Machine Learning

Ensembles: Bagging

Ensembles: Gradient Boosting

Ensembles: Ada Boost

Clustering

Ensemble methods

Why learn one classifier when you can learn many?

Ensemble: combine many predictors

- (Weighted) combinations of predictors
- May be same type of learner or different

Who wants to be a millionaire?

Various options for getting help:

https://www.youtube.com/watch?v=EMe2E-o7jMM

Simple ensembles

"Committees"

- Unweighted average / majority vote:
- Take several trained models, and report their average prediction

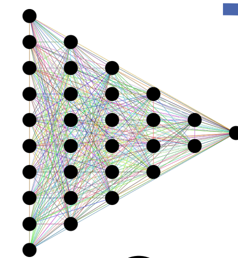
Weighted averages

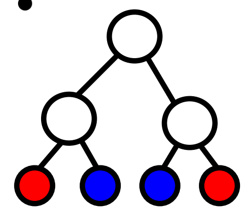
- Up-weight "better" predictors
- Ex: Classes: +1 , -1 , weights alpha:

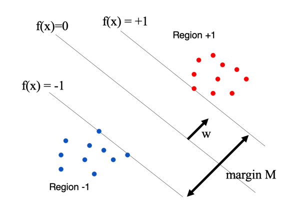
$$\hat{y}_1 = f_1(x_1, x_2, \ldots)$$

$$\hat{y}_2 = f_2(x_1, x_2, \ldots) \qquad \Rightarrow \qquad \hat{y}_e = \mathrm{sign}\left(\sum \alpha_i \, \hat{y}_i\right)$$

…







“Stacked” ensembles

Train a “predictor of predictors”

- Treat individual predictors as features

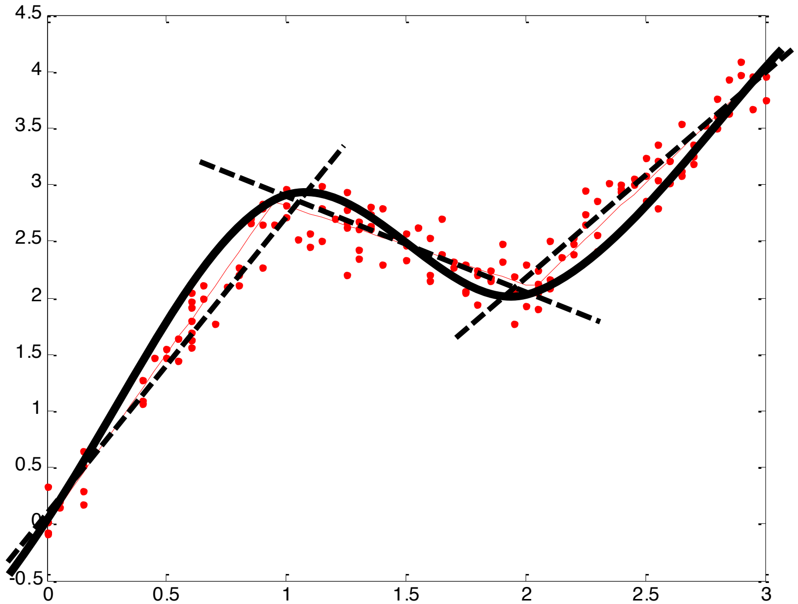
$$\hat{y}_1 = f_1(x_1, x_2, \ldots)$$
$$\hat{y}_2 = f_2(x_1, x_2, \ldots) \quad \Rightarrow \quad \hat{y}_e = f_e(\hat{y}_1, \hat{y}_2, \hat{y}_3, \hat{y}_4, ..)$$
$$\ldots$$

- Similar to multi-layer perceptron idea
- For example, if f_e is a linear classifier:
  - Weighted vote: $\hat{y}_e = sign(\sum_i \alpha_i \hat{y}_i)$, but with learned weights
- Can train stacked learner f_e on validation data
  - Avoids giving high weight to overfit models

Mixtures of experts

Can make weights depend on x

- Weight $\alpha_z(x)$ indicates "expertise"
- Combine using weighted average (or even just pick largest)



Mixture of three linear predictor experts

Weighted average:

$$f(x;\omega,\theta) = \sum_z \alpha_z(x;\omega)\ f_z(x;\theta_z)$$

Weights: (multi) logistic regression

$$\alpha_z(x;\omega) = \frac{\exp(x \cdot \omega^z)}{\sum_c \exp(x \cdot \omega^c)}$$

If loss, learners, weights are all differentiable, can train jointly…

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Ensemble methods

Why learn one classifier when you can learn many?

