

Twin Boosting: Improved Feature Selection and Prediction

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Abstract

We propose Twin Boosting which has much better feature selection behavior than boosting. In addition, for cases with a few important effective and many noise features, Twin Boosting also substantially improves the predictive accuracy of boosting. Twin Boosting is as general and generic as boosting. It can be used with general weak learners and in a wide variety of situations, including generalized regression, classification or survival modeling. Furthermore, it is computationally feasible for large problems with potentially many more features than observed samples. Finally, for the special case of orthonormal linear models, we prove equivalence of Twin Boosting to the adaptive Lasso which yields a theoretical basis for some properties of Twin Boosting.

Key Words: Classification, Gradient descent, High-dimensional data, Regression, Regularization

Running Title: Twin Boosting

1 Introduction

Twin boosting is a very generic boosting-based method which most often yields better feature or variable selection than boosting while keeping or even increasing the prediction accuracy. Twin boosting proceeds roughly as follows. A first round of “classical” boosting is done (the first twin); then, in a second round, another boosting process is run (the second twin) which is forced to resemble the one from the first round. Thus, the two rounds are similar, like twins, and hence the name Twin Boosting. Boosting itself has attracted much attention in the machine learning community (cf. Schapire, 2002; Meir and Rätsch, 2003, and the references therein) as well as in related areas in statistics (Breiman, 1998, 1999; Friedman et al., 2000), mainly because of its excellent performance and computational attractiveness for large datasets.

There have been some attempts to make boosting or also related Lasso-methods (Tibshirani, 1996) more powerful, in particular in terms of feature or variable selection but also for prediction. The potential for improvement is mainly given for cases with many ineffective and a few effective covariates. To deal with many ineffective features, a strong

regularization is employed in boosting or in related Lasso-methods, creating a large estimation bias. Proposals to effectively avoid such large biases include Sparse Boosting (Bühlmann and Yu, 2006), conjugate direction boosting (Lutz and Bühlmann, 2006), Lasso with relaxation (Meinshausen, 2005) or the adaptive Lasso (Zou, 2006). Our approach has some similarity to the latter as it encompasses the adaptive Lasso in the very special case of an orthonormal linear model. An aspect of success of some of these methods is their greater flexibility than what is possible with a single regularization parameter in boosting (the number of iterations) or in related Lasso-methods (the penalty parameter). Our new Twin Boosting involves two tuning parameters which can be chosen sequentially rather than simultaneously optimizing over a two-dimensional space of regularization parameters.

All these recently proposed methods mentioned above, aiming to improve over boosting or Lasso, are far less general and generic than our Twin Boosting approach. The latter can be easily used with any real-valued weak learner which is a (possibly crude) estimator of the conditional mean function. Secondly, Twin Boosting can be used for a rich class of loss functions, including squared and absolute error for regression, logistic or exponential loss for classification or Poisson-loss for count data. Therefore, Twin Boosting is essentially as general and generic as boosting.

2 Boosting algorithms

Boosting is used in supervised learning from data $(X_i, Y_i), \dots, (X_n, Y_n)$, where $X_i \in \mathcal{X}$ is a p -dimensional predictor variable and $Y_i \in \mathcal{Y}$ is a univariate response variable. The space of predictor variables \mathcal{X} is often a subset of \mathbb{R}^p and the space of response variables often a subspace of \mathbb{R} , e.g. $\mathcal{Y} = \{-1, +1\}$ for binary classification or $\mathcal{Y} = \mathbb{R}$ for Gaussian regression.

A boosting algorithm needs the specification of a loss function and a weak learner. Regarding the former, consider a loss function

$$\rho : \mathcal{Y} \times \mathcal{X} \rightarrow \mathbb{R},$$

(or a subset of \mathbb{R} ; and we exclude here the case where the range of $\rho(\cdot, \cdot)$ is multivariate). The loss function is assumed to be differentiable (almost everywhere) and typically convex with respect to the second argument. Examples include squared error loss $\rho(y, f) = |y - f|^2/2$ with $y \in \mathbb{R}$ for regression or the logistic loss $\rho(y, f) = \log_2(1 + \exp(-2yf))$ with $y \in \{-1, +1\}$ for binary classification. The weak learner is in our setting a real-valued function estimator:

$$(X_1, U_1), \dots, (X_n, U_n) \xrightarrow{\text{weak learner}} \hat{g}(\cdot),$$

where X_i is the p -dimensional predictor variable and $U_i \in \mathbb{R}$ a pseudo-response variable. The notion of a pseudo-response variable will become clear in the description of the generic boosting algorithm below. An example of a weak learner is a regression tree yielding a regression function estimate $\hat{g}(\cdot)$.

It is instructive to look at the population minimizer of the loss function:

$$f^*(\cdot) = \operatorname{argmin}_{f(\cdot)} \mathbf{E}[\rho(Y, f(X))], \quad (1)$$

It is itself a function and it is the target of the boosting algorithm. For example, the squared error loss $\rho(y, f) = |y - f|^2/2$ yields the well-known population minimizer $f^*(x) = \mathbf{E}[Y|X = x]$ and boosting algorithms using the squared error loss are estimators of the regression function $f^*(\cdot)$.

2.1 The generic boosting algorithm

Boosting is based on the empirical risk $n^{-1} \sum_{i=1}^n \rho(Y_i, f(X_i))$ and pursuing iterative steepest descent in function space as described below for estimating the unknown function $f^*(\cdot)$. This very general and useful view of boosting has been pioneered by Breiman (1998, 1999) and further developed by Friedman et al. (2000), Rätsch et al. (2001) and Friedman (2001).

Variable or feature selection is pursued in this paper without any statistical significance testing. The selected features is the set of variables which enter explicitly (via the boosting algorithm) in the final function estimate $\hat{f}(\cdot)$.

Generic boosting algorithm

1. Initialize $\hat{f}^{[0]}$: typical values are $\hat{f}^{[0]} \equiv \bar{Y} = n^{-1} \sum_{i=1}^n Y_i$ or $\hat{f}^{[0]} \equiv 0$. Set $m = 0$.
2. Increase m by 1. Compute negative gradient $-\frac{\partial}{\partial f} \rho(Y, f)$ and evaluate at $\hat{f}_{m-1}(X_i)$:

$$U_i = -\frac{\partial}{\partial f} \rho(Y, f)|_{f=\hat{f}_{m-1}(X_i)}, \quad i = 1, \dots, n.$$

3. Fit negative gradient vector U_1, \dots, U_n by the weak learner

$$(X_1, U_1), \dots, (X_n, U_n) \xrightarrow{\text{weak learner}} \hat{g}^{[m]}(\cdot),$$

Thus, $\hat{g}^{[m]}(\cdot)$ can be viewed as an approximation of the negative gradient vector.

4. Up-date $\hat{f}^{[m]} = \hat{f}^{[m-1]}(\cdot) + \nu \cdot \hat{g}^{[m]}(\cdot)$, where $0 < \nu \leq 1$ is a step-length, i.e. proceed along an estimate of the negative gradient vector.
5. Iterate steps 2 - 4 until $m = m_{stop}$ for some stopping iteration m_{stop} .

The stopping iteration, which is the main tuning parameter, can be estimated via cross-validation. The choice of the step-size ν in step 4. is of minor importance, as long as it is “small” such as $\nu = 0.1$. A smaller value of ν typically requires a larger number of boosting iterations, and thus more computing time, while the predictive accuracy has been found to be potentially better for ν being “sufficiently small”, e.g. $\nu = 0.1$ (Friedman, 2001). Friedman (2001) suggests to use an additional line search between steps 3 and 4 (in case of different loss functions $\rho(\cdot, \cdot)$ than squared error): it yields a slightly different algorithm but the additional line search seems unnecessary to pursue for achieving a good estimator $\hat{f}^{[m_{stop}]}(\cdot)$.

2.2 L_2 Boosting

L_2 Boosting is the generic boosting algorithm when using the squared error loss $\rho(y, f) = |y - f|^2/2$. It has been proposed by Friedman (2001) and further developed and analyzed in Bühlmann and Yu (2003).

