Lecture 10: Boosting and Stacking

S-109A Introduction to Data Science

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Outline

- General Review
- Review of Ensemble Methods
- Boosting
  - Set-up and intuition
  - Connection to Gradient Descent
  - The Algorithm
- Stacking

Bags and Forests of Trees

Last time we examined how the short-comings of single decision tree models can be overcome by ensemble methods - making one model out of many trees.

We focused on the problem of training large trees, these models have low bias but high variance.

We compensated by training an ensemble of full decision trees and then averaging their predictions - thereby reducing the variance of our final model.

Bags and Forests of Trees (cont.)

Bagging:

- create an ensemble of full trees, each trained on a bootstrap sample of the training set;
- average the predictions

Random forest:

- create an ensemble of full trees, each trained on a bootstrap sample of the training set;
- in each tree and each split, randomly select a subset of predictors, choose a predictor from this subset for splitting;
- average the predictions

Note that the ensemble building aspects of both method are embarrassingly parallel!

Motivation for Boosting

Could we address the shortcomings of single decision trees models in some other way?

For example, rather than performing variance reduction on complex trees, can we decrease the bias of simple trees - make them more expressive?

A solution to this problem, making an expressive model from simple trees, is another class of ensemble methods called ***boosting***.

Boosting Algorithms

Gradient Boosting

The key intuition behind boosting is that one can take an ensemble of simple models $\{T_h\}_{h\in H}$ and additively combine them into a single, more complex model.

Each model T_h might be a poor fit for the data, but a linear combination of the ensemble

$$T = \sum_h \lambda_h T_H$$

can be expressive/flexible.

But which models should we include in our ensemble? What should the coefficients or weights in the linear combination be?

Gradient Boosting: the algorithm

Gradient boosting is a method for iteratively building a complex regression model T by adding simple models. Each new simple model added to the ensemble compensates for the weaknesses of the current ensemble.

1. Fit a simple model $T^{(0)}$ on the training data

$$\{(x_1, y_1), ..., (x_N, y_N)\}$$

Set $T \leftarrow T^{(0)}$. Compute the residuals $\{r_1, \ldots, r_N\}$ for T.