- "Committee": learn K classifiers, average their predictions

Bagging = bootstrap aggregation

- Learn many classifiers, each with only part of the data
- Combine through model averaging

Remember overfitting: "memorize" the data

- Used test data to see if we had gone too far
- Cross-validation
  - Make many splits of the data for train & test
  - Each of these defines a classifier
  - Typically, we use these to check for overfitting
  - Instead of checking if we overfit, we combine these classifiers to produce a better classdifier

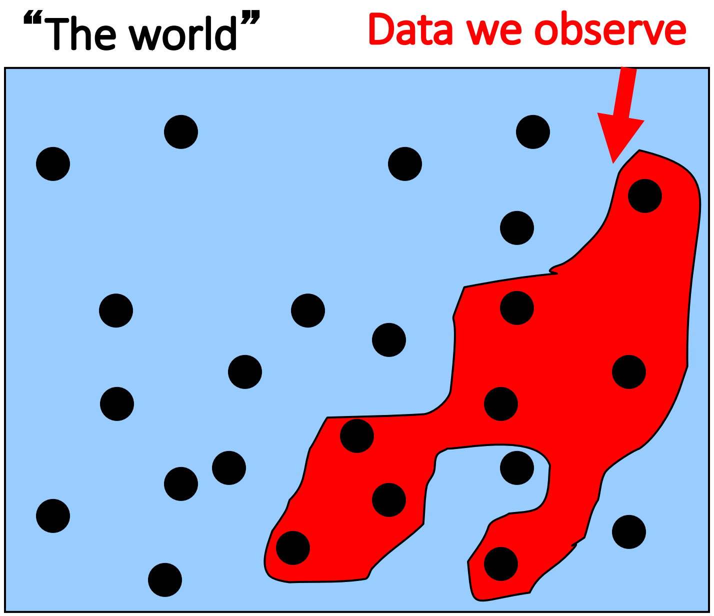
Bagging

Bootstrap
- Create a random subset of data by sampling
- Draw m’ of the m samples, with replacement (some variants w/o)
  - Some data left out; some data repeated several times

Bagging
- Repeat K times
  - Create a training set of m’ < m examples
  - Train a classifier on the random training set
- To test, run each trained classifier
  - Each classifier votes on the output, take majority
  - For regression: each regressor predicts, take average

Some complexity control: harder for each to memorize data
  - Each learner has data set where data points are missing, thus memorization is suppressed
  - Doesn’t work for linear models (average of linear functions is linear function…)
  - Perceptrons OK (linear + threshold = nonlinear)

