Ensemble Methods

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Decision Trees …

- Simple learning algorithm(s)
- Both classification and regression forms
- For some implementations, features values can be "unknown"
- Classification models easily handle multiple classes
- Models can be intuitive for human experts
  - Naturally give us a sense of the most important features

Decision Tree Challenges

- Splits are most often based on individual features
- Crisp region boundaries
  - Most common regression architecture: end up with a piecewise constant function (so, it is discontinuous)
- Deep trees are necessary to capture complex models
- Deeper models:
  - > Fewer samples in the leaf nodes
  - > Brittle when it comes to generalization

Sir Francis Galton (1822-1911)

- Meteorology: first weather maps
- Statistics: regression
- Psychology
- Heredity
- …

Weighing a Cow

Weighing a Cow

- Individually, non-experts are generally not good at guessing the weight of a cow
- However, the distribution is ~Normal, with a mean very close to the true weight

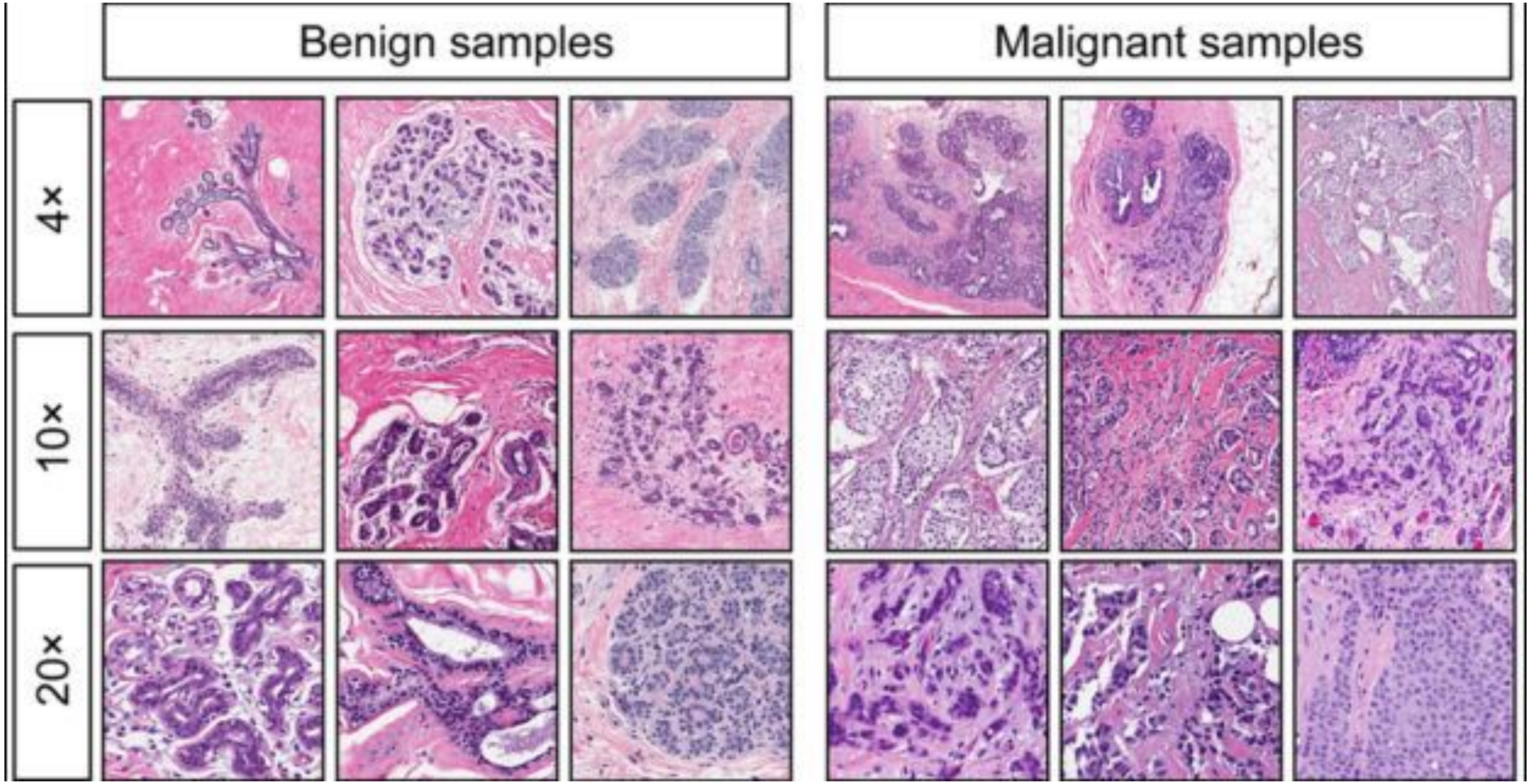
Message: Measures from a large set of ***independent***, poor-quality predictors can give us a high-quality prediction

