Lecture 14: Boosting

Machine Learning, Summer Term 2019

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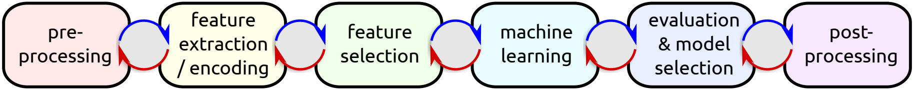
The Big Picture



- Lecture 1: overview
- Lecture 2-6: linear methods
- Lecture 7-9: algorithm-independent principles
- Lectures 10-15: nonlinear methods
  - Lecture 10-12: kernel-based methods
  - Lectures 13-14: tree-based methods and ensembles
  - Lecture 15: neural networks

Motivation for Boosting

Winning Methods of 10 Kaggle competitions in 2016 with non-image input (Competitions with images: deep neural networks dominate)

Almost all winners were large ensembles prominently using boosting:

Competition	Winners
Expedia Hotel Recommendations	1st: XGB
Santander Customer Satisfaction	3rd: XGB, RF, AdaBoost & others
Home Depot Product Search Relevance	1st and 3rd: XGB and RF
BNP Paribas Cardif Claims Management	1st and 2nd: XGB, RF & others
March Machine Learning Mania 2016	1st: RF and logarithmic regression
Telstra Network Disruptions	1st: sklearn, XGB, NN
Prudential Life Insurance Assessment	Top 3 used XGB (2nd and 3rd also others)
Airbnb New User Bookings	2nd: XGB; 3rd: XGB, NN, RF, ET
Homesite Quote Conversion	1st and 2nd: XGB & others; 3rd: others

XGB = Extreme Gradient Boosting
Places not listed: choice of method not released

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- Similar to random forests, boosting has often been called the best off-the-shelf model (e.g., by Leo Breiman, inventor of random forests)

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- Similar advantages as random forests (we'll boost trees)
  - Trees: easy to interpret
  - Directly handle categorical features
  - Scalable to many data points (can be fast)
  - Scalable to many features (automated feature selectors)
  - Robust performance even for small datasets

Lecture Overview

1. Introduction to Boosting
2. AdaBoost
3. Gradient Boosting

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- A weak learner is a learning algorithm that does at least slightly better than random (e.g., strictly better than 50% error for binary classification)
  - E.g., email spam filter: occurence of 'buy now' would already let us classify better than random
  - Often, these simple rules already yield reasonable classification performance

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- Boosting combines many weak learners into a highly accurate decision model.
- In this lecture, we use decision trees as our class of weak learners (even single-level trees, 'stumps', are sometimes used)

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Two approaches to boosting

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In this lecture, we will consider two algorithms that implement boosting:

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- Adaboost, where mistakes are identified by weightings on more "difficult" data points
  - Each submodel also gets a different weight, based on how "good" it is

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In this lecture, we will consider two algorithms that implement boosting:

- Adaboost, where mistakes are identified by weightings on more "difficult" data points
  - Each submodel also gets a different weight, based on how "good" it is
- Gradient Boosting, where mistakes are identified by the gradient of our loss function
  - Each submodel gets the same weight

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AdaBoost [Freund and Schapire, 1995]

Basic idea: iteratively construct submodels G_m that fix previous errors

- We'll have a weight w_i for each data point i
  - w_i measures how hard data point x_i is to predict
  - Start with uniform weights $w_i^{(1)}$, adapt across iterations m: $w_i^{(m)}$
  - In each iteration m,
    exponentially increase weights of data points x_i misclassified by G_m:

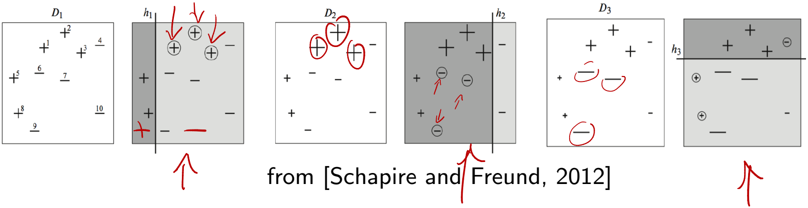

Figure from [Schapire and Freund, 2012]

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$$w_i^{(m+1)} := \begin{cases} w_i^{(m)} \times \exp(\alpha_m) & , \quad \text{if } y_i \neq G_m(x_i) \\ w_i^{(m)} & , \quad \text{otherwise} \end{cases}$$

