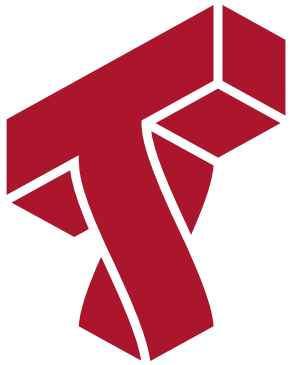

Lecture 13: Boosting

Applied Machine Learning

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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*.

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.

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.

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.

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.

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.

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 $f = g$.

1. 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.

1. Fit another weak learner g_1 on $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$ with weights $w^{(i)}$.

1. Set $f_1 = g_0 + \alpha_1 g$ for some weight α_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)
```

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.

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.

Defining Adaboost

One of the first practical boosting algorithms was *Adaboost*.

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

1. Fit weak learner g_t on $\mathcal{D}$ with weights $w^{(i)}$.

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

1. Compute model weight $\alpha_t = \log[(1 - e_t)/e_t]$. Set $f \leftarrow f + \alpha_t g_t$.

1. Compute new data weights $w^{(i)} \leftarrow w^{(i)} \exp\left[\alpha_t \mathbb{I}\{y^{(i)} \neq f(x^{(i)})\}\right]$.

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.

In [1]:
```
# https://scikit-learn.org/stable/auto_examples/ensemble/plot_adaboost_twoclass.html
import numpy as np
from sklearn.datasets import make_gaussian_quantiles

# Construct dataset
X1, y1 = make_gaussian_quantiles(cov=2., n_samples=200, n_features=2, n_classes=2,
random_state=1)
X2, y2 = make_gaussian_quantiles(mean=(3, 3), cov=1.5, n_samples=300, n_features=2
, n_classes=2, random_state=1)
X = np.concatenate((X1, X2))
y = np.concatenate((y1, - y2 + 1))
```

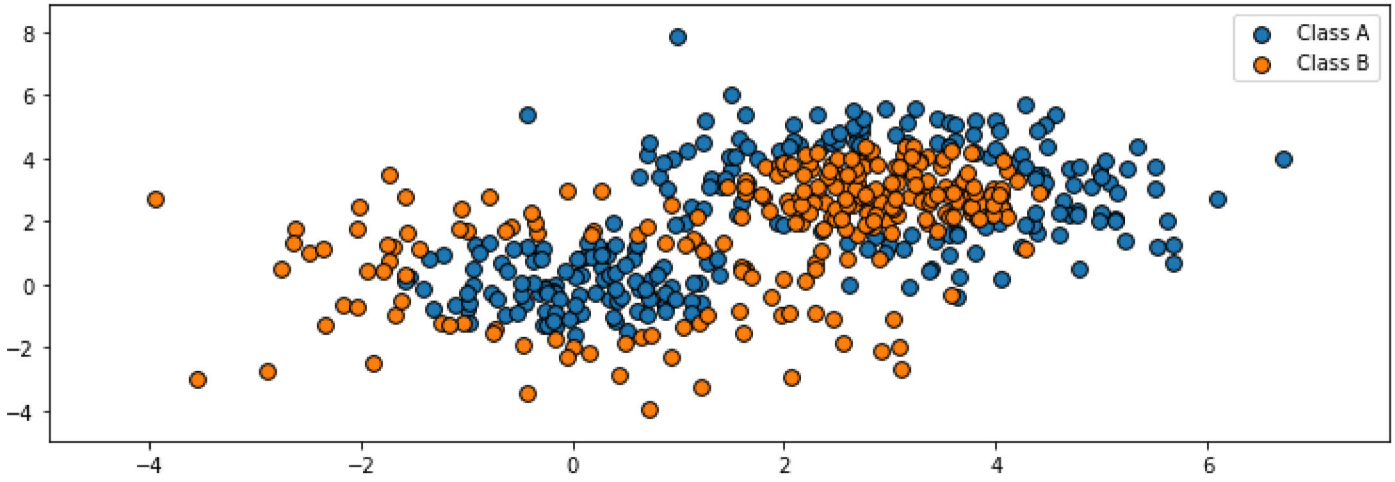
We can visualize this dataset using `matplotlib` .

In [15]:
```
import matplotlib.pyplot as plt
plt.rcParams['figure.figsize'] = [12, 4]

