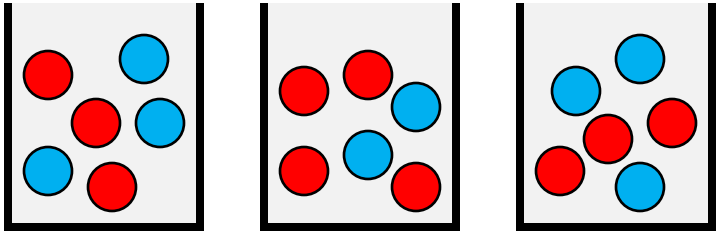
COMP 432 Machine Learning

Bagging & Boosting

Computer Science & Software Engineering
Concordia University, Fall 2021

Bagging



Bagging

- Bootstrap aggregation (B-agg-ing => Bagging) is a simple technique for combining "unstable" models and making them more "stable"
- *Unstable:* a small change in training data can lead to a large change in predictions.
  - Decision trees, high-degree polynomials, …
  - Hard-margin SVM unstable inside margin, stable outside
- Random forests are just "bagged decision trees"

Bagging predictors

L Breiman - Machine learning, 1996 - Springer

Bagging predictors is a method for generating multiple versions of a predictor and using these to get an aggregated predictor. The aggregation averages over the versions when predicting a numerical outcome and does a plurality vote when predicting a class. The …

☆ 99 Cited by 21633 Related articles All 65 versions »

Bootstrap sampling

- **Idea:** Train a model that is insensitive to dropping or duplicating individual training examples
  - After all, the observed training data is just *one* possible sampling from the true data distribution.
- Remember considerations for random forests?...
  - Should we *perturb* the data? Possible, but hard to know what perterbations help or 'corrupt' in harmful ways.
  - Should we *subsample* the data? Reasonable! But each new training set is smaller than N, and by how much?
  - Should we *re-sample* the data *with replacement*? Good! Some $(\mathbf{x}_i, y_i)$ get duplicated, but no parameters to choose.

This is called "bootstrap sampling" and each re-sampling is called a "bootstrap sample"

Proposed for statistical analyses *by Brad Efron* in 1979-1982

Sampling with replacement in Python

- See slide from prev lecture on how to sample data for random forests:

```
print(X)
print(y)
```

```
[[0. 0.]
 [1. 1.]
 [2. 2.]
 [3. 3.]
 [4. 4.]]
[0 1 2 3 4]
```

```
sample_indices = np.random.randint(0, N, N)
print(sample_indices)
```

```
[2 4 2 1 3]
```

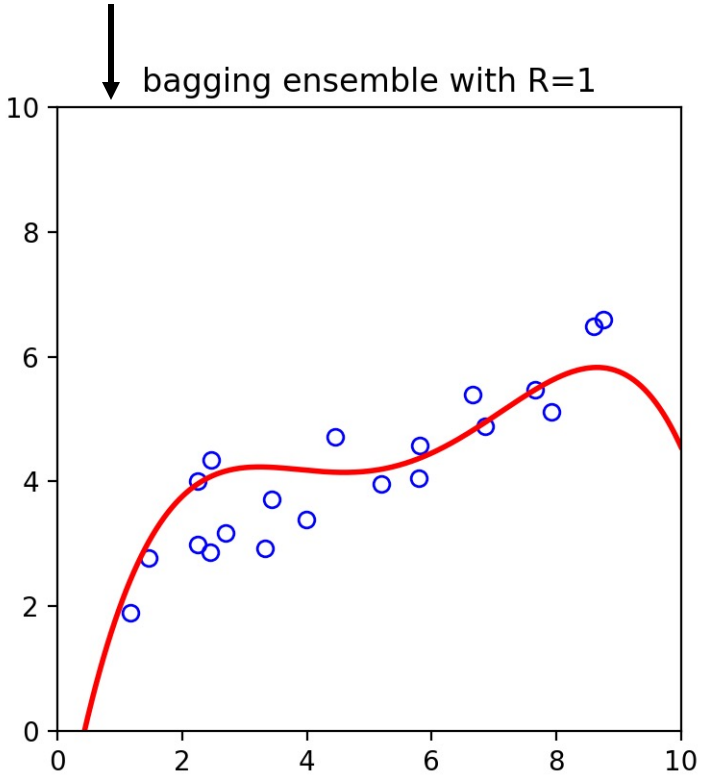
```
X_resampled = X[sample_indices]
y_resampled = y[sample_indices]
print(X_resampled)
print(y_resampled)
```

```
[[2. 2.]
 [4. 4.]
 [2. 2.]
 [1. 1.]
 [3. 3.]]
[2 4 2 1 3]
```

- Bootstrap is a *general idea* from statistics, *not* specific to random forests!

Bagging Example 1

One model trained on a *bootstrap sample* of the training data.

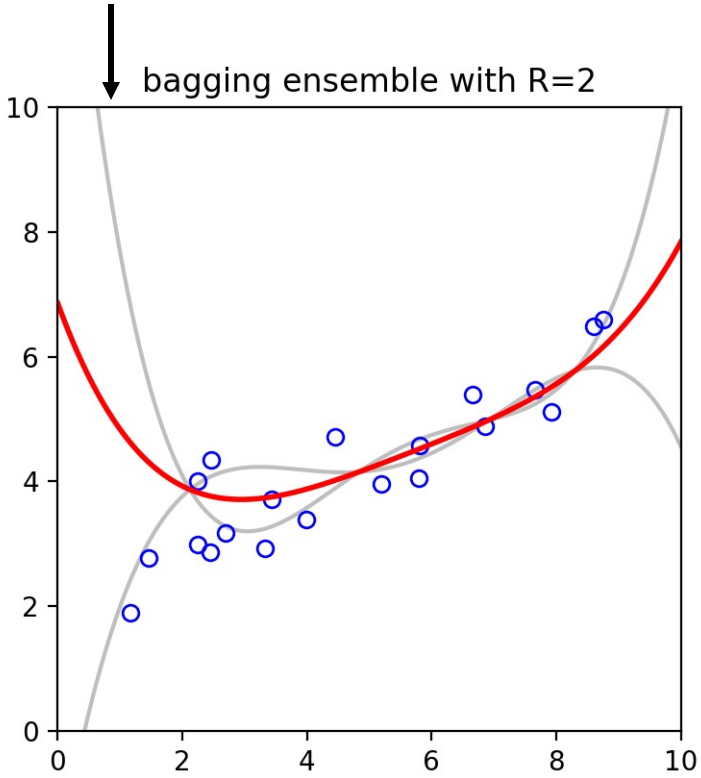


Fit polynomial to this data by using linear regression on feature transformation

$$\phi(x) = \begin{bmatrix} 1 & x & x^2 & x^3 & x^4 \end{bmatrix}^T$$

Bagging Example 1

Average of *R*=2 models, each trained on a different bootstrap sample of the training data.



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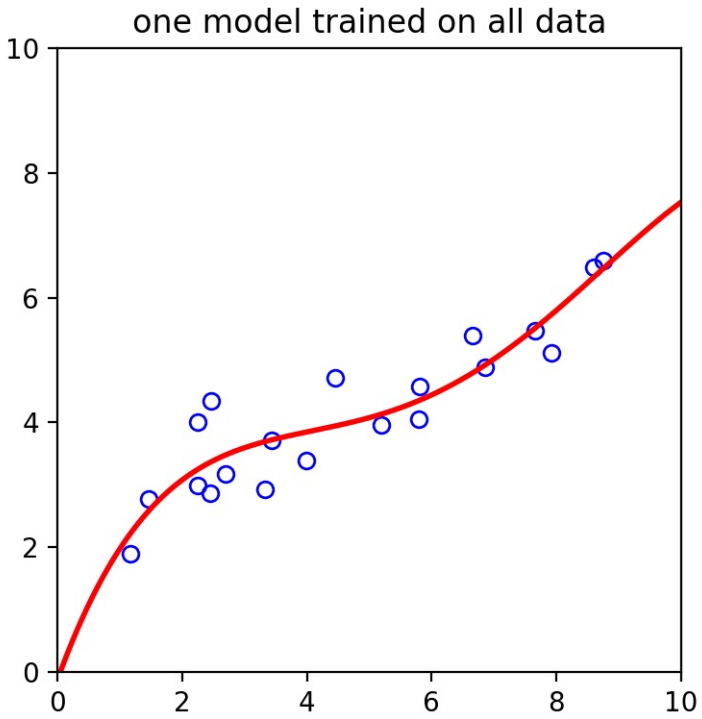

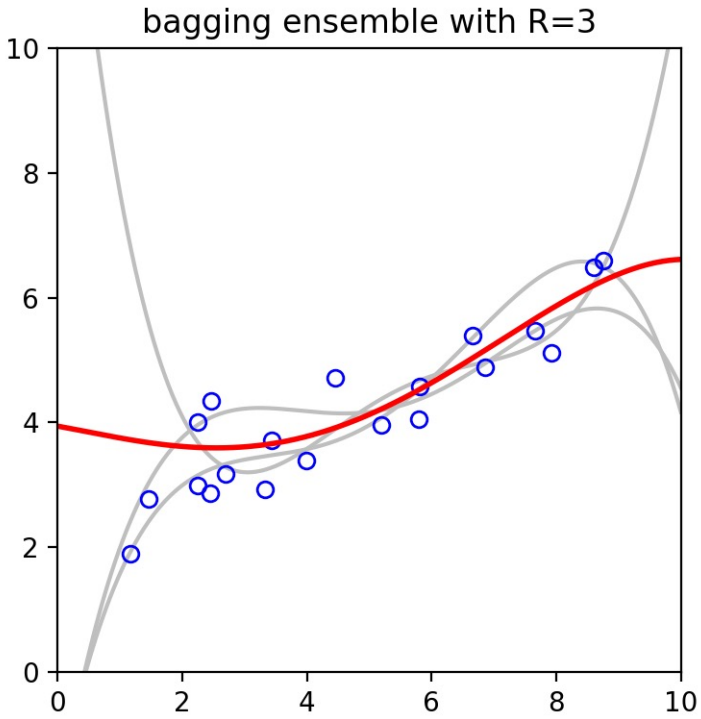

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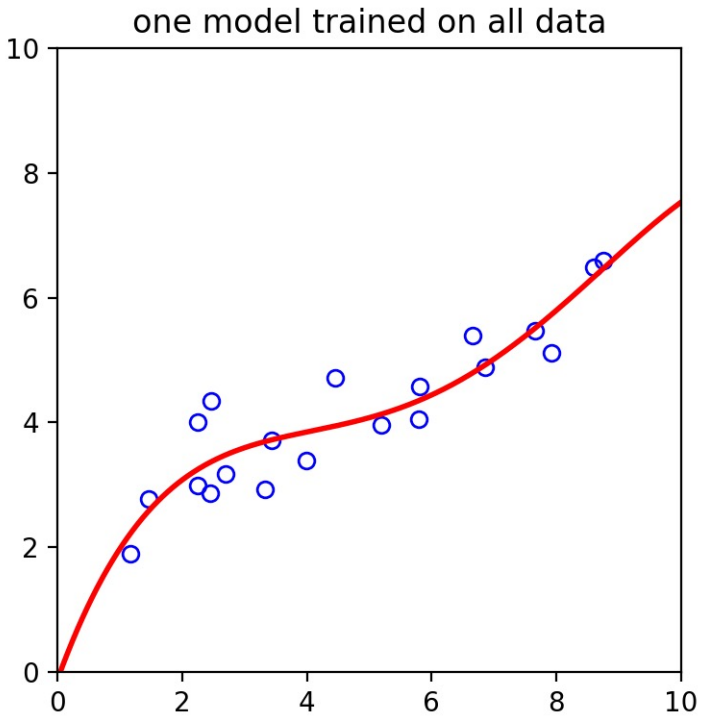

