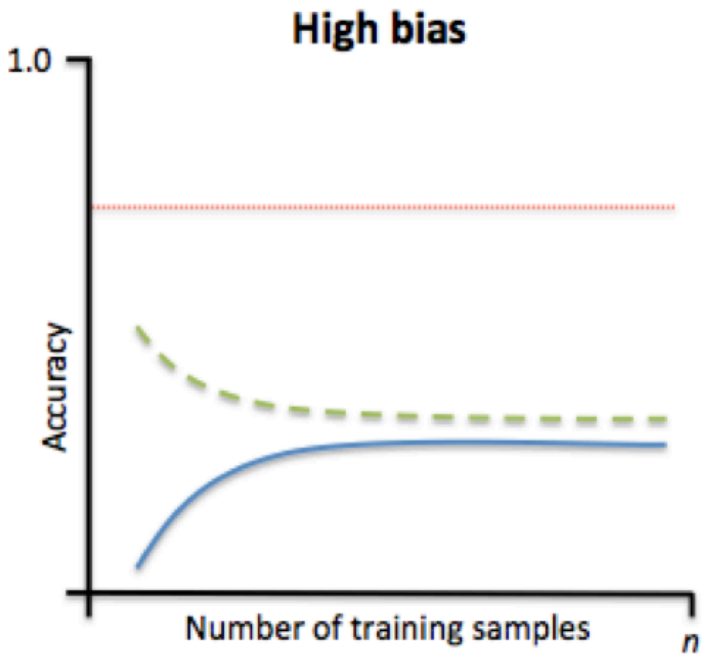
# Learning Curves

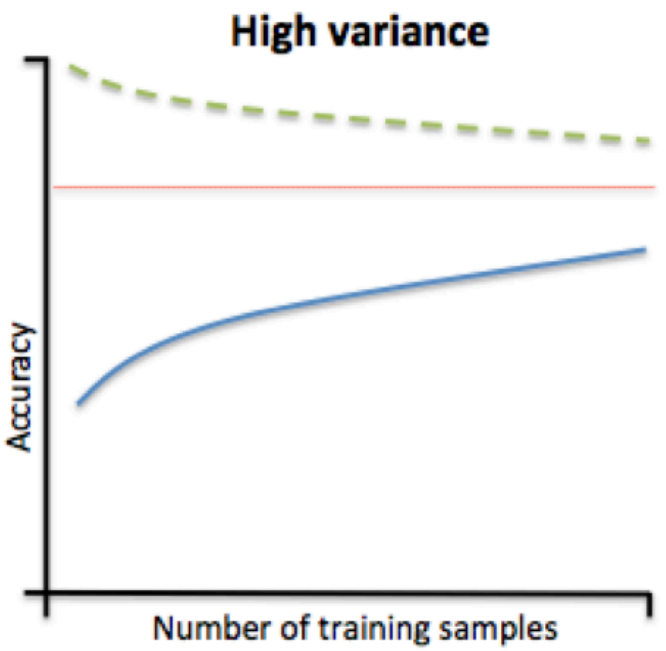
A typical pattern is that:

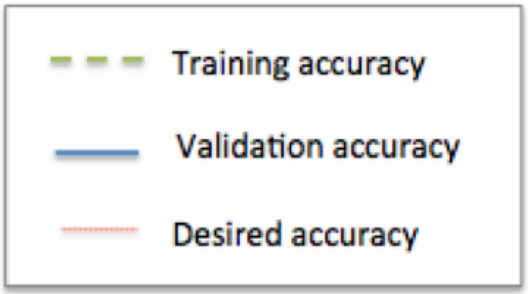
- Training accuracy decreases with more data
- Validation accuracy increases
- The two accuracies should converge to be similar

