Iterated Regularization for High-Dimensional Data: from Boosting to Twin Boosting

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The starting points

Regarding iterated regularization

1 tuning parameter (as in e.g. Lasso, Ridge, etc.) may not be sufficient to regularize in 1000-dimensional space

2-3 tuning parameters may be (much) better

Regarding Boosting: with a version of LogitBoost

Roman Lutz

Statistics, ETH Zurich

winner of the prediction/classification challenge

World Congress of Computational Intelligence 2006

$\rightsquigarrow$ Boosting is not an "out-dated" method

competitors were: weighted LS-SVM (S. Cawley)

Bayesian Neural Networks (R. Neal)

Random Forests (C. Dahinden)

SVM/Gaussian process classifier (W. Chu)

High-dimensional data setting

$(X_1, Y_1), \ldots, (X_n, Y_n)$ i.i.d. or stationary

X_i p-dimensional predictor variable

Y_i univariate response variable, e.g. $Y_i \in \mathbb{R}$ or $Y_i \in \{0, 1\}$

high-dimensional: $p \gg n$

areas of application: astronomy, biology, imaging, marketing research, text classification,...

sometimes n is large as well (and $p \approx n$ or $p \gg n$)
$\rightsquigarrow$ computational challenges

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Examples from molecular biology

- Microarray data
  $p \approx 5'000 - 20'000$, $n \approx 10 - 200$
- Motif finding with motif regression
  $p \approx 4'000 - 10'000$, $n \approx 4'000 - 30'000$
- Dynamic (w.r.t. time) motif regression
  $p \approx 4'000 - 10'000$ and $n \approx 40'000 - 300'000$

Boosting

AdaBoost (Freund & Schapire, 1996): ensemble method

Breiman (1998) has demystified boosting as a
functional gradient descent method

Aim: find $f^*(\cdot) = \text{argmin}_{f(\cdot)} \mathbb{E}[\rho(Y, f(X))]$
e.g. for $\rho(y, f) = |y - f|^2 \rightsquigarrow f^*(x) = \mathbb{E}[Y|X = x]$

FGD solution: consider empirical risk $n^{-1} \sum_{i=1}^n \rho(Y_i, f(X_i))$ and
do iterative steepest descent in function space

with the use of a base procedure (weak learner)

$$(X_1, U_1), \ldots, (X_n, U_n) \longrightarrow \hat{\theta}(\cdot) \approx \mathbb{E}[U|X = \cdot]$$

e.g. regression tree, componentwise smoothing spline, etc ...

Functional gradient descent: the concept

empirical risk functional: $C(f) = n^{-1} \sum_{i=1}^{n} \rho(Y_i, f(X_i))$
inner product: $\langle f, g \rangle = n^{-1} \sum_{i=1}^{n} f(X_i) g(X_i)$

rough idea:

1. Initialize $\hat{f}_0(\cdot)$; then, for $m = 1, 2, \ldots m_{stop}$:
2. Calculate negative gradient (negative Gateaux derivative):

$$-dC(f)(x) = \frac{\partial}{\partial \alpha} - C(f + \alpha 1_x)|_{\alpha=0}$$

Approximate

$$-dC(\hat{f}_{m-1})(\cdot) \text{ by base procedure fit } \hat{\theta}_m(\cdot)$$

3. Up-date

$$\hat{f}_m(\cdot) = \hat{f}_{m-1}(\cdot) + \underbrace{\nu}_{\text{step-length}} \cdot \hat{\theta}_m(\cdot)$$

Computational implementation: Generic FGD algorithm

Step 1. $\hat{f}_0 \equiv 0$ (or $\equiv \overline{Y}$); set $m = 0$.

Step 2. Increase m by 1. Compute negative gradient $-\frac{\partial}{\partial f}\rho(Y, f)$ and evaluate at $f = \hat{f}_{m-1}(X_i) = U_i$ $(i = 1, \ldots, n)$

Step 3. Fit negative gradient vector $U_1, \ldots, U_n$ by base proced.

$$(X_i, U_i)_{i=1}^n \xrightarrow{\text{base proced.}} \hat{\theta}_m(\cdot)$$

i.e. $\hat{\theta}_m(\cdot)$ is an approximation of the negative gradient vector

Step 4. Up-date $\hat{f}_m(\cdot) = \hat{f}_{m-1}(\cdot) + \nu \cdot \hat{\theta}_m(\cdot)$
$(0 < \nu \leq 1$ step-length)
i.e: proceed along an estimate of the negative gradient vector