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- We'll also compute a weight α_m for each submodel G_m
  - This depends on how good the model is
  - We'll use these weights α_m for a weighted majority vote in the end

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- Final model $G(x)$ combines individual submodels $G_1, \ldots, G_M$ through a weighted majority vote with weights $\alpha_1, \ldots, \alpha_M$:

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- Submodels G_m are weighted depending on their error err_m:

$$\alpha_m := \log \frac{1 - err_m}{err_m}$$

  - E.g., $err_m = 0.1 \rightarrow \alpha_m = 2.197$
  - E.g., $err_m = 0.4 \rightarrow \alpha_m = 0.41$
  - E.g., $err_m = 0.5 \rightarrow \alpha_m = 0$

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  - This choice of α_m can be shown to minimize an upper bound of the final hypothesis error (see [Schapire, 2003] for details)

AdaBoost [Freund and Schapire, 1995]

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- As mentioned, these weighted training error rates are used for computing the model weights:

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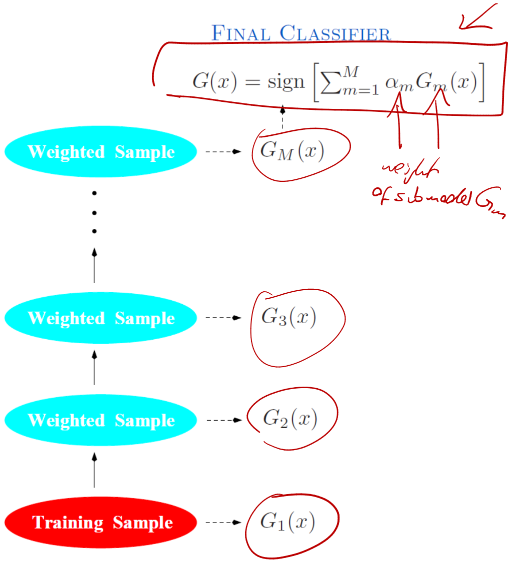
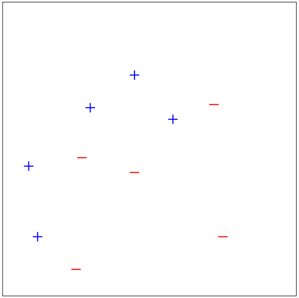
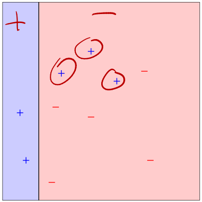


from [Hastie, Tibshirani and Friedman]

AdaBoost Example (step $m = 1$)

Example taken from [Schapire, 2003]
Model class: simple axis-aligned splits (decision stumps)





How large is the error err_1 of this first model?

★ 0.3 ★ 0.2 ★ 0.5 ★ 0.7

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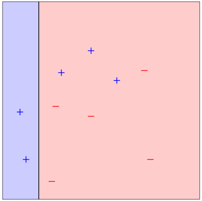

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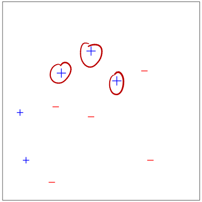

AdaBoost Example (step $m = 1$ details)

- Model error and model weight:

$$err_1 = \sum_{i=1}^{N} w_i^{(1)} \, \mathbb{I}(G_1(x_i) \neq y_i) = \frac{1}{10} \times 3 = 0.3$$

$$\underline{\alpha_1} = \log \frac{1 - err_1}{err_1} = \underline{\log \frac{1 - 0.3}{0.3}} \approx \underline{0.847}$$

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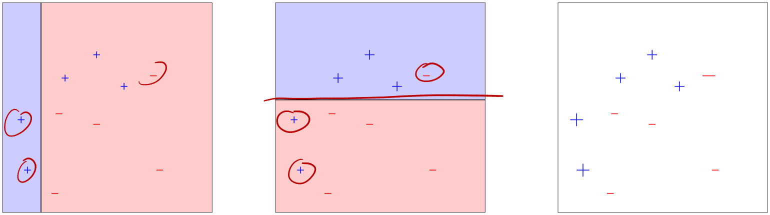
- Weight adaptation for data points:

$$w_i^{(m+1)} = w_i^{(m)} \exp(\alpha_m \, \mathbb{I}(y_i \neq G_m(x_i)))$$

  - Misclassified data point: $w_i^{(2)} \leftarrow w_i^{(1)} \exp(\alpha_1) \approx 0.1 \exp(0.847) \approx 0.233$
  - Correctly classified data points: $w_i^{(2)} \leftarrow w_i^{(1)} = 0.1$