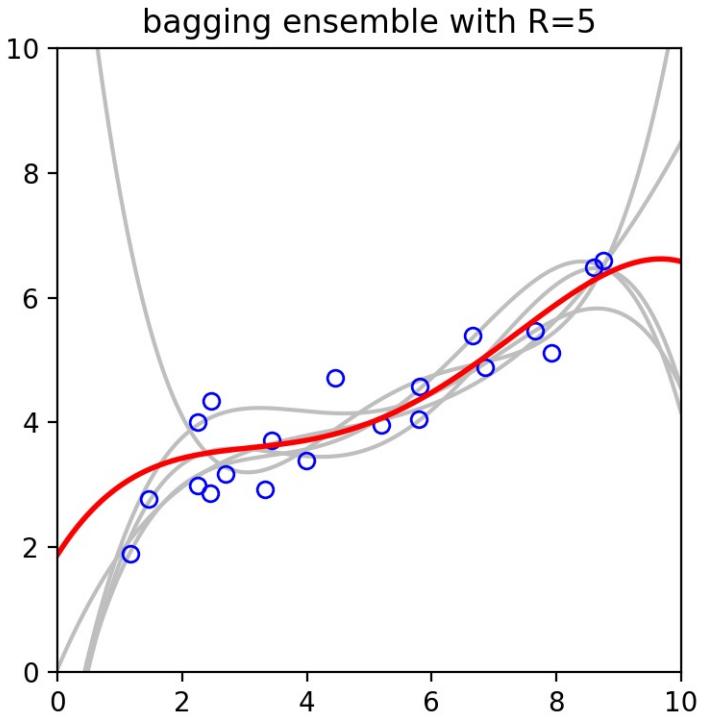

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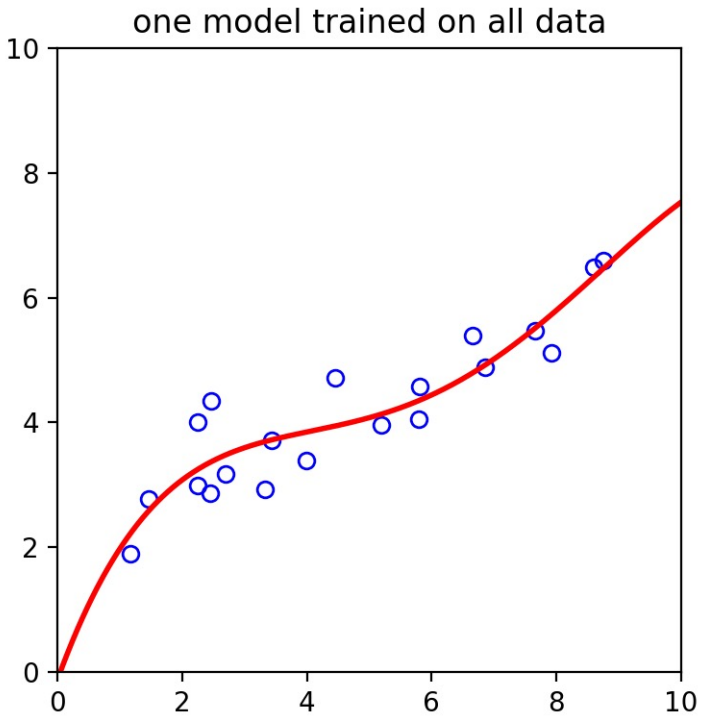
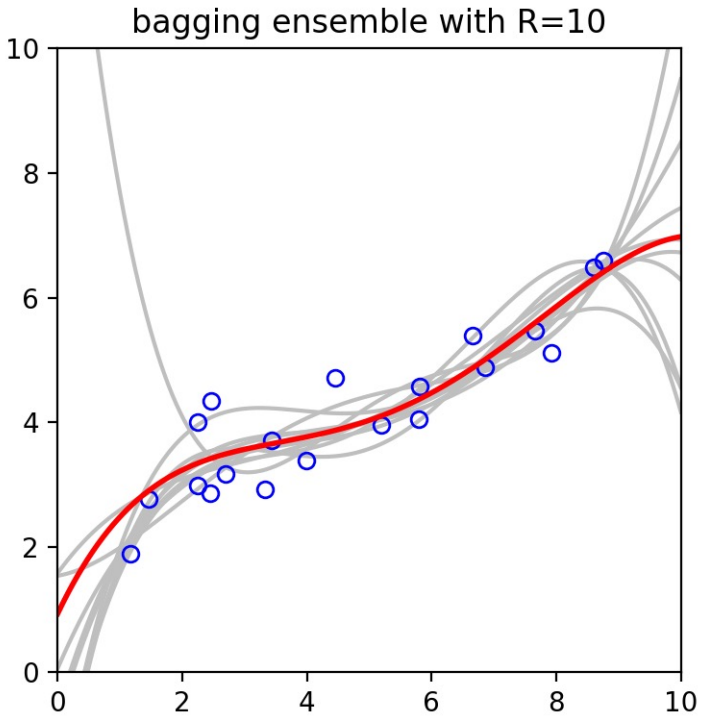
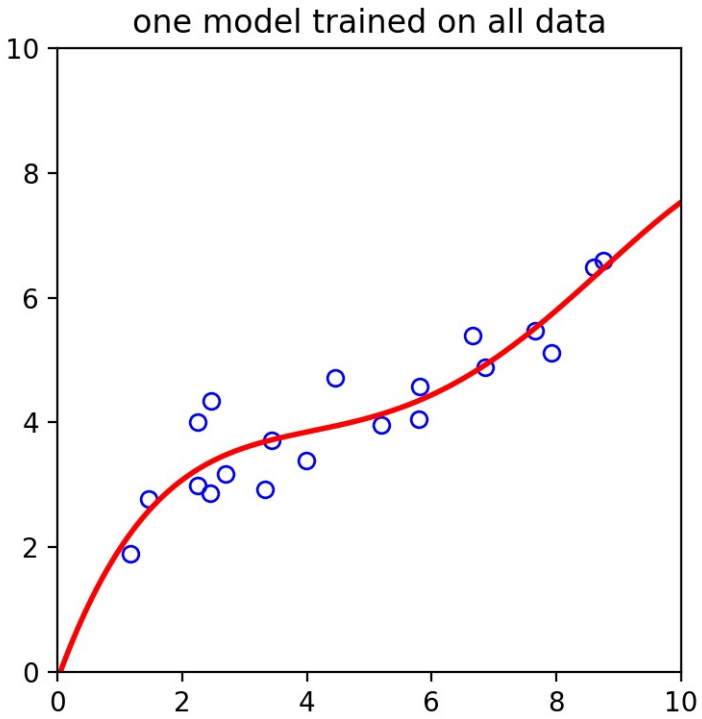


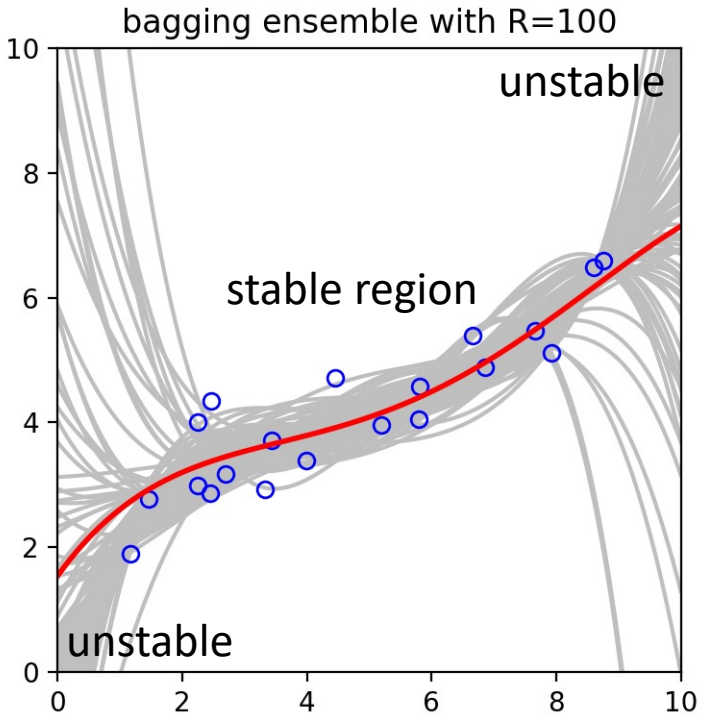


Fit polynomial to this data by using linear regression on feature transformation

$$\boldsymbol{\phi}(x) = \begin{bmatrix} 1 & x & x^2 & x^3 & x^4 \end{bmatrix}^T$$