L_2 Boosting algorithm

1. Initialize $\hat{f}^{[0]}$: the default value is $\hat{f}^{[0]} \equiv \bar{Y} = n^{-1} \sum_{i=1}^n Y_i$. Set $m = 0$.
2. Increase m by 1. Compute the residuals $U_i = Y_i - \hat{f}^{[m-1]}(X_i)$ for $i = 1, \dots, n$.
3. Fit the residual vector U_1, \dots, U_n by the weak learner

$$(X_1, U_1), \dots, (X_n, U_n) \xrightarrow{\text{weak learner}} \hat{g}^{[m]}(\cdot).$$

4. Up-date $\hat{f}^{[m]}(\cdot) = \hat{f}^{[m-1]}(\cdot) + \nu \cdot \hat{g}^{[m]}(\cdot)$, where $0 < \nu \leq 1$ is a step-length factor.
5. Iterate steps 2 to 4 until $m = m_{stop}$ for some stopping iteration m_{stop} .

The stopping iteration m_{stop} is the main tuning parameter which can be selected using cross-validation.

Other loss functions, e.g. the logistic loss for classification, and corresponding boosting algorithms are described in Section 5. For reasons of clarity, we will first describe all the ideas and motivation for Twin Boosting for the case of the squared error loss. We will then show in Section 5 that the concepts easily generalize to general loss functions.

3 Twin L_2 Boosting for linear models

For expository simplicity, we first describe Twin Boosting for linear models:

$$Y_i = \sum_{j=1}^p \beta_j X_i^{(j)} + \varepsilon_i, \tag{2}$$

where $\varepsilon_1, \dots, \varepsilon_n$ are independent, identically distributed (i.i.d.), independent from X_1, \dots, X_n , with $\mathbf{E}[\varepsilon_i] = 0$. We sometimes write in short:

$$\mathbf{Y} = \mathbf{X}\beta + \varepsilon$$

with $\mathbf{Y}_{n \times 1} = (Y_1, \dots, Y_n)^T$, $\varepsilon_{n \times 1} = (\varepsilon_1, \dots, \varepsilon_n)^T$ and $\mathbf{X}_{n \times p} = [X_1, \dots, X_n]^T$.

Fitting of the linear model in (2) with boosting or Twin Boosting is based on the squared error loss (L_2 Boosting) and the componentwise linear least squares weak learner, as described in Section 3.1 below. Already L_2 Boosting itself has been proven to be very useful for fitting linear models with potentially many more covariates than samples (Friedman, 2001; Bühlmann, 2006; Bühlmann and Yu, 2006) and we will argue here in which circumstances Twin Boosting is even better.

In the sequel, we will extensively use the following notation:

$$\langle u, v \rangle = \sum_{i=1}^n u_i v_i \text{ for some vectors } u, v \in \mathbb{R}^n,$$

$$\|u\|^2 = \langle u, u \rangle = \sum_{i=1}^n u_i^2 \text{ for some vector } u \in \mathbb{R}^n.$$

Moreover, denote by $\mathbf{X}^{(j)}$ the j th $n \times 1$ column vector of \mathbf{X} .

3.1 Componentwise linear least squares as weak learner

Consider the following weak learner based on data $(X_1, U_1), \dots, (X_n, U_n)$:

$$\hat{g}(x) = \hat{\gamma}_{\hat{\mathcal{S}}} x^{\hat{\mathcal{S}}},$$

$$\hat{\gamma}_j = \langle \mathbf{U}, \mathbf{X}^{(j)} \rangle / \|\mathbf{X}^{(j)}\|^2, \quad \hat{\mathcal{S}} = \arg \min_{1 \leq j \leq p} \sum_{i=1}^n (U_i - \hat{\gamma}^{(j)} X_i^{(j)})^2. \quad (3)$$

It selects and fits the best predictor variable in a simple linear model in the sense of ordinary least squares fitting. For computational implementation as well as for the construction our Twin Boosting, it is useful to represent the selected predictor variable as:

$$\hat{\mathcal{S}} = \arg \min_{1 \leq j \leq p} |\langle \mathbf{U}, \mathbf{X}^{(j)} \rangle|^2 / \|\mathbf{X}^{(j)}\|^2. \quad (4)$$

The derivation of (4) is straightforward.

When using L_2 Boosting with this base procedure, we select in every iteration one predictor variable, not necessarily a different one for each iteration, and we up-date the function $\hat{f}^{[m]}(\cdot)$ linearly as described in Section 2.2. For componentwise linear least squares, we can simply up-date the parameter vector of a linear model.

L_2 Boosting with componentwise linear least squares

1. Initialize $\hat{\beta}^{[0]}$. Set $m = 0$.
2. Increase m by 1. Compute the residuals $U_i = Y_i - \bar{Y} - (\mathbf{X}\hat{\beta}^{[m-1]})_i$ for $i = 1, \dots, n$.
3. Compute $\hat{\mathcal{S}}_m$ as in (4) and $\hat{\gamma}_{\hat{\mathcal{S}}_m}$ as in (3).
4. Up-date

$$\hat{\beta}^{[m]} = \hat{\beta}^{[m-1]} + \nu \cdot \hat{\gamma}_{\hat{\mathcal{S}}_m}.$$

The notation should be read that only the $\hat{\mathcal{S}}_m$ th component of the coefficient estimate is up-dated.

5. Iterate steps 2 to 4 until $m = m_{stop}$ for some stopping iteration m_{stop} .

The selected variables are corresponding to the indices j for which $\hat{\beta}^{[m_1]} \neq 0$.

3.2 Twin L_2 Boosting with componentwise linear least squares

Twin Boosting for linear models uses the squared error loss and componentwise linear least squares as weak learner. For expository simplicity, we consider standardized data where $n^{-1} \sum_{i=1}^n Y_i = 0$, $n^{-1} \sum_{i=1}^n X_i^{(j)} = 0$ and $\sum_{i=1}^n (X_i^{(j)})^2 = 1$ for all $j = 1, \dots, p$ (for unstandardized data, the algorithm has to be slightly re-formulated). This can always be achieved by centering with the empirical mean and scaling with the empirical standard deviation.

Twin L_2 Boosting with componentwise linear least squares

1. Run a first round of L_2 Boosting with componentwise linear least squares, using m_1 iterations. Denote the estimated parameter by $\hat{\beta}_{init}^{[m_1]}$.
2. For the second round, run L_2 Boosting with componentwise linear least squares but replace formula (4) by

$$\hat{\mathcal{S}} = \operatorname{argmax}_{1 \leq j \leq p} |\langle \mathbf{U}, \mathbf{X}^{(j)} \rangle|^2 |\hat{\beta}_{init,j}^{[m_1]}|^2. \quad (5)$$

Note that $\|X^{(j)}\|^2 = 1$ because of standardized data. Use m_2 iterations and denote the Twin L_2 Boosting estimator by $\hat{\beta}_{TWB}^{[m_2]}$.

Two tuning parameters m_1 and m_2 are involved. Instead of optimizing (e.g. cross-validating) over both parameters simultaneously, we use the following, computationally much faster sequential approach: first, an estimate \hat{m}_1 is obtained from cross-validation for L_2 Boosting and then, cross-validation for Twin Boosting with fixed \hat{m}_1 in the initial estimator yields an estimate \hat{m}_2 .

3.3 Connections to the Lasso and the adaptive Lasso

There is an intriguing connection between L_2 Boosting with componentwise linear least squares and the Lasso (Tibshirani, 1996). The latter is an ℓ^1 -penalty method for regression defined by

$$\hat{\beta}(\lambda) = \operatorname{argmin}_{\beta} n^{-1} \sum_{i=1}^n (Y_i - \beta_0 - \sum_{j=1}^p \beta_j X_i^{(j)})^2 + \lambda \sum_{j=1}^p |\beta_j|. \quad (6)$$

Efron et al. (2004) consider a version of L_2 Boosting, called forward stagewise linear regression (FSLR), and they show that FSLR with infinitesimally small step-sizes (i.e. the value ν) produces a set of solutions which is approximately equivalent to the set of Lasso solutions when varying the regularisation parameter λ in Lasso (see also (6) above). The approximate equivalence is derived by representing FSLR and Lasso as two different modifications of their computationally efficient least angle regression (LARS) algorithm. In special cases where the design matrix satisfies a “positive cone condition”, FSLR, Lasso and LARS all coincide (Efron et al., 2004, p.425).