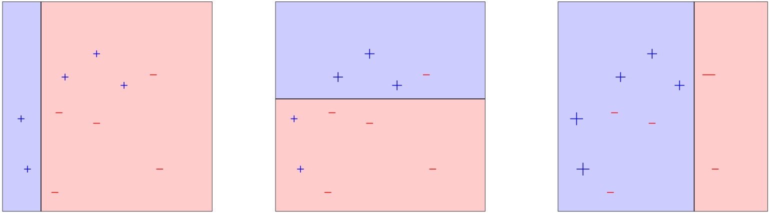
AdaBoost Example (step $m = 2$)



$$err_2 = \frac{\sum_{i=1}^{N} w_i^{(2)} \, \mathbb{I}(G_m(x_i) \neq y_i)}{\sum_{i=1}^{N} w_i^{(2)}} \approx \frac{0.1 + 0.1 + 0.1}{1.4} \approx 0.21$$

$$\alpha_2 = \log \frac{1 - err_2}{err_2} \approx \log \frac{1 - 0.21}{0.21} \approx 1.3$$

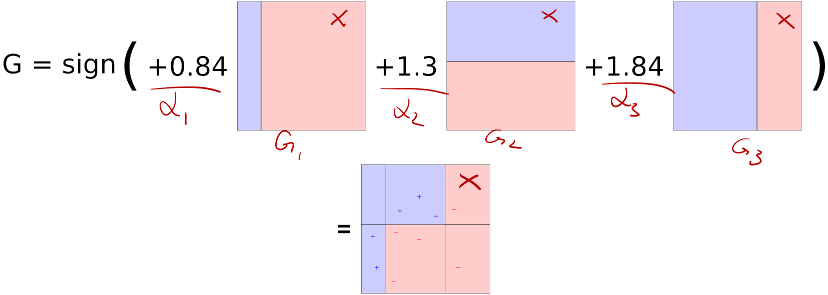
AdaBoost Example (step $m = 3$)



$err_3 \approx 0.14, \alpha_3 \approx 1.84$

AdaBoost Example

Final classifier:

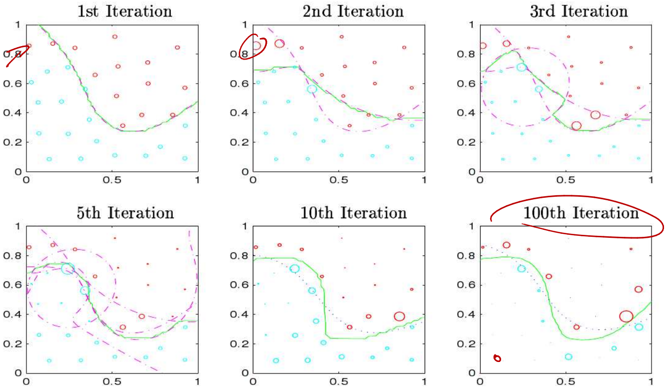


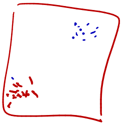
Algorithm 10.1 *AdaBoost.M1.*

1. Initialize the observation weights $w_i = 1/N$, $i = 1, 2, \ldots, N$.
2. For $m = 1$ to M:
   (a) Fit a classifier $G_m(x)$ to the training data using weights w_i.
   (b) Compute
   $$\text{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
   (c) Compute $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$.
   (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))]$, $i = 1, 2, \ldots, N$.
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

from [Hastie, Tibshirani and Friedman]

AdaBoost: Focus on Hardest Data Points





Taken from [Meir, Raetsch, 2003]: AdaBoost on a 2D toy data set: color indicates the label, diameter is proportional to the weight of the example. Purple dashed lines: decision boundaries of the single classifiers (up to 5th iteration). Solid green line: decision boundary of the combined classifier. In the last two plots the decision line of Bagging is plotted for a comparison.