Mixing Many Imperfect "Experts"

Ensemble-based methods:

- Create many models
- Combine the predictions of these models
  - Classifiers: voting
  - Regression: some mechanism for blending the predictions (e.g., computing a mean)

Example: Breast Cancer Classification



Levenson et al. (2015), PLOS One

Breast Cancer Classification

Levenson et al:

- Trained individuals to label images of tumors as either malignant or benign
- After 2 weeks, these individuals could classify the images with an accuracy of 85%
- Hard voting classifier: the votes across the individuals were tallied
- Accuracy increased to 99%!

Breast Cancer Classification

Hard voting classifier:

- This improvement in performance requires independence of the individuals
- The law of large numbers: combining a large number of independent random variable samples gives us the correct answer with high probability

Breast Cancer Classification

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And, the individuals in this case were pigeons…

Ensemble Predictions

- Set of trained classifiers
- Can be different types of classifiers: decision tree, logistic regression, support vector machine…
  - Different model types often capture different trends in the training set
- Combine the labels from the classifiers:
  - Hard voting: crisp answers are counted across the ensemble
  - Soft voting: average class probabilities & select the highest one

Example: Voting Classifier

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Ensemble Predictions

sklearn.ensemble: VotingClassifier

- Constructor:
  - List of classifiers
    - We have generally already chosen hyperparameters
  - Hard or soft voting
    - Soft voting requires predict_proba() to be available
- fit() will fit each model in sequence
- predict() will query all models and combine the results

Example: Multiple Classifiers

```
classifier1 = DecisionTreeClassifier(max_leaf_nodes=3)
classifier2 = SVC(kernel='poly', C=100.0, degree=2,gamma='auto')
classifier3 = LogisticRegression(random_state=None,
                                 max_iter=10000,
                                    tol=1e-3, solver='newton-cg',
                                    penalty='l2', C=100000)
```

Example: Combining Multiple Classifiers

```
voting_classifier = VotingClassifier([('tree', classifier1),
                                      ('SVC', classifier2),
                                      ('Logistic Regression',
                                                    classifier3)],
                                        voting='hard', n_jobs=-1)
```

Bagging and Pasting

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Ensemble Methods

- Success of ensemble methods relies on independence of the individual models
- Can we achieve this if the models are all of the same type?

Forcing Independence

- Train each model instance with a subsample of the training set:
  - Pasting: sample without replacement
  - Bagging (bootstrap aggregation): sample with replacement

- Models can be trained in parallel

Forcing Independence

- Pasting: sample without replacement
  - All ensemble members have different training data
  - Effective training sets may not be large enough
- Bagging (bootstrap aggregation): sample with replacement
  - A single training sample may be used by multiple ensemble members -> less independence
  - But, allows us to have larger training sets

Forcing Independence

After training, a new query is addressed by asking each model to provide an answer

- Classifier: voting
- Regression: average the predictions of the individual models

Example: Bagging Classifier

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Random Subspaces

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Forcing Independence

- So far:
  - Bagging & pasting take random subsets of the training data
  - These are ***Random Patches*** of the data
- Sampling features:
  - ***Random Subspaces***: only use a subset of the available features for a given model
  - Support for this also in BaggingClassifier