# Plot the training points
plot_colors, plot_step, class_names = "br", 0.02, "AB"
x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1

for i, n, c in zip(range(2), class_names, plot_colors):
    idx = np.where(y == i)
    plt.scatter(X[idx, 0], X[idx, 1], cmap=plt.cm.Paired, s=60, edgecolor='k', lab
el="Class %s" % n)
plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)
plt.legend(loc='upper right')
```

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



Let's now train Adaboost on this dataset.

In [12]:
```
from sklearn.ensemble import AdaBoostClassifier
from sklearn.tree import DecisionTreeClassifier

# Create and fit an AdaBoosted decision tree
bdt = AdaBoostClassifier(DecisionTreeClassifier(max_depth=1),
                         algorithm="SAMME",
                         n_estimators=200)
bdt.fit(X, y)
```

Out[12]:
```
AdaBoostClassifier(algorithm='SAMME',
                   base_estimator=DecisionTreeClassifier(max_depth=1),
                   n_estimators=200)
```

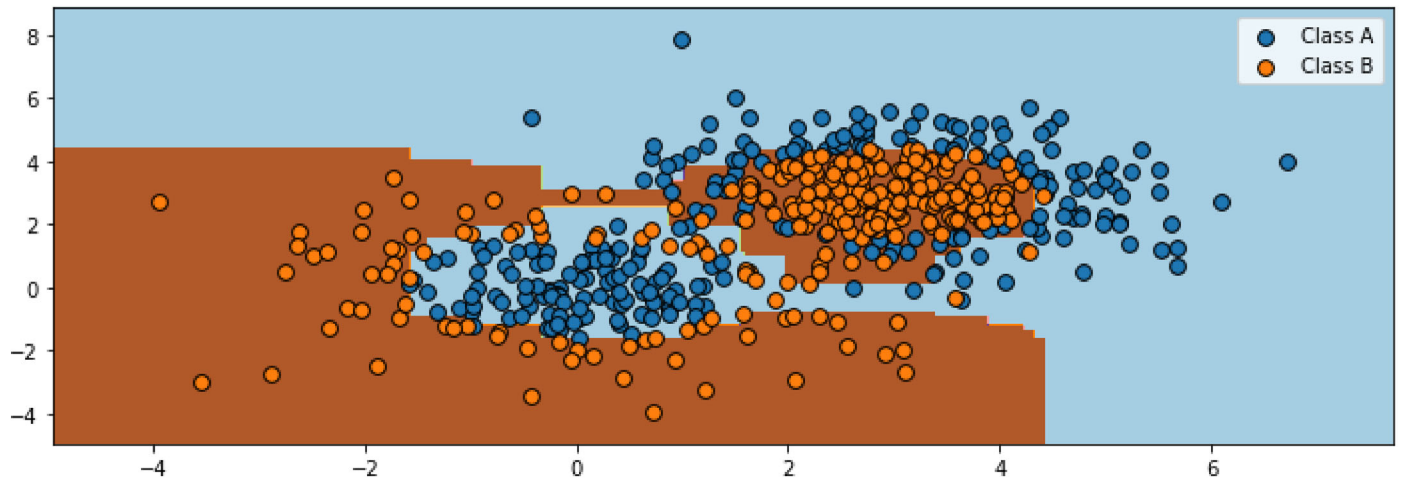
Visualizing the output of the algorithm, we see that it can learn a highly non-linear decision boundary to separate the two classes.

In [14]:
```
xx, yy = np.meshgrid(np.arange(x_min, x_max, plot_step), np.arange(y_min, y_max, p
lot_step))

# plot decision boundary
Z = bdt.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
cs = plt.contourf(xx, yy, Z, cmap=plt.cm.Paired)