2. Fit a simple model, T^i, to the current ***residuals***, i.e. train using

$$\{(x_1, r_1), ..., (x_N, r_N)\}$$

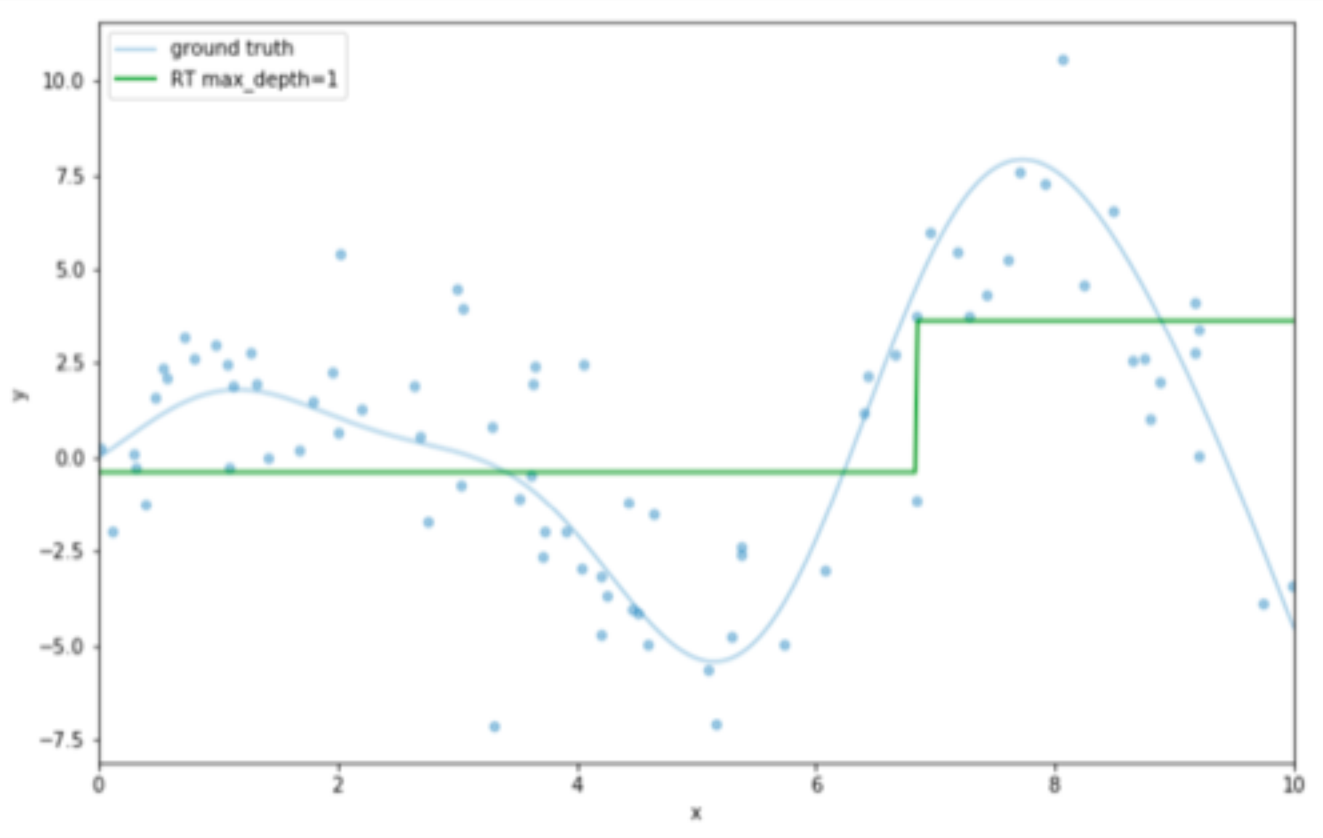
3. Set $T \leftarrow T + \lambda T^i$

4. Compute residuals, set $r_n \leftarrow r_n - \lambda T^i(x_n)$, $n = 1,\ldots,N$

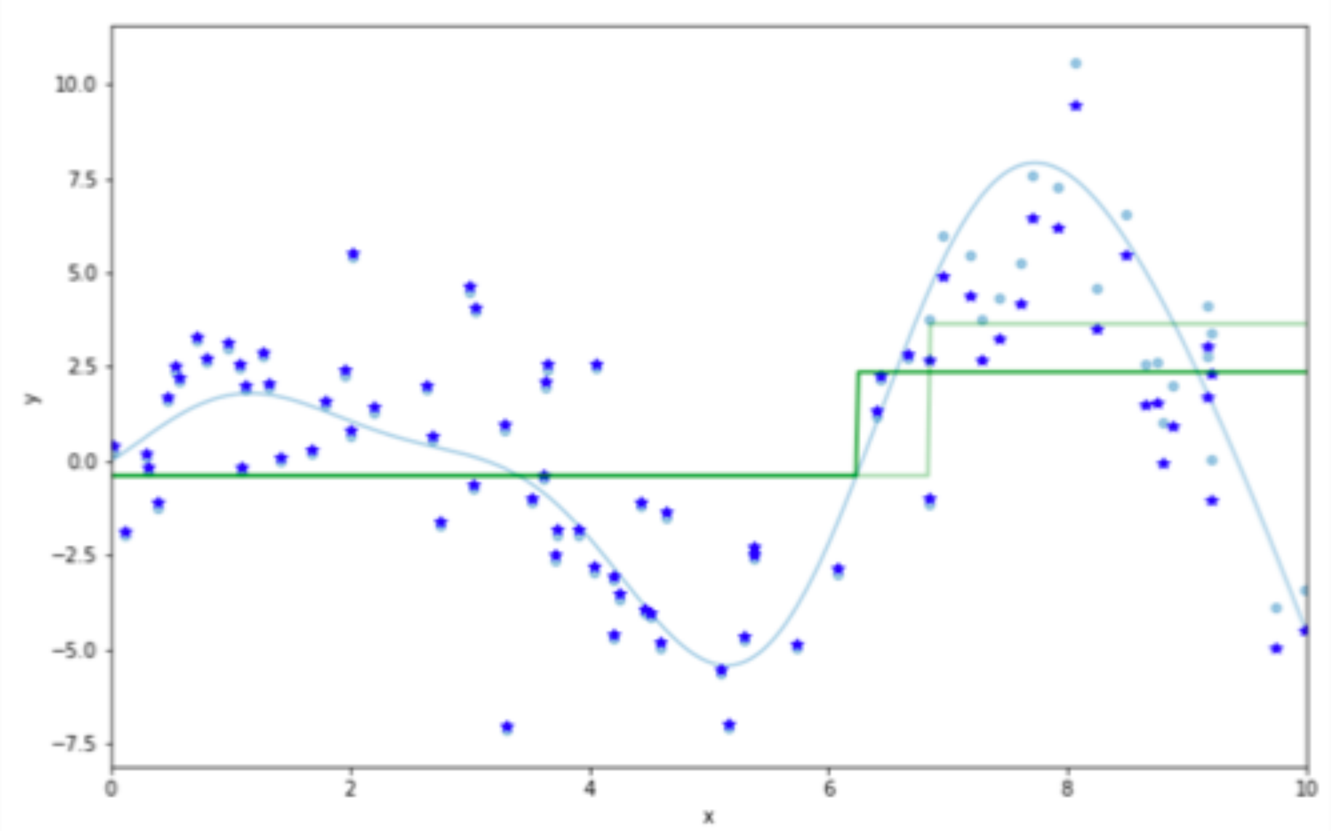
5. Repeat steps 2-4 until ***stopping*** condition met.

where λ is a constant called the ***learning rate***.