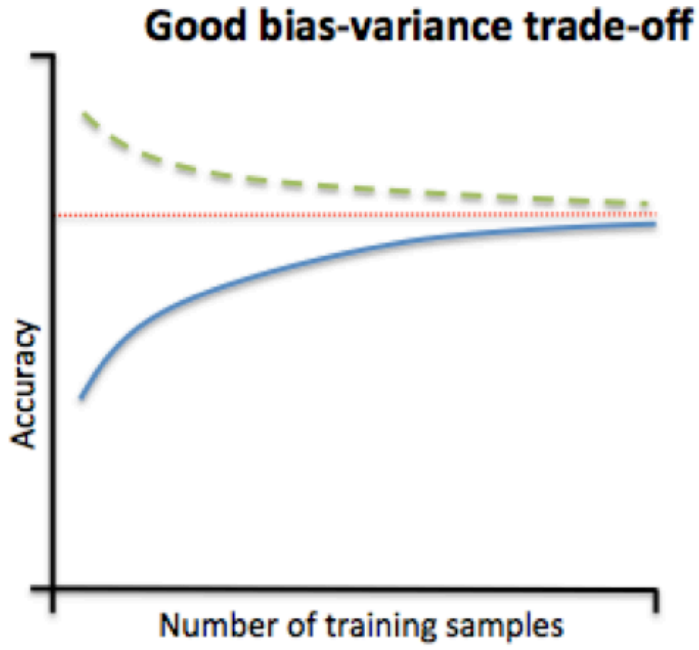
Something to look for:

- If gap between train/validation performance isn't closing, probably too much variance (overfitting)
- If gap between train/validation closes quickly, might suggest high bias (underfitting)


High bias
1.0
Accuracy
Number of training samples
n

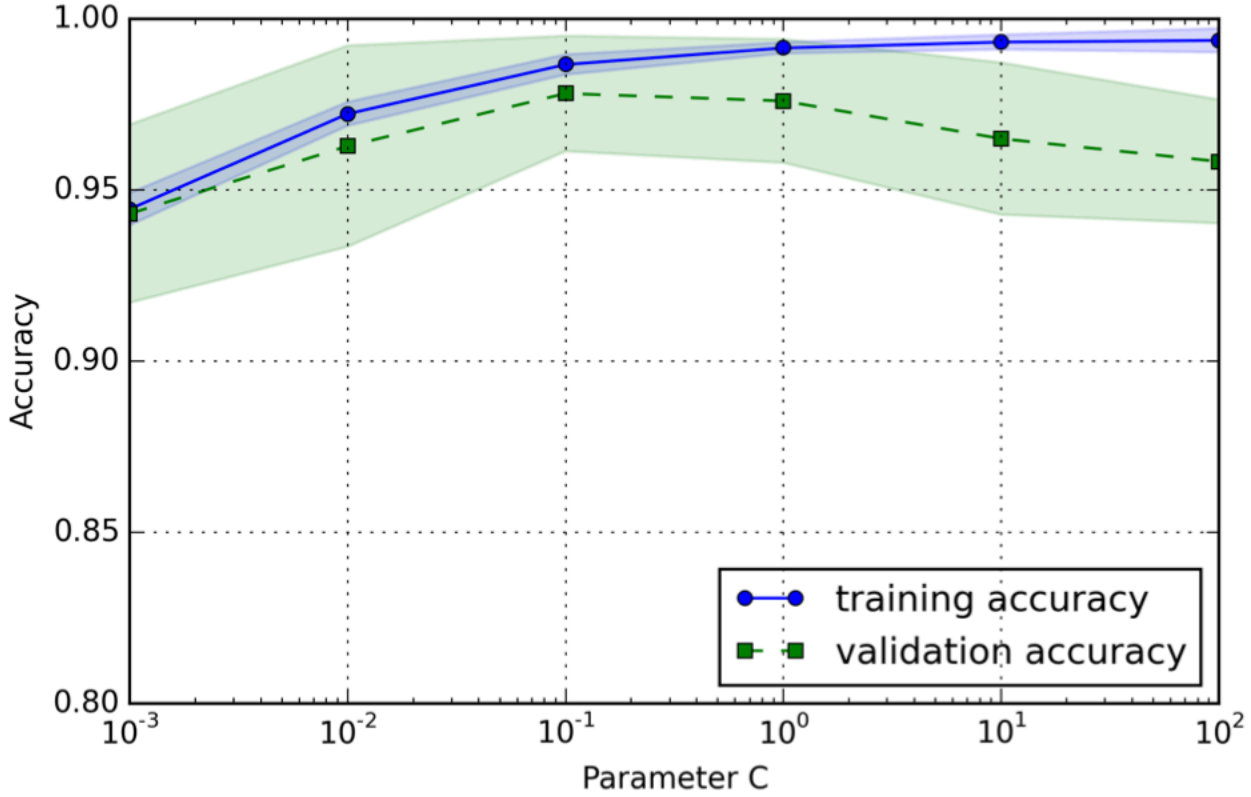

High variance
Accuracy
Number of training samples


Training accuracy
Validation accuracy
Desired accuracy


Good bias-variance trade-off
Accuracy
Number of training samples

# Validation Curves

A **validation curve** measures the performance of a model at different hyperparameter settings

