# lecture13-boosting

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## 1 Lecture 13: Boosting

### 1.0.1 Applied Machine Learning

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## 2 Part 1: Boosting and Ensembling

We are now going to look at ways in which multiple machine learning can be combined. In particular, we will look at a way of combining models called *boosting*.

# 3 Review: Components of A Supervised Machine Learning Problem

At a high level, a supervised machine learning problem has the following structure:

# 4 Review: Overfitting

Overfitting is one of the most common failure modes of machine learning. \* A very expressive model (a high degree polynomial) fits the training dataset perfectly. \* The model also makes wildly incorrect prediction outside this dataset, and doesn't generalize.

# 5 Review: Bagging

The idea of *bagging* is to reduce *overfitting* by averaging many models trained on random subsets of the data.

```
for i in range(n_models):
    # collect data samples and fit models
    X_i, y_i = sample_with_replacement(X, y, n_samples)
    model = Model().fit(X_i, y_i)
    ensemble.append(model)

# output average prediction at test time:
y_test = ensemble.average_prediction(y_test)
```

The data samples are taken with replacement and known as bootstrap samples.

## 6 Review: Underfitting

Underfitting is another common problem in machine learning. \* The model is too simple to fit the data well (e.g., approximating a high degree polynomial with linear regression). \* As a result, the model is not accurate on training data and is not accurate on new data.

## 7 Boosting

The idea of boosting is to reduce underfitting by combining models that correct each others' errors.

- As in bagging, we combine many models  $g_t$  into one ensemble f.
- Unlike bagging, the  $g_t$  are small and tend to underfit.
- Each  $g_t$  fits the points where the previous models made errors.

### 8 Weak Learners

A key ingredient of a boosting algorithm is a weak learner.

- Intuitively, this is a model that is slightly better than random.
- Examples of weak learners include: small linear models, small decision trees.

# 9 Structure of a Boosting Algorithm

The idea of boosting is to reduce underfitting by combining models that correct each others' errors.

- 1. Fit a weak learner  $g_0$  on dataset  $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$ . Let f = g.
- 2. Compute weights  $w^{(i)}$  for each i based on model predictions  $f(x^{(i)})$  and targets  $y^{(i)}$ . Give more weight to points with errors.
- 3. Fit another weak learner  $g_1$  on  $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$  with weights  $w^{(i)}$ .
- 4. Set  $f_1 = g_0 + \alpha_1 g$  for some weight  $\alpha_1$ . Go to Step 2 and repeat.

In Python-like pseudocode this looks as follows:

```
weights = np.ones(n_data,)
for i in range(n_models):
    model = SimpleBaseModel().fit(X, y, weights)
    predictions = model.predict(X)
    weights = update_weights(weights, predictions)
    ensemble.add(model)

# output consensus prediction at test time:
y_test = ensemble.consensus_prediction(y_test)
```

## 10 Origins of Boosting

Boosting algorithms were initially developed in the 90s within theoretical machine learning.

- Originally, boosting addressed a theoretical question of whether weak learners with >50% accuracy can be combined to form a strong learner.
- Eventually, this research led to a practical algorithm called *Adaboost*.

Today, there exist many algorithms that are considered types of boosting, even though they were not derived from a theoretical angle.

## 11 Algorithm: Adaboost

- **Type**: Supervised learning (classification).
- Model family: Ensembles of weak learners (often decision trees).
- Objective function: Exponential loss.
- Optimizer: Forward stagewise additive model building.

## 12 Defining Adaboost

One of the first practical boosting algorithms was Adaboost.

We start with uniform  $w^{(i)} = 1/n$  and f = 0. Then for t = 1, 2, ..., T:

- 1. Fit weak learner  $g_t$  on  $\mathcal{D}$  with weights  $w^{(i)}$ .
- 2. Compute misclassification error  $e_t = \frac{\sum_{i=1}^n w^{(i)} \mathbb{I}\{y^{(i)} \neq f(x^{(i)})\}}{\sum_{i=1}^n w^{(i)}}$
- 3. Compute model weight  $\alpha_t = \log[(1 e_t)/e_t]$ . Set  $f \leftarrow f + \alpha_t g_t$ .
- 4. Compute new data weights  $w^{(i)} \leftarrow w^{(i)} \exp[\alpha_t \mathbb{I}\{y^{(i)} \neq f(x^{(i)})\}]$ .