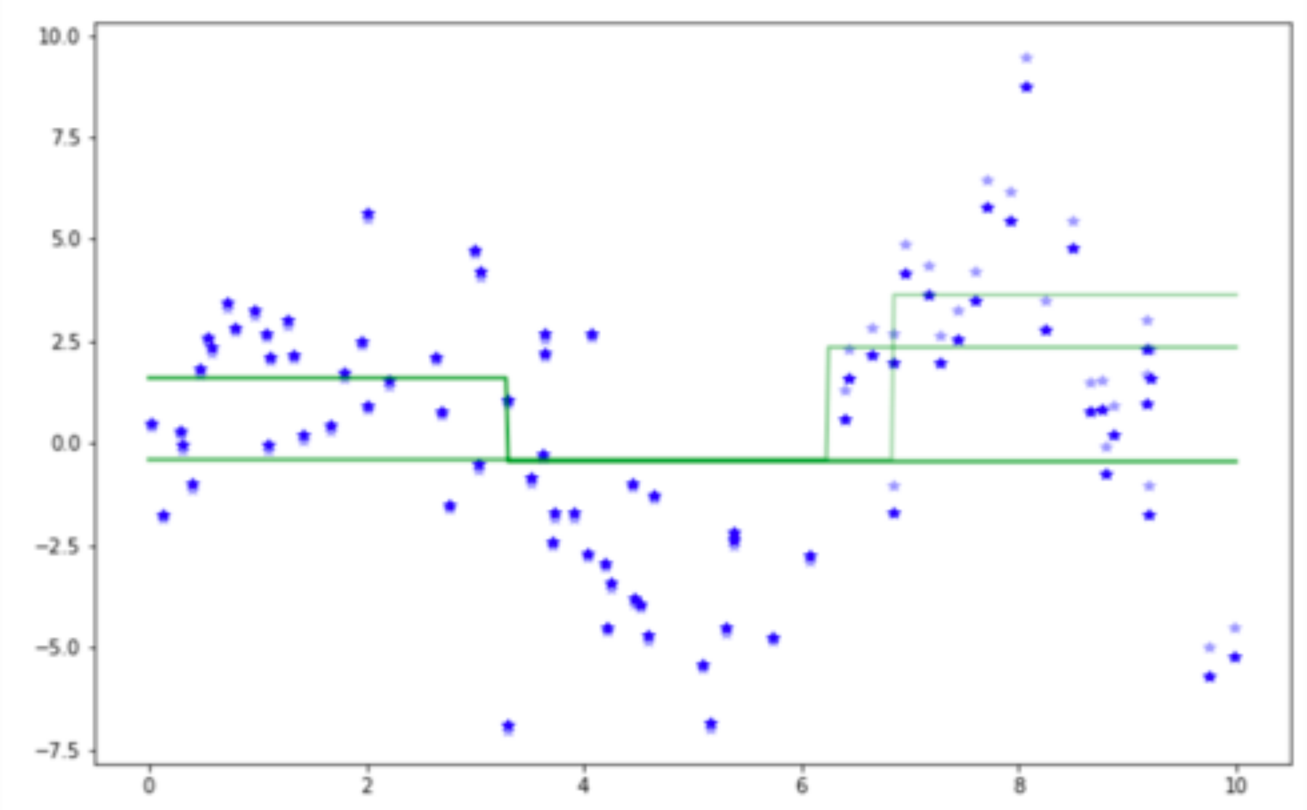
Gradient Boosting: illustration (0)



