Boosting

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Objectives

1. Discuss model averaging and other ensemble methods
2. Introduce an example
3. Adaboost
4. Gradient boosting
5. Summarize the important points with room for discussion

Machine learning algorithms

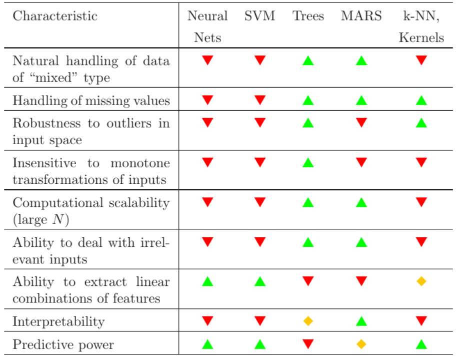
There are always advantages and disadvantages

Algorithm	Strengths	Challenges
GLMs	fast,interpretable	non-linearity,high-dimensionality
KNNs	simple, non-linear	does not scale well, distance function
Decision trees	fast,robust to noise	not competitive in terms of accuracy
Neural Networks	very flexible	prone to overfit, black-box, runtime
SVM's	scales well	parameter and kernel choices
...	...	...
...	...	...
Bayesian networks	probabilistic, priors	not always tractable
Genetic algorithms	mimics natural selection	unsuited for discrete decisions

There is no free lunch in statistics...
Or we could say that no one method outperforms all others given all possible data sets

see http://www.no-free-lunch.org for more on the theorems

TABLE 10.1. *Some characteristics of different learning methods. Key:* ▲ *= good,* ◆ *=fair, and* ▼ *=poor.*



Characteristic	Neural Nets	SVM	Trees	MARS	k-NN, Kernels
Natural handling of data of "mixed" type	▼	▼	▲	▲	▼
Handling of missing values	▼	▼	▲	▲	▲
Robustness to outliers in input space	▼	▼	▲	▼	▲
Insensitive to monotone transformations of inputs	▼	▼	▲	▼	▼
Computational scalability (large N)	▼	▼	▲	▲	▼
Ability to deal with irrelevant inputs	▼	▼	▲	▲	▼
Ability to extract linear combinations of features	▲	▲	▼	▼	◆
Interpretability	▼	▼	◆	▲	▼
Predictive power	▲	▲	▼	◆	▲

[Hastie et al., 2009]

Combining models

- **Committees** - train some number of models and use, for example, the average of the predictions
- **Boosting** - a variant on committees, where models are **trained in sequence** and the **error function** for a given model depends on the previous one
- **Decision trees** - instead of averaging let the model choice be a function of the input variables
- **Mixture of experts** - instead of hard partitioning of the input space we can move to a **probabilistic framework** for partitioning
- **Model stacking** - a method to combine models of different types

To learn more about model stacking see the Kaggle guide

Model averaging

In the **mixture of experts** we combine K models as follows

$$p(t|\mathbf{x}) = \sum_{k=1}^{K} \pi_k(\mathbf{x}) p(t|\mathbf{x}, k) \tag{1}$$

where $\mathbf{x}$ are the inputs, t are the targets and $\pi_k(\mathbf{x}) = p(k|\mathbf{x})$

An example of **model combination** is the density of a Gaussian mixture model

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k), \text{where } p(\mathbf{X}) = \prod_{n=1}^{N} p(\mathbf{x}_n) \tag{2}$$

Bayesian model averaging has a similar form

$$p(\mathbf{X}) = \sum_{k=1}^{K} p(\mathbf{X}|k) p(k) \tag{3}$$

except each data point in the former has a weight (π_k) where each model has weight $(p(k))$ in the latter.

Model averaging

Ensemble learning or committees

Use multiple predictive models and combine the predictions

- **Bagging** or Bootstrap aggregation [Breiman, 1996]
  - Bootstrap the training data and grow a tree from each bootstrap sample
  - Average the bootstrapped trees $\rightarrow$ reduces variance
  - Pruning adds bias so do not prune the trees just average them
- **Random Forests** [Breiman et al., 1999]
  - Bagging except we randomly select predictors at each split
  - Decorrelates the trees
- **Boosting** [Freund and Schapire, 1996]
  - Each subsequent tree is grown based on a reweighted version of the training data
  - Decorrelates the trees

But why do we want to do this again?

