9.520: Class 24

Bagging and Boosting

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(based on notes from Theodoros Evgeniou)

About this class

Theme We discuss *bagging* and *boosting* and provide some attempts to justify them.

Web The slides and all what concerns this class can be found on the web.

Plan

- ⋄ Bagging
- ⋄ Bias-Variance Decomposition
- ⋄ Combinations of Kernel Machines (i.e. SVM)
- ⋄ Boosting and Adaboost
- ⋄ Bounds for Boosting
- ⋄ Additive Logistic Regression

Some motivations for combining Learning Machines

- Suppose you have many "easy rules": combining them may be a good idea.

- Parameter Estimation: combine many machines each with different parameters?

- Bootstrap: maybe helps with "variance"?

Bagging (Bootstrap AGGregatING)

Given a training set $D = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_\ell, y_\ell)\}$,

- sample N sets of ℓ elements from D (with replacement) $D_1, D_2, \dots D_N \rightarrow N$ quasi replica training sets;

- train a machine on each D_i, $i = 1, ..., N$ and obtain a sequence of N outputs $f_1(\mathbf{x}), \dots f_N(\mathbf{x})$.

Bagging (cont.)

The final aggregate classifier can be

- for regression

$$\bar{f}(\mathbf{x}) = E\{f_i(\mathbf{x})\},$$

  the average of f_i for $i = 1, ..., N$;

- for classification

$$\bar{f}(\mathbf{x}) = \theta(E\{f_i(\mathbf{x})\})$$

  the majority vote from $f_i(\mathbf{x})$.

Theoretical analysis

Breiman (1996) studies the average generalization performance of a learning algorithm with respect to the training set. It is possible to relate this quantity to the distance or **bias** between the Bayes optimal solution and the average solution of the learning algorithm and the **variance** of the solution.

Bias - Variance for Regression

Let

$$I[f] = \int (f(\mathbf{x}) - y)^2 p(\mathbf{x}, y) d\mathbf{x} dy$$

be the expected risk and f_0 the regression function. With $\bar{f}(\mathbf{x}) = E\{f_i(\mathbf{x})\}$, if we define the *bias* as

$$\int (f_0(\mathbf{x}) - \bar{f}(\mathbf{x}))^2 p(\mathbf{x}) d\mathbf{x}$$

and the *variance* as

$$E\left\{\int (f_i(\mathbf{x}) - \bar{f}(\mathbf{x}))^2 p(\mathbf{x}) d\mathbf{x}\right\},$$

we have the decomposition

$$E\{I[f_i]\} = I[f_0] + bias + variance.$$

Bias-Variance for Classification

No unique decomposition for classification exists. In the binary case, with $\bar{f}(\mathbf{x}) = \theta(E\{f_i(\mathbf{x})\})$, the decomposition suggested by Kong and Dietterich (1995) is

$$I[\bar{f}] - I[f_0]$$

for the *bias*, and

$$E\{I[f_i]\} - I[\bar{f}]$$

for the *variance*, which (again) gives

$$E\{I[f_i]\} = I[f_0] + bias + variance.$$

Bagging reduces variance

If each single classifier is **unstable** – that is, it has **high variance**, the aggregated classifier $\bar{f}$ has a smaller **variance** than a single original classifier.

The aggregated classifier $\bar{f}$ can be thought of as an approximation to the true average f obtained by replacing the probability distribution p with the bootstrap approximation to p obtained concentrating mass $1/\ell$ at each point $(\mathbf{x}_i, y_i)$.

Ensembles of Kernel Machines

What happens when combining kernel machines (i.e. SVM)?

- Different subsamples of training data (bagging)
- Different kernels or different features
- Different parameters (i.e. regularization parameter)

Combination of SVM Machines

Let $f_1(\mathbf{x}), \ldots, f_N(\mathbf{x})$ be SVM machines we want to combine and let

$$f(\mathbf{x}) = \sum_{n=1}^{N} c_n f_n(\mathbf{x})$$

for some fixed $c_n > 0$ with $\sum c_n = 1$.