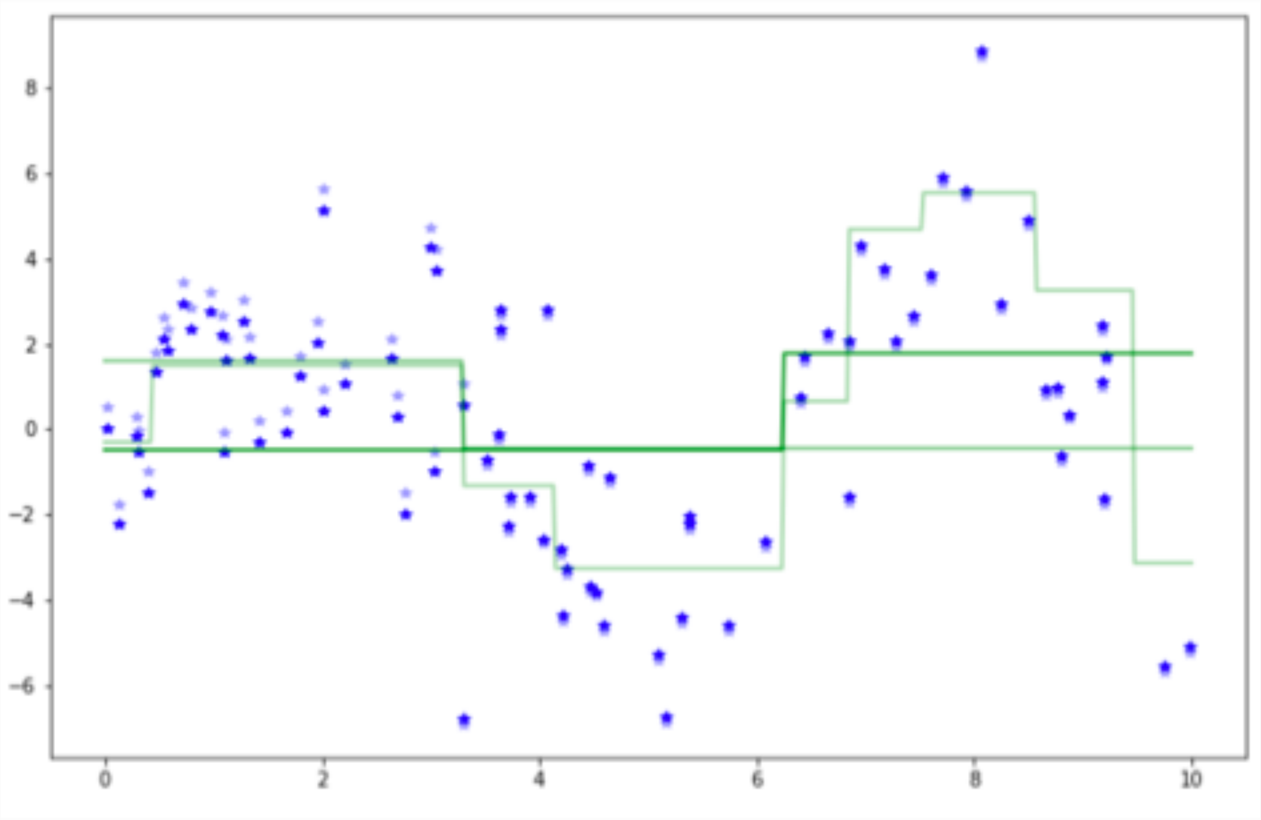
Gradient Boosting: illustration 1



Gradient Boosting: illustration 2



Gradient Boosting: illustration 3



Why Does Gradient Boosting Work?

Intuitively, each simple model $T^{(i)}$ we add to our ensemble model *T*, models the errors of *T*.

Thus, with each addition of $T^{(i)}$, the residual is reduced

$$r_n - \lambda T^{(i)}(x_n)$$

Note that gradient boosting has a tuning parameter, λ.

If we want to easily reason about how to choose λ and investigate the effect of λ on the model *T*, we need a bit more mathematical formalism.

In particular, how can we effectively descend through this optimization via an iterative algorithm?

We need to formulate gradient boosting as a type of ***gradient descent***.

Review: A Brief Sketch of Gradient Descent

In optimization, when we wish to minimize a function, called the ***objective function***, over a set of variables, we compute the partial derivatives of this function with respect to the variables.

If the partial derivatives are sufficiently simple, one can analytically find a common root - i.e. a point at which all the partial derivatives vanish; this is called a ***stationary point.***

If the objective function has the property of being ***convex***, then the stationary point is precisely the min.

Review: A Brief Sketch of Gradient Descent the Algorithm

In practice, our objective functions are complicated and analytically find the stationary point is intractable.