If we use simple linear regression as an example model and imagine we knew the true regression function $h(\mathbf{x})$. From bagging we had

$$y_b(\mathbf{x}) = h(\mathbf{x}) + \epsilon_b(\mathbf{x}) \tag{4}$$

we could compute the average sum of squares error as

$$E_{\mathrm{AV}} = \frac{1}{B} \sum_{b=1}^{B} \mathbb{E}_{\mathbf{x}} \left[\{ y_b(\mathbf{x}) - h(\mathbf{x}) \}^2 \right] \tag{5}$$

$$E_{\mathrm{COM}} = \mathbb{E}_{\mathbf{x}} \left[\left\{ \frac{1}{B} \sum_{b=1}^{B} y_b(\mathbf{x}) - h(\mathbf{x}) \right\}^2 \right] \tag{6}$$

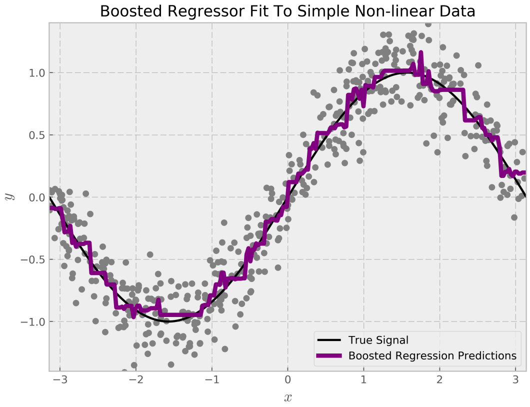
If we assume that the errors have zero mean and they are uncorrelated

$$E_{\mathrm{COM}} = \frac{1}{B} E_{\mathrm{AV}} \tag{7}$$

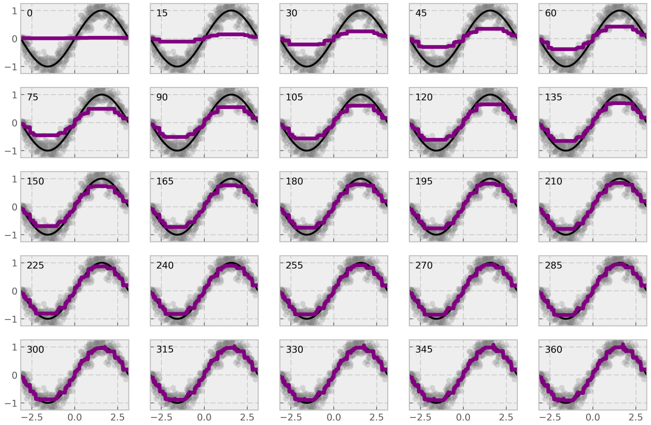
So in a perfect world the average error is reduced by a factor of B

see [Bishop, 2006][Chapter 14] for more details

A simple example

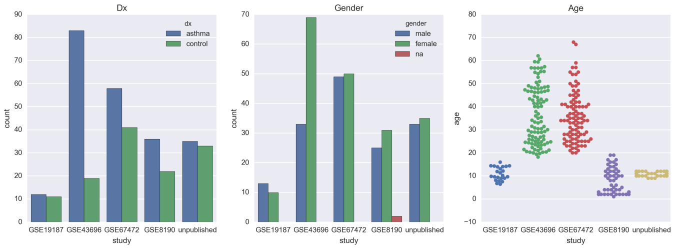


Boosting Stages Over Time

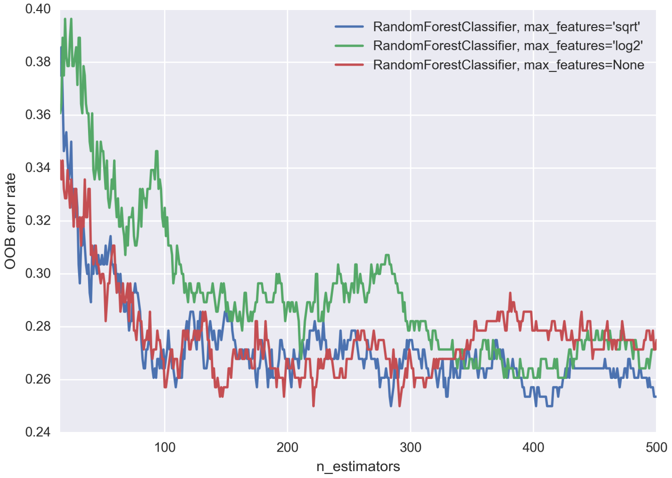


Predicting asthma with gene expression data

dx	study	age	gender	gene-1	gene-2	...	...	gene-N
asthma	study1	10	male	0.24381	-0.14274	...	...	-0.04381
control	study3	8	female	0.17981	0.42480	...	...	-0.05456
...	...	...	...	...	...	...	...	...
control	study2	14	female	0.19933	-0.57384	...	...	0.403921



350 samples, filtered by variance from 11523 to 200 genes



see the sklearn example

A return to random forests

```
import numpy as np
from sklearn.cross_validation import train_test_split

data = train_test_split(X, y, test_size=0.20,random_state=1)
X_train, X_test, y_train, y_test = data
X_train = X_train[:,np.argsort(X_train.var(axis=0))[::-1][:200]]
```