We want to study the generalization performance of $f(\mathbf{x})$

Leave-one-out error

The leave-one-out error is computed in three steps

1. Leave a training point out
2. Train the remaining points and test the point left out
3. Repeat for each training point and count "errors"

Theorem (Luntz and Brailovski, 1969)

$$E\{I[f_\ell]\} = E\{\text{CV error of } f_{\ell+1}\}$$

Leave-one-out of a kernel machine

The leave-one-out error of a kernel machine (without b) is upper bounded by

$$\sum_{i=1}^{\ell} \theta(\alpha_i K(\mathbf{x}_i, \mathbf{x}_i) - y_i f(\mathbf{x}_i))$$

(Jaakkola and Haussler, 1998)

Proof (SVM case)

Given ℓ examples we have

$$L(\boldsymbol{\alpha}) = \sum_j \alpha_j - \frac{1}{2} \sum_{j,k} \alpha_j \alpha_k y_j y_k K_{jk}.$$

If $\boldsymbol{\alpha}^*$ denotes the maximizer we clearly have

$$L(\boldsymbol{\alpha}^*) \geq L(\boldsymbol{\alpha}) \quad \forall \boldsymbol{\alpha}.$$

If we leave the i-th point out, denoting with L' the new objective function and with α' the $\ell - 1$-dimensional vector of Lagrangian multipliers, we can write

$$L'(\alpha') = \sum_{j \neq i} \alpha_j - \frac{1}{2} \sum_{j,k \neq i} \alpha_j \alpha_k y_j y_k K_{jk}.$$

If $\bar{\alpha}'$ denotes the maximizer we have

$$L'(\bar{\alpha}') \geq L'(\alpha') \quad \forall \alpha'.$$

Proof (cont.)

Consider the objective function L with $\alpha_i = \alpha_i^*$,

$$L(\boldsymbol{\alpha}'; \alpha_i^*) = L'(\boldsymbol{\alpha}') - \alpha_i^* y_i \sum_{j \neq i} \alpha_j y_j K_{ij} + \alpha_i^*.$$

Since $\boldsymbol{\alpha}^*$ is a maximizer for L we have that

$$L(\boldsymbol{\alpha}'^*; \alpha_i^*) \geq L(\bar{\boldsymbol{\alpha}}'; \alpha_i^*)$$

which can be rewritten as

$$L'(\boldsymbol{\alpha}'^*) - \alpha_i^* y_i \sum_{j \neq i} \alpha_j^* y_j K_{ij} \geq L'(\bar{\boldsymbol{\alpha}}') - \alpha_i^* y_i \sum_{j \neq i} \bar{\alpha}_j y_j K_{ij}.$$

Proof (cont.)

Since $\bar{\alpha}'$ is a maximizer for L' we have

$$L'(\bar{\alpha}') \geq L'(\alpha'^*)$$

and hence we obtain

$$y_i f'(\mathbf{x}_i) = y_i \sum_{j \neq i} \bar{\alpha}_j y_j K_{ij} \geq y_i \sum_{j \neq i} \alpha_j^* y_j K_{ij}.$$

On the other hand we have

$$y_i f(\mathbf{x}_i) = y_i \sum_{j \neq i} \alpha_j^* y_j K_{ij} + \alpha_i^* K_{ii},$$

and therefore we can conclude that

$$y_i f'(\mathbf{x}_i) \geq y_i f(\mathbf{x}_i) - \alpha_i^* K_{ii}.$$

Leave-one-out bound for an SVM

For SVM classification we can also write

$$\sum_{i=1}^{\ell} \theta(\alpha_i K(\mathbf{x}_i, \mathbf{x}_i) - y_i f(\mathbf{x}_i)) \leq \frac{r^2}{\rho^2}$$

where r is the radius of the smallest sphere containing the Support Vectors and ρ the **true** margin (*different from the boosting margin!*

Leave-one-out bound for a kernel machine ensemble

The leave-one-out error of a kernel machine ensemble

$$f(\mathbf{x}) = c_1 f_1(\mathbf{x}) + c_2 f_2(\mathbf{x}) + ... + c_N f_N(\mathbf{x})$$

is upper bounded by

$$\sum_{i=1}^{\ell} \theta(\sum_{n=1}^{N} (\alpha_i K^{(n)}(\mathbf{x}_i, \mathbf{x}_i)) - y_i f(\mathbf{x}_i))$$