# plot training points
for i, n, c in zip(range(2), class_names, plot_colors):
    idx = np.where(y == i)
    plt.scatter(X[idx, 0], X[idx, 1], cmap=plt.cm.Paired, s=60, edgecolor='k', lab
el="Class %s" % n)
plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)
plt.legend(loc='upper right')
```

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



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 $P(\theta \mid \mathcal{D})$.

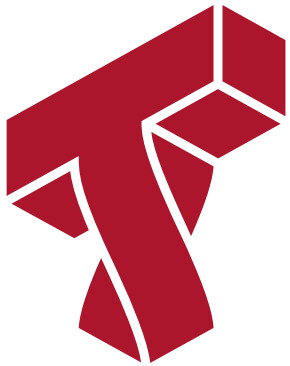
Pros and Cons of Ensembling

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.

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.

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.

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 α_t and paramaters ϕ_t.
- The parameters are the α_t plus the parameters ϕ_t of each g.

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

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 $f = g$.

1. 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.

1. Fit another weak learner g_1 on $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$ with weights $w^{(i)}$.

1. Set $f_1 = g_0 + \alpha_1 g$ for some weight α_1. Go to Step 2 and repeat.

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 $f_0 = \arg\min_\phi \sum_{i=1}^n L(y^{(i)}, g(x^{(i)}; \phi))$.

Practical Considerations

- Popular choices of g 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.

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.

In [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()
```

Special Case: Adaboost

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

At each step t we minimize

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

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:

$$\begin{aligned} L_t &= e^{\alpha} \sum_{y^{(i)} \neq g(x^{(i)})} w^{(i)} + e^{-\alpha} \sum_{y^{(i)} = g(x^{(i)})} w^{(i)} \\ &= (e^{\alpha} - e^{-\alpha}) \sum_{i=1}^{n} w^{(i)} \mathbb{I}\{y^{(i)} \neq g(x^{(i)})\} + e^{-\alpha} \sum_{i=1}^{n} w^{(i)}. \end{aligned}$$

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.

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 $t - 1$.

Logistic Loss

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

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

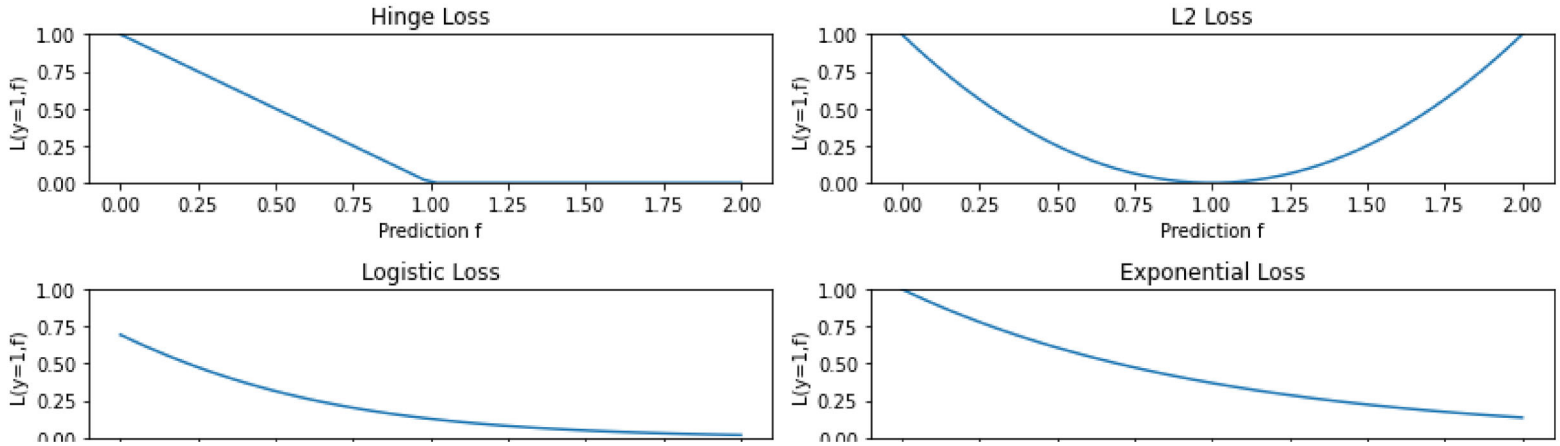
This looks like the log of the exponential loss; it is less sensitive to outliers since it doesn't penalize large errors as much.