RandomForestClassifier/Regressor

- sklearn.ensemble
- `n_estimators` - the trees
- `max_features` - modulates *m*
- `oob_score`

The sklearn implementation averages the probabilistic prediction (not votes)

OOB

out-of-bag observations - those not used by a given bootstrapped tree

- Convenient to estimate test error
- For ea. observation predict the response for all trees where it was OOB
- Essentially, a free version of leave one out cross validation

sklearn.model_selection.cross_val_score

```
from sklearn.model_selction import cross_val_score
clf = RandomForestClassifier(n_estimators=100,
                             max_features='sqrt',
                             random_state=42)
scores = cross_val_score(clf, X, y, cv=5,scoring=None)
print("Accuracy: %0.2f (+/- %0.2f)"%(scores.mean(),scores.std()*2))

scores = cross_val_score(clf, X, y, cv=5,
                                          scoring='f1_weighted')
print("F1_weighted: %0.2f (+/- %0.2f)"%(scores.mean(),scores.std()*2))
```

```
Accuracy: 0.71 (+/- 0.11)
F1_weighted: 0.68 (+/- 0.14)
```

There are iterators and other convenience classes for CV i.e. KFold

sklearn.model_selection.grid_search.GridSearchCV

```
from sklearn.model_selection import GridSearchCV

random_forest_grid = {'max_depth': [3, None],
                      'max_features': ['sqrt', 'log2', None],
                      'min_samples_split': [1, 2, 4],
                      'min_samples_leaf': [1, 2, 4],
                      'bootstrap': [True, False],
                      'n_estimators': [20, 40, 60, 80, 100, 120],
                      'random_state': [42]}

rf_gridsearch = GridSearchCV(RandomForestClassifier(),
                             random_forest_grid,
                             n_jobs=-1,verbose=True,
                             scoring='f1_weighted')
rf_gridsearch.fit(X_train, y_train)
print "best parameters:", rf_gridsearch.best_params_
```

```
 best parameters: {'bootstrap': True, 'min_samples_leaf': 1, '
     n_estimators': 100, 'min_samples_split': 1, 'random_state': 42, '
     max_features': 'sqrt', 'max_depth': None}
```

1. Initialize data weighting coefficients $\{w_n\}$ by setting them equal to $1/N$
2. For each classifier:
   - Fit the classifier to the training data by minimizing the weighted error function

$$J_m = \sum_{n=1}^{N} w_n^{(m)} I(y_m(\mathbf{x}_n) \neq t_n) \tag{8}$$

   - Then evaluate

$$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^{(m)} I(y_m(\mathbf{x}_n) \neq t_n)}{\sum_{n=1}^{N} w_n^{(m)}} \tag{9}$$

   - to get

$$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\} \tag{10}$$

   - Update the weighting coefficients

$$w_n^{(m+1)} = w_n^{(m)} \exp\{\alpha_m I(y_m(\mathbf{x}_n) \neq t_n)\} \tag{11}$$

3. Make predictions using the final model

$$Y_M(\mathbf{x}) = \mathrm{sign}\left[\sum_{m=1}^{M} \alpha_m C_m(x)\right] \tag{12}$$

Adaboost [Freund and Schapire, 1996]

Adaptive boosting

- Strives to create a *strong* classifier out of multiple *weak* ones
- Weak learners are often decision trees in practice
- Works on both classification and regression problems
- Classifiers are trained in sequence
- Training occurs on **weighted** data dependent on the previous classifier
- With each iteration the next classifier is more focused on the problematic data
- Predictions are made with a weighted majority vote