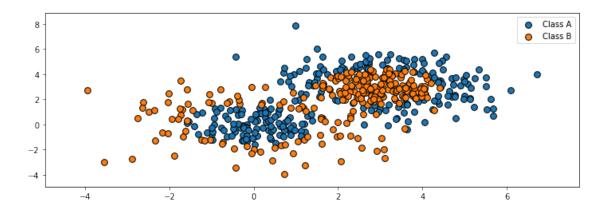
## 13 Adaboost: An Example

Let's implement Adaboost on a simple dataset to see what it can do.

Let's start by creating a classification dataset.

We can visualize this dataset using matplotlib.

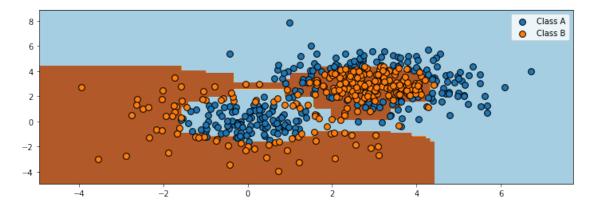
[15]: <matplotlib.legend.Legend at 0x12afda198>



Let's now train Adaboost on this dataset.

Visualizing the output of the algorithm, we see that it can learn a highly non-linear decision boundary to separate the two classes.

#### [14]: <matplotlib.legend.Legend at 0x12b3b8438>



## 14 Ensembling

Boosting and bagging are special cases of *ensembling*.

The idea of ensembling is to combine many models into one. Bagging and Boosting are ensembling techniques to reduce over- and under-fitting.

- In stacking, we train m independent models  $g_j(x)$  (possibly from different model classes) and then train another model f(x) to prodict y from the outputs of the  $g_j$ .
- The Bayesian approach can also be seen as form of ensembling

$$P(y \mid x) = \int_{\theta} P(y \mid x, \theta) P(\theta \mid \mathcal{D}) d\theta$$

where we average models  $P(y \mid x, \theta)$  using weights  $P(\theta \mid \mathcal{D})$ .

# 15 Pros and Cons of Ensembling

Ensembling is a useful tecnique in machine learning. \* It often helps squeeze out additional performance out of ML algorithms. \* Many algorithms (like Adaboost) are forms of ensembling.

Disadvantages include: \* It can be computationally expensive to train and use ensembles.

# Part 2: Additive Models

Next, we are going to see another perspective on boosting and derive new boosting algorithms.

# 16 The Components of A Supervised Machine Learning Algorithm

We can define the high-level structure of a supervised learning algorithm as consisting of three components: \* A model class: the set of possible models we consider. \* An objective function,

which defines how good a model is. \* An **optimizer**, which finds the best predictive model in the model class according to the objective function

## 17 Review: Underfitting

Underfitting is another common problem in machine learning. \* The model is too simple to fit the data well (e.g., approximating a high degree polynomial with linear regression). \* As a result, the model is not accurate on training data and is not accurate on new data.

## 18 Review: Boosting

The idea of boosting is to reduce underfitting by combining models that correct each others' errors.

- As in bagging, we combine many models  $g_i$  into one ensemble f.
- Unlike bagging, the  $g_i$  are small and tend to underfit.
- Each  $g_i$  fits the points where the previous models made errors.

### 19 Additive Models

Boosting can be seen as a way of fitting an additive model:

$$f(x) = \sum_{t=1}^{T} \alpha_t g(x; \phi_t).$$

- The main model f(x) consists of T smaller models g with weights  $\alpha_t$  and parameters  $\phi_t$ .
- The parameters are the  $\alpha_t$  plus the parameters  $\phi_t$  of each g.

This is more general than a linear model, because g can be non-linear in  $\phi_t$  (therefore so is f).

## 20 Example: Boosting Algorithms

Boosting is one way of training additive models.

- 1. Fit a weak learner  $g_0$  on dataset  $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$ . Let f = g.
- 2. Compute weights  $w^{(i)}$  for each i based on model predictions  $f(x^{(i)})$  and targets  $y^{(i)}$ . Give more weight to points with errors.
- 3. Fit another weak learner  $g_1$  on  $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$  with weights  $w^{(i)}$ .
- 4. Set  $f_1 = g_0 + \alpha_1 g$  for some weight  $\alpha_1$ . Go to Step 2 and repeat.