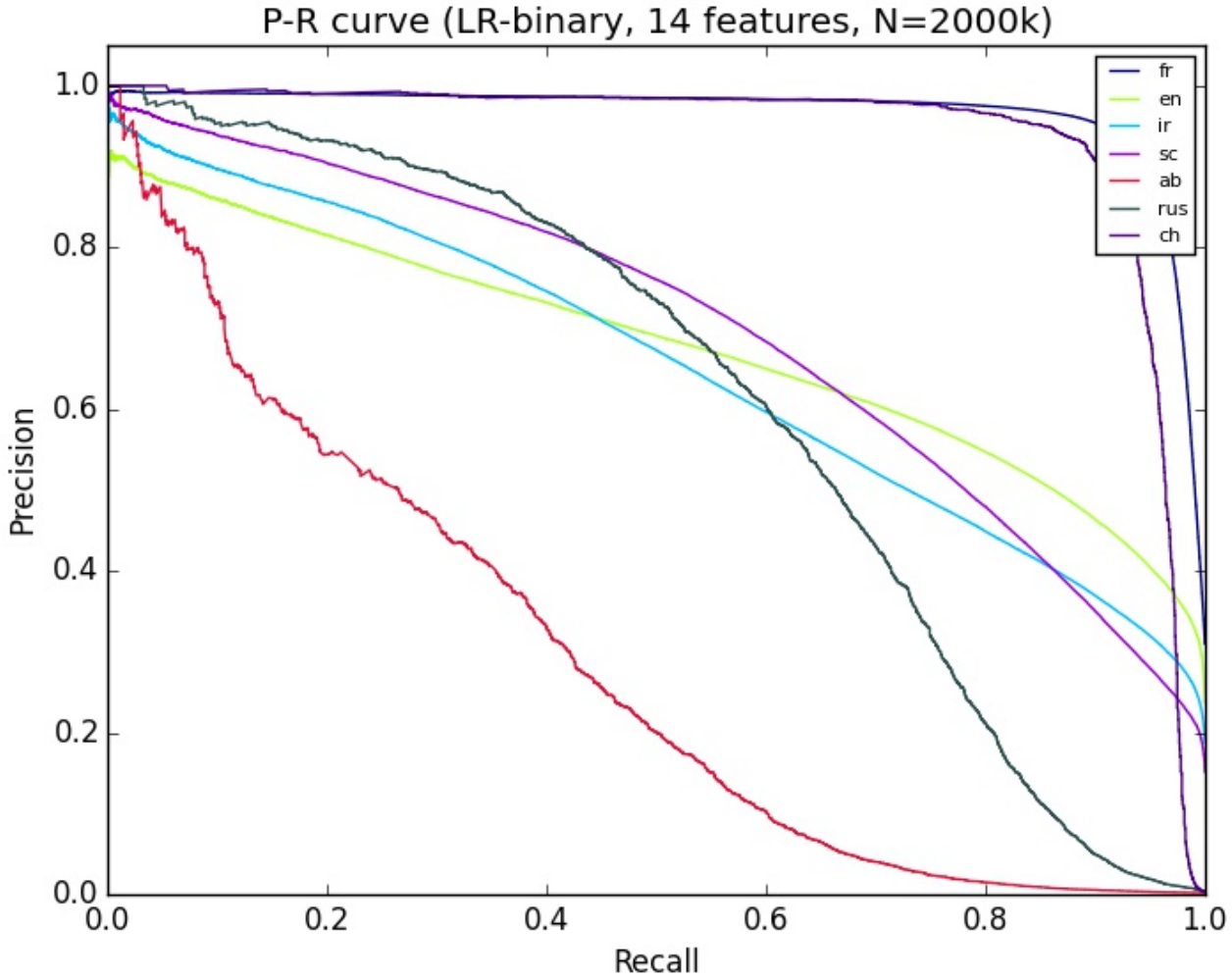


# Validation Curves

Validation curves help you understand the effect of hyperparameters, and also help understand the bias/variance tradeoff