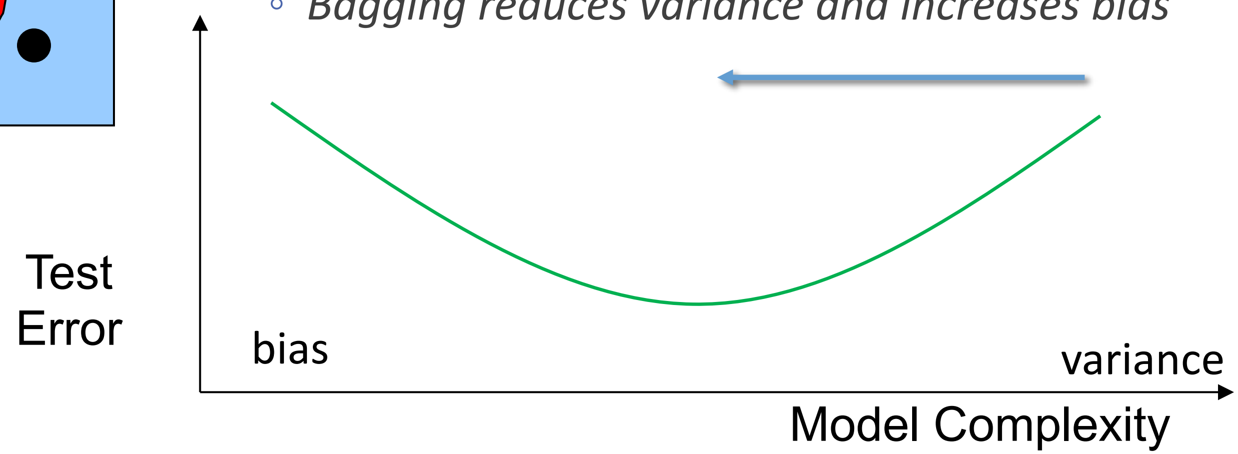
Bias / variance



We only see a little bit of data

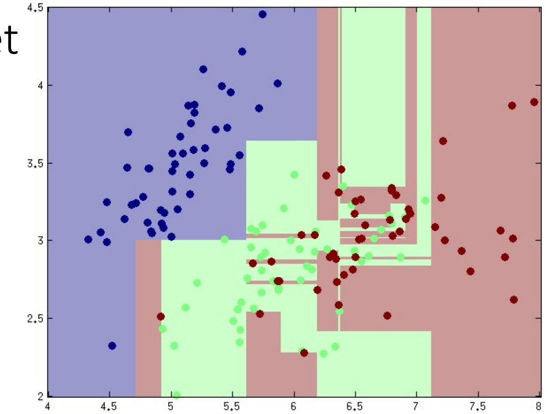
Can decompose error into two parts

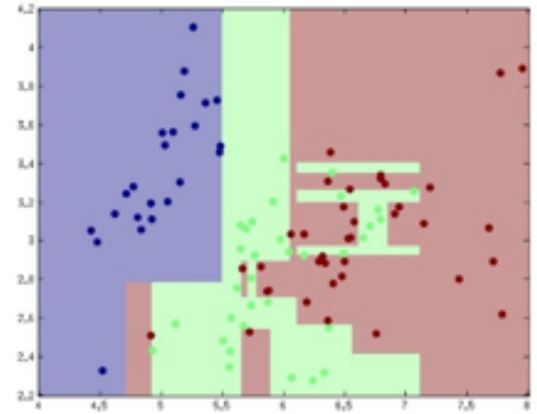
- Bias – error due to model choice
  - Inability of model class to represent the best function
  - Gets better with more model complexity
- Variance – randomness due to data size
  - Better w/ more data, worse w/ complexity
- *Bagging reduces variance and increases bias*



Bagged decision trees

Full data set

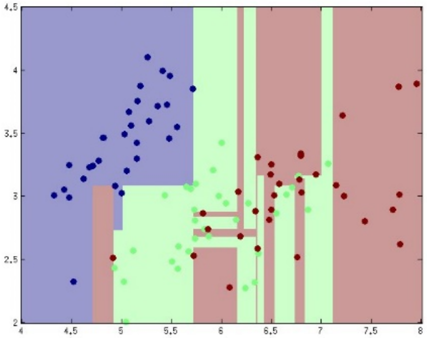


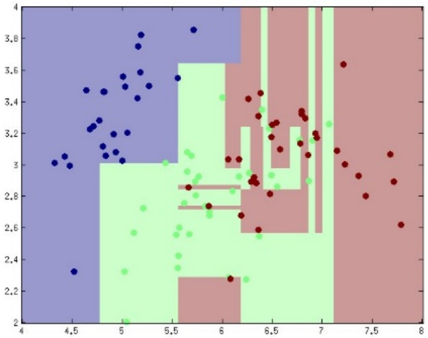


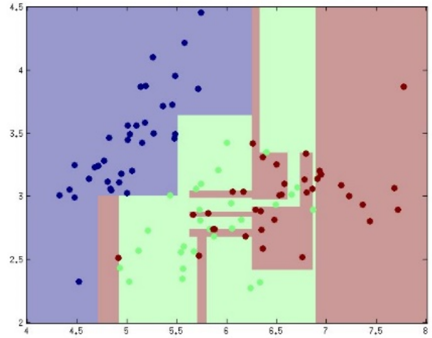
Randomly resample data

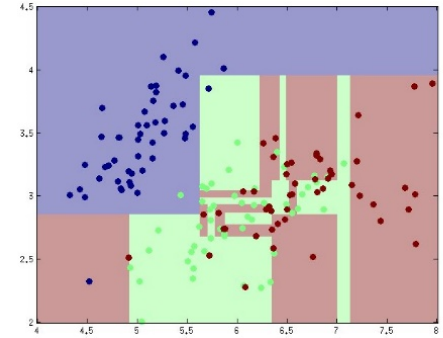
Learn a decision tree for each

- No max depth = very flexible class of functions
- Learner is low bias, but high variance
- Sampling:
  - simulates “equally likely” data sets we could have observed
  - train decision tree on every sampled data set