## 21 Forward Stagewise Additive Modeling

A general way to fit additive models is the forward stagewise approach.

- Suppose we have a loss  $L: \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$ .
- Start with  $f_0 = \arg\min_{\phi} \sum_{i=1}^n L(y^{(i)}, g(x^{(i)}; \phi)).$
- At each iteration t we fit the best addition to the current model.

$$\alpha_t, \phi_t = \arg\min_{\alpha, \phi} \sum_{i=1}^n L(y^{(i)}, f_{t-1}(x^{(i)}) + \alpha g(x^{(i)}; \phi))$$

### 22 Practical Considerations

- Popular choices of q include cubic splines, decision trees and kernelized models.
- We may use a fix number of iterations T or early stopping when the error on a hold-out set no longer improves.
- An important design choice is the loss L.

## 23 Exponential Loss

Give a binary classification problem with labels  $\mathcal{Y} = \{-1, +1\}$ , the exponential loss is defined as

$$L(y, f) = \exp(-y \cdot f).$$

- When y = 1, L is small when  $f \to \infty$ .
- When y = -1, L is small when  $f \to -\infty$ .

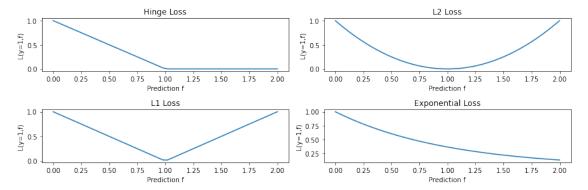
Let's visualize the exponential loss and compare it to other losses.

```
[23]: from matplotlib import pyplot as plt
  import numpy as np
  plt.rcParams['figure.figsize'] = [12, 4]

# define the losses for a target of y=1
losses = {
    'Hinge' : lambda f: np.maximum(1 - f, 0),
    'L2': lambda f: (1-f)**2,
    'L1': lambda f: np.abs(f-1),
    'Exponential': lambda f: np.exp(-f)
}

# plot them
f = np.linspace(0, 2)
fig, axes = plt.subplots(2,2)
for ax, (name, loss) in zip(axes.flatten(), losses.items()):
```

```
ax.plot(f, loss(f))
ax.set_title('%s Loss' % name)
ax.set_xlabel('Prediction f')
ax.set_ylabel('L(y=1,f)')
plt.tight_layout()
```



## 24 Special Case: Adaboost

Adaboost is an instance of forward stagewise additive modeling with the expoential loss.

At each step t we minimize

$$L_t = \sum_{i=1}^n e^{-y^{(i)}(f_{t-1}(x^{(i)}) + \alpha g(x^{(i)};\phi))} = \sum_{i=1}^n w^{(i)} \exp\left(-y^{(i)} \alpha g(x^{(i)};\phi)\right)$$

with 
$$w^{(i)} = \exp(-y^{(i)} f_{t-1}(x^{(i)})).$$

We can derive the Adaboost update rules from this equation.

Suppose that  $g(y; \phi) \in \{-1, 1\}$ . With a bit of algebraic manipulations, we get that:

$$L_{t} = e^{\alpha} \sum_{y^{(i)} \neq g(x^{(i)})} w^{(i)} + e^{-\alpha} \sum_{y^{(i)} = g(x^{(i)})} w^{(i)}$$
$$= (e^{\alpha} - e^{-\alpha}) \sum_{i=1}^{n} w^{(i)} \mathbb{I} \{ y^{(i)} \neq g(x^{(i)}) \} + e^{-\alpha} \sum_{i=1}^{n} w^{(i)}.$$

where  $\mathbb{I}\{\cdot\}$  is the indicator function.

From there, we get that:

$$\phi_t = \arg\min_{\phi} \sum_{i=1}^{n} w^{(i)} \mathbb{I} \{ y^{(i)} \neq g(x^{(i)}; \phi) \}$$

$$\alpha_t = \log[(1 - e_t)/e_t]$$

where 
$$e_t = \frac{\sum_{i=1}^n w^{(i)} \mathbb{I}\{y^{(i)} \neq f(x^{(i)})\}}{\sum_{i=1}^n w^{(i)}\}}.$$

These are update rules for Adaboost, and it's not hard to show that the update rule for  $w^{(i)}$  is the same as well.