⇝ Main problem of AdaBoost: if the data is very noisy, it can overfit badly / it it very sensitive to outliers

Lecture Overview

1 Introduction to Boosting

2 AdaBoost

3 Gradient Boosting

Break: Teaching evaluations

- Teaching evaluations are running
  - Evaluations are our only formal reward
  - We redesigned much of the course, so feedback is very valuable

- Let's take a 10-minute break to do the evaluation right now

An alternative formulation of boosting

- With AdaBoost, we took the sign of a weighted majority vote of M submodels, for binary classification:

$$G(x) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m G_m(x)\right)$$

- Let's now generalise to a real-valued prediction, and remove the weights on each submodel:

$$G(x) = \sum_{m=1}^{M} G_m(x)$$

- Again, we will fit these M submodels sequentially.

An alternative formulation of boosting

Suppose that $M-1$ submodels have already been fitted, and our task is to fit the Mth submodel.

$$G(x) = \sum_{m=1}^{M-1} G_m(x) + G_M(x)$$

An alternative formulation of boosting

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$$G(x) \;=\; \sum_{m=1}^{M-1} G_m(x) + G_M(x)$$

As always, our objective is to minimise the loss over all data points:

$$\sum_{i=1}^{N} L(y_i, \boxed{\sum_{m=1}^{M-1} G_m(x_i) + \underline{G_M(x_i)}})$$

An alternative formulation of boosting

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$$y_i - \sum_{m=1}^{M-1} G_m(x)$$

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As always, our objective is to minimise the loss over all data points:

$$\sum_{i=1}^{N} L(y_i, \sum_{m=1}^{M-1} G_m(x_i) + G_M(x_i))$$

Question: What method have we seen for iteratively minimising the loss of a model's predictions?

★ PCA ★ ICA ★ Talking to domain experts ★ Gradient descent

Gradient Boosting: Idea

- We can use **any** differentiable loss function L, and find the gradient g_i of our model's predictions (with M submodels) with respect to our predictions for each data point i:

$$g_i = \frac{\partial L(y_i, G(x_i))}{\partial G(x_i)}$$

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- We then fit our new weak learner G_{M+1} with parameters θ_{M+1} using a gradient descent step $-\nu \cdot g$ as our target variable y.
  - ν is our gradient descent step size, or learning rate. In the context of gradient boosting, ν is also known as shrinkage.

$$\boxed{\theta_{M+1} = \arg\min_{\theta} \sum_{i=1}^{N} L(\overbrace{-\nu \cdot g_i}^{y_i}, G(x_i; \theta))}$$

Gradient Boosting Algorithm (Simplified)

1. Initialize G = best constant prediction for y.
2. For $m = 1$ to M
   (a) For $i = 1$ to N: $g_i = \frac{\partial L(y_i, G(x_i))}{\partial G(x_i)}$
   (b) Fit weak learner G_m to data $\langle x_i, -\nu \cdot g_i \rangle_{i=1}^{N}$
   (c) Update $G(x) \leftarrow G(x) + G_m(x)$
3. Output final prediction $G(x)$

Gradient Boosting: Plugging in decision trees

1. Initialize $G =$ best constant prediction for y.
2. For $m = 1$ to M
   (a) For $i = 1$ to N: $g_i = \frac{\partial L(y_i, G(x_i))}{\partial G(x_i)}$
   (b) Fit decision tree G_m to data $\langle x_i, -\nu \cdot g_i \rangle_{i=1}^{N}$
   (c) Update $G(x) \leftarrow G(x) + G_m(x)$
3. Output final prediction $G(x)$

Each of these lines is basically one line in Python (using a tree building library)

Gradient Boosting: Plugging in Squared Error Loss

- Plugging in squared error loss to our gradient function, we get a familiar result:

$$
\begin{aligned}
g_i &= \frac{\partial L(y_i, G(x_i))}{\partial G(x_i)} \\
&= \frac{\partial \frac{1}{2}(y_i - G(x_i))^2}{\partial G(x_i)} \\
&= -(y_i - G(x_i))
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$$

$\rightarrow$ Doing a step w.r.t. the negative gradient: Fit a submodel with the previous model's residuals $y_i - G(x_i)$ as targets.

- Review: why do we use the *negative* gradient?