Bagging Example 1



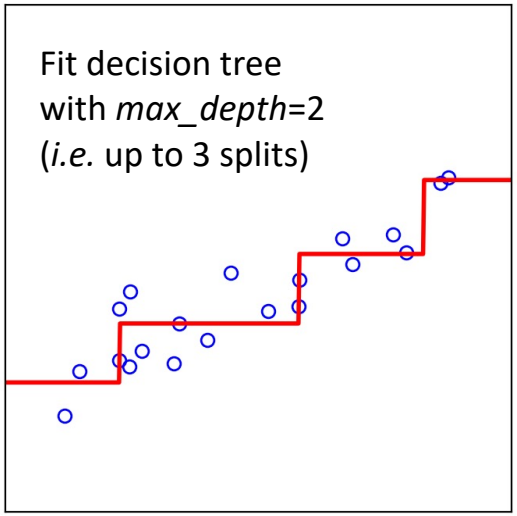


Fit polynomial to this data by using linear regression on feature transformation

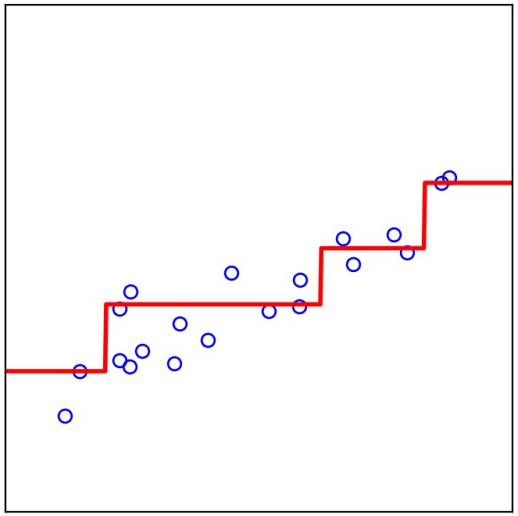
$$\phi(x) = \begin{bmatrix} 1 & x & x^2 & x^3 & x^4 \end{bmatrix}^T$$

Example 2: Decision Tree Regression

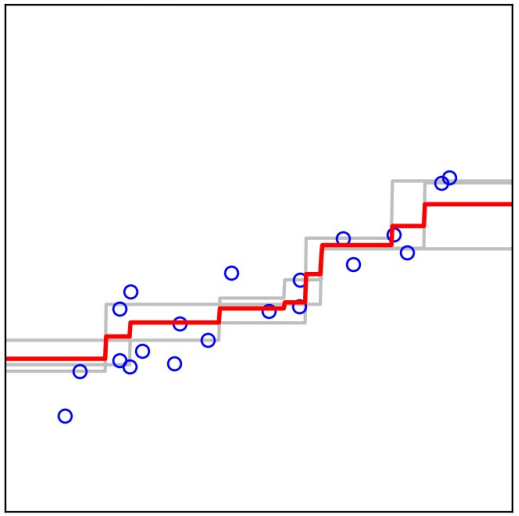
one model trained on all data



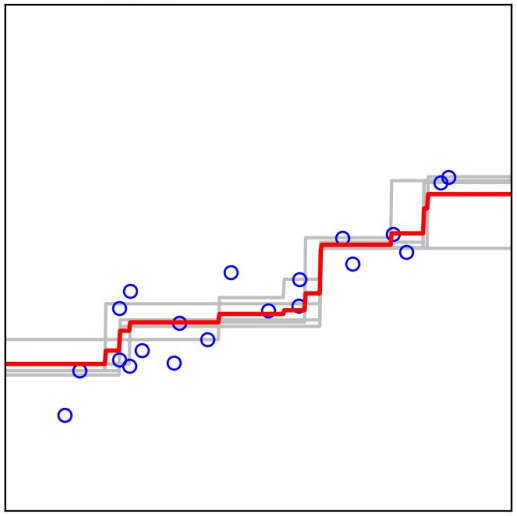
bagging ensemble with R=1



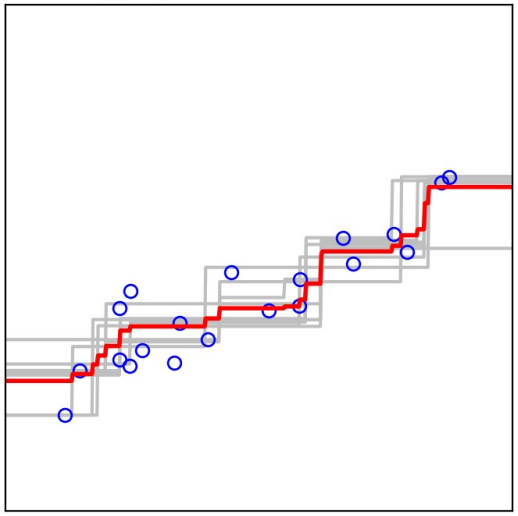
bagging ensemble with R=3



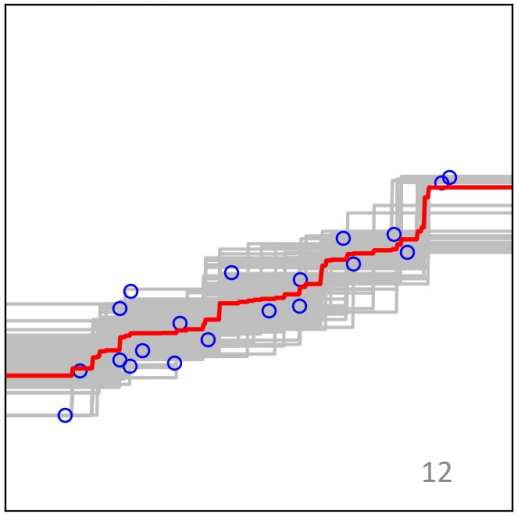
bagging ensemble with R=5



bagging ensemble with R=10



bagging ensemble with R=100



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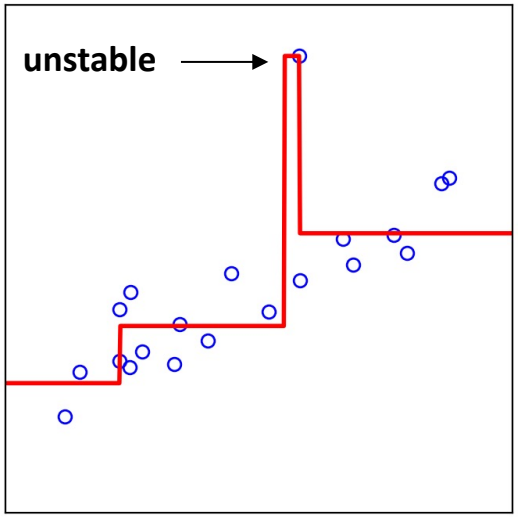
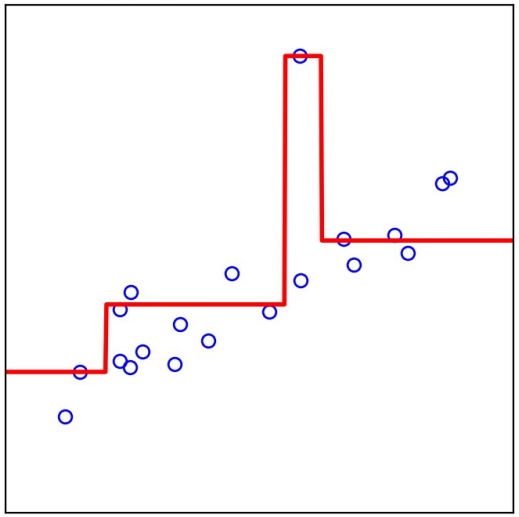
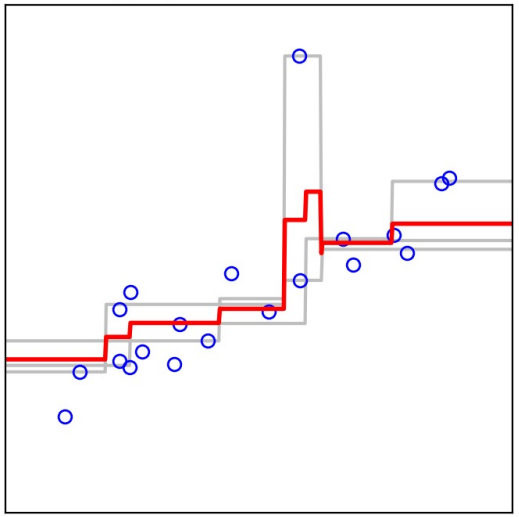