Despite the fact that L_2 Boosting and Lasso are not equivalent methods in general, the connection between boosting (as a forward, greedy method) and the Lasso (involving convex optimization) is interesting.

Recently, Zou (2006) has proposed the adaptive Lasso, defined as

$$\hat{\beta}(\lambda) = \arg \min_{\beta} n^{-1} \sum_{i=1}^n (Y_i - \beta_0 - \sum_{j=1}^p \beta_j X_i^{(j)})^2 + \lambda \sum_{j=1}^p \frac{|\beta_j|}{|\beta_{init,j}|}, \quad (7)$$

where β_{init} is an initial estimator. Zou (2006) mainly uses ordinary least squares as initial estimator (for cases with reasonable ratio n/p) and he mentions the Ridge estimator as one among several possible alternatives. In addition, he proposed a more general class of estimators, but the specific form in (7) is useful and often sufficient. The adaptive Lasso has two advantages over the Lasso. It yields consistent variable selection without imposing severe restriction on the design matrix, at least for the case with fixed predictor dimension p (Zou, 2006), whereas the Lasso is inconsistent (typically yields too large models) if the design is roughly speaking “strongly correlated” (Meinshausen and Bühlmann, 2006; Zou, 2006; Zhao and Yu, 2006). Secondly, adaptive Lasso yields better predictions if the true underlying model has many ineffective (noise) predictor variables. Both of these advantages are closely related to the motivation of our Twin Boosting, see Section 1.

In case of an orthonormal linear model, i.e. the model (2) with $\sum_{i=1}^n X_i^{(j)} X_i^{(k)} = \delta_{jk}$ (Kronecker $\delta_{jk} = 1$ if $j = k$ and 0 otherwise), explicit connections between boosting and Lasso exist. It has been shown (constructively) that L_2 Boosting with componentwise linear least squares approximates the solution from Lasso (as $\nu > 0$ tends to zero) which equals the soft-threshold estimator (Bühlmann and Yu, 2006). For Twin Boosting, the following holds.

Proposition 1 *In an orthonormal linear model, Twin Boosting with componentwise linear least squares approximates the adaptive Lasso described in (7) with $\hat{\beta}_{init}^{[m_1]}$ as initial estimator. In particular, when stopping the second round of Twin Boosting after m_2 iterations, there is a corresponding $\lambda > 0$ such that the following holds: for step-size factor $\nu \rightarrow 0$,*

$$\hat{\beta}_{TWB;j}^{[m_2]} \rightarrow \text{sign}(Z_j) \left(Z_j - \frac{\lambda}{|\hat{\beta}_{init,j}^{[m_1]}|} \right)_+ \quad (\nu \rightarrow 0),$$

where $(x)_+ = \max(0, x)$ denotes the positive part and $Z_j = (\mathbf{X}^T \mathbf{Y})_j$.

A proof is given in the Appendix. Proposition 1 illustrates that in the simple case of an orthonormal linear model, Twin Boosting yields the adaptive Lasso which equals here the adaptive soft-threshold estimator (as given in Proposition 1 as the limiting case for $\nu \rightarrow 0$). The connection is interesting but the real power of Twin Boosting is its generic applicability to very general weak learners and loss functions.

4 Twin L_2 Boosting with trees and general weak learners

The most popular weak learners for boosting are decision trees. Our proposal for Twin Boosting with trees is simple, easy to implement and effective. We could represent trees

in terms of basis functions (with indicator functions of rectangles) and then employ Twin Boosting methodology as for linear models. However, such an approach becomes computationally very impractical due to the huge number of basis functions (particularly for larger trees) and in addition, such an approach would (adaptively) encourage sparseness in the space of basis functions rather than sparseness in the space of predictor variables; the latter is often much more interesting for many datasets and scientific problems.

Twin Boosting with any real-valued (regression-type) weak learner is defined as follows.

Twin L_2 Boosting with general weak learner

1. Run a first round of L_2 Boosting and denote by $\hat{\mathbf{f}}_{init}^{[m_1]} = (\hat{f}_{init}^{[m_1]}(X_1), \dots, \hat{f}_{init}^{[m_1]}(X_n))$ the fitted function at the data points and by $\hat{\mathcal{V}}^{[m_1]} \subseteq \{1, \dots, p\}$ the subset of indices corresponding to selected predictor variables, both based on m_1 boosting iterations. (If the weak learner is not doing any variable selection, then $\hat{\mathcal{V}}^{[m_1]} = \{1, \dots, p\}$ is the full set).
2. For the second round, initialize $\hat{f}^{[0]}$: the default value is $\hat{f}^{[0]} \equiv \bar{Y} = n^{-1} \sum_{i=1}^n Y_i$. Set $m = 0$.
3. Increase m by 1. Compute the residuals $U_i = Y_i - \hat{f}^{[m-1]}(X_i)$ for $i = 1, \dots, n$.
4. For every subset $\mathcal{W} \subseteq \hat{\mathcal{V}}^{[m_1]}$,¹ fit the residual vector U_1, \dots, U_n to X_1, \dots, X_n with the weak learner. Denote this fitted function by $\hat{h}_{\mathcal{W}}(\cdot)$ and by $\hat{\mathbf{h}}_{\mathcal{W}} = (\hat{h}_{\mathcal{W}}(X_1), \dots, \hat{h}_{\mathcal{W}}(X_n))$. Then, choose the best \mathcal{W} according to:

$$\begin{aligned} \widehat{\mathcal{W}} &= \operatorname{argmax}_{\mathcal{W}} C_{\mathcal{W}}^2 (2\langle \mathbf{U}, \hat{\mathbf{h}}_{\mathcal{W}} \rangle - \|\hat{\mathbf{h}}_{\mathcal{W}}\|^2), \\ C_{\mathcal{W}} &= \langle \hat{\mathbf{f}}_{init}^{[m_1]} - \overline{\hat{f}_{init}^{[m_1]}}, \hat{\mathbf{h}}_{\mathcal{W}} \rangle / \|\hat{\mathbf{h}}_{\mathcal{W}}\|, \quad \overline{\hat{f}_{init}^{[m_1]}} = n^{-1} \sum_{i=1}^n \hat{f}_{init}^{[m_1]}(X_i). \end{aligned} \quad (8)$$

Denote by $\hat{g}^{[m]}(\cdot) = \hat{h}_{\widehat{\mathcal{W}}}(\cdot)$.

5. Up-date $\hat{f}^{[m]} = \hat{f}^{[m-1]}(\cdot) + \nu \cdot \hat{g}^{[m]}(\cdot)$, where $0 < \nu \leq 1$ is a step-length factor.
6. Iterate steps 3 to 5 until $m = m_2$ for some stopping iteration m_2 .

The stopping iteration m_2 is the main tuning parameter (for a given boosting estimator of the first round) which can be selected using cross-validation.

From a computational point of view, it seems awkward to consider all subsets $\mathcal{W} \subseteq \hat{\mathcal{V}}^{[m_1]}$ in step 4. However, if the weak learner does variable selection, selecting at most d predictor variables (e.g. a tree with at most $d + 1$ terminal nodes), we only have to consider in step 4 all subsets \mathcal{W} having cardinality $|\mathcal{W}| = d$. For example, when using stumps, $d = 1$ and step 4 becomes:

step 4 for stumps. For every $j \in \hat{\mathcal{V}}^{[m_1]}$, fit the residual vector with a stump and denote it by $\hat{h}_j(\cdot)$. The remaining part of step 4 is then as above.

¹See also the discussion after the description of the algorithm.

The selected variables from Twin Boosting arise from the set of variables which occur in $\widehat{\mathcal{W}}$ from step 4 for at least one iteration. For example with trees as weak learner, the selected variables arise from variable selection of the tree-type weak learner during the Twin Boosting iterations.