## 25 Squared Loss

Another popular choice of loss is the squared loss.

$$L(y, f) = (y - f)^2.$$

The resulting algorithm is often called L2Boost. At step t we minimize

$$\sum_{i=1}^{n} (r_t^{(i)} - g(x^{(i)}; \phi))^2,$$

where  $r_t^{(i)} = y^{(i)} - f(x^{(i)})_{t-1}$  is the residual from the model at time t-1.

## 26 Logistic Loss

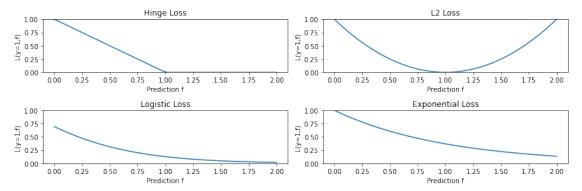
Another common loss is the log-loss. When  $\mathcal{Y} = \{-1, 1\}$  it is defined as:

$$L(y, f) = \log(1 + \exp(-2 \cdot y \cdot f)).$$

This looks like the log of the exponential loss; it is less sensitive to outliers since it doesn't penalize large errors as much.

```
[25]: from matplotlib import pyplot as plt
      import numpy as np
      plt.rcParams['figure.figsize'] = [12, 4]
      # define the losses for a target of y=1
      losses = {
          'Hinge' : lambda f: np.maximum(1 - f, 0),
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      # plot them
      f = np.linspace(0, 2)
      fig, axes = plt.subplots(2,2)
      for ax, (name, loss) in zip(axes.flatten(), losses.items()):
          ax.plot(f, loss(f))
          ax.set_title('%s Loss' % name)
```

```
ax.set_xlabel('Prediction f')
ax.set_ylabel('L(y=1,f)')
ax.set_ylim([0,1])
plt.tight_layout()
```



In the context of boosting, we minimize

$$J(\alpha, \phi) = \sum_{i=1}^{n} \log \left( 1 + \exp\left(-2y^{(i)}(f_{t-1}(x^{(i)}) + \alpha g(x^{(i)}; \phi)\right) \right).$$

This give a different weight update compared to Adabost. This algorithm is called LogitBoost.

## 27 Pros and Cons of Boosting

The boosting algorithms we have seen so far improve over Adaboost. \* They optimize a wide range of objectives. \* Thus, they are more robust to outliers and extend beyond classification.

Cons: \* Computational time is still an issue. \* Optimizing greedily over each  $\phi_t$  can take time. \* Each loss requires specialized derivations.

## 28 Summary

• Additive models have the form

$$f(x) = \sum_{t=1}^{T} \alpha_t g(x; \phi_t).$$

- These models can be fit using the forward stagewise additive approach.
- This reproduces Adaboost and can be used to derive new boosting-type algorithms.

# Part 3: Gradient Boosting

We are now going to see another way of deriving boosting algorithms that is inspired by gradient descent.

## 29 Review: Boosting

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This is not a linear model, because g can be non-linear in  $\phi_t$  (therefore so is f).

## 31 Review: Forward Stagewise Additive Modeling

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- Suppose we have a loss  $L: \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$ .
- Start with  $f_0 = \arg\min_{\phi} \sum_{i=1}^n L(y^{(i)}, g(x^{(i)}; \phi)).$
- At each iteration t we fit the best addition to the current model.

$$\alpha_t, \phi_t = \arg\min_{\alpha, \phi} \sum_{i=1}^n L(y^{(i)}, f_{t-1}(x^{(i)}) + \alpha g(x^{(i)}; \phi))$$

#### 32 Losses for Additive Models

We have seen several losses that can be used with the forward stagewise additive approach. \* The exponential loss  $L(y, f) = \exp(-yf)$  gives us Adaboost. \* The log-loss  $L(y, f) = \log(1 + \exp(-2yf))$  is more robust to outliers. \* The squared loss  $L(y, f) = (y - f)^2$  can be used for regression.

## 33 Limitations of Forward Stagewise Additive Modeling

Forward stagewise additive modeling is not without limitations. \* There may exist other losses for which it is complex to derive boosting-type weight update rules. \* At each step, we may need to solve a costly optimization problem over  $\phi_t$ . \* Optimizing each  $\phi_t$  greedily may cause us to overfit.