Random Forests

Ensemble of Decision Trees

- Can continue to use the Bagging Classifier
- RandomForestClassifier class does the same thing, but is optimized for classifying with decision trees
  – Hyper-parameters for this class include Decision Tree hyper-parameters and the ensemble hyper-parameters
- RandomForestRegressor also optimized for ensemble of regression trees

Forcing Independence

Adding noise to tree construction. For each possible split:

- Random forest: consider only a small subset of the available features
  - This is the Random Subspaces idea!
  - Particularly useful when there are many features possible or many possible questions
- Extra trees: consider only a subset of possible thresholds (or question parameters)
  - ExtraTreesClassifier class
  - Reduces search during each leaf node split

Ensemble Methods

- Allow us to combine many ***weak learners***
  - Each does not have to perform very well
  - The ensemble model often performs better than the weak learners
- Bigger implications:
  - We can specifically choose simpler models (e.g., trees that are heavily regularized)
  - Cheaper to compute and leaf node predictions are based on a larger number of samples (compared to deeper trees)

Feature Importance

- Feature Importance:
  - Which of our input features are useful in constructing our models?

- Getting this right can:
  - Help domain scientists focus their models
  - Allow us to more efficiently construct models in the future
  - Refine our data collection / storage processes

Feature Importance

Common approaches:

- How often does a feature occur in a tree?
- Where does a feature occur in a tree?
- Measure for questions involving specific features
  - Support built into the RandomForestClassifier & other models
  - model.feature_importances_:
    - Measure for each feature of its importance in the tree
    - Change of impurity or entropy, depending on your split metric

Feature Importance

Another approach: ***Importance sampling***: how does the model perform when an individual feature is corrupted?

- Typical approach:
  - For a given feature, shuffle the values for that feature across the entire data set.
  - Measure the difference in model performance for the original data set and the corrupted data set
  - Big differences are indicative of that feature playing an important role in the tree

Boosting

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Forests

So far: training of one tree is handled independently of other trees

- Natural parallelization
- Independence to varying degrees
  - True independence: can easily combine the output of the different models
  - In general:
    - We don't necessarily achieve true independence
    - If a part of the sample space is not well represented in the training set, then it will often be ignored by all of the constituent models

Boosting

Alternative approach:

- Grow ensemble incrementally
- The model currently being learned attempts to repair prediction errors of the prior models
  - Want each new model to solve a new piece of the problem
  - With the set of models, we attempt to cover all of the training set (even the sparsely represented regions of the sample space)

AdaBoost

- Prior algorithms: all training samples have been treated with equal weight in computing the cost function
- In boosting, we adjust these weights depending on how well the current ensemble performs

Example: AdaBoost

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Boosting

- Advantage: at each step, we learn a new model that tries to repair problems with the prior model(s)

- The cost: we lose parallelization

Gradient Boosting

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Gradient Boosting

- Focus: regression
- Learn a sequence of regression models
  - Each model in the sequence: try to predict the errors from the previous model
  - Then, this model's output is added to the rest of the model outputs

Example: Gradient Boosting

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Example: Gradient Boosting

GradientBoostingRegressor class

- learning_rate: total contribution by each tree (***shrinkage***)
- n_estimators: maximum number of trees
- subsample: fraction of the number of training samples to use for a given tree
- validation_fraction: fraction of samples to hold out to detect overfitting

- Can overfit the training data
  - Cut-off training at some number of trees based on performance
  - We can do this after the fact or dynamically

Stacking

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Stacking

So far: we have combined the outputs of the individual models through some fixed method

- Voting, averaging …
- Ignores the fact that some models are better than others

- Exception: Boosting

Stacking

We can ask another model to do this combination

- Split the training set
- First training set:
  - Train the individual models
- Second training set:
  - Each model makes predictions for the samples in the 2nd training set
  - New learner (***the blender*** or ***meta-learner***):
    - Inputs: predictions made by the individual models
    - Outputs: outputs from the 2nd training set