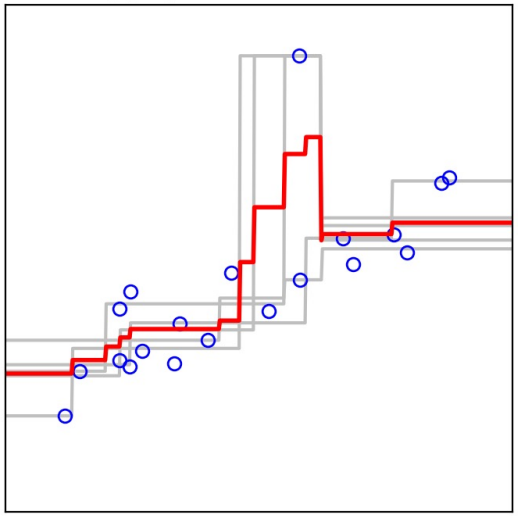
bagging ensemble with R=1



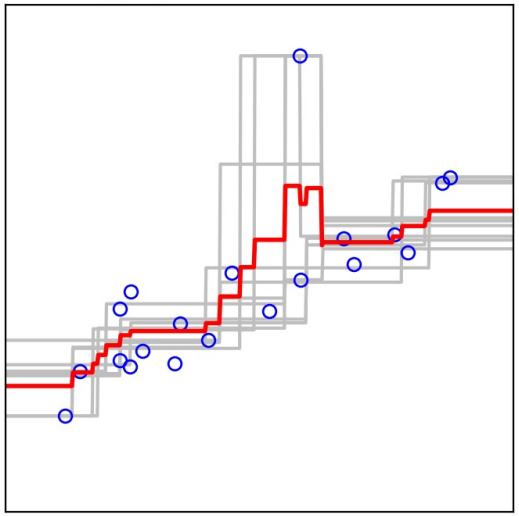
bagging ensemble with R=3



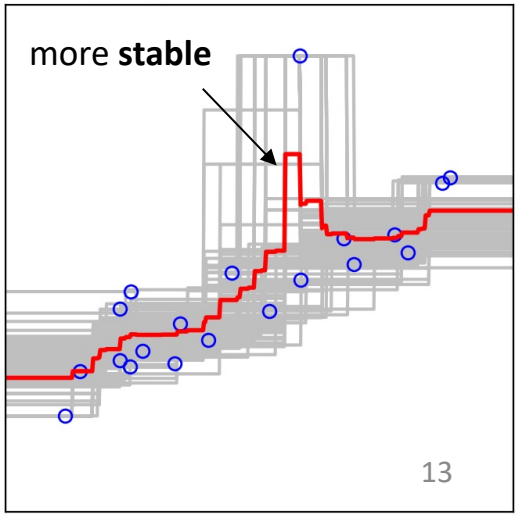
bagging ensemble with R=5



bagging ensemble with R=10

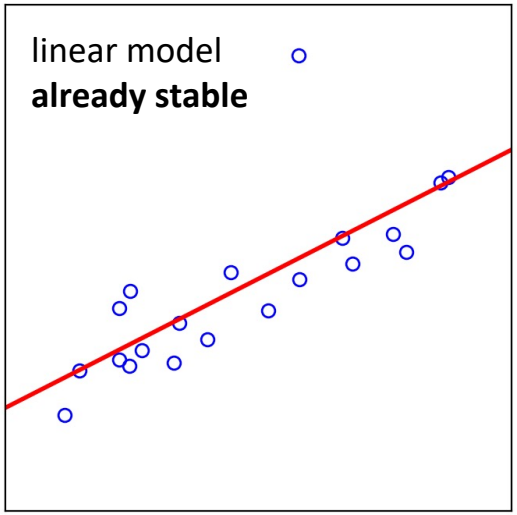


bagging ensemble with R=100

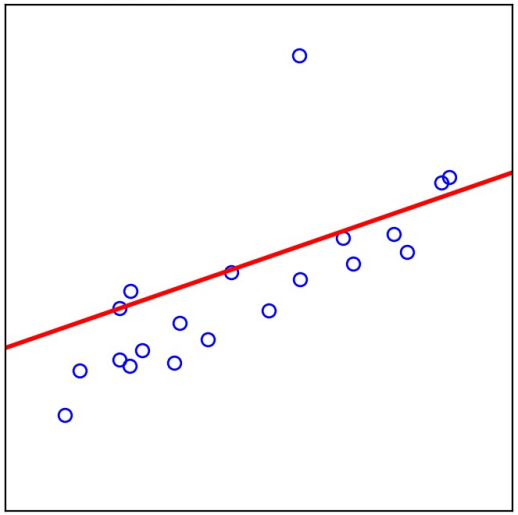


Example 3: Linear Regression

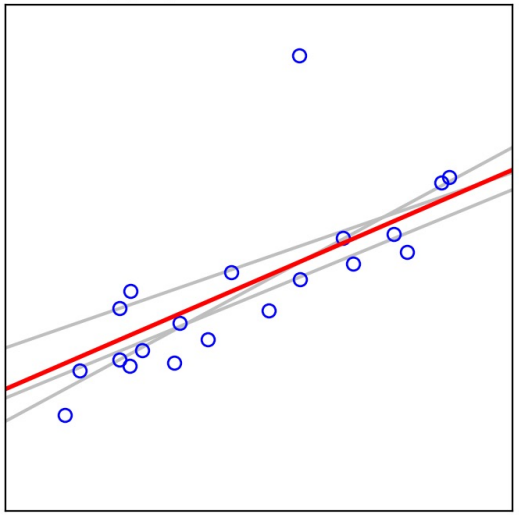
one model trained on all data



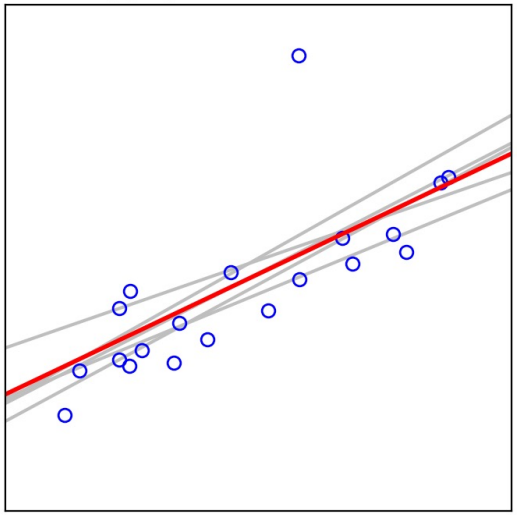
bagging ensemble with R=1



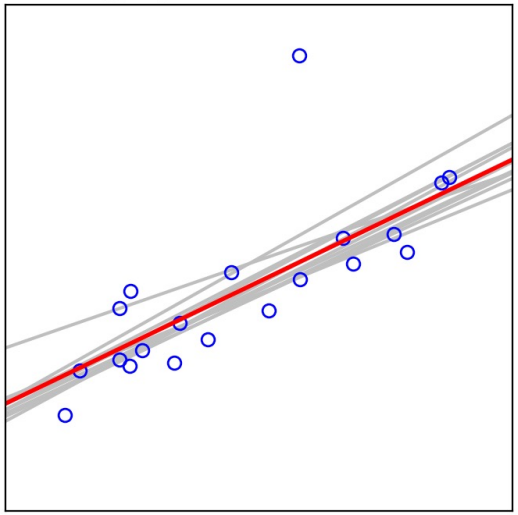
bagging ensemble with R=3



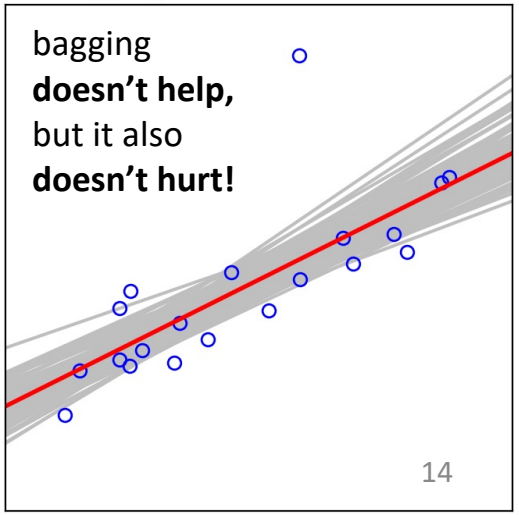
bagging ensemble with R=5



bagging ensemble with R=10



bagging ensemble with R=100



Scikit-learn makes bagging easy!

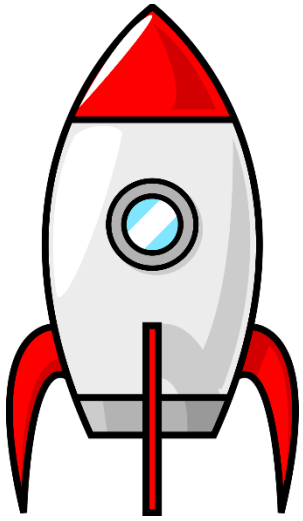
```
# Create a prototype of the kind of model we want BaggingRegressor to fit
tree = DecisionTreeRegressor(max_depth=2)

# Create a model with 10 separate DecisionTreeRegressor instances inside
model = BaggingRegressor(n_estimators=10,
                         base_estimator=tree)

# Train 10 separate decision trees, each on a different bootstrap sample of rows of X, y.
model.fit(X, y)
```

```
BaggingRegressor(base_estimator=DecisionTreeRegressor(criterion='mse',
                                                      max_depth=2,
                                                      max_features=None,
                                                      max_leaf_nodes=None,
                                                      min_impurity_decrease=0.0,
                                                      min_impurity_split=None,
                                                      min_samples_leaf=1,
                                                      min_samples_split=2,
                                                      min_weight_fraction_leaf=0.0,
                                                      presort=False,
                                                      random_state=None,
                                                      splitter='best'),
                 bootstrap=True, bootstrap_features=False, max_features=1.0,
                 max_samples=1.0, n_estimators=10, n_jobs=None, oob_score=False,
                 random_state=None, verbose=0, warm_start=False)
```

If you have CPU time to spare, it is often worth trying a BaggingRegressor/Classifier.

But remember, the best hyperparameters (regularization, depth, polynomial degree, etc.) for a non-bagged estimator might not be the best hyperparameters for the bagged version. version can only benefit if there is a little extra 'instability' in the underlying estimator!

Boosting



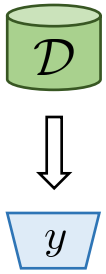
Bagging vs Boosting

- In *bagging*, we train models $\{1, \ldots, R\}$ *independently*
- In *boosting*, we train models $\{1, \ldots, R\}$ *sequentially*
- **General idea of boosting:** If we train the models sequentially, then we can train the r^{th} model to *fix the errors* that models $\{1, \ldots, r-1\}$ are currently making on the training set, "boosting" performance.
- **AdaBoost:** The r^{th} model focuses on the data $(\mathbf{x}_i, y_i)$ that are still 'hard' after combining $\{1, \ldots, r-1\}$
- **Gradient boosting:** The r^{th} model learns to fix the residual errors after combining $\{1, \ldots, r-1\}$

General idea of boosting

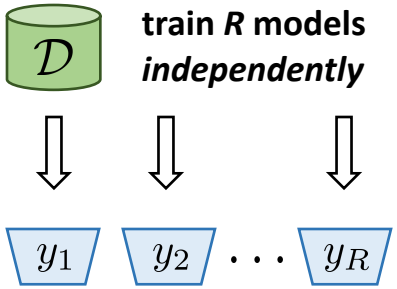
We can keep increasing *R* to aim for higher training accuracy, unlike bagging.

Single model



train one model $y(\mathbf{x})$

Bagging



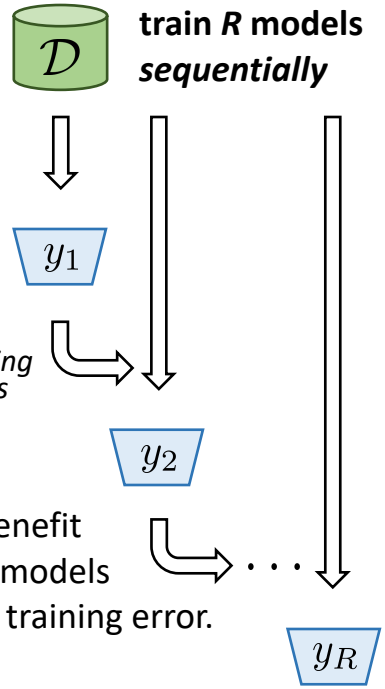
train *R* models *independently*

Can be done in parallel.

Models that are *unstable* benefit the most.

Models don't have to be 'weak', to benefit, *e.g.* helps stabilize decision trees even if deep.