Using trees as weak learner, $d = 1$ (stumps) or $d = 2$ is often a good choice (see also the discussion below in Section 4.1). More generally, for a tree with $d + 1$ terminal nodes (d splits), the computation in step 4 is of the order $O(dnp|\hat{\mathcal{V}}^{[m_1]}|^d)$. It should be noted here that usually $|\hat{\mathcal{V}}^{[m_1]}| \leq \min(n, p)$, often even $\ll \min(n, p)$.

In case of large trees as weak learner, we could also take random subsets \mathcal{W} of cardinality d and proceed then as above in step 4.

We give now a motivation for the construction in step 4. Consider Twin L_2 Boosting for linear models, described in Section 3.2. There, it happens automatically that the second round of Twin Boosting considers only the set of predictor variables $\hat{\mathcal{V}}^{[m_1]}$ which has been chosen in the first round. Next, we consider the formula (8). The residual sum of squares is

$$\|\mathbf{U} - \hat{\mathbf{h}}_{\mathcal{W}}\|^2 = \|\mathbf{U}\|^2 - 2\langle \mathbf{U}, \hat{\mathbf{h}}_{\mathcal{W}} \rangle + \|\hat{\mathbf{h}}_{\mathcal{W}}\|^2 = \text{const.} - (2\langle \mathbf{U}, \hat{\mathbf{h}}_{\mathcal{W}} \rangle - \|\hat{\mathbf{h}}_{\mathcal{W}}\|^2).$$

L_2 Boosting would proceed by choosing the best \mathcal{W} maximizing

$$G(\mathcal{W}) = 2\langle \mathbf{U}, \hat{\mathbf{h}}_{\mathcal{W}} \rangle - \|\hat{\mathbf{h}}_{\mathcal{W}}\|^2. \quad (9)$$

For Twin Boosting, we want to multiply weights $C_{\mathcal{W}}$ into the criterion $G(\mathcal{W})$. For the form of these weights, it is instructive to consider Twin Boosting for linear models with normed predictor variables having $\|\mathbf{X}^{(j)}\|^2 = 1$: there, \mathcal{W} is an element of $\{1, \dots, p\}$ and $\hat{h}_j(X_i) = \langle \mathbf{U}, \mathbf{X}^{(j)} \rangle X_i^{(j)}$. Using this, we easily obtain for $\mathcal{W} = j$,

$$G(\mathcal{W}) = G(j) = |\langle \mathbf{U}, \mathbf{X}^{(j)} \rangle|^2. \quad (10)$$

Twin Boosting for linear models does nothing else than multiplying $G(j)$ by the weights $\beta_{init,j}^2$. Therefore, we want to multiply $G(\mathcal{W})$ in (9) with the square of a suitable regression coefficient. Our $C_{\mathcal{W}}$ in formula (8) is the standardized regression coefficient when regressing the fitted function from the first round of Twin Boosting $\hat{\mathbf{f}}^{[m_1]}$ against the candidate estimate $\hat{\mathbf{h}}_{\mathcal{W}}$; the standardization is a multiplication by $\|\hat{\mathbf{h}}_{\mathcal{W}}\|$. The standardization is useful as it implicitly measures the regression coefficient on a scale where $\hat{\mathbf{h}}_{\mathcal{W}}$ would have been standardized to $\|\hat{\mathbf{h}}_{\mathcal{W}}\| \equiv 1$ for all \mathcal{W} . We end our motivation of step 3 with the following result.

Proposition 2 *Consider the general Twin L_2 Boosting algorithm and choose the componentwise linear least squares weak learner. Then, this algorithm coincides exactly with Twin L_2 Boosting for linear models, as described in Section 3.2, provided that the underlying regression model is orthonormal as specified in (2) with $\sum_{i=1}^n X_i^{(j)} X_i^{(k)} = \delta_{jk}$.*

A proof is given in the Appendix.

4.1 Stumps and larger trees as weak learners

The choice of the weak learner is usually driven by optimizing the prediction performance. In addition, some structural properties can be another useful criterion as well.

The generic boosting and Twin Boosting estimator is a linear combination of weak learners

$$\hat{f}^{[m]}(\cdot) = \nu \sum_{k=1}^m \hat{g}^{[k]}(\cdot).$$

Therefore, structural properties of the boosting function estimator are given by linear combination of structural characteristics of the weak learner.

Trees are among the most popular base procedures in machine learning. They have the advantage to be invariant under monotone transformations of predictor variables, i.e., we do not need to search for good data transformations.

When using stumps, i.e., a tree with two terminal nodes, the boosting and Twin Boosting estimate will be an additive model in the original predictor variables, because every stump-estimate is a function of a single predictor variable only. Similarly, boosting trees with (at most) $d+1$ terminal nodes results in a nonparametric model having at most interactions of order $d-1$: e.g. for $d=2$, we would pick up interaction terms between pairs of predictor variables. Thus, if we want to constrain the degree of interactions, we can easily do this by constraining the (maximal) number of nodes in the tree learner. For many real datasets, it seems that low-order interaction (or even additive) models are sufficiently rich for good prediction and interpretation. For example, the naive Bayes classifier or linear discriminant analysis, based on an additive or linear decision function respectively, works surprisingly well in many applications (Jamain and Hand, 2005; Hand, 2006). Also boosting with stumps, yielding an additive model, has proven to be successful in many areas, e.g. winning the performance prediction challenge of the IEEE World Congress on Computational Intelligence 2006 (Lutz, 2006). Thus, we often get good performance with trees having 2 or 3 terminal nodes ($d=1$ or 2 , respectively). With such small values of d , Twin Boosting is computationally fast, as discussed after the description of the Twin Boosting algorithm in Section 4.

5 Other loss functions and generic Twin Boosting

For other loss functions than squared error (i.e. other boosting algorithms than L_2 Boosting) we can use the general functional gradient descent approach as described in Section 2.1.

Interesting examples of loss functions include the following. For binary classification with $y \in \{-1, +1\}$, the logistic loss is

$$\rho_{logit}(y, f) = \log_2(1 + \exp(-2yf)), \quad (11)$$

and the exponential loss is

$$\rho_{exp}(y, f) = \exp(-yf). \quad (12)$$

Boosting with the logistic loss or exponential loss function is essentially LogitBoost (Friedman et al., 2000) (also called BinomialBoosting) or AdaBoost (Freund and Schapire, 1996), respectively. For both loss function, the population minimizer is

$$f^*(x) = \frac{1}{2} \log\left(\frac{p(x)}{1-p(x)}\right), \quad p(x) = \mathbb{P}[Y = 1|X = x].$$

For cases where $Y \in \{0, 1, 2, \dots\}$, the Poisson log-likelihood is often appropriate:

$$\rho(y, f) = -yf + \exp(f), \quad f = \log(\lambda).$$

In survival analysis, we can derive the loss function from the partial likelihood in the Cox model (Cox, 1975).

5.1 Generic Twin Boosting with general weak learners

If the loss function $\rho(\cdot, \cdot)$ is differentiable (almost everywhere) with respect to the second argument, the generic boosting algorithm from Section 2.1 can be used.

Generic Twin Boosting is exactly as Twin L_2 Boosting from Section 3.2, except that in step 3, instead of using residuals U_i we will use

$$U_i = -\frac{\partial}{\partial f} \rho(Y, f)|_{f=\hat{f}_{m-1}(X_i)}, \quad i = 1, \dots, n,$$

exactly as in the generic boosting algorithm from Section 2.1. Therefore, from an implementation point of view, Twin Boosting with general loss functions is as simple as Twin L_2 Boosting.

6 Empirical results

We report here some results on Twin Boosting for regression and classification and we compare them with boosting. We will demonstrate that Twin Boosting has a clear advantage over boosting if the truth has many ineffective predictor variables. Given the success of boosting algorithms in many application areas, Twin Boosting exhibits a substantial potential for further improvements over boosting. All our results are displayed in Figures, giving a better summary how the methods behave as a function of boosting iterations.

6.1 Regression

The response variables Y_i are real-valued and the goal is estimation of the function $\mathbb{E}[Y|X = x]$ or prediction of new observations Y .