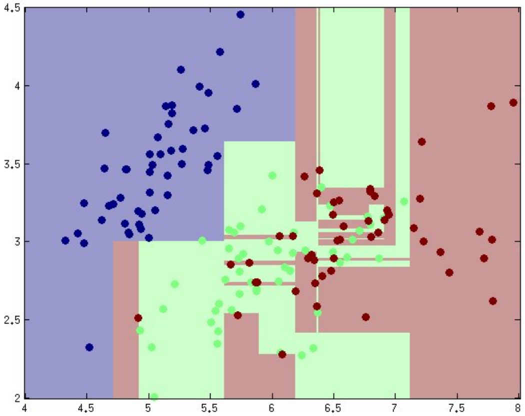








Bagged decision trees



Full data set

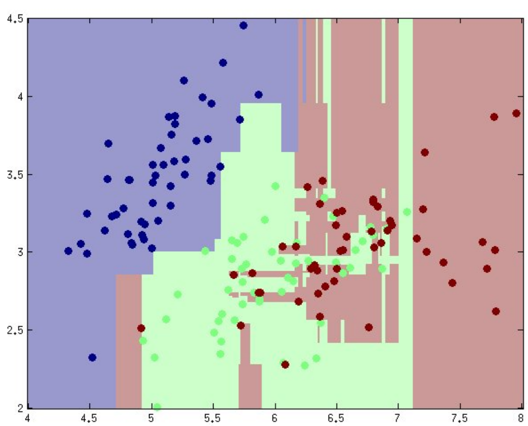
Average over collection

- Classification: majority vote

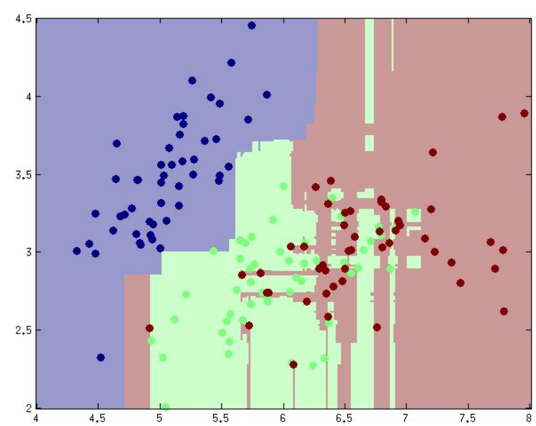
Reduces memorization effect

- Not every predictor sees each data point
- Lowers effective “complexity” of the overall average
- Usually, better generalization performance
- Intuition: reduces variance while keeping bias low

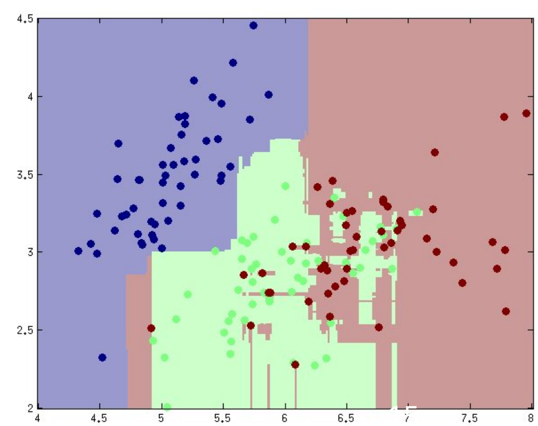
Avg of 5 trees



Avg of 25 trees



Avg of 100 trees



Bagging in Python

```
# Load data set X, Y for training the ensemble…
m,n = X.shape
classifiers = [ None ] * nBag                # Allocate space for learners
for i in range(nBag):
    ind = np.floor( m * np.random.rand(nUse)) # Bootstrap sample a data set:
    Xi, Yi  =  X[ind,:], Y[ind]               # select the data at those indices
    classifiers[i] = ml.MyClassifier(Xi, Yi)  # Train a model on data Xi, Yi
```

```
# test on data Xtest
mTest = Xtest.shape[0]
predict = np.zeros( (mTest, nBag) )    # Allocate space for predictions from each model
for i in range(nBag):
    predict[:,i] = classifiers[i].predict(Xtest)   # Apply each classifier

# Make overall prediction by majority vote
predict = np.mean(predict, axis=1) > 0 # if +1 vs -1
```

Random forests

Bagging applied to decision trees

Problem

- With lots of data, we usually learn the same classifier
- Averaging over these doesn't help!

Introduce extra variation in learner

- At each step of training, only allow a subset of features
- Enforces diversity ("best" feature not available)
- Keeps bias low (every feature available eventually)
- Average over these learners (majority vote)

```
# in FindBestSplit(X,Y):
for each of a subset of features
   for each possible split
       Score the split  (e.g. information gain)
Pick the feature & split with the best score
Recurse on left & right splits
```

Summary

Ensembles: collections of predictors

- Combine predictions to improve performance

Bagging

- "Bootstrap aggregation"
- Reduces complexity of a model class prone to overfit
- In practice: Resample the data many times
  - For each, generate a predictor on that resampling
- Plays on bias / variance trade off
- Price: more computation per prediction

Machine Learning

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Clustering

Ensembles

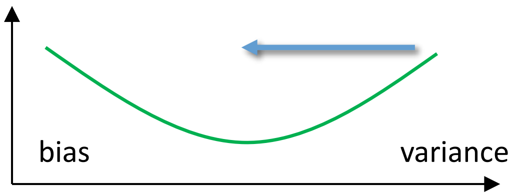
Weighted combinations of predictors

"Committee" decisions

- Trivial example
- Equal weights (majority vote / unweighted average)
- Might want to weight unevenly – up-weight better predictors

Bagging

- Bootstrapping: subsampling with replacement
- Train classifiers on bootstraps, average the results
- Reduces complexity of a model class prone to overfit
  - Plays on bias / variance trade off



Ensembles

Weighted combinations of predictors

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- Trivial example
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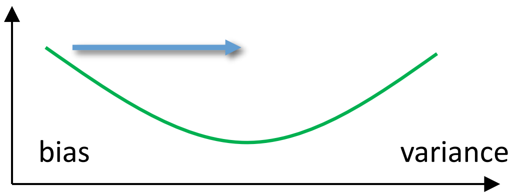
Boosting

- Focus new learners on examples that others get wrong
- Train learners sequentially
- Errors of early predictions indicate the "hard" examples
- Focus later predictions on getting these examples right
- Combine the whole set in the end
- Convert many "weak" learners into a complex predictor