Boosting



train *R* models *sequentially*

'Weak' models benefit the most; strong models already have low training error.

Subsequent models are trained to focus on *fixing errors* that remain after combining previous models.

Depiction of boosting from Bishop

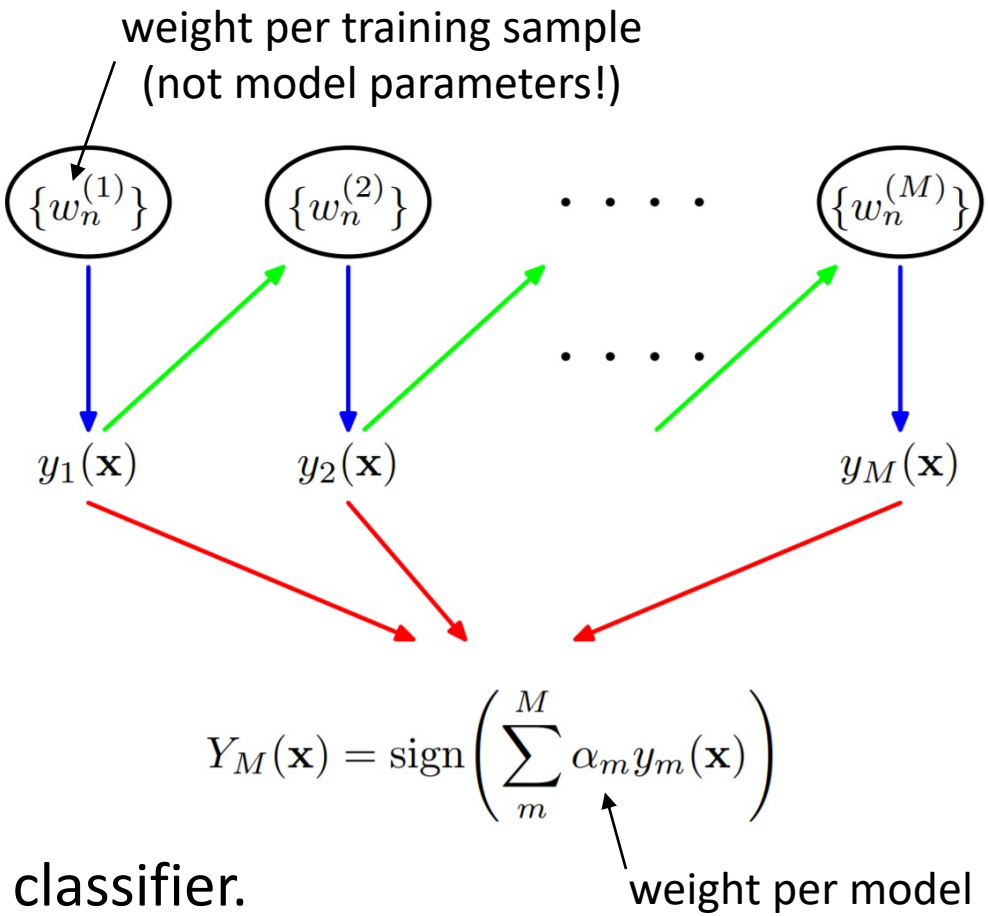


Figure 14.1 Schematic illustration of the boosting framework. Each base classifier $y_m(\mathbf{x})$ is trained on a weighted form of the training set (blue arrows) in which the weights $w_n^{(m)}$ depend on the performance of the previous base classifier $y_{m-1}(\mathbf{x})$ (green arrows). Once all base classifiers have been trained, they are combined to give the final classifier $Y_M(\mathbf{x})$ (red arrows).

This depicts "boosting" a binary classifier.
(Boosting can be generalized to multi-class too.)

Image credit: Christopher M. Bishop

fit(*X*, *y*, *sample_weight=None*)

If you specify your own "sample weights," they just get multiplied by AdaBoost's internal ones. $\{w_1, \ldots, w_N\}$

AdaBoost

- Adaptive boosting (AdaBoost) is a classic algorithm
- Tries to find weights $\{\alpha_1, \ldots, \alpha_R\}$ that can combine 'weak' models into a 'strong' one:

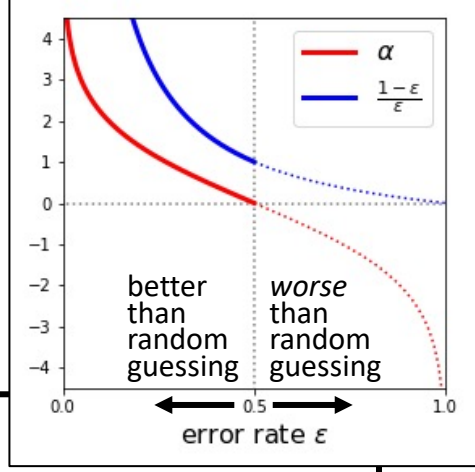
$$\underbrace{y(\mathbf{x})}_{\text{collectively strong}} = \sum_{r=1}^{R} \alpha_r \underbrace{y_r(\mathbf{x})}_{\text{individually weak}}$$

Notice that bagging assumes $\alpha_r = \frac{1}{R}$

- Works by 'adaptively' re-weighting the training cases so that later models focus on harder examples.
  - Maintains per-training sample weights $\{w_1, \ldots, w_N\}$
  - At training iteration r, sample weight w_i captures how poorly the combination of models $\{1, \ldots, r-1\}$ was at predicting the target for training sample $\mathbf{x}_i$.
  - The r^{th} model then knows which samples to "focus" on.

AdaBoost algorithm (binary)

$\mathcal{D} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_N, t_N)\}$ where $t_i \in \{-1, +1\}$



initialize $w_i = \frac{1}{N}$ for $i = 1, \ldots, N$

weighted equally

for $r = 1, \ldots, R$:

weighted loss function
error i weighted by w_i

train y_r to minimize $\epsilon = \sum_{i=1}^{N} w_i \left[y_r(\mathbf{x}_i) \neq t_i\right]$

notation $[P] = \begin{cases} 1 & \text{if } P \text{ true} \\ 0 & \text{if } P \text{ false} \end{cases}$

compute $\alpha_r = \ln\left(\frac{1-\epsilon}{\epsilon}\right)$ weight of model r

compute $w_i' = w_i e^{\alpha_r [y_r(\mathbf{x}_i) \neq t_i]}$ scale w_i by $\frac{1-\epsilon}{\epsilon}$ if $\mathbf{x}_i$ classified incorrectly, otherwise no change

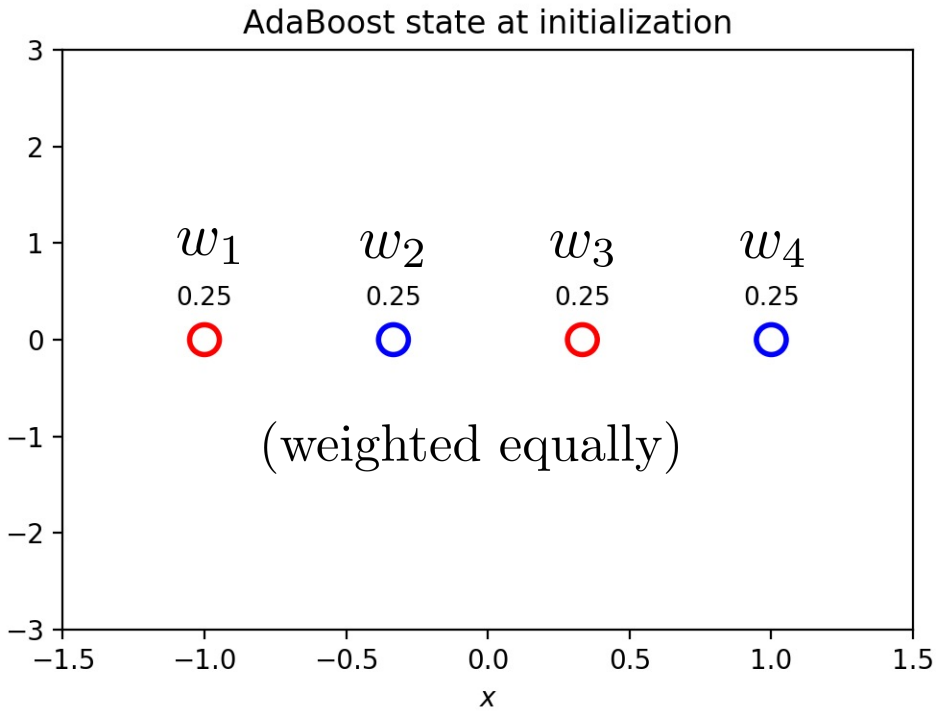
update $w_i \leftarrow \frac{w_i'}{\sum_i w_i'}$ re-normalize weights so that $\sum_i w_i = 1$

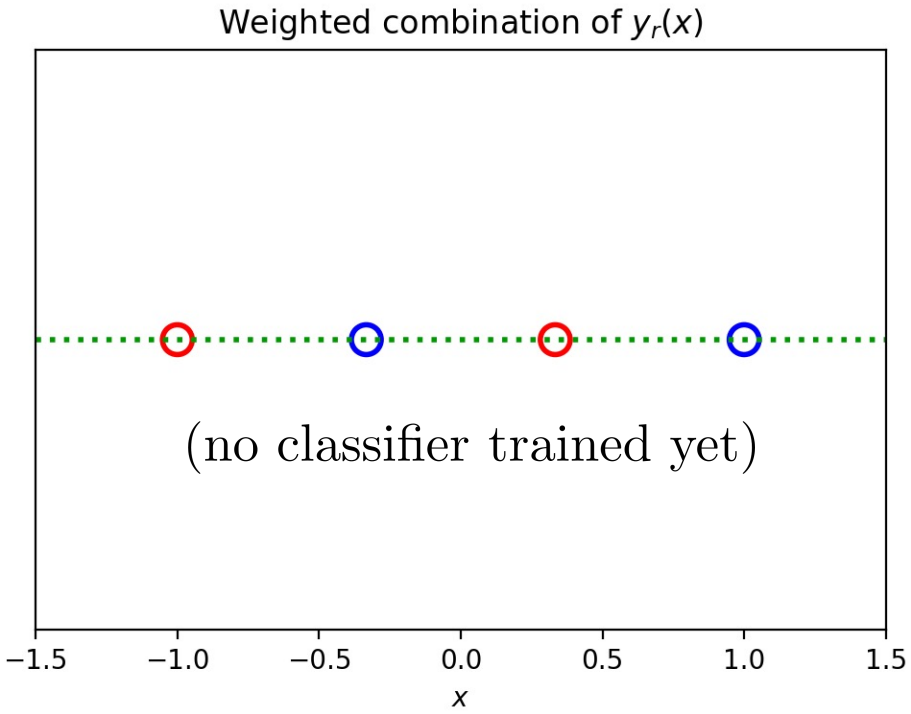
predict class by $y(\mathbf{x}) = \text{sign}\left(\sum_{r=1}^{R} \alpha_r y_r(\mathbf{x})\right)$

sklearn normalizes its decision function, so slightly different (lab 6)

AdaBoost algorithm (binary)

Example using a decision tree with *max_depth*=1 (one split) as the "weak learner," also called a "decision stump." This is very popular, and the default in sklearn.