6.1.1 Simulated data

Consider the linear model:

$$\begin{aligned} \text{model in (2) with} \quad p &= 500, \quad \beta_1 = 5, \quad \beta_j = 0 \quad (j = 2, \dots, p), \\ X_i &\sim \mathcal{N}_p(0, I) \text{ and } \varepsilon_i \sim \mathcal{N}(0, 1). \end{aligned} \tag{13}$$

Sample size is chosen as $n = 50$ and the number of independent simulation runs is 100.

We first use L_2 Boosting and Twin L_2 Boosting for linear models, using the componentwise linear least squares weak learner. The step-length factor is chosen as $\nu = 0.1$ and the number of boosting iterations in the first round of Twin Boosting is chosen as $m_1 = 50$ which is a reasonable value according to the performance of L_2 Boosting. Figure 1 displays the mean squared error (MSE) $\mathbb{E}[(\hat{\beta} - \beta)^T X_{new}]^2 = \sum_{j=1}^p \mathbb{E}[(\hat{\beta}_j - \beta_j)^2]$ (i.e. generalization error) and the number of selected and incorrectly selected predictor variables, as a function of boosting iterations. Figure 1 is an impressive demonstration how much can be gained by using Twin Boosting instead of boosting, particularly in terms of variable selection.

Figure 1 about here.

Next, we consider L_2 Boosting and Twin L_2 Boosting with stumps. The results are displayed in Figure 2; for Twin Boosting, we used $m_1 = 50$ iterations in the first round.

Figure 2 about here.

Although boosting (and Twin Boosting) with stumps yields an additive model fit, the weak learner is “mis-specified” (as is often the case in practice). This explains why the mean squared error is much larger than with componentwise linear least squares. Also here, L_2 Boosting selects way too many predictor variables while Twin Boosting is very effective and substantially reduces the number of selected variables.

The results here are quite representative for many other simulation settings.

6.1.2 Real data

We consider two real data sets: ozone concentration and motif regression from molecular biology. Both data sets are available from

`ftp://ftp.stat.math.ethz.ch/Research-Reports/Other-Manuscripts/buhlmann/ozone.dat`
`ftp://ftp.stat.math.ethz.ch/Research-Reports/Other-Manuscripts/buhlmann/motif.dat`
 respectively.

The ozone data is about daily ozone concentration in the Los Angeles basin as a function of $p = 8$ meteorological predictor variables. Sample size is $n = 330$. From a prediction point of view, the componentwise linear least squares weak learner is inferior than stumps. Thus, Figure 3 reports only for boosting and Twin Boosting (with $m_1 = 100$ iterations in the first round) with stumps.

Figure 3 about here.

In addition, we look at a synthetically enlarged problem. We add 500 additional, ineffective noise predictor variables $X_{add} \sim \mathcal{N}_{500}(0, I)$. The problem has then dimension $p = 508$ with at most 8 effective predictors. This will enable us to see whether and how many from the obviously ineffective variables will be selected; we do not know whether all of the 8 original predictor variables are effective or not. We refer to an obviously incorrectly selected predictor variable if it is one of the 500 synthetically added predictors. Figure 4 reports the results (with $m_1 = 100$ iterations in the first round of Twin Boosting). Twin

L_2 Boosting has slightly better prediction performance than L_2 Boosting and is much better with respect to obviously incorrectly selected variables.

Figure 4 about here.

The motif regression data models gene expression as a function of MDSCAN motif scores (Conlon et al., 2003, p. 3343: Spellman et al. data, 15th time point). This data is representative for many gene expression - motif scores data-sets, all of them being very noisy. Our data has $p = 4312$ motif scores (predictor variables) and sample size (number of genes) is $n = 4443$. Figure 5 displays the results for the componentwise linear least squares weak learner.

Figure 5 about here.

Although L_2 Boosting is performing as well as Twin L_2 Boosting from a prediction point of view, the sparsity of Twin L_2 Boosting in terms of selected variables is crucial in this application. When using about 600-800 boosting iterations, L_2 Boosting selects 144-178 predictors while Twin Boosting uses 41-53 variables only. Biological validation of about 50 potential motifs (cis-regulatory elements) is much more realistic than for 3 times as many candidates. L_2 Boosting and Twin L_2 Boosting with trees did not improve prediction performance while it selected more predictor variables than what is reported above for componentwise linear least squares.

6.2 Classification

We consider some binary classification problems and use exclusively the logistic loss in (11) for boosting, i.e. Binomial- or LogitBoosting. The classifier is given by $sign(\hat{f}(x))$ where $\hat{f}(\cdot)$ is the estimated function from boosting or Twin Boosting, respectively. This rule is equivalent to classify to the label with larger (conditional) class-probability.

6.2.1 Simulated data

We modify model (13) as follows:

$$p = 500, \beta_1 = 2, \beta_j = 0 \ (j = 2, \dots, p),$$

$$X_i \sim \mathcal{N}_p(0, I), \log(\pi_i/(1 - \pi_i)) = \sum_{j=1}^p \beta_j X_i^{(j)}, Y_i \sim \text{Bernoulli}(\pi_i). \quad (14)$$

Sample size is again chosen as $n = 50$ and the number of independent simulation runs is 100. We reduced the size of the coefficient β_1 in comparison to model (13) to decrease the signal to noise ratio in the problem.

Figure 6 reports the results for Binomial/LogitBoosting and its Twin Boosting version (with $m_1 = 10$ iterations in the first round of Twin Boosting) with componentwise linear least squares (which yields a logistic linear model). The results are qualitatively comparable to the case of regression in Figure 1, demonstrating a clear advantage of Twin Boosting.

Figure 6 about here.

6.2.2 Real data

We consider the sonar dataset ($n = 208$, $p = 60$) from the Statlog project, available from `ftp://ftp.stat.math.ethz.ch/Research-Reports/Other-Manuscripts/buhlmann/sonar.dat` and the ionosphere dataset ($n = 351$, $p = 34$) from the UCI machine learning repository (`http://www.ics.uci.edu/mllearn/MLSummary.html`). For both cases, we also consider synthetically enlarged predictor spaces where we add 500 ineffective predictor variables. We use boosting and Twin Boosting with stumps; logistic linear models, fitted by using the componentwise linear least squares weak learner, were not competitive for both data-sets.

For the sonar data, we use $m_1 = 100$ iterations in the first round of Twin Boosting. The results are displayed in Figure 7. The classification accuracy is about the same for boosting and Twin Boosting while the latter selects about 30% fewer variables (when using reasonable stopping iterations which differ for the two methods).

Figure 7 about here.

We enlarge the number of features by adding 500 additional, ineffective noise predictor variables $X_{add} \sim \mathcal{N}_{500}(0, I)$. Then, the classification problem involves dimension $p = 560$ with at most 60 effective predictors. We refer to an obviously incorrectly selected predictor variable if it belongs to one of the 500 synthetically added features. Results are given in Figure 8.

Figure 8 about here.

The interpretation is similar (even more in favor of Twin Boosting) as for the original sonar data. In addition, Twin Boosting is much better in terms of obviously incorrectly selected variables.

For the ionosphere data, $m_1 = 500$ iterations in the first round of Twin Boosting is a reasonable value. The results are displayed in Figure 9.

Figure 9 about here.

Twin Boosting has marginally better prediction power while being more sparse in the selected variables. When adding 500 additional, ineffective noise predictor variables $X_{add} \sim \mathcal{N}_{500}(0, I)$ the problem has dimension $p = 534$ with at most 34 effective predictors. Results are displayed in Figure 10, based on $m_1 = 200$ iterations in the first round of Twin Boosting; as above for the sonar data, the obviously incorrectly selected variables can be determined.

Figure 10 about here.

Interestingly, the classification performance does not degrade for both boosting and Twin Boosting. The reason is probably due to the increased resistance of overfitting (e.g. when selecting wrong features) when using the misclassification error (Friedman et al., 2000, p.400-404) and having a situation with low noise (low misclassification error). Regarding the quality of feature selection, however, Twin Boosting is much better than boosting in terms of selecting obviously incorrect predictor variables.