Instead, we use an iterative method called ***gradient descent***:

1. Initialize the variables at any value:

$$x = [x_1, ..., x_J]$$

2. Take the gradient of the objective function at the current variable values:

$$\nabla f(x) = \left[\frac{\partial f}{\partial x_1}(x), \ldots, \frac{\partial f}{\partial x_J}(x)\right]$$

3. Adjust the variables values by some negative multiple of the gradient:

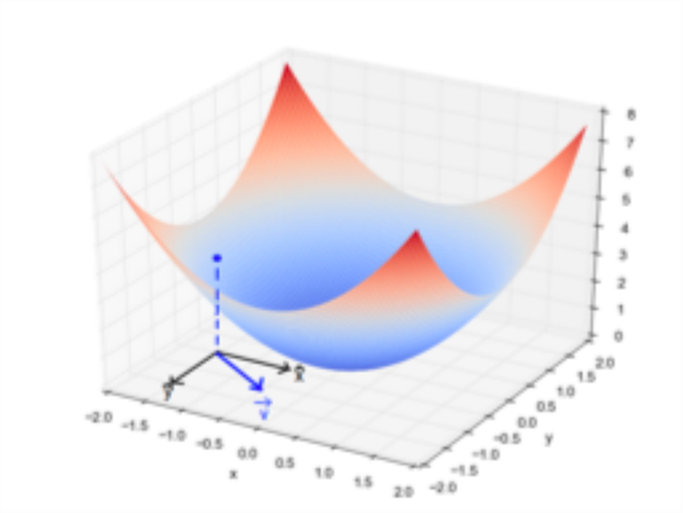
$$x \leftarrow x - \lambda \nabla f(x)$$

The factor λ is often called the learning rate.

Why Does Gradient Descent Work?

Claim: If the function is convex, this iterative methods will eventually move x close enough to the minimum, for an appropriate choice of λ.

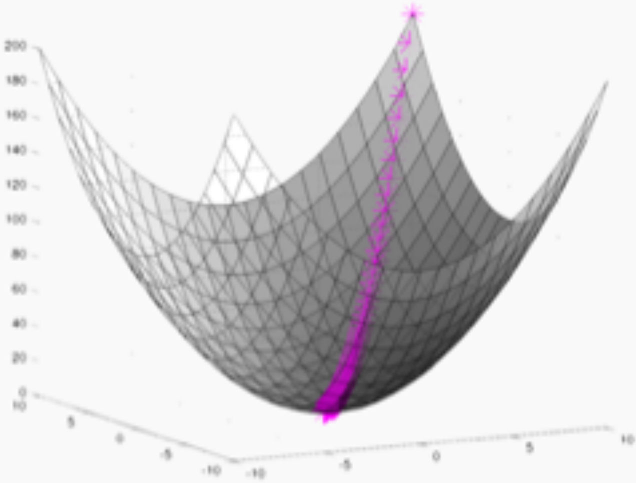
Why does this work? Recall, that as a vector, the gradient at at point gives the direction for the greatest possible rate of increase.



Why Does Gradient Descent Work?

Subtracting a λ multiple of the gradient from x, moves x in the ***opposite*** direction of the gradient (hence towards the steepest decline) by a step of size λ.

If f is convex, and we keep taking steps descending on the graph of f, we will eventually reach the minimum.



Gradient Boosting as Gradient Descent

Often in regression, our objective is to minimize the MSE

$$\mathsf{MSE}(\hat{y}_1, \ldots, \hat{y}_N) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

Treating this as an optimization problem, we can try to directly minimize the MSE with respect to the predictions

$$\begin{aligned} \nabla \mathsf{MSE} &= \left[\frac{\partial \mathsf{MSE}}{\partial \hat{y}_1}, \ldots, \frac{\partial \mathsf{MSE}}{\partial \hat{y}_N}\right] \\ &= -2\left[y_1 - \hat{y}_1, \ldots, y_N - \hat{y}_N\right] \\ &= -2\left[r_1, \ldots, r_N\right] \end{aligned}$$

The update step for gradient descent would look like

$$\hat{y}_n \leftarrow \hat{y}_n + \lambda r_n, \quad n = 1, \ldots, N$$

Gradient Boosting as Gradient Descent (cont.)

There are two reasons why minimizing the MSE with respect to $\hat{y}_n$'s is not interesting:

- We know where the minimum MSE occurs: $\hat{y}_n = y_n$, for every n.
- Learning sequences of predictions, $\hat{y}_n^1, \dots, \hat{y}_n^i, \dots$, does not produce a model. The predictions in the sequences do not depend on the predictors!

Gradient Boosting as Gradient Descent (cont.)

The solution is to change the update step in gradient descent. Instead of using the gradient - the residuals - we use an ***approximation*** of the gradient that depends on the predictors:

$$\hat{y} \leftarrow \hat{y}_n + \lambda \hat{r}_n(x_n), \quad n = 1, \ldots, N$$

In gradient boosting, we use a simple model to approximate the residuals, $\hat{r}_n(x_n)$, in each iteration.