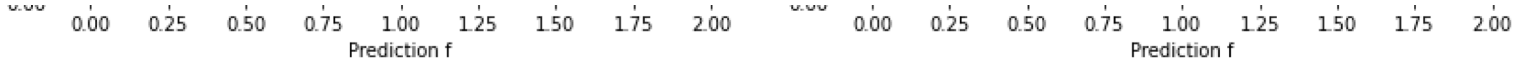
In [25]:

```
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),
    'L2': lambda f: (1-f)**2,
    'Logistic': lambda f: np.log(1+np.exp(-2*f)),
    '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)')
    ax.set_ylim([0,1])
plt.tight_layout()
```




0.00
0.25
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Prediction f
0.00
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0.50
0.75
1.00
1.25
1.50
1.75
2.00
Prediction f

In the context of boosting, we minimize

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

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

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:

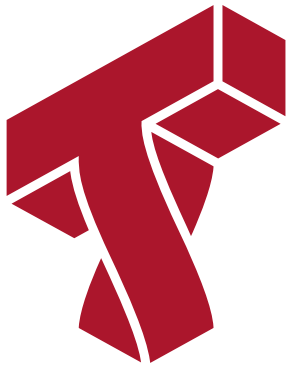
- Computational time is still an issue.
- Optimizing greedily over each ϕ_t can take time.
- Each loss requires specialized derivations.

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.

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.

Review: 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 α_t and paramaters ϕ_t.
- The parameters are the α_t plus the parameters ϕ_t of each g.

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

Review: 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 $f_0 = \arg$.

$$\min_\phi \sum_{i=1}^n L(y^{(i)}, g(x^{(i)}; \phi))$$

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.

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 ϕ_t.
- Optimizing each ϕ_t greedily may cause us to overfit.

Functional Optimization

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

- Consider optimizing a loss over arbitrary functions $f : \mathcal{X} \to \mathcal{Y}$.
- Functional optimization consists in solving the problem
$$\min_f \sum_{i=1}^{n} L(y^{(i)}, f(x^{(i)})).$$
over the space of all possible f.
- It's easiest to think about f as an infinite dimensional vector indexed by $x \in \mathcal{X}$.

To simplify our explanations, we will assume that there exists a true deterministic mapping
$$f^* : \mathcal{X} \to \mathcal{Y}$$
between $\mathcal{X}$ and $\mathcal{Y}$, but the algorithm shown here works perfectly without this assumption.

Functional Gradients

Consider solving the optimization problem using gradient descent:

$$J(f) = \min_f \sum_{i=1}^{n} L(y^{(i)}, f(x^{(i)})).$$

We may define the functional gradient of this loss at f_0 as a function $\nabla J(f_0) : \mathcal{X} \to \mathbb{R}$

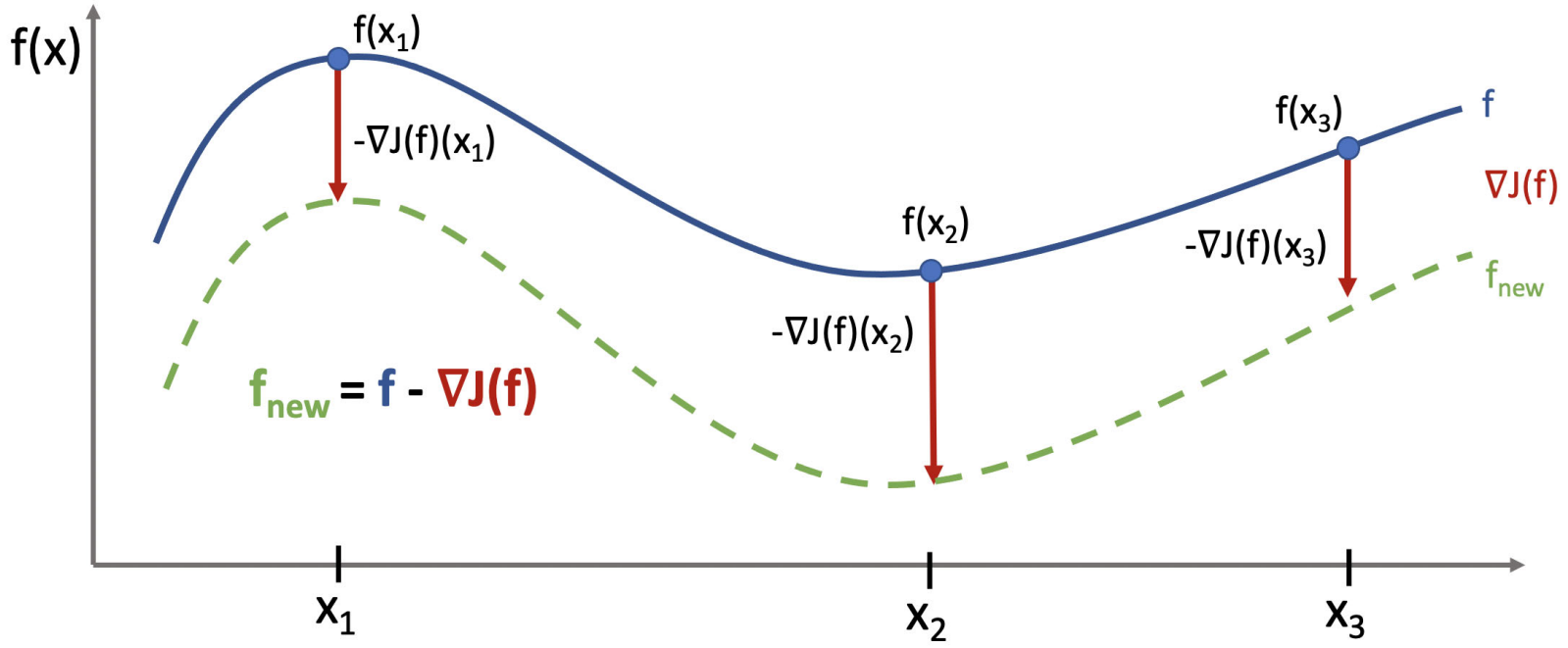
$$\nabla J(f_0)(x) = \left. \frac{\partial L(\mathrm{y}, \mathrm{f})}{\partial \mathrm{f}} \right|_{\mathrm{f}=f_0(x), \mathrm{y}=f^*(x)}.$$