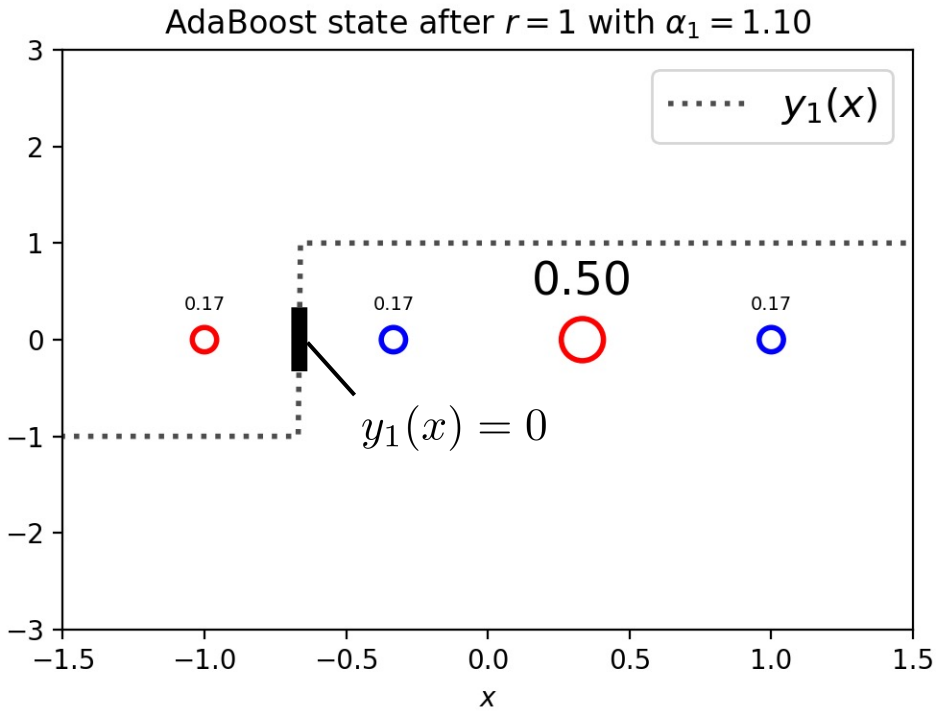
$$y(x) = \text{sign}\,(0)$$

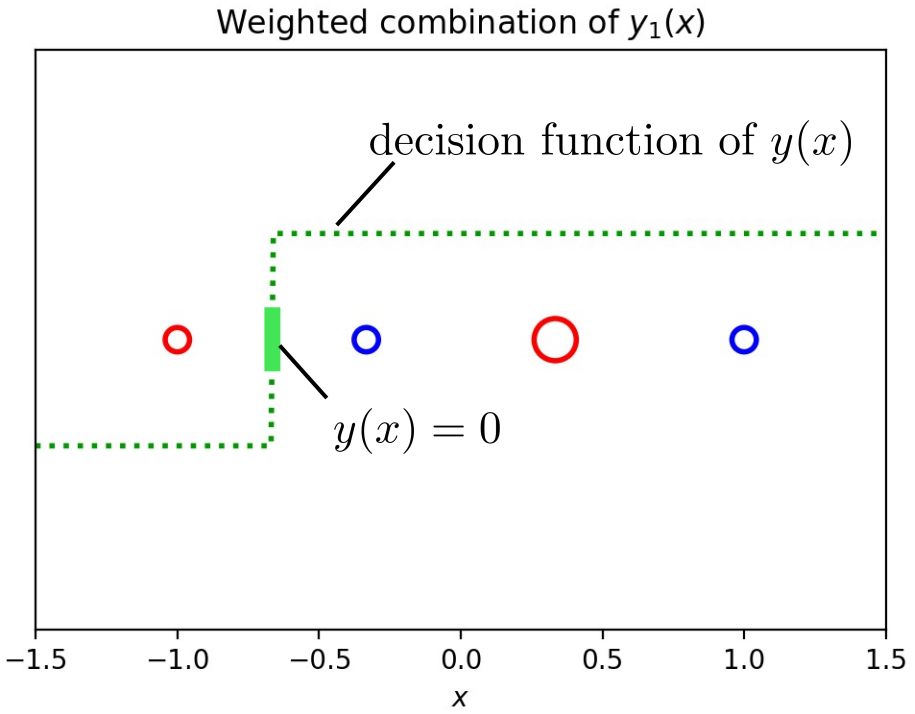
(This example uses a 1-dimensional feature space. The *y*-axis shows decision function value, not x_2!)

$$\mathcal{D} = \{(-1, -1), (-\tfrac{1}{3}, +1), (\tfrac{1}{3}, -1), (1, +1)\}$$

AdaBoost algorithm (binary)

Example using a decision tree with *max_depth*=1 (one split) as the "weak learner," also called a "decision stump." This is very popular, and the default in sklearn.



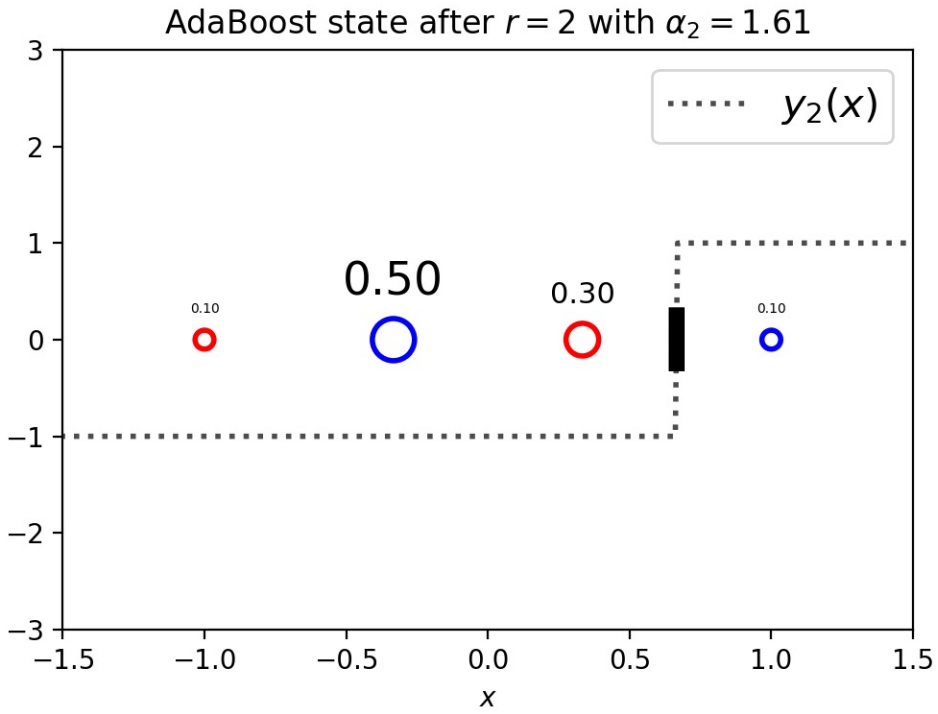


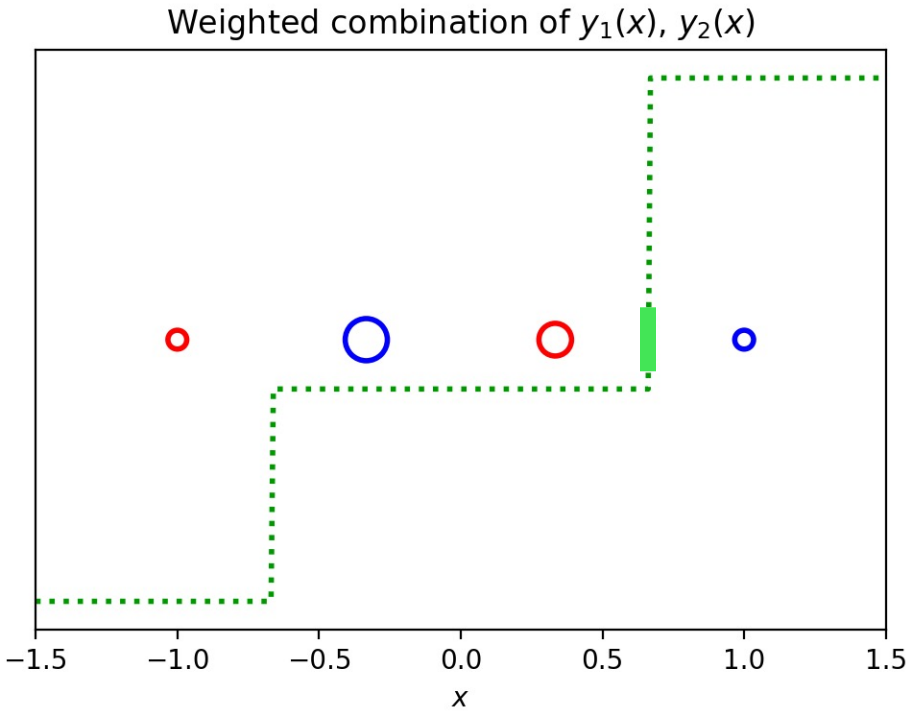
$$y(x) = \text{sign}\left(1.10 y_1(x)\right)$$

$$\mathcal{D} = \{(-1, -1), (-\tfrac{1}{3}, +1), (\tfrac{1}{3}, -1), (1, +1)\}$$

AdaBoost algorithm (binary)

Example using a decision tree with *max_depth*=1 (one split) as the "weak learner," also called a "decision stump." This is very popular, and the **default in sklearn**.