Motto: gradient boosting is a form of gradient descent with the MSE as the objective function.

Technical note: note that gradient boosting is descending in a space of models or functions relating x_n to y_n!

Gradient Boosting as Gradient Descent (cont.)

But why do we care that gradient boosting is gradient descent?

By making this connection, we can import the massive amount of techniques for studying gradient descent to analyze gradient boosting.

For example, we can easily reason about how to choose the learning rate λ in gradient boosting.

Choosing a Learning Rate

Under ideal conditions, gradient descent iteratively approximates and converges to the optimum.

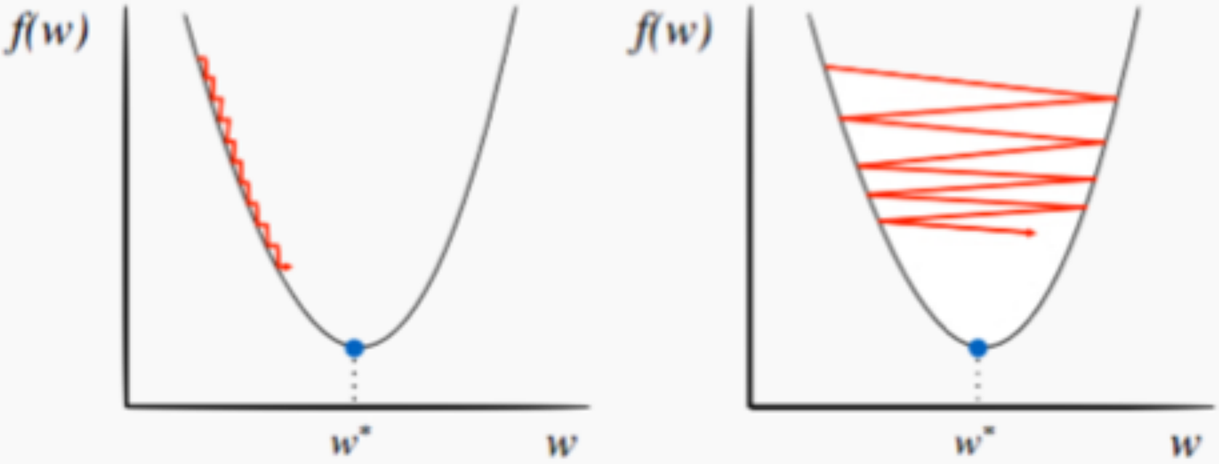
When do we terminate gradient descent?

- We can limit the number of iterations in the descent. But for an arbitrary choice of maximum iterations, we cannot guarantee that we are sufficiently close to the optimum in the end.
- If the descent is stopped when the updates are sufficiently small (e.g. the residuals of T are small), we encounter a new problem: the algorithm may never terminate!

Both problems have to do with the magnitude of the learning rate, λ.

Choosing a Learning Rate

For a constant learning rate, λ, if λ is too small, it takes too many iterations to reach the optimum.



If λ is too large, the algorithm may ‘bounce’ around the optimum and never get sufficiently close.

Choosing a Learning Rate

Choosing λ:

- If λ is a constant, then it should be tuned through cross validation.
- For better results, use a variable λ. That is, let the value of λ depend on the gradient

$$\lambda = h(\|\nabla f(x)\|),$$

where $\|\nabla f(x)\|$ is the magnitude of the gradient, $\nabla f(x)$. So

- around the optimum, when the gradient is small, λ should be small
- far from the optimum, when the gradient is large, λ should be larger

Motivation for AdaBoost

Using the language of gradient descent also allow us to connect gradient boosting for regression to a boosting algorithm often used for classification, AdaBoost.

In classification, we typically want to minimize the classification error:

$$\text{Error} = \frac{1}{N}\sum_{n=1}^{N} \mathbb{1}(y_n \neq \hat{y}_n), \quad \mathbb{1}(y_n \neq \hat{y}_n) = \begin{cases} 0, & y_n = \hat{y}_n \\ 1, & y_n \neq \hat{y}_n \end{cases}$$

Naively, we can try to minimize Error via gradient descent, just like we did for MSE in gradient boosting.

Unfortunately, Error is not differentiable with respect to the predictions, $\hat{y}_n$ ☹

Motivation for AdaBoost (cont.)

Our solution: we replace the Error function with a differentiable function that is a good indicator of classification error.