Let's make a few observations about the functional gradient

$$\nabla J(f_0)(x) = \left.\frac{\partial L(\mathrm{y}, \mathrm{f})}{\partial \mathrm{f}}\right|_{\mathrm{f}=f_0(x), \mathrm{y}=f^*(x)}.$$

- It's an object indexed by $x \in \mathcal{X}$.
- At each $x \in \mathcal{X}$, $\nabla J(f_0)(x)$ tells us how to modify $f_0(x)$ to make $L(f^*(x), f_0(x))$ smaller.

This is best understood via a picture.



Functional Gradient Descent

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

$$f \leftarrow f - \alpha \nabla J(f).$$

As defined, this is not a practical algorithm:

- Minimizing the objective is easy because it's unconstrained.
- The optimal f only fits the training data, and doesn't generalize.
- We only know $J(f)$ at n training points.

Modeling Functional Gradients

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

- In supervised learning, we only have access to n data points that describe the true $\mathcal{X} \to \mathcal{Y}$ mapping.
- We learn a *model* $f_\theta : \mathcal{X} \to \mathcal{Y}$ within a class $\mathcal{M}$ to approximate f^*.
- The model extrapolates beyond the training set. Given enough datapoints, f_θ learns a true mapping.

We will apply the same idea to gradients.

- We assume a model $g_\theta : \mathcal{X} \to R$ of the functional gradient $\nabla J(f)$ within a class $\mathcal{M}$.

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

- The model extrapolates beyond the training set. Given enough datapoints, g_θ learns $\nabla J(f)$.

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 $f \leftarrow f - \alpha \nabla J(f)$.

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

$$\frac{\partial L(\mathrm{y}, \mathrm{f})}{\partial \mathrm{f}}\bigg|_{\mathrm{f}=f_0(x), \mathrm{y}=f^*(x)}.$$

at any $x \in \mathcal{X}$\$

1. We define a loss L_g (e.g., L2 loss) measure how well $g \approx \nabla J(f)$.

1. We compute $\nabla_{\mathbf{f}} J(\mathbf{f})$ on the training dataset:

$$\mathcal{D}_g = \left\{ \left(x^{(i)}, \underbrace{\left. \frac{\partial L(y^{(i)}, \mathrm{f})}{\partial \mathrm{f}} \right|_{\mathrm{f}=f(x^{(i)})}}_{\text{functional derivative } \nabla_{\mathbf{f}} J(\mathbf{f})_i \text{ at } f(x^{(i)})} \right), i = 1, 2, \ldots, n \right\}$$

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

$$g(x) \approx \left. \frac{\partial L(\mathrm{y}, \mathrm{f})}{\partial \mathrm{f}} \right|_{\mathrm{f}=f_0(x), \mathrm{y}=f^*(x)}.$$

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:

$$g_t(x) \approx \left. \frac{\partial L(\mathrm{y}, \mathrm{f})}{\partial \mathrm{f}} \right|_{\mathrm{f}=f_0(x), \mathrm{y}=f^*(x)}.$$

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

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

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.