Gradient boosting

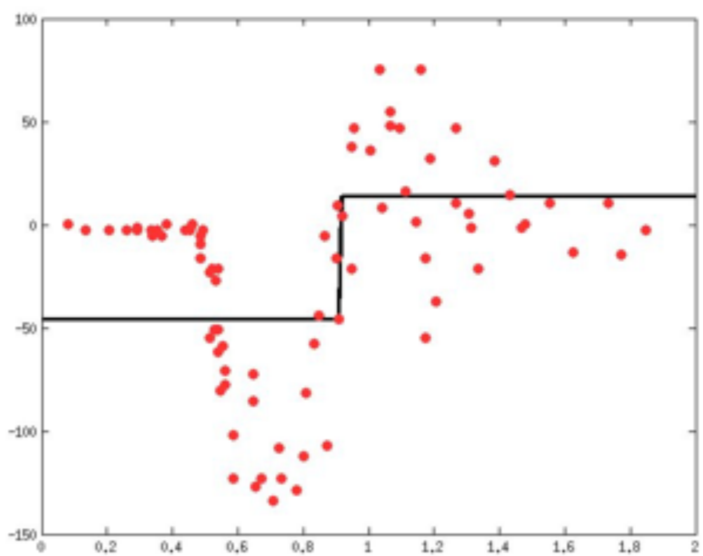
Learn a regression predictor $f_1(x^{(i)}) \approx y^{(i)}$

Compute the error residual $\epsilon^{(i)} = y^{(i)} - f_1(x^{(i)})$

Learn to predict the residual $f_2(x^{(i)}) \approx \epsilon^{(i)}$

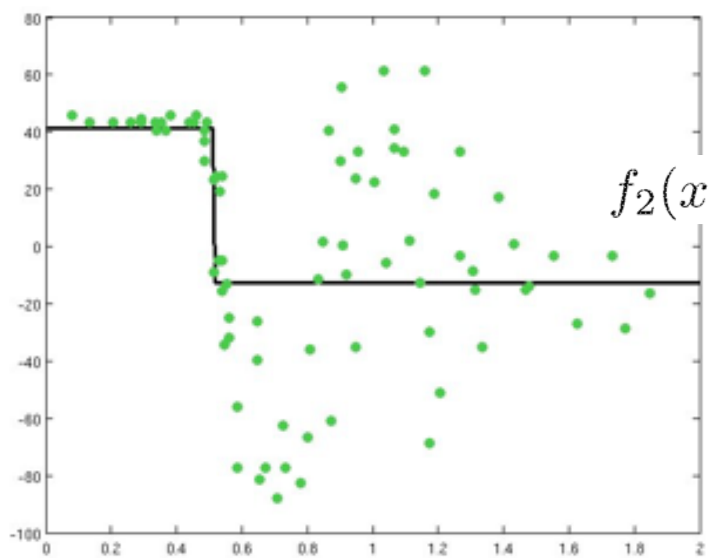
Learn a simple predictor…

$$f_1(x^{(i)}) \approx y^{(i)}$$



Then try to correct its errors

$$\epsilon^{(i)} = y^{(i)} - f_1(x^{(i)})$$



$$f_2(x^{(i)}) \approx \epsilon^{(i)}$$

Gradient boosting

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Compute the error residual $\epsilon^{(i)} = y^{(i)} - f_1(x^{(i)})$

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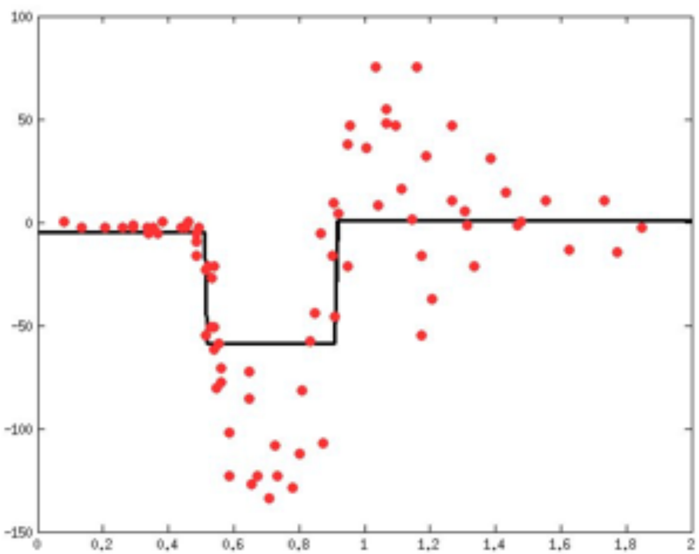
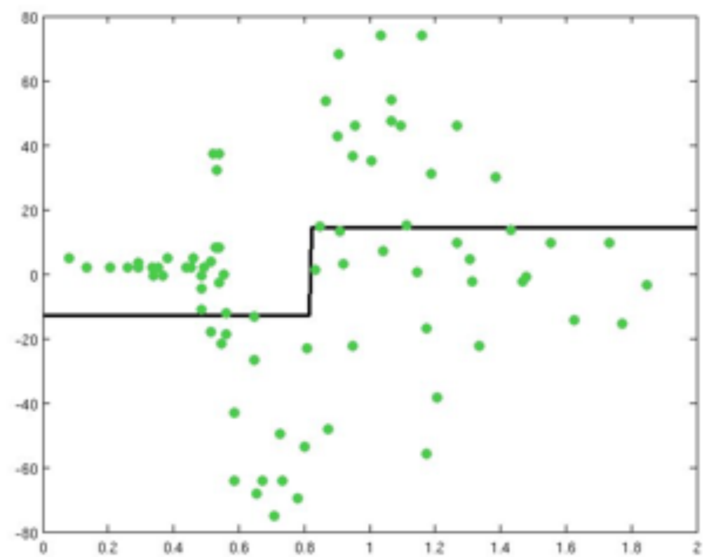
Combining gives a better predictor…