## 34 Functional Optimization

Functional optimization offers a different angle on boosting algorithms and a recipe for new algorithms.

- Consider optimizing a loss over abitrary functions  $f: \mathcal{X} \to \mathcal{Y}$ .
- Since we only have n datapoints, this reduces to optimizing over vectors  $\mathbf{f} \in \mathbb{R}^n$
- Thus, functional optimization consists in solving the problem

$$\min_{\mathbf{f}} \sum_{i=1}^{n} L(y^{(i)}, \mathbf{f}_i).$$

### 35 Functional Gradients

Consider solving the optimization problem using gradient descent:

$$J(\mathbf{f}) = \min_{\mathbf{f}} \sum_{i=1}^{n} L(y^{(i)}, \mathbf{f}_i).$$

We may define the functional gradient of this loss as

$$\nabla_{\mathbf{f}} J(\mathbf{f}) = \begin{bmatrix} \frac{\partial L(y^{(1)}, \mathbf{f}_1)}{\partial \mathbf{f}_1} \\ \frac{\partial L(y^{(2)}, \mathbf{f}_2)}{\partial \mathbf{f}_2} \\ \vdots \\ \frac{\partial L(y^{(n)}, \mathbf{f}_n)}{\partial \mathbf{f}_n} \end{bmatrix}.$$

### 36 Functional Gradient Descent

We can optimize our objective using gradient descent in functional space via the usual update rule:

$$\mathbf{f} \leftarrow \mathbf{f} - \alpha \nabla_{\mathbf{f}} J(\mathbf{f}).$$

As defined, this is not a practical algorithm: \* Minimizing the objective is easy because it's unconstrained. \* The optimal  $\mathbf{f}$  only fits the training data, and doesn't generalize. \* We want a way to optimize  $J(\mathbf{f})$  at any n training points.

# 37 Modeling Functional Gradients

We will address this problem by learning a *model* of gradients.

In supervised learning, we define a model  $f: \mathcal{X} \to \mathcal{Y}$  for  $\mathbf{f}$  within a class  $\mathcal{M}$ .

$$f \in \mathcal{M}$$
  $f \approx \mathbf{f}$ 

The model extrapolates beyond the training set and ensures we generalize.

We will apply the same idea to gradients. We assume a model  $g: \mathcal{X} \to R$  of the functional gradient  $\nabla_{\mathbf{f}} J(\mathbf{f})$  within a class  $\mathcal{M}$ .

$$g \in \mathcal{M}$$
  $g \approx \nabla_{\mathbf{f}} J(\mathbf{f})$ 

Our model of gradients can generalize beyond the training set.

Functional descent then has the form:

$$\underbrace{f(x)}_{\text{new function}} \leftarrow \underbrace{f(x) - \alpha g(x)}_{\text{old function - gradient step}}.$$

If g generalizes, this approximates  $\mathbf{f} \leftarrow \mathbf{f} - \alpha \nabla_{\mathbf{f}} J(\mathbf{f})$  at any n points.

## 38 Fitting Functional Gradients

What does it mean to approximate a functional gradient  $g \approx \nabla_{\mathbf{f}} J(\mathbf{f})$  in practice? We can use standard supervised learning.

Suppose we have a fixed function f and we want to estimate the functional gradient of L

$$\frac{\partial L(y, \mathbf{f})}{\partial \mathbf{f}} \bigg|_{\mathbf{f} = f(x)}$$

at any value of f(x).

- 1. We define a loss  $L_g$  (e.g., L2 loss) measure how well  $g \approx \nabla_{\mathbf{f}} J(\mathbf{f})$ .
- 2. We compute  $\nabla_{\mathbf{f}} J(\mathbf{f})$  on the training dataset:

$$\mathcal{D}_{g} = \left\{ \left( x^{(i)}, \underbrace{\frac{\partial L(y, \mathbf{f})}{\partial \mathbf{f}}} \Big|_{\mathbf{f} = f(x^{(i)})}, i = 1, 2, \dots, n \right\}$$
functional derivative  $\nabla_{\mathbf{f}} J(\mathbf{f})_{i}$  at  $f(x^{(i)})$ 

3. We train a model  $g: \mathcal{X} \to \mathbb{R}$  on  $\mathcal{D}_g$  to predict functional gradients at any x:

$$g(x) \approx \frac{\partial L(y, \mathbf{f})}{\partial \mathbf{f}} \bigg|_{\mathbf{f} = f(x)}$$

# 39 Gradient Boosting

Gradient boosting is a procedure that performs functional gradient descent with approximate gradients.