Boosting vs. Gradient Boosting

Consider, for example, L2Boost, which optimizes the L2 loss

$$L(y, f) = \frac{1}{2}(y - f)^2.$$

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 $t-1$.

Observe that the residual

$$r_t^{(i)} = y^{(i)} - f(x^{(i)})_{t-1}$$

is also the gradient of the $L2$ loss with respect to f as $f(x^{(i)})$

$$r_t^{(i)} = \frac{\partial L(y^{(i)}, \mathrm{f})}{\partial \mathrm{f}}\Big|_{\mathrm{f}=f_0(x)}$$

Most boosting algorithms are special cases of gradient boosting in this way.

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.

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 α, 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).

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.

Gradient Boosting: An Example

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

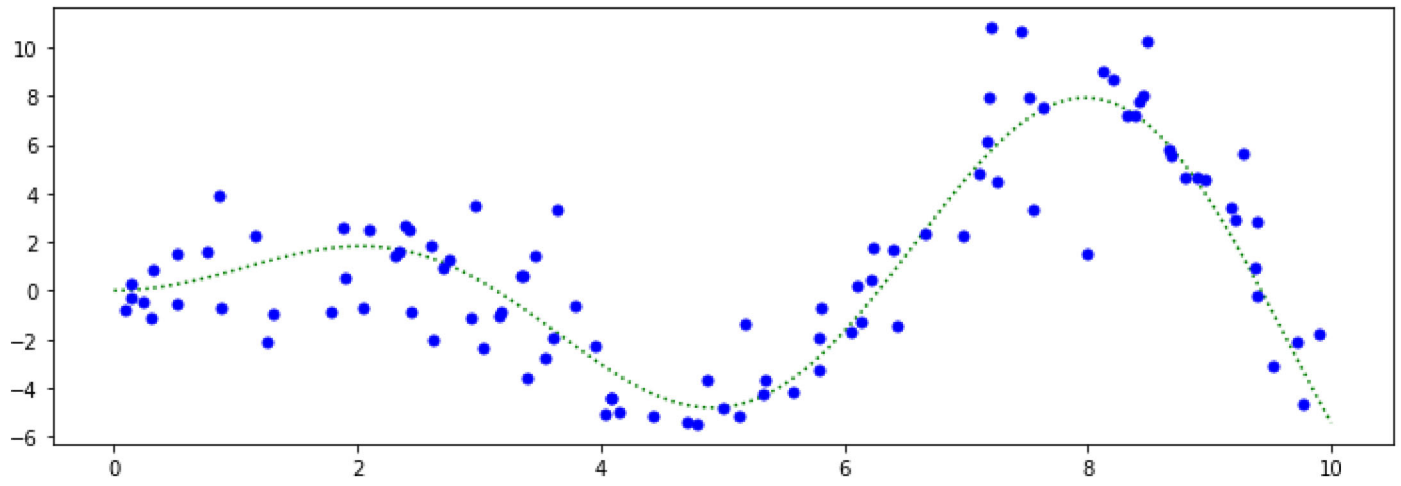
First we create the dataset.

In [21]:
```
# https://scikit-learn.org/stable/auto_examples/ensemble/plot_gradient_boosting_quantile.html
X = np.atleast_2d(np.random.uniform(0, 10.0, size=100)).T
X = X.astype(np.float32)

# Create dataset
f = lambda x: x * np.sin(x)
y = f(X).ravel()
dy = 1.5 + 1.0 * np.random.random(y.shape)
noise = np.random.normal(0, dy)
y += noise

# Visualize it
xx = np.atleast_2d(np.linspace(0, 10, 1000)).T
plt.plot(xx, f(xx), 'g:', label=r'$f(x) = x\,\sin(x)$')
plt.plot(X, y, 'b.', markersize=10, label=u'Observations')
```

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



Next, we train a GBDT regressor.