$$\Rightarrow \quad f_1(x^{(i)}) + f_2(x^{(i)}) \approx y^{(i)}$$



Can try to correct its errors also, & repeat

$$\epsilon_2^{(i)} = y^{(i)} - f_1(x^{(i)} - f_2(x^{(i)}) \quad \ldots$$



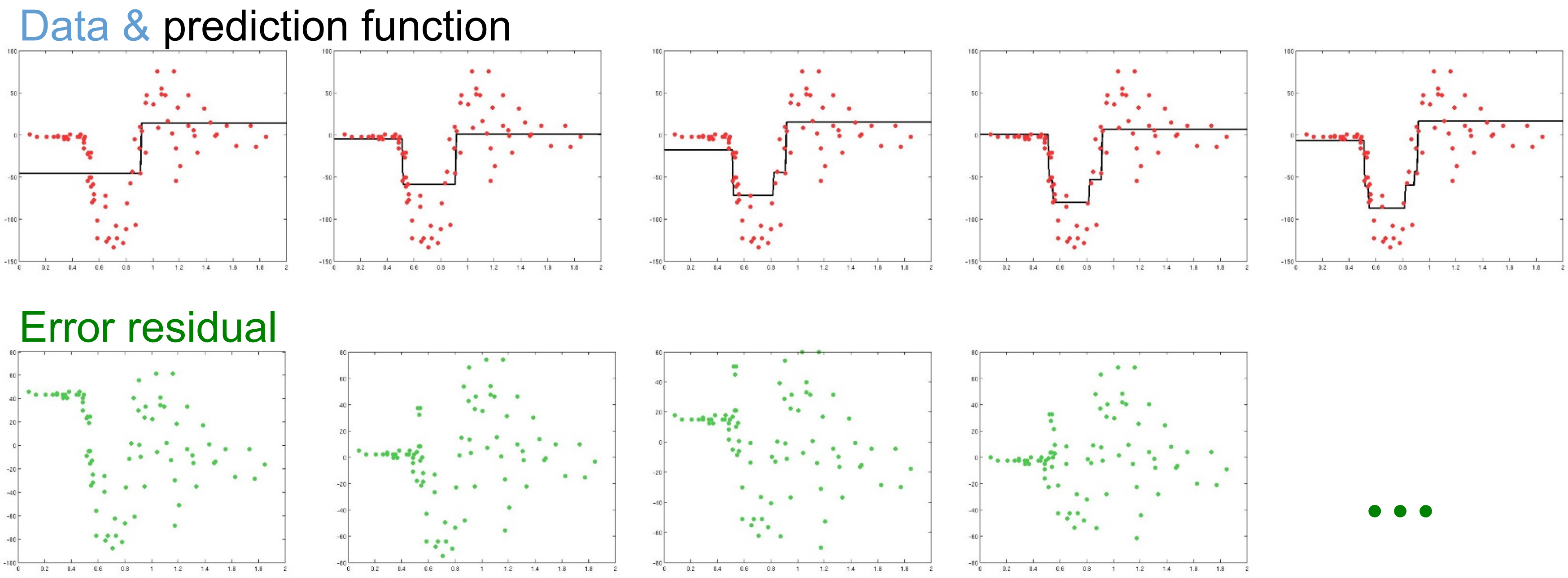
Gradient boosting

Learn sequence of predictors

Sum of predictions is increasingly accurate

Predictive function is increasingly complex

$$y^{(i)} \approx \sum_z f_z(x^{(i)})$$



Gradient boosting

Make a set of predictions $\hat{y}[i]$

The "error" in our predictions is $J(y,\hat{y})$

- For MSE: $J(.) = \sum (y[i] - \hat{y}[i])^2$

We can "adjust" $\hat{y}$ to try to reduce the error

- $\hat{y}[i] = \hat{y}[i] + \alpha \, f[i]$
- $f[i] \approx \nabla J(y, \hat{y})$ $= (y[i]-\hat{y}[i])$ for MSE