The function we choose is called ***exponential loss***

$$\text{ExpLoss} = \frac{1}{N}\sum_{n=1}^{N} \exp\left(-y_n \hat{y}_n\right), \;\; y_n \in \{-1, 1\}$$

Exponential loss is differentiable with respect to $\hat{y}_n$ and it is an upper bound of Error.

Gradient Descent with Exponential Loss

We first compute the gradient for ExpLoss:

$$\nabla \text{Exp} = [-y_1 \exp(-y_1 \hat{y}_1), \ldots, -y_N \exp(-y_N \hat{y}_N)]$$

It’s easier to decompose each $y_n \exp(-y_n \hat{y}_n)$ as $w_n y_n$, where $w_n = \exp(-y_n \hat{y}_n)$.

This way, we see that the gradient is just a re-weighting applied the target values

$$\nabla \text{Exp} = [-w_1 y_1, \ldots, -w_N y_N]$$

Notice that when $y_n = \hat{y}_n$, the weight w_n is small; when $y_n \neq \hat{y}_n$, the weight is larger.

Gradient Descent with Exponential Loss

The update step in the gradient descent is

$$\hat{y}_n \leftarrow \hat{y}_n - \lambda w_n y_n, \quad n = 1, \ldots, N$$

Just like in gradient boosting, we approximate the gradient, $\lambda w_n y_n$with a simple model, *T*$^{(i)}$, that depends on x_n.

This means training *T*$^{(i)}$ on a re-weighted set of target values,

$$\{(x_1, w_1 y_1), ..., (x_N, w_N, y_N)\}$$

That is, gradient descent with exponential loss means iteratively training simple models that ***focuses on the points misclassified by the previous model.***

AdaBoost

With a minor adjustment to the exponential loss function, we have the algorithm for gradient descent:

1. Choose an initial distribution over the training data, $w_n = 1/N$.
2. At the i^{th} step, fit a simple classifier $T^{(i)}$ on weighted training data

$$\{(x_1, w_1 y_1), ..., (x_N, w_N, y_N)\}$$

3. Update the weights:

$$w_n \leftarrow \frac{w_n \exp(-\lambda^{(i)} y_n T^{(i)}(x_n))}{Z}$$

where Z is the normalizing constant for the collection of updated weights

4. Update T: $T \leftarrow T + \lambda^{(i)} T^{(i)}$

where λ is the learning rate.

Choosing the Learning Rage

Unlike in the case of gradient boosting for regression, we can analytically solve for the optimal learning rate for AdaBoost, by optimizing:

$$\underset{\lambda}{\text{argmin}} \frac{1}{N} \sum_{n=1}^{N} \exp\left[-y_n(T + \lambda^{(i)} T^{(i)}(x_n))\right]$$

Doing so, we get that

$$\lambda^{(i)} = \frac{1}{2} \ln \frac{1-\epsilon}{\epsilon}, \quad \epsilon = \sum_{n=1}^{N} w_n \mathbb{1}(y_n \neq T^{(i)}(x_n))$$

Boosting in sklearn

Python has boosting algorithms implemented for you:

- `sklearn.ensemble.AdaBoostClassifier`
- `sklearn.ensemble.AdaBoostRegressor`
- With arguments of **base_estimator** (what models to use), **n_estimators** (max number of models to use), **learning_rate** (λ), etc…

Stacking

Motivation for Stacking

Recall that in boosting, the final model *T*, we learn is a weighted sum of simple models, T_h,

$$T = \sum_h \lambda_h T_H$$

where λ_h is the learning rate. In AdaBoost for example, we can analytically determine the optimal values of λ_h for each simple model T_h.

On the other hand, we can also determine the final model *T* implicitly by ***learning any model, called meta-learner, that transforms the outputs of*** T_h ***into a prediction***.

Stacked Generalization

The framework for ***stacked generalization*** or ***stacking*** (Wolpert 1992) is:

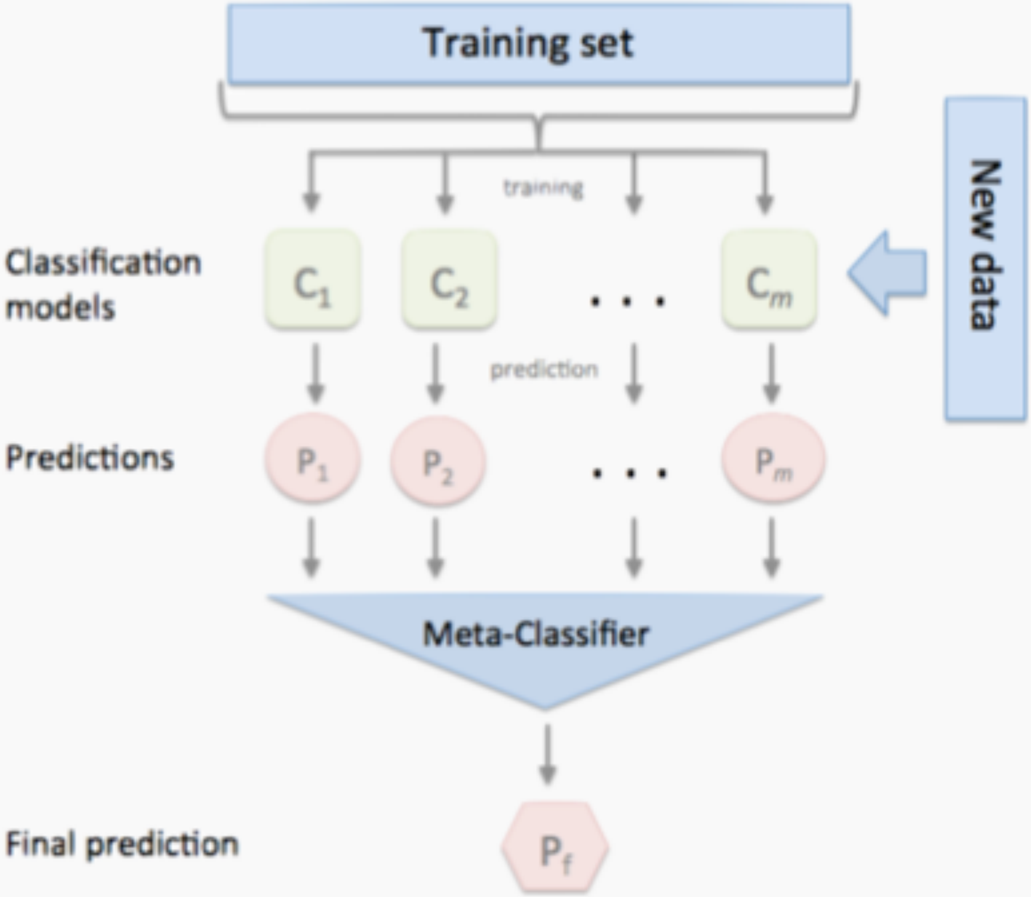
- train L number of models, T_l on the training data

$$\{(x_1, y_1), ..., (x_N, y_N)\}$$

- train a meta-learner $\tilde{T}$ on the predictions of the ensemble of models, i.e. train using the data

$$\{(T_1(x_1), ..., T_L(x_1), y_1), ..., (T_1(x_N), ..., T_L(x_N), y_N)\}$$

Stacking: an Illustration



Stacked Generalization

Stacking is a very general method,

- the models, T_l, in the ensemble can come from different classes. The ensemble can contain a mixture of logistic regression models, trees etc.
- the meta-learner, T, can be of any type. **Note:** we want to train T on the ***out of sample***

predictions of the ensemble. For example we train T on

$$\{(T_1(x_1), ..., T_L(x_1), y_1), ..., (T_1(x_N), ..., T_L(x_N), y_N)\}$$

where $T_l(x_n)$ is generated by training T_l on

$$\{(x_1, y_1), ..., (x_{n-1}, y_{n-1}), (x_{n+1}, y_{n+1}), ...(x_N, y_N)\}$$

Stacking: General Guidelines

The flexibility of stacking makes it widely applicable but difficult to analyze theoretically. Some general rules have been found through empirical studies:

- models in the ensemble should be diverse, i.e. their errors should not be uncorrelated
- for classification, each model in the ensemble should have error rate < 1/2
- if models in the ensemble outputs probabilities, it’s better to train the meta-learner on probabilities rather than predictions
- apply regularization to the meta-learner to avoid overfitting

Stacking: Subsemble Approach

We can extend the stacking framework to include ensembles of models that specialize on small subsets of data (Sapp et. al. 2014), for de-correlation or improved computational efficiency:

- divide the data in to J subsets
- train models, T_j , on each subset
- train a meta-learner $\tilde{T}$ on the predictions of the ensemble of models, i.e. train using the data

$$\{(T_1(x_1), ..., T_J(x_1), y_1), ..., (T_1(x_N), ..., T_J(x_N), y_N)\}$$

Again, we want to make sure that each $T_j(x_i)$ is an out of sample prediction.

Stacking in sklearn

Unfortunately, Python does not have stacking algorithms implemented for you ☹

So how can we do it?

We can set it up by ‘manually’ fitting several base models, take the outputs of those models, and fitting the meta model on the outputs of those base models.

It’s a model on models!

Example