Gradient Tree Boosting with L2 Error

1. Initialize $G =$ best constant prediction for y.
2. For $m = 1$ to M
   (a) For $i = 1$ to N: $r_i = y_i - G(x_i)$
   (b) Fit decision tree G_m to data $\langle x_i, -\nu \cdot r_i \rangle_{i=1}^{N}$
   (c) Update $G(x) \leftarrow G(x) + G_m(x)$
3. Output final prediction $G(x)$

- Computationally very simple!
- This is related to forward stagewise additive modelling, which fits an additive model by greedily fitting one component at a time

Gradient Boosting: Plugging in Absolute Error

- Plugging in absolute error loss to our gradient function, we get another effective algorithm:

$$\begin{aligned} g_i &= \frac{\partial L\left(y_i, G(x_i)\right)}{\partial G(x_i)} \\ &= \frac{\partial |y_i - G(x_i)|}{\partial G(x_i)} \\ &= \underline{\text{sign}(y_i - G(x_i))} \end{aligned}$$

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$$

- Review: when would you expect this to perform better than squared error loss? 

The link between Gradient Boosting and Adaboost

- What if we plug in the exponential loss function $L(y_i, G(x_i)) = \exp(-y_i \times G(x_i))$?

The link between Gradient Boosting and Adaboost

- What if we plug in the exponential loss function $L(y_i, G(x_i)) = \exp(-y_i \times G(x_i))$?
- It turns out that we recover the Adaboost algorithm!
  - The optimal G_m minimizes weighted error:

$$G_m = \arg\min_G \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}(y_i \neq G(x_i))$$

  - Reintroduce a model weight α_m as in Adaboost:

$$\alpha_m = \log \frac{1 - err_m}{err_m}$$

  - The weight update rule is as in Adaboost:

$$w_i^{(m+1)} \propto w_i^{(m)} \cdot \exp(\alpha_m \mathbb{I}(y_i \neq G_m(x_i)))$$

  - (More info on ILIAS; these details will not be examinable)

Regularisation for Tree Complexity

- Recall our formal definition of a tree $G(x_i; \theta)$, where:

$$\theta = \langle \underbrace{\{R_1, \ldots, R_J\}}_{\text{leaf regions}}, \underbrace{\{w_1, \ldots, w_J\}}_{\text{leaf scores}} \rangle$$

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- We can impose a complexity penalty Ω on each submodel G_m
  - hyperparameters γ and λ penalise tree complexity J and leaf score magnitude $\|\mathbf{w}_m\|$ respectively:

$$\Omega(G_m) = \gamma J_m + \frac{1}{2}\lambda \left\|\mathbf{w}_m\right\|_2^2$$

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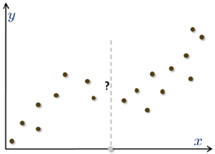
- Our method for fitting each submodel then becomes:

$$\theta_m = \arg\min_{\theta} \left[\sum_{i=1}^{N} L(-\nu \cdot g_i, G(x_i;\theta)) + \Omega(G_m) \right]$$

Regularisation for Tree Complexity

- Suppose we have a prior belief that:
  - there should be few divisions along the axes of our input space . . .
  - . . . but that these divisions should separate highly different samples



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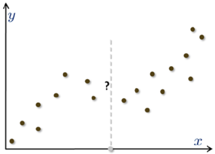


- What would be an appropriate hyperparameter setting?

$$\Omega(G_m) = \gamma J_m + \frac{1}{2}\lambda \|\mathbf{w}_m\|_2^2$$

★ High γ, High λ ★ High γ, Low λ
★ Low γ, High λ ★ Low γ, Low λ

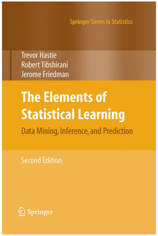
Summary by learning goals

Having heard this lecture, you can now . . .

- explain the principles of boosting, and how it differs from bagging
- describe the steps of the AdaBoost algorithm
- describe the steps of the gradient boosting approach
- Explain the relationship between gradient boosting, gradient descent, and Adaboost
- Describe the role of shrinkage and regularisation in gradient boosting

Further Reading

- Main source: Hastie, Tibshirani and Friedman
  - Chapter 10: Boosting and Additive Trees



- Wikipedia article on boosting
- Specialized literature
  - Schapire: A boosting tutorial
    `www.cs.princeton.edu/~schapire`
  - Meir and Raetsch, 2003: An introduction to boosting
  - Raetsch: Tutorial at MLSS 2003

Preview of Assignment 9

In the 9^{th} assignment, you will

- Implement the AdaBoost algorithm
- Implement the gradient boosting algorithm