Each learner is estimating the gradient of the loss function

Gradient descent: take sequence of steps to reduce J

- Sum of predictors, weighted by step size α

Gradient boosting in Python

```
# Load data set X, Y …
learner = [None] * nBoost   # storage for ensemble of models
alpha = [1.0] * nBoost # and weights of each learner
mu = Y.mean()      # often start with constant ”mean” predictor
dY = Y – mu        # subtract this prediction away
for k in range( nBoost ):
    learner[k] = ml.MyRegressor( X, dY )     # regress to predict residual dY using X
    alpha[k] = 1.0     # alpha: ”learning rate” or ”step size”
    # smaller alphas need more classifiers, but may predict better given enough of them

    # compute the residual given our new prediction:
    dY = dY – alpha[k] * learner[k].predict(X)
```

```
# test on data Xtest
mTest = Xtest.shape[0]
predict = np.zeros( (mTest,) ) + mu  # Allocate space for predictions & add 1st (mean)
for k in range(nBoost):
    predict += alpha[k] * learner[k].predict(Xtest) # Apply next predictor & accum
```

Summary

Ensemble methods

- Combine multiple classifiers to make "better" one
- Committees, average predictions
- Can use weighted combinations
- Can use same or different classifiers

Gradient Boosting

- Use a simple regression model to start
- Subsequent models predict the error residual of the previous predictions
- Overall prediction given by a weighted sum of the collection

Demo Time

http://arogozhnikov.github.io/2016/06/24/gradient_boosting_explained.html

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Ensembles

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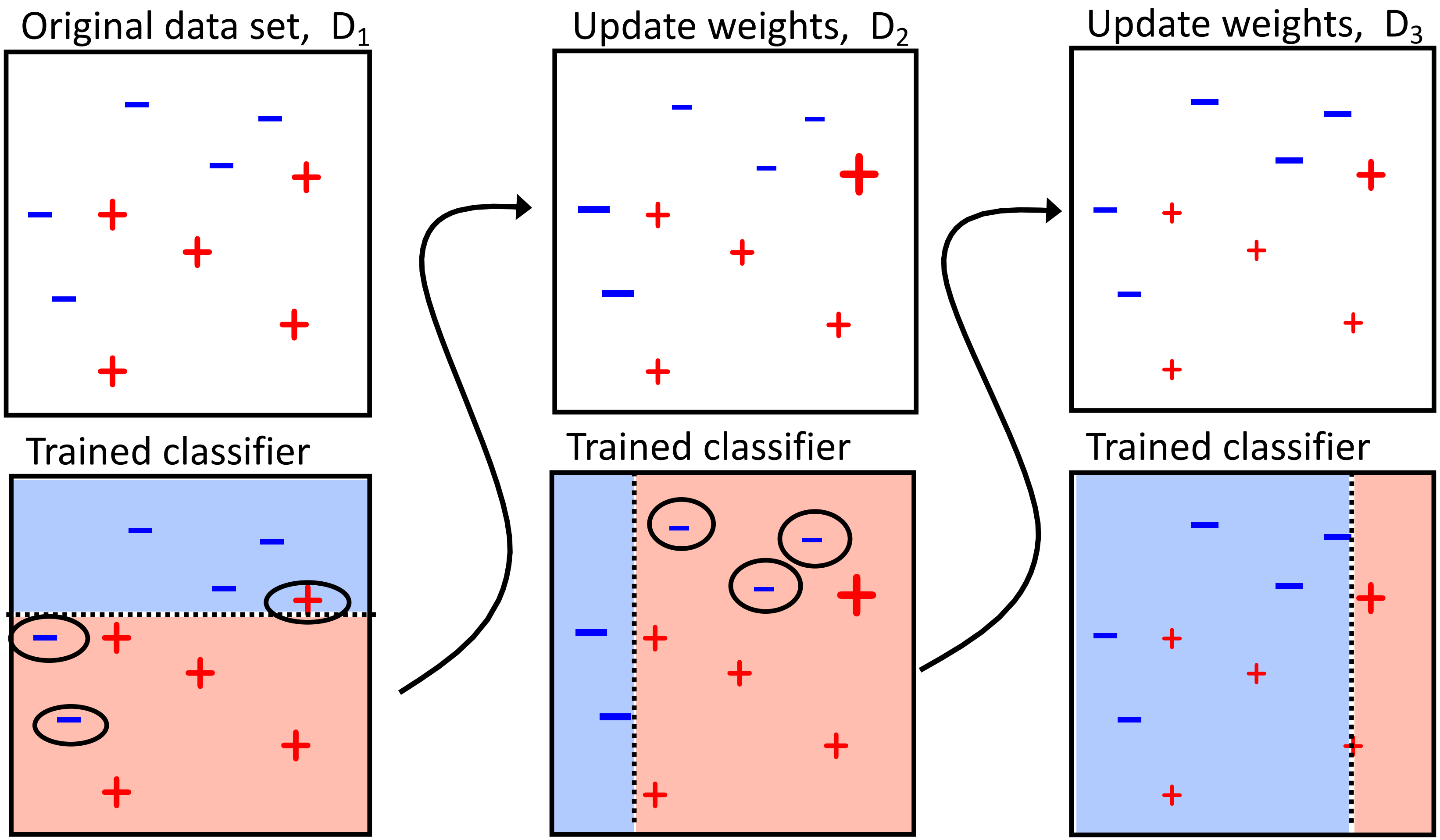
Boosting example



Minimizing Weighted Error

So far we've mostly minimized unweighted error

Minimizing weighted error is no harder!