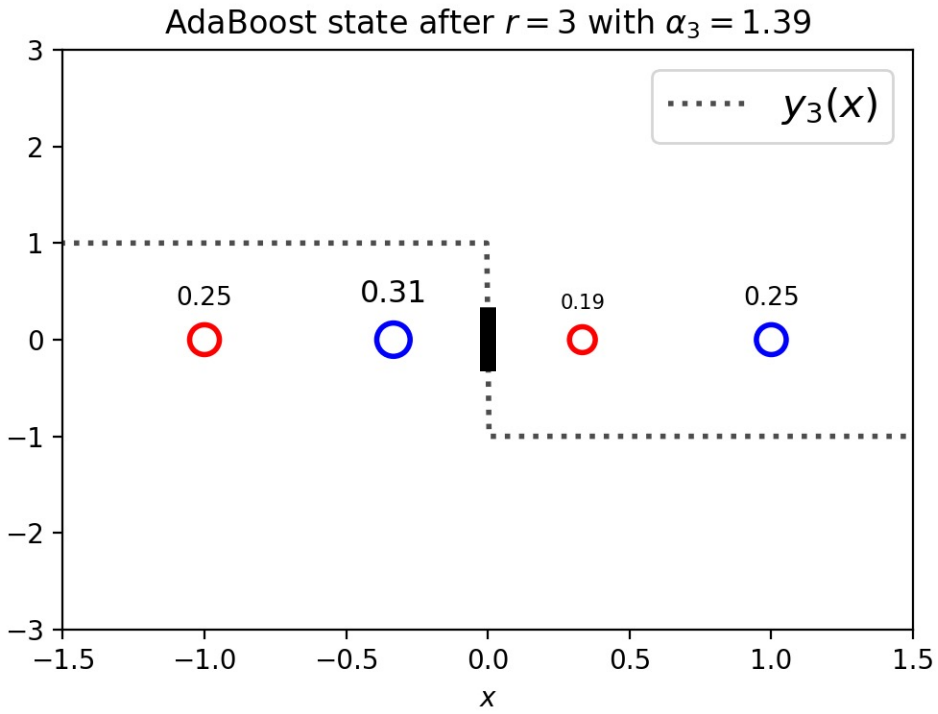


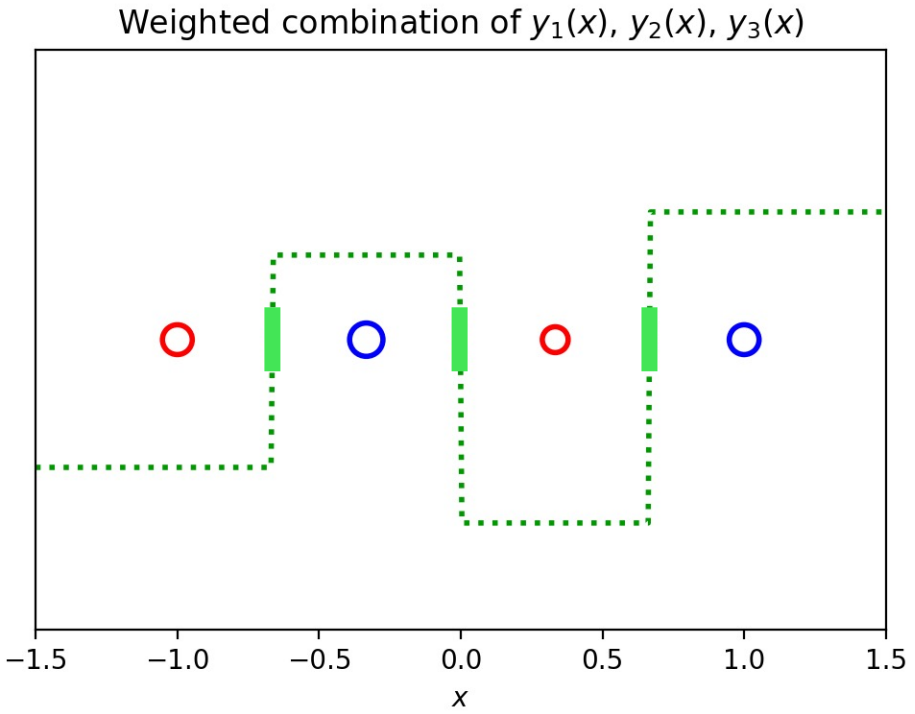
$$y(x) = \text{sign}\left(1.10 y_1(x) + 1.61 y_2(x)\right)$$

$$\mathcal{D} = \{(-1, -1), (-\tfrac{1}{3}, +1), (\tfrac{1}{3}, -1), (1, +1)\}$$

AdaBoost algorithm (binary)

Example using a decision tree with *max_depth*=1 (one split) as the "weak learner," also called a "decision stump." This is very popular, and the default in sklearn.



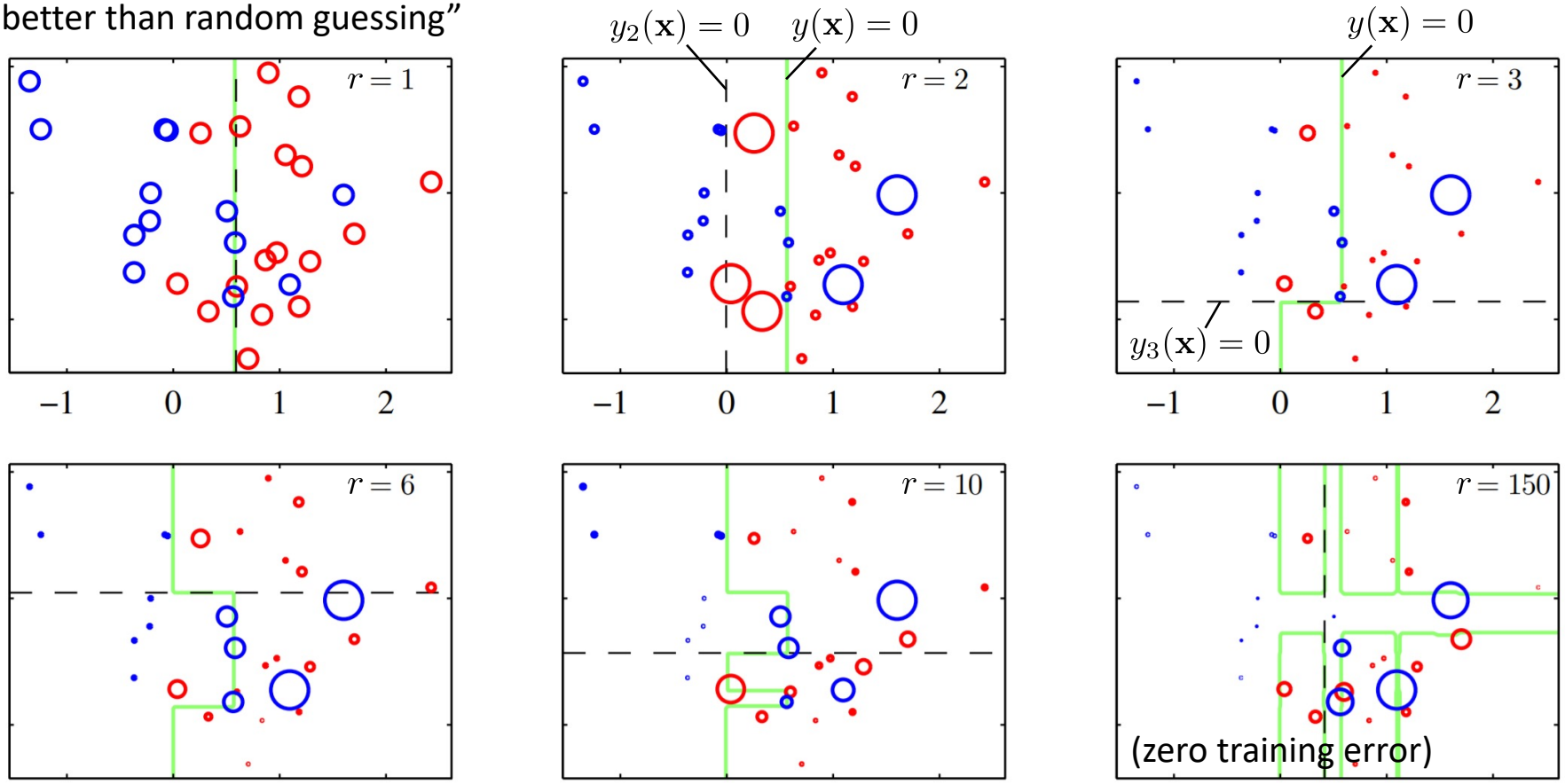


$$y(x) = \text{sign}\left(1.10y_1(x) + 1.61y_2(x) + 1.39y_3(x)\right)$$

$$\mathcal{D} = \{(-1, -1), (-\tfrac{1}{3}, +1), (\tfrac{1}{3}, -1), (1, +1)\}$$

These weights are not identical to sklearn's because there are slight variants of AdaBoost.

"not perfect separation, but better than random guessing"



i.e. "decision stumps"

Figure 14.2 Illustration of boosting in which the base learners consist of simple thresholds applied to one or other of the axes. Each figure shows the number r of base learners trained so far, along with the decision boundary of the most recent base learner (dashed black line) and the combined decision boundary of the ensemble (solid green line). Each data point is depicted by a circle whose radius indicates the weight assigned to that data point when training the most recently added base learner. Thus, for instance, we see that points that are misclassified by the $r = 1$ base learner are given greater weight when training the $r = 2$ base learner.

Image credit: Christopher M. Bishop

Gradient boosting

- Also searches over weights $\{\alpha_1, \ldots, \alpha_R\}$ that could combine 'weak' models into a 'strong' one:

$$y(\mathbf{x}) = \sum_{r=1}^{R} \alpha_r y_r(\mathbf{x})$$

any number, not just -1 or +1

- A regression example on $(\mathbf{x}_i, t_i)$ gives a sense for idea:

mean of targets (a constant)

1. choose $y_0(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} t_i$
2. train $y_1(\mathbf{x})$ on data $(\mathbf{x}_i, t_i - y_0(\mathbf{x}_i))$

try to predict this residual

3. predict $y(\mathbf{x}) = \underbrace{y_0(\mathbf{x})}_{\text{initial guess (a constant)}} + \underbrace{y_1(\mathbf{x})}_{\text{correction}} + \cdots$ corrections on corrections on corrections?

But wait, here all the $\alpha_r = 1$. Where do the α_r come in??