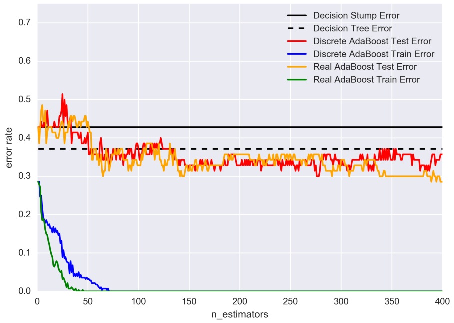
sklearn.ensemble.AdaBoostClassifier

Parameter	Default	Comment
base_estimator	DecisionTreeClassifier	By far the most commonly used
n_estimators	50	Plotting OOB error can help
learning_rate	1.0	Shrinks the contribution of each classifier
max_depth	3	Maximum depth limit for number of nodes in tree
loss	'ls'	Loss function to be optimized (regressor only)

```
from sklearn.ensemble import AdaBoostClassifier
from sklearn.tree import DecisionTreeClassifier

clf = AdaBoostClassifier(DecisionTreeClassifier(max_depth=1),
                         n_estimators=100)

scores = cross_validation.cross_val_score(clf,X,y,cv=5,
                                          scoring='f1_weighted')
print("F1_weighted:%0.2f(+/- %0.2f)"%(scores.mean(),scores.std()*2))
```

```
F1_weighted: 0.73 (+/- 0.08)
```

```
dt_stump = DecisionTreeClassifier(max_depth=1, min_samples_leaf=1)
ada_discrete = AdaBoostClassifier(base_estimator=dt_stump,
                                  n_estimators=n_estimators,
                                  algorithm="SAMME")
ada_real = AdaBoostClassifier(base_estimator=dt_stump,
                              n_estimators=n_estimators,
                              algorithm="SAMME.R")
```



Modified from [Hastie et al., 2009] and the adaboost sklearn example

Gradient boosting

It is a generalization of boosting to arbitrary differentiable loss functions

- Typically uses fixed trees
- Adaboost uses a exponential loss function
- Loss function can be used with both regression and classification
- It uses parameter optimization function **Gradient Decent**

Gradient boosting creates learners as a process. Subsequent learners use the previous step to (i.e. residuals) to weight observations.

Adaboost requires users to specify a set of weak learners where observation weights are continually updated.

sklearn.ensemble.GradientBoostingClassifier

Parameter	Default	Comment
base_estimator	DecisionTreeClassifier	By far the most commonly used
n_estimators	100	Plotting OOB error can help
learning_rate	0.1	Shrinks the contribution of each classifier
max_depth	3	Maximum depth limit for number of nodes in tree
loss	'ls'	Loss function to be optimized

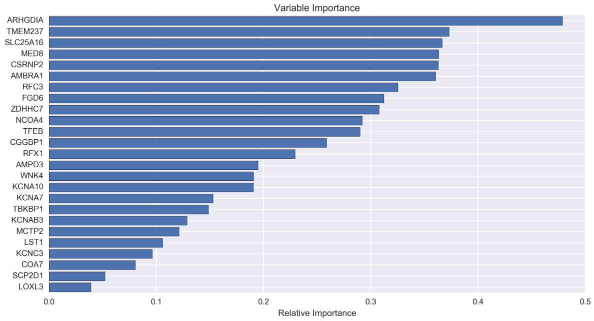
```
params = {'n_estimators': 400, 'max_depth': 4, 'min_samples_split': 1,
          'learning_rate': 0.01}
clf = ensemble.GradientBoostingClassifier(**params)
clf.fit(X_train, y_train)

scores = cross_validation.cross_val_score(clf, X, y, cv=5, scoring='
     f1_weighted')
print("F1_weighted: %0.2f (+/- %0.2f)"%(scores.mean(),scores.std()*2))
```

```
F1_weighted: 0.65 (+/- 0.14)
```

Feature importance

- In regression - Total amount of RSS decreased due to splits for a given predictor
- In classification - Add the total amount the Gini index is decreased due to splits for a given predictor

```
feature_importance = clf.feature_importances_
feature_importance = 100.0*(feature_importance/feature_importance.max())
```



Modified from gradient boosting regression example

Summary

- Bagging provided a major methodological step forward
- Bayesian model averaging in that conceptually it is a single model
- Random Forests reduce the correlation among trees
- Boosting also reduces the correlation among trees
- Bagging and RFs are ensemble methods that use **averaging**
- Boosting is a sequential method **averaging**

- Bagging is improved by using more complex base estimators (i.e. trees)
- Boosting on the other hand works best with simple ones

- Random Forests reduce the correlation among trees
- Boosting also reduces the correlation among trees
- Bagging and RFs are ensemble methods that use **averaging**
- Boosting is a sequential method **averaging**

Resources

Videos

- Hastie and Tibshirani ISLR book video
- Patrick Winston's chalk talk

Other

- A well-written paper about Bayesian model averaging in density estimation
- The new elements of statistical learning book
- Presentation on gradient boosting

Bishop, C. M. (2006).
Pattern Recognition and Machine Learning.
Springer.

Breiman, L. (1996).
Bagging predictors.
Machine Learning, 24(2):123–140.

Breiman, L., Friedman, J. H., Olshen, R. A., and Stone, C. J. (1999).
Classification and Regression Trees.
CRC Press, New York.

Freund, Y. and Schapire, R. E. (1996).
Experiments with a new boosting algorithm.
In Saitta, L., editor, *Proceedings of the Thirteenth International Conference on Machine Learning (ICML 1996)*, pages 148–156. Morgan Kaufmann.

Hastie, T., Tibshirani, R., and Friedman, J. (2009).
The elements of statistical learning: data mining, inference and prediction.
Springer, 2 edition.