Start with f(x) = 0. Then, at each step t > 1:

1. Create a training dataset  $\mathcal{D}_g$  and fit  $g_t(x^{(i)})$  using loss  $L_g$ :

$$g_t(x) \approx \frac{\partial L(y, \mathbf{f})}{\partial \mathbf{f}} \bigg|_{\mathbf{f} = f(x)}.$$

2. Take a step of gradient descent using approximate gradients:

$$f_t(x) = f_{t-1}(x) - \alpha \cdot g_t(x).$$

## 40 Interpreting Gradient Boosting

Notice how after T steps we get an additive model of the form

$$f(x) = \sum_{t=1}^{T} \alpha_t g_t(x).$$

This looks like the output of a boosting algorithm!

- This works for any differentiable loss L.
- It does not require any mathematical derivations for new L.

## 41 Losses for Gradient Boosting

Gradient boosting can optimize a wide range of losses.

- 1. Regression losses:
  - L2, L1, and Huber (L1/L2 interpolation) losses.
  - Quantile loss: estimates quantiles of distribution of p(y|x).
- 2. Classification losses:
  - Log-loss, softmax loss, exponential loss, negative binomial likelihood, etc.

### 42 Practical Considerations

When using gradient boosting these additional facts are useful: \* We most often use small decision trees as the learner  $g_t$ . Thus, input pre-processing is minimal. \* We can regularize by controlling tree size, step size  $\alpha$ , and using early stopping. \* We can scale-up gradient boosting to big data by subsampling data at each iteration (a form of stochastic gradient descent).

# 43 Algorithm: Gradient Boosting

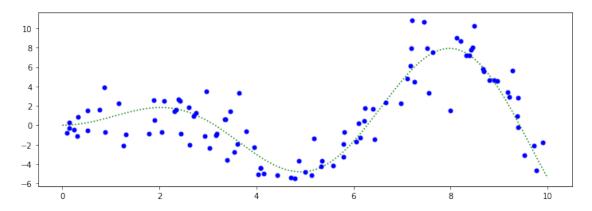
- Type: Supervised learning (classification and regression).
- Model family: Ensembles of weak learners (often decision trees).
- Objective function: Any differentiable loss function.
- Optimizer: Gradient descent in functional space. Weak learner uses its own optimizer.
- Probabilistic interpretation: None in general; certain losses may have one.

# 44 Gradient Boosting: An Example

Let's now try running Gradient Boosted Decision Trees on a small regression dataset.

First we create the dataset.

#### [21]: [<matplotlib.lines.Line2D at 0x12ed61898>]



Next, we train a GBDT regressor.

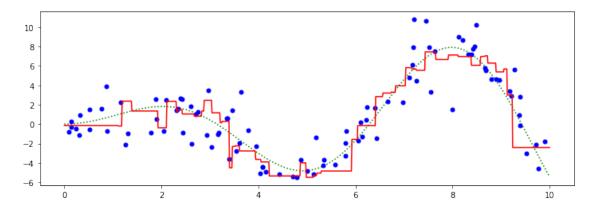
```
clf.fit(X, y)
```

[19]: GradientBoostingRegressor(alpha=0.95, min\_samples\_leaf=9, min\_samples\_split=9, n\_estimators=250)

We may now visualize its predictions

```
[22]: y_pred = clf.predict(xx)
plt.plot(xx, f(xx), 'g:', label=r'\f(x) = x\,\sin(x)\f(x)\)
plt.plot(X, y, 'b.', markersize=10, label=u'Observations')
plt.plot(xx, y_pred, 'r-', label=u'Prediction')
```

[22]: [<matplotlib.lines.Line2D at 0x12c98e438>]



# 45 Pros and Cons of Gradient Boosting

Gradient boosted decision trees (GBTs) are one of the best off-the-shelf ML algorithms that exist, often on par with deep learning. \* Attain state-of-the-art performance. GBTs have won the most Kaggle competitions. \* Require little data pre-processing and tuning. \* Work with any objective, including probabilistic ones.

Their main limitations are: \* GBTs don't work with unstructured data like images, audio. \* Implementations not as flexible as modern neural net libraries.