Step 5. Iterate Steps 2-4 until $m = m_{stop}$

ν small will be good, e.g. $\nu = 0.1$

L_2Boosting (Friedman, 2001; PB & Yu, 2003)

loss function $\rho(y, f) = |y - f|^2$
population minimizer: $f^*(x) = \mathbb{E}[Y|X = x]$
FGD with base procedure $\hat{\theta}(\cdot)$: repeated fitting of residuals

$$
\begin{aligned}
m = 1: \ & (X_i, Y_i)_{i=1}^n \rightsquigarrow \hat{\theta}_1(\cdot), \ \hat{f}_1 = \nu\hat{\theta}_1 && \rightsquigarrow \text{ resid. } U_i = Y_i - \hat{f}_1(X_i) \\
m = 2: \ & (X_i, U_i)_{i=1}^n \rightsquigarrow \hat{\theta}_2(\cdot), \ \hat{f}_2 = \hat{f}_1 + \nu\hat{\theta}_2 && \rightsquigarrow \text{ resid. } U_i = Y_i - \hat{f}_2(X_i) \\
& \ldots && \ldots
\end{aligned}
$$

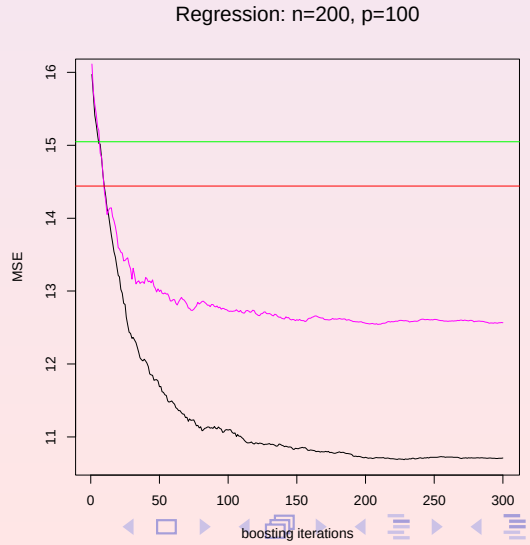
$$\hat{f}_{m_{stop}}(\cdot) = \nu \sum_{m=1}^{m_{stop}} \hat{\theta}_m(\cdot) \quad \text{(greedy fitting of residuals)}$$

Tukey (1977): twicing for $m_{stop} = 2$ and $\nu = 1$

any gain over classical methods?

- not at all if n/p is reasonable

- substantial gain if n/p is small



Componentwise linear least squares base procedure

linear ordinary least squares against the one predictor variable which reduces RSS most

$$\hat{\theta}(x) = \hat{\beta}_{\hat{S}} x^{(\hat{S})}, \ \hat{\beta}_j = \sum_{i=1}^n Y_i X_i^{(j)} / \sum_{i=1}^n (X_i^{(j)})^2, \ \ \hat{S} = \text{argmin}_j \sum_{i=1}^n (Y_i - \hat{\beta}_j X_i^{(j)})^2$$

first round: selected predictor variable $X^{(\hat{S}_1)}$ (e.g. $= X^{(3)}$)
corresponding $\hat{\beta}_{\hat{S}_1} \rightsquigarrow$ fitted function $\hat{f}_1(x)$

2nd round: selected predictor variable $X^{(\hat{S}_2)}$ (e.g.$= X^{(21)}$)
corresponding $\hat{\beta}_{\hat{S}_2} \rightsquigarrow$ fitted function $\hat{f}_2(x)$

etc.

L_2Boosting: $\hat{f}_m(x) = \hat{f}_{m-1}(x) + \nu \cdot \hat{\theta}(x)$
$\rightsquigarrow$ linear model fit, including variable selection

i.e. a structured model fit

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for $\nu = 1$, this is known as
Matching Pursuit (Mallat and Zhang, 1993)
Weak greedy algorithm (deVore & Temlyakov, 1997)
a version of Boosting (Schapire, 1992; Freund & Schapire, 1996)

Gauss-Southwell algorithm

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Binary lymph node classification using gene expressions:
a high noise problem
$n = 49$ samples, $p = 7129$ gene expressions