Leave-one-out bound for an SVM ensemble (Evgeniou et al., 2000)

For an SVM ensemble, the leave-one-out error can be bounded using geometry

$$\sum_{i=1}^{\ell} \theta\Big(\sum_{n=1}^{N} (\alpha_i K^{(n)}(\mathbf{x}_i, \mathbf{x}_i)) - y_i f(\mathbf{x}_i)\Big) \leq \sum_{n=1}^{N} \frac{r_{(n)}^2}{\rho_{(n)}^2}$$

where $r_{(n)}$ is the radius of the smallest sphere containing the SVs of machine n and $\rho_{(n)}$ the margin of SVM n. This suggests that bagging SVMs can be a good idea!

Recent developments (Evgeniou et al, 2001)

Through a modified version of the notion of stability, it is possible to study conditions under which **bagging** should or should not improve performances...

The original Boosting (Schapire, 1990)

1. Train a first classifier f_1 on a training set drawn from a probability $p(\mathbf{x}, y)$. Let ϵ_1 be the obtained performance;

2. Train a second classifier f_2 on a training set drawn from a probability $p_2(\mathbf{x}, y)$ such that it has half its measure on the event that h_1 makes a mistake and half on the rest. Let ϵ_2 be the obtained performance;

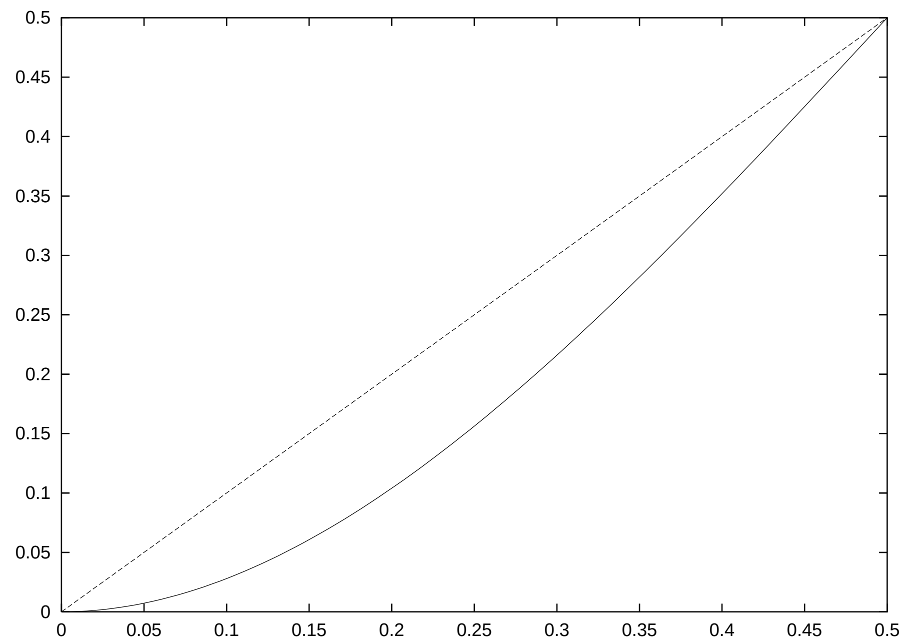
3. Train a third classifier f_3 on disagreements of the first two – that is, drawn from a probability $p_3(\mathbf{x}, y)$ which has its support on the event that h_1 and h_2 disagree. Let ϵ_3 be the obtained performance.

Boosting (cont.)

Main result: If $\epsilon_i < p$ for all i, the boosted hypothesis

$$f = MajorityVote\ (f_1, f_2, f_3)$$

has performance no worse than $\epsilon = 3p^2 - 2p^3$



Adaboost (Freund and Schapire, 1996)

The idea is of *adaptively* resampling the data

- Maintain a probability distribution over training set;

- Generate a sequence of classifiers in which the "next" classifier focuses on sample where the "previous" classifier failed;

- *Weigh* machines according to their performance.