7 Conclusions

We proposed Twin Boosting which is as general and generic as boosting. It can be used with general weak learners and in a wide variety of situations, including regression, classification, Poisson regression or survival analysis (using the loss function from the partial likelihood in the Cox model). Furthermore, it is easy to implement and computationally feasible for large problems with potentially very many features (or predictors or covariates) and/or large sample size. In particular, it is useful for high-dimensional situations where the number of features is much larger than sample size.

We have empirically shown that Twin Boosting has much better feature or variable selection behavior than boosting. For cases with a few important effective covariates and many noise features, Twin Boosting also improves the predictive accuracy of boosting; for other situations, we never found it worse for prediction than boosting. For the special case of orthonormal linear models, we prove equivalence to the adaptive Lasso (Zou, 2006) which yields a theoretical basis for explaining our general empirical findings for Twin Boosting.

8 Appendix

Proof of Proposition 1.

The proof of Theorem 2 in Bühlmann and Yu (2006) can be adapted. The main modification is needed for formula (22) and its previous 5 lines. We denote in short by $\beta_{init} = \hat{\beta}_{init}^{[m_1]}$ and $\hat{\beta}^{[m]} = \hat{\beta}_{TWB}^{[m]}$.

The residual sum of squares of Twin L_2 Boosting at iteration m , denoted by RSS_m , decreases monotonically in m . The difference in residual sum of squares is:

$$RSS_m - RSS_{m+1} = |\langle \mathbf{U}, \mathbf{X}^{(\mathcal{S}_{m+1})} \rangle|^2,$$

where \mathbf{U} denotes the residual vector $\mathbf{Y} - \mathbf{X}\hat{\beta}^{[m]}$ and \mathcal{S}_{m+1} the selected variable in iteration $m+1$. In every step of Twin L_2 Boosting, a maximal reduction of the weighted difference in residual sum of squares is used:

$$G_{m+1} = (RSS_m - RSS_{m+1})|\beta_{init, \mathcal{S}_{m+1}}|^2 = |\langle \mathbf{U}, \mathbf{X}^{(\mathcal{S}_{m+1})} \rangle|^2 |\beta_{init, \mathcal{S}_{m+1}}|^2,$$

and the sequence $G_{m+1}, m = 1, 2, \dots$ is monotonically decreasing (because of the definition of Twin L_2 Boosting, the independence of fitting the i th component of β from the j th component ($i \neq j$) and the form of the decay of differences of residual sum of squares). Therefore, every stopping iteration corresponds to a tolerance δ^2 as in formula (22) in Bühlmann and Yu (2006), using here G_{m+1} instead of $RSS_m - RSS_{m+1}$. The remaining part of the proof is exactly as in Bühlmann and Yu (2006): the additional factor $|\beta_{init, i}|^2$ leads to the assertion of Proposition 1. \square

Proof of Proposition 2.

By formula (10), we only have to deal with the form of the coefficient $C_{\mathcal{W}} = C_j$ in (8). Denote by $\hat{\gamma}_j = \langle \mathbf{U}, \mathbf{X}^{(j)} \rangle$ the estimated regression coefficient of \mathbf{U} versus $\mathbf{X}^{(j)}$. Then,

$$C_j = \langle \hat{\mathbf{f}}_{init}^{[m_1]}, \hat{\gamma}_j \mathbf{X}^{(j)} \rangle / \|\hat{\gamma}_j \mathbf{X}^{(j)}\|$$

$$= \left\langle \sum_{k=1}^p \hat{\beta}_{init,k}^{[m_1]} \mathbf{X}^{(k)}, \hat{\gamma}_j \mathbf{X}^{(j)} \right\rangle / \|\hat{\gamma}_j \mathbf{X}^{(j)}\| = \hat{\beta}_{init,j}^{[m_1]} \hat{\gamma}_j / |\hat{\gamma}_j|.$$

Hence,

$$C_j^2 = (\hat{\beta}_{init,j}^{[m_1]})^2,$$

equaling the factor in formula (5). This completes the proof. \square

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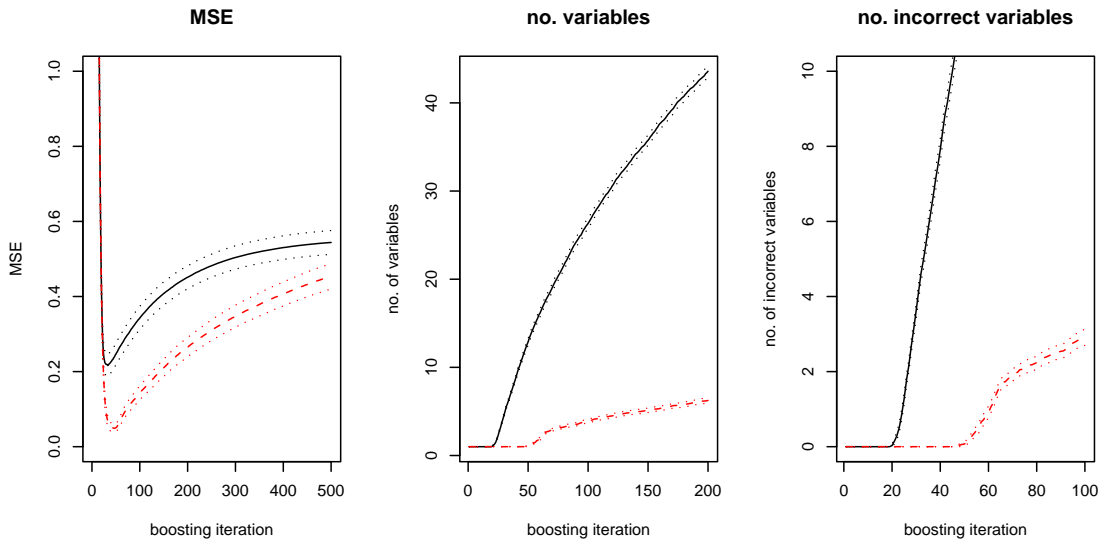


Figure 1: L_2 Boosting (solid line) and Twin Boosting (dashed line) with componentwise linear least squares in model (13). Mean squared error (MSE) (left), average number of selected predictor variables (middle) and number of incorrectly selected predictor variables (right) as a function of boosting iterations (or iterations from the second round in Twin Boosting, respectively). Simulation accuracy is indicated by dotted lines as 95% confidence intervals.

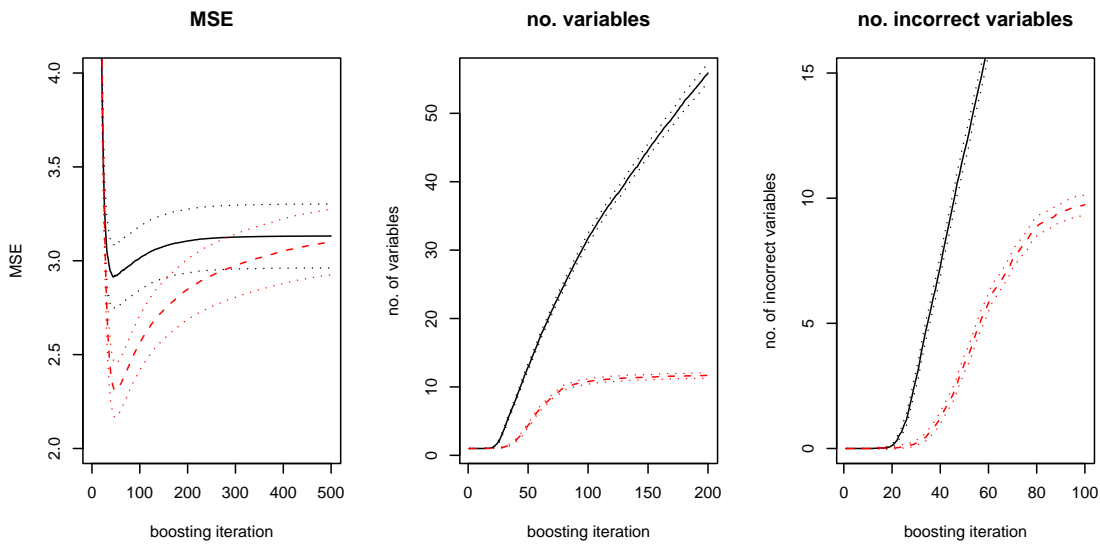


Figure 2: L_2 Boosting (solid line) and Twin L_2 Boosting (dashed line) with stumps for model (13). Other specifications as in Figure 1.