Unweighted average loss:

$$J(\theta) = \frac{1}{m} \sum_i J_i(\theta, x^{(i)})$$

Weighted average loss:

$$J(\theta) = \sum_i w_i J_i(\theta, x^{(i)})$$

For any loss (logistic MSE, hinge, …)

$$J(\theta, x^{(i)}) = \left(\sigma(\theta x^{(i)}) - y^{(i)}\right)^2$$

$$J(\theta, x^{(i)}) = \max\left[0\,,\, 1 - y^{(i)}\, \theta x^{(i)}\right]$$

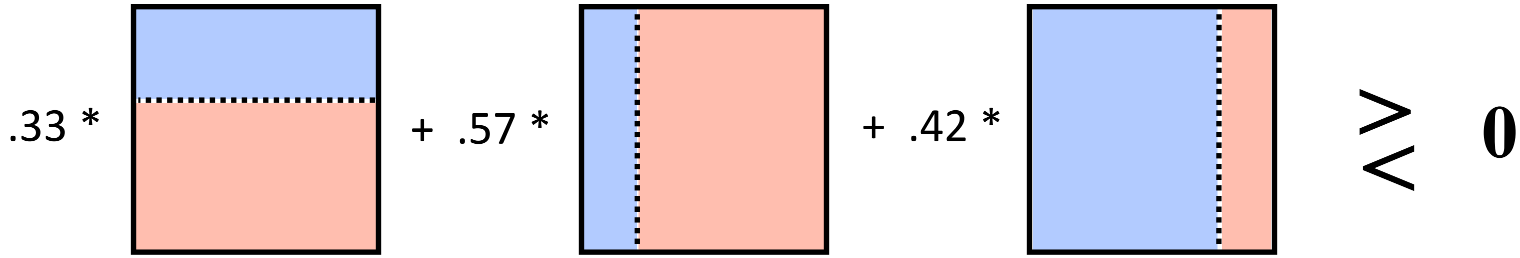
For e.g. decision trees, compute weighted information gain:

$p(+1) \propto$ total weight of data with class +1

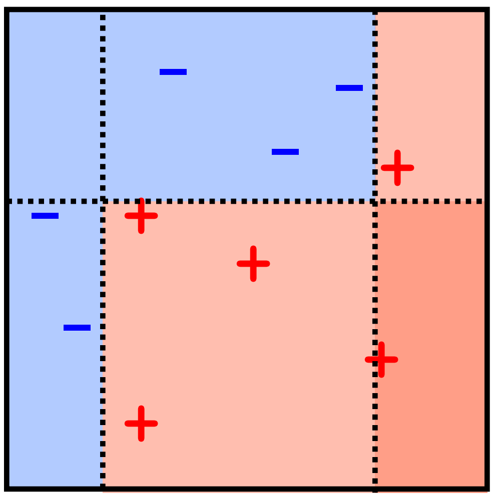
$p(-1) \propto$ total weight of data with class -1 => $H(p)$ = entropy

Boosting example

Weight each classifier and combine them:



Combined classifier



1-node decision trees
"decision stumps"
very simple classifiers

AdaBoost: "Adaptive boosting"

```
# Load data set X, Y … ; Y assumed +1 / -1
for i in range(nBoost):
  learner[i] = ml.MyClassifier( X,Y, weights=wts ) # train a weighted classifier
  Yhat = learner[i].predict(X)
  e = wts.dot( Y != Yhat )              # compute weighted error rate
  alpha[i] = 0.5 * np.log( (1-e)/e )
  wts *= np.exp( -alpha[i] * Y * Yhat )        # update weights
  wts /= wts.sum()                 #    and normalize them
```

Notes

- e > .5 means classifier is not better than random guessing
- if Y == Yhat, Y * Yhat > 0 and weights decrease
- Otherwise, they increase

```
# Final classifier:
predict = np.zeros( (mTest,) )
for i in range(nBoost):
    predict += alpha[i] * learner[i].predict(Xtest)# compute contribution of each
predict = np.sign(predict)             # and convert to +1 / -1 decision
```

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- Combine multiple classifiers to make "better" one
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- Weighted combinations
- Can use same or different classifiers

Boosting

- Train sequentially; later predictors focus on mistakes by earlier

Boosting for classification (e.g., AdaBoost)

- Use results of earlier classifiers to know what to work on
- Weight "hard" examples so we focus on them more
- Example: Viola-Jones for face detection