Adaboost (pseudocode)

Given a learning method that can use weights on the data, initialize the distribution as $P_1(i) = 1/\ell$.
Then, for $n = 1, \ldots N$:

1. Train a machine with weights $P_n(i)$ and get f_n;

2. Compute the *weighted* error $\epsilon_n = \sum_{i=1}^{\ell} P_n(i)\theta(-y_i f_n(\mathbf{x}_i))$;

3. Compute the *importance* of f_n as $\alpha_n = 1/2 \ln\left(\frac{1-\epsilon_n}{\epsilon_n}\right)$;

4. Update the distribution $P_{n+1}(i) \propto P_n(i) e^{-\alpha_n y_i f_n(\mathbf{x}_i)}$.

Adaboost (cont.)

Adopt as final hypothesis

$$f(\mathbf{x}) = \text{sign}\left(\sum_{n=1}^{N} \alpha_n f_n(\mathbf{x})\right)$$

Theory of Boosting

We define the margin of $(\mathbf{x}_i, y_i)$ according to *the real value* function f to be

$$\text{margin}(\mathbf{x}_i, y_i) = y_i f(\mathbf{x}_i).$$

Note that this notion of margin is **different** from the SVM margin. This defines a margin for each training point!

A first theorem on boosting

Theorem *(Schapire et al, 1997)*

If running **adaboost** generates functions with errors:

$$\epsilon_1, \ldots \epsilon_N$$

Then for $\forall \gamma$

$$\sum_{i=1}^{\ell} \theta(\gamma - y_i f(\mathbf{x}_i)) \leq \prod_{n=1}^{N} \sqrt{4\epsilon_n^{1-\gamma}(1-\epsilon_n)^{1+\gamma}}.$$

Thus, the **training** margin error drops exponentially fast if $\epsilon_n < 0.5$

A second theorem on boosting

Let H be an hypothesis space with VC-dimension d and C the convex hull of H

$$C = \left\{ f : f(\mathbf{x}) = \sum_{h \in H} \alpha_h h(\mathbf{x}) \;\mid\; \alpha_h \geq 0; \;\; \sum_h \alpha_h = 1 \right\}$$

Theorem *(Schapire et al, 1997)*
For $\forall f \in C$ and $\forall \gamma > 0$:

$$I[f] \leq \sum_{i=1}^{\ell} \theta(\gamma - y_i f(\mathbf{x}_i)) + O\left(\frac{d/\ell}{\gamma}\right).$$

This holds for *any voting method!*

Are these theorems really useful?

- The first theorem simply ensures that the training error goes to zero...

- The second gives a loose bound which does not account for the success of boosting as a learning technique...

Additive Logistic Regression (Friedman, Hastie, Tibshirani 1999)

A possibly better insight can be gained by interpreting particular versions of adaboost as fitting an additive model using a certain loss function.

For example, in the *discrete* case ($f_n \in \{-1, 1\}$), it can be shown that adaboost builds an additive logistic regression model via Newton-like updates for approximately minimizing the functional

$$I[f] = \int e^{-yf(\mathbf{x})} p(\mathbf{x}, y) d\mathbf{x} dy.$$

Additive Logistic Regression (cont.)

The functional $I[f]$ is minimized at

$$f(\mathbf{x}) = \frac{1}{2} \log \frac{P(y = 1|\mathbf{x})}{P(y = -1|\mathbf{x})}.$$

Hence,

$$P(y = 1|\mathbf{x}) = \frac{e^{f(\mathbf{x})}}{e^{-f(\mathbf{x})} + e^{f(\mathbf{x})}}$$

$$P(y = -1|\mathbf{x}) = \frac{e^{-f(\mathbf{x})}}{e^{-f(\mathbf{x})} + e^{f(\mathbf{x})}}$$

Note that the usual logistic transform would not have the factor 1/2.

Why this loss? (Shapire and Singer, 1998)

The loss

$$V(f(\mathbf{x}), y) = e^{-yf(\mathbf{x})}$$

- is a differentiable upper bound to the $0-1$ loss
- it has similar flavor to the SVM loss

Where is the regularizing term in this case?