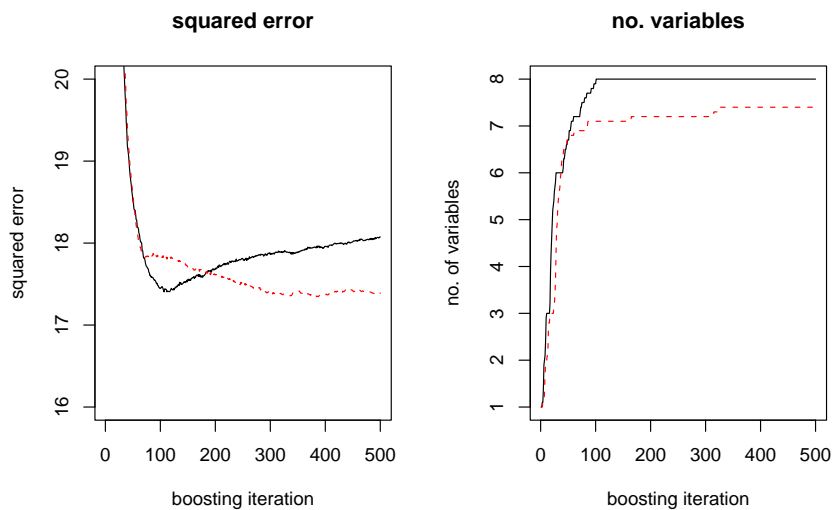


Figure 3: L_2 Boosting (solid line) and Twin Boosting (dashed line) with stumps for ozone data. 10-fold cross-validation of: Squared error (left) and number of selected predictor variables (right), as a function of boosting iterations (or iterations from the second round in Twin Boosting, respectively).

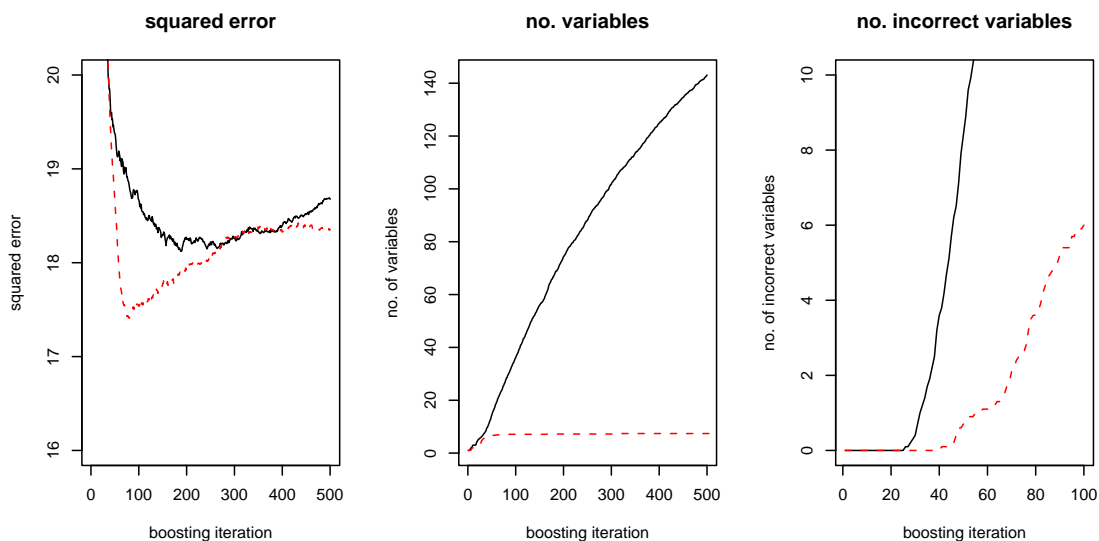


Figure 4: L_2 Boosting (solid line) and Twin Boosting (dashed line) with stumps for ozone data with synthetically enlarged predictor space ($p = 508$). 10-fold cross-validation of: Squared error (left), number of selected predictor variables (middle) and number of obviously incorrectly selected variables (right), as a function of boosting iterations (or iterations from the second round in Twin Boosting, respectively).

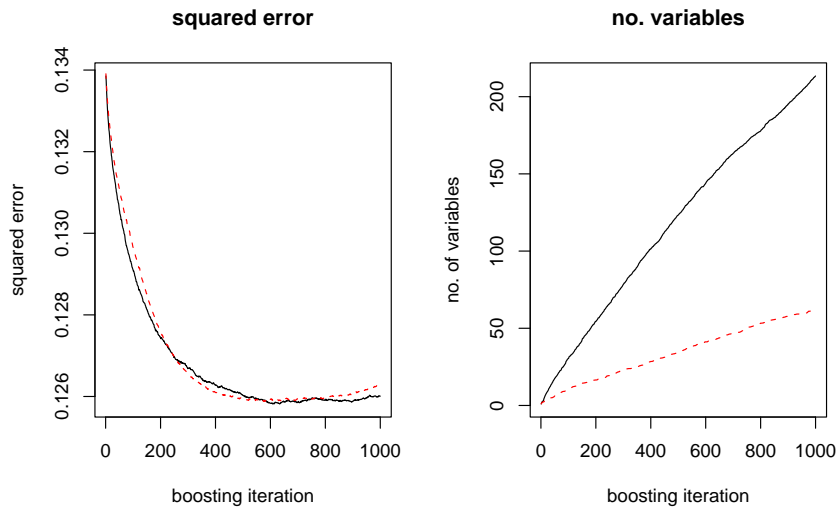


Figure 5: L_2 Boosting (solid line) and Twin L_2 Boosting (dashed line) with componentwise linear least squares for motif regression data. Other specifications as in Figure 3.

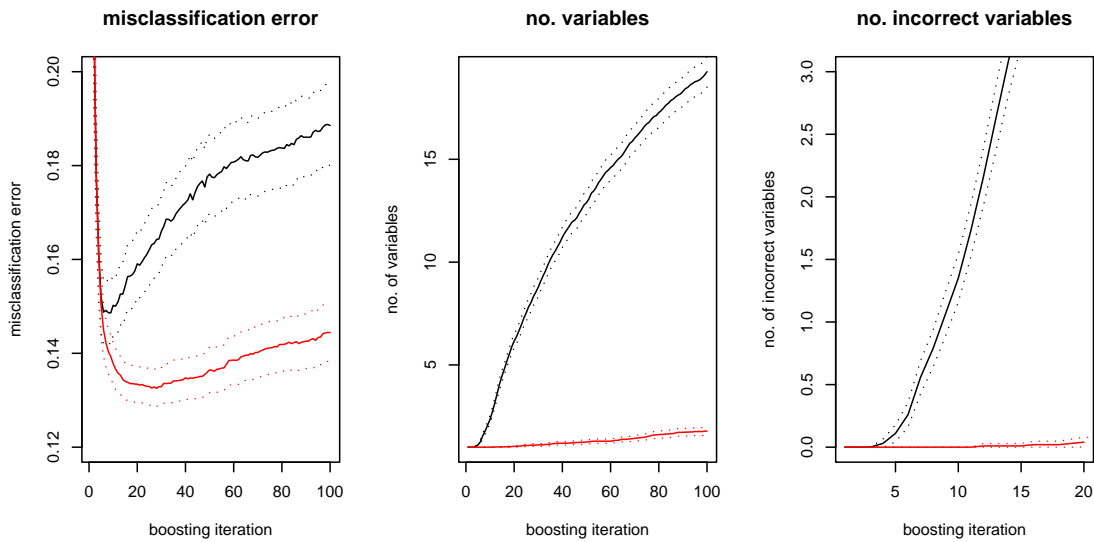


Figure 6: LogitBoosting (solid line) and corresponding Twin Boosting (dashed line) with componentwise linear least squares in model (14). Misclassification error (left), average number of selected predictor variables (middle) and average number of incorrectly selected predictor variables (right) as a function of boosting iterations (or iterations from the second round in Twin Boosting, respectively). Simulation accuracy is indicated by dotted lines as 95% confidence intervals.