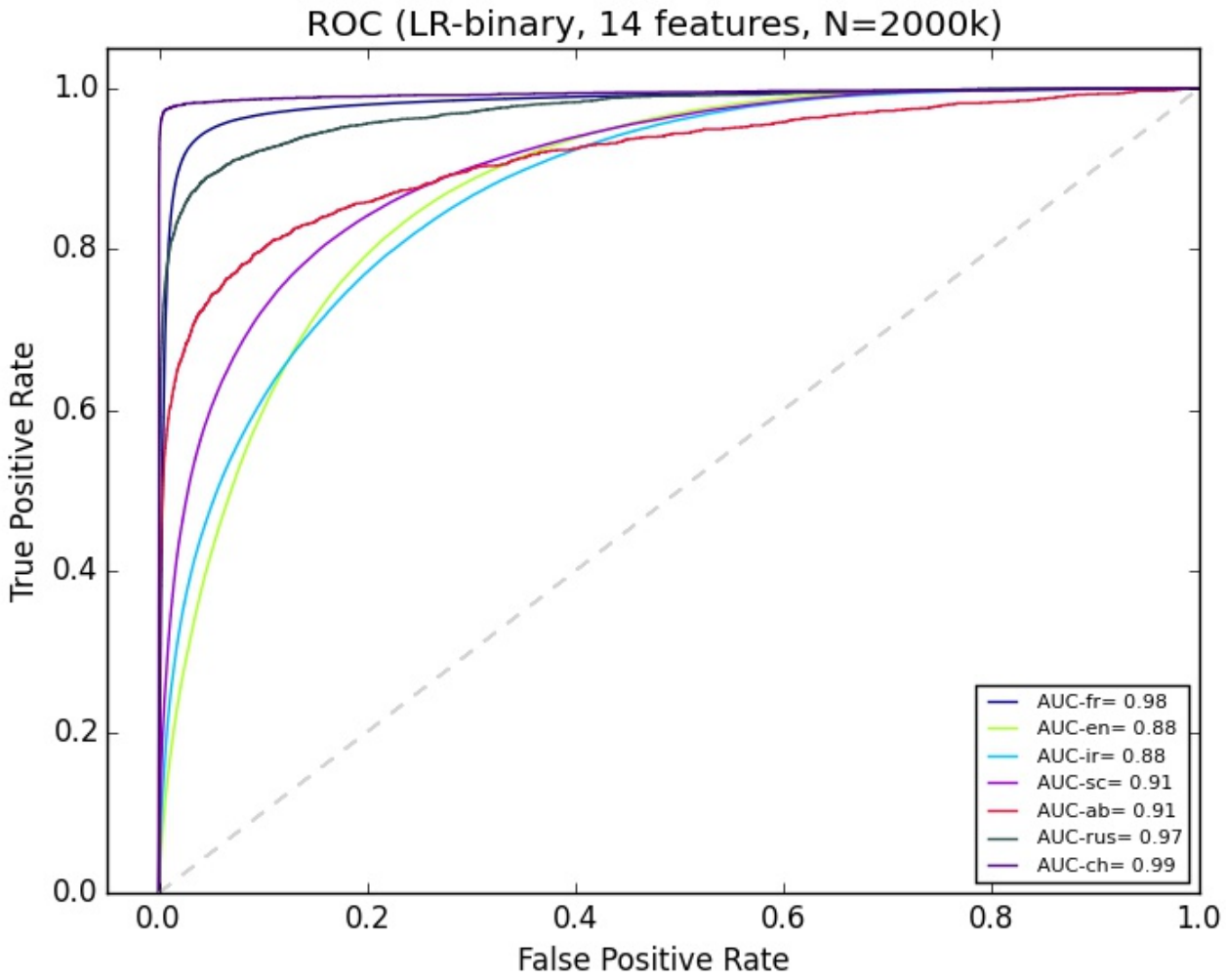
- Want to find a setting where train/validation performance is similar (low variance)
- Of the settings where train/validation performance are similar, pick the one with the highest validation accuracy (low bias)

# Precision-Recall Curve




From: https://stackoverflow.com/questions/33294574/good-roc-curve-but-poor-precision-recall-curve

# ROC Curve




From: https://stackoverflow.com/questions/33294574/good-roc-curve-but-poor-precision-recall-curve

# Debugging

Lots of places in the pipeline where there could be an implementation mistake:

- Data preprocessing
- Feature engineering
- Training algorithm
- Validation pipeline

Best to start simple, compare to existing data/systems, then expand from there