In [19]:
```
from sklearn.ensemble import GradientBoostingRegressor

alpha = 0.95
clf = GradientBoostingRegressor(loss='ls', alpha=alpha,
                                n_estimators=250, max_depth=3,
                                learning_rate=.1, min_samples_leaf=9,
                                min_samples_split=9)
clf.fit(X, y)
```

Out[19]:
```
GradientBoostingRegressor(alpha=0.95, min_samples_leaf=9, min_samples_split=9,
                          n_estimators=250)
```

We may now visualize its predictions

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.

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Functional Optimization

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

- Consider optimizing a loss over arbitrary 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

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

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

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

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.

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 $\mathcal{M}$.

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

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 $\mathcal{M}$.

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

Our model of gradients can generalize beyond the training set.

Functional descent then has the form:

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

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

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

$$\left.\frac{\partial L(y, \mathrm{f})}{\partial \mathrm{f}}\right|_{\mathrm{f}=f(x)}$$

at any value of $f(x)$.

1. We define a loss L_g (e.g., L2 loss) measure how well $g \approx \nabla_{\mathbf{f}} J(\mathbf{f})$.

1. We compute $\nabla_{\mathbf{f}} J(\mathbf{f})$ on the training dataset:

$$\mathcal{D}_g = \left\{ \left(x^{(i)}, \underbrace{\left.\frac{\partial L(y, \mathrm{f})}{\partial \mathrm{f}}\right|_{\mathrm{f}=f(x^{(i)})}}_{\text{functional derivative } \nabla_{\mathbf{f}} J(\mathbf{f})_i \text{ at } f(x^{(i)})} \right), i = 1, 2, \ldots, n \right\}$$

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

$$g(x) \approx \left.\frac{\partial L(y, \mathrm{f})}{\partial \mathrm{f}}\right|_{\mathrm{f}=f(x)}$$

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:

$$g_t(x) \approx \left. \frac{\partial L(y, \mathrm{f})}{\partial \mathrm{f}} \right|_{\mathrm{f}=f(x)}.$$

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

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

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.

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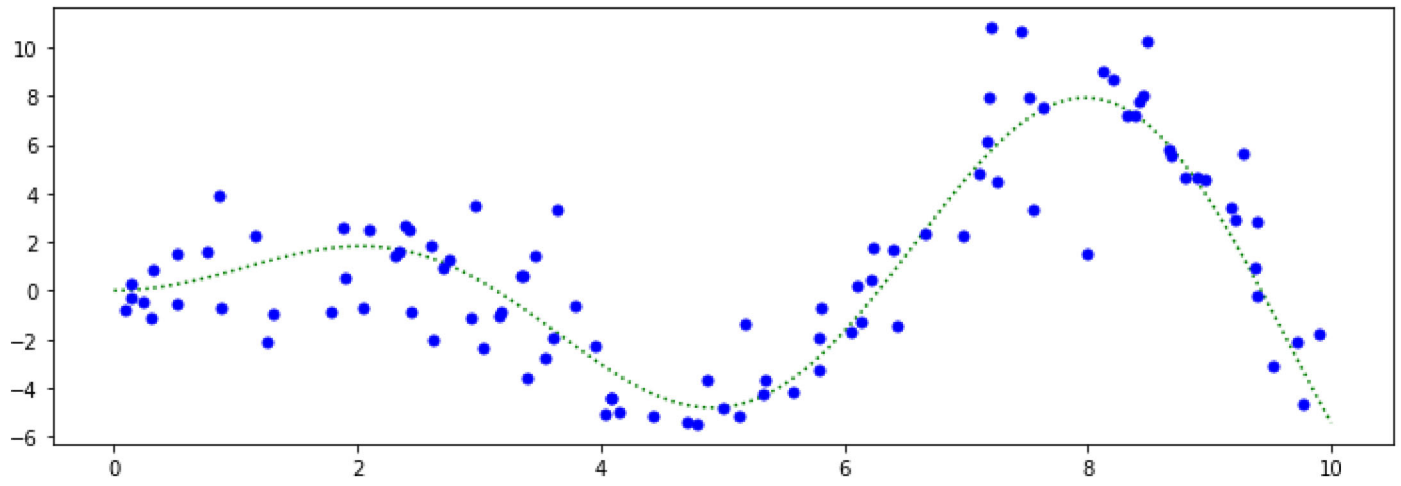

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