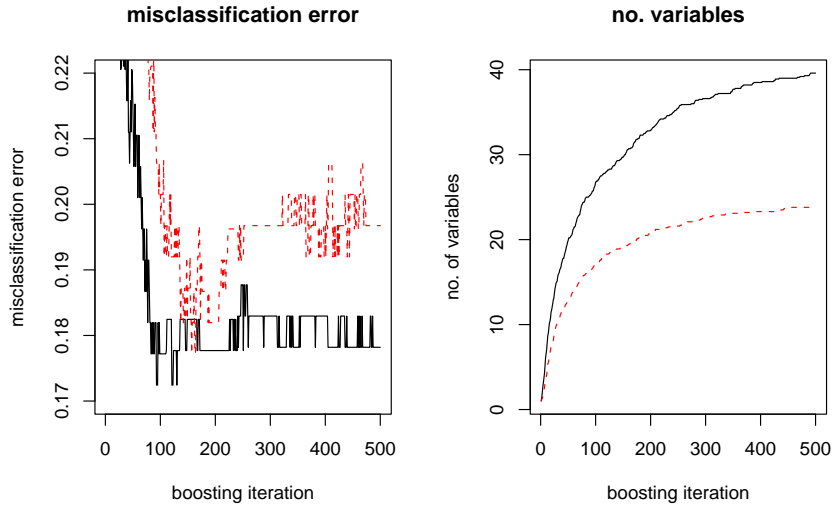


Figure 7: LogitBoosting (solid line) and corresponding Twin Boosting (dashed line) with stumps for sonar data. 10-fold cross-validation of: Misclassification error rate (left) and number of selected predictor variables (right, as a function of boosting iterations (or iterations from the second round in Twin Boosting, respectively)).

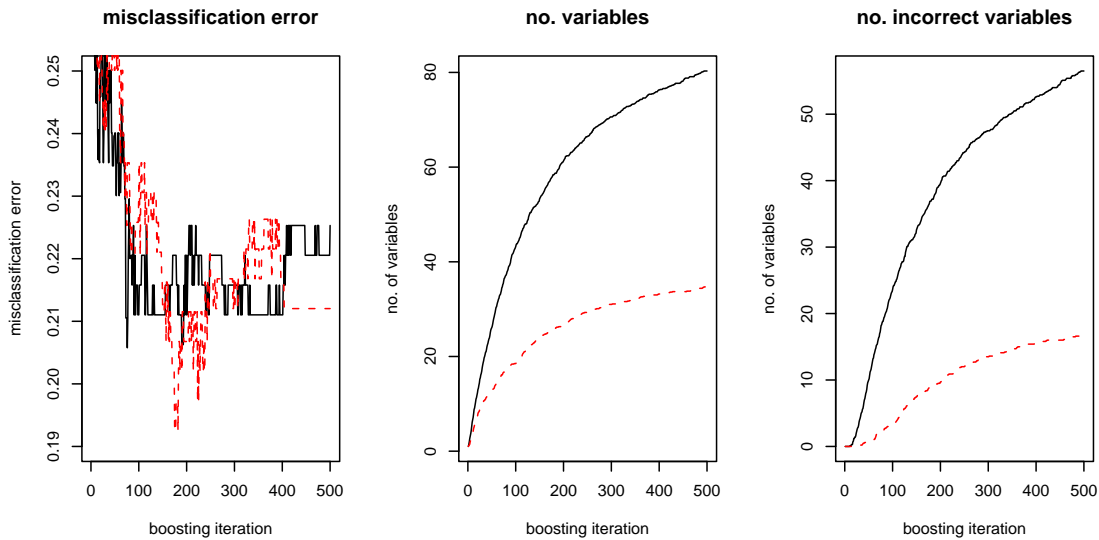


Figure 8: LogitBoosting (solid line) and corresponding Twin Boosting (dashed line) with stumps for sonar data with synthetically enlarged predictor space. 10-fold cross-validation of: Misclassification error rate (left), number of selected predictor variables (middle) and number of obviously incorrectly selected variables (right), as a function of boosting iterations (or iterations from the second round in Twin Boosting, respectively).

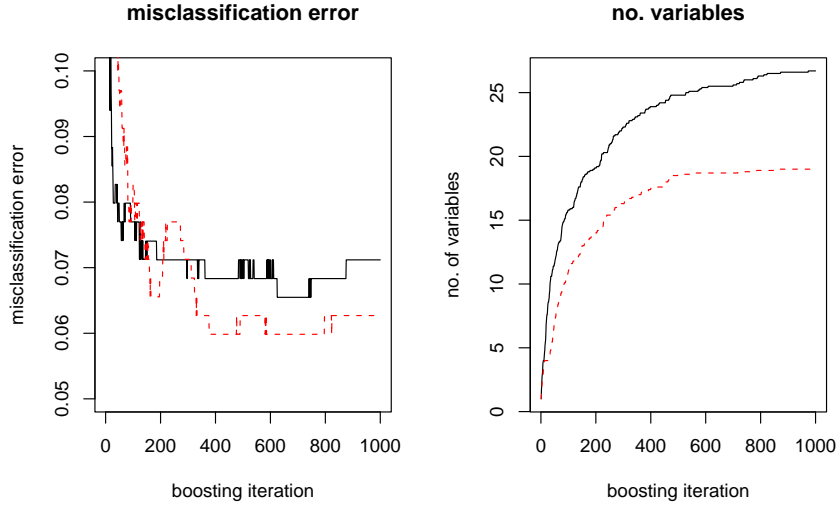


Figure 9: LogitBoosting (solid line) and corresponding Twin Boosting (dashed line) with stumps for ionosphere data. Other specifications as in Figure 7.

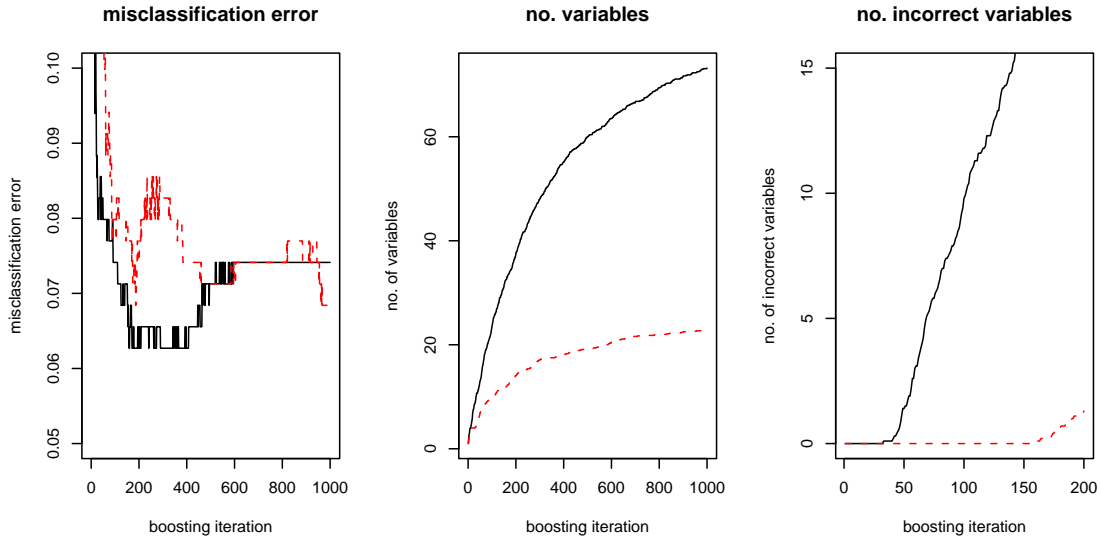


Figure 10: LogitBoosting (solid line) and corresponding Twin Boosting (dashed line) with stumps for ionosphere data with synthetically enlarged predictor space. Other specifications as in Figure 8.