Gradient boosting

- Suppose overall training goal is to minimize squared error $\ell(\mathbf{t}, \mathbf{y}) = \frac{1}{2}\sum_{i=1}^{N}(t_i - y(\mathbf{x}_i))^2$ of the *strong* model

  vector of all strong predictions $y(\mathbf{x}_i)$, short for $\mathbf{y}(\mathbf{X})$

- Given current strong model $y(\mathbf{x})$, what change to that function would most rapidly reduce strong training loss $\ell(\mathbf{t}, \mathbf{y})$?
- **Idea:** Change $y(\mathbf{x})$ in a 'direction' (in function space) that gives a *steepest descent* step w.r.t. $\ell(\mathbf{t}, \mathbf{y})$!
  - Wait, we somehow compute $\nabla_{\mathbf{y}}\,\ell(\mathbf{t}, \mathbf{y})$? ... um, what? 🤨
  - It's OK! For squared error loss:

$$\frac{\partial}{\partial y(\mathbf{x}_i)}\left[\frac{1}{2}\sum_{i=1}^{N}(t_i - y(\mathbf{x}_i))^2\right] = \overbrace{y(\mathbf{x}_i) - t_i}^{\text{just negative of } i^{\text{th}} \text{ residual}}$$

😯

Let's re-do our example:

1. let $y(\mathbf{x}) = y_0$ where $y_0 = \frac{1}{N}\sum_{i=1}^{N} t_i$

2a. compute $\nabla_{\mathbf{y}}\ell(\mathbf{t}, \mathbf{y}) = \begin{bmatrix} y(\mathbf{x}_1) - t_1 \\ \vdots \\ y(\mathbf{x}_N) - t_N \end{bmatrix}$ on training data

Key: this is only defined for the training points $\mathbf{x}_i$

2b. train $y_1(\mathbf{x})$ on data $(\mathbf{x}_i, t_i - y(\mathbf{x}_i))$ so that $y_1(\mathbf{x}) \approx -\frac{\partial \ell}{\partial y(\mathbf{x})}$

... whereas y_1 is defined for *any* $\mathbf{x}$ can use to predict!

3. let $y^{\text{new}}(\mathbf{x}) = y(\mathbf{x}) - \eta\frac{\partial \ell}{\partial y(\mathbf{x})}$ for step size $\eta \geq 0$ or, equivalently, choose some step size $\alpha_1 \geq 0$ for

$$y^{\text{new}}(\mathbf{x}) = \underbrace{y_0}_{\text{initial guess}} + \underbrace{\alpha_1 y_1(\mathbf{x})}_{\text{correction}}$$

for squared error loss, this is just the predicted training residual at $\mathbf{x}$, *i.e.* residual $\mathbf{x}$ *would have had* were it included in the original training set.

Gradient boosting: why defined like this?

- **Why** must we define gradient boosting in terms of this fancy $\nabla_{\mathbf{y}} \ell(\mathbf{t}, \mathbf{y})$ thing? *What's wrong with just training each "corrector" directly on residuals?*
- Our overall training goal is to minimize loss $\ell(\mathbf{t}, \mathbf{y})$ that we chose for the *strong model* $y(\mathbf{x})$.
  - Loss could be squared error $\ell(\mathbf{t}, \mathbf{y}) = \frac{1}{2} \sum_{i=1}^{N} (t_i - y(\mathbf{x}_i))^2$, or *anything else* that we want to train strong model on.
  - **Key:** Want ability to use *any* weak model $y_r(\mathbf{x})$, even if its usual training algorithm minimizes some <u>other</u> loss ℓ_{weak}.
    - Treat $y_r(\mathbf{x})$ as **<u>black box</u>**, can't assume it directly minimizes ℓ!
  - By asking $y_r(\mathbf{x})$ to mimick $\frac{\partial \ell}{\partial y(\mathbf{x})}$ at each $\mathbf{x}_i$, it can use whatever loss function it wants. After y_r is trained, we just need to find a good step size α_r to "boost" with!

Gradient boosting algorithm

let $y(\mathbf{x}) = y_0$ where $y_0 = \arg\min_{y_0' \in \mathbb{R}} \ell(\mathbf{t}, \mathbf{y}_0')$

find constant y_0 that minimizes ℓ

for $r = 1, \ldots, R$:

compute $\boldsymbol{\delta} = \nabla_{\mathbf{y}} \ell(\mathbf{t}, \mathbf{y})$ on the training set

$\frac{\partial \ell}{\partial y(\mathbf{x}_i)}$ *i.e.* rate of change in $\ell(\mathbf{t}, \mathbf{y})$ per unit change in $y(\mathbf{x}_i)$

train $y_r(\mathbf{x})$ on data $(\mathbf{x}_i, -\delta_i)$ using ℓ_{weak}

all current predictions

predicted gradient (predicted $\boldsymbol{\delta}$)

find $\alpha_r = \arg\min_{\alpha} \ell(\mathbf{t}, \mathbf{y} + \alpha \mathbf{y}_r)$ by line search

or just use a fixed learning rate

easy 1D optimization method (don't need to know for course)

update $y(\mathbf{x}) \leftarrow y(\mathbf{x}) + \alpha_r y_r(\mathbf{x})$ add 'best' correction term

predict $y(\mathbf{x}) = \sum_{r=1}^{R} \alpha_r y_r(\mathbf{x})$

Scikit-learn supports several loss functions but only *tree* learners

1.11.4.1. Classification

`GradientBoostingClassifier` supports both binary and multi-class classification. The following example shows how to fit a gradient boosting classifier with 100 decision stumps as weak learners:

```
>>> from sklearn.datasets import make_hastie_10_2
>>> from sklearn.ensemble import GradientBoostingClassifier

>>> X, y = make_hastie_10_2(random_state=0)
>>> X_train, X_test = X[:2000], X[2000:]
>>> y_train, y_test = y[:2000], y[2000:]

>>> clf = GradientBoostingClassifier(n_estimators=100, learning_rate=1.0,
...     max_depth=1, random_state=0).fit(X_train, y_train)
>>> clf.score(X_test, y_test)
0.913...
```

1.11.4.2. Regression

`GradientBoostingRegressor` supports a number of different loss functions for regression which can be specified via the argument `loss`; the default loss function for regression is least squares (`'ls'`).

```
>>> import numpy as np
>>> from sklearn.metrics import mean_squared_error
>>> from sklearn.datasets import make_friedman1
>>> from sklearn.ensemble import GradientBoostingRegressor

>>> X, y = make_friedman1(n_samples=1200, random_state=0, noise=1.0)
>>> X_train, X_test = X[:200], X[200:]
>>> y_train, y_test = y[:200], y[200:]
>>> est = GradientBoostingRegressor(n_estimators=100, learning_rate=0.1,
...     max_depth=1, random_state=0, loss='ls').fit(X_train, y_train)
>>> mean_squared_error(y_test, est.predict(X_test))
5.00...
```

sklearn.ensemble.HistGradientBoostingClassifier

class `sklearn.ensemble.` **`HistGradientBoostingClassifier`**(*loss='auto', *, learning_rate=0.1, max_iter=100, max_leaf_nodes=31, max_depth=None, min_samples_leaf=20, l2_regularization=0.0, max_bins=255, categorical_features=None, monotonic_cst=None, warm_start=False, early_stopping='auto', scoring='loss', validation_fraction=0.1, n_iter_no_change=10, tol=1e-07, verbose=0, random_state=None*) [source]

Histogram-based Gradient Boosting Classification Tree.

This estimator is much faster than `GradientBoostingClassifier` for big datasets (n_samples >= 10 000).

HistGradientBoostingClassifier was inspired by LightGBML

LightGBM

Welcome to LightGBM's documentation!

LightGBM is a gradient boosting framework that uses tree based learning algorithms. It is designed to be distributed and efficient with the following advantages:

- Faster training speed and higher efficiency.
- Lower memory usage.
- Better accuracy.
- Support of parallel, distributed, and GPU learning.
- Capable of handling large-scale data.

XGBoost designed for huge datasets, too big to train on a single computer

XGBoost Documentation

XGBoost is an optimized distributed gradient boosting library designed to be highly **efficient**, **flexible** and **portable**. It implements machine learning algorithms under the Gradient Boosting framework. XGBoost provides a parallel tree boosting (also known as GBDT, GBM) that solve many data science problems in a fast and accurate way. The same code runs on major distributed environment (Hadoop, SGE, MPI) and can solve problems beyond billions of examples.

Classic paper showing how to interpret AdaBoost and may others as "gradient descent in function space"

Boosting Algorithms as Gradient Descent

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Abstract

We provide an abstract characterization of boosting algorithms as gradient decsent on cost-functionals in an inner-product function space. We prove convergence of these functional-gradient-descent algorithms under quite weak conditions.

(not on exam!)

https://papers.nips.cc/paper/1766-boosting-algorithms-as-gradient-descent.pdf

Summary of bagging, boosting

- **Bagging** can be run in parallel; main goal is remove the errors caused by instability (sensitivity to training set, or "variance"); a *variance reduction* technique.
- **Boosting** is run sequentially; main goal is to reduce the systematic errors (prediction "bias") made by "weak learners"; a *bias reduction* technique that also inherits some of the *variance reduction* of bagging.
- AdaBoost and Gradient Boosting are both **greedy** algorithms. Neither guarantees that the returned combination of $\{\alpha_1, \ldots, \alpha_R\}$ and trained weak learners is the best possible for a budget of R.

Ensembling in general

Ensembles are consistently better than single models, in research and in almost all Kaggle competitions!

- When we take multiple models and combine their predictions to create a new model, that's called *ensembling* and the new model is called an *ensemble*.
- Bagging and boosting are both "ensemble methods" because the model that they return is an *ensemble*.
- Ensembling is a very broad concept:
  - Combining the predictions of any collection of sub-models (SVMs, trees, neural nets, etc) trained for the task.
- **Stacking:** train models $\{1, \ldots, R\}$, then use their predictions as features to train a final model (still on original targets) that is "stacked on top" of the others.

***Bagging** is **stacking** but where the final model has no parameters: just take average! Sometimes training a model "on top" helps more than taking average.*

PRML Readings

- 3rd paragraph on p.23 ("One approach to determining frequentist error bars is the *bootstrap*")
- §14.2.0 Committees
- §14.3.0 Boosting

OPTIONAL:

- §14.3.1 Minimizing exponential error

  (Only if curious about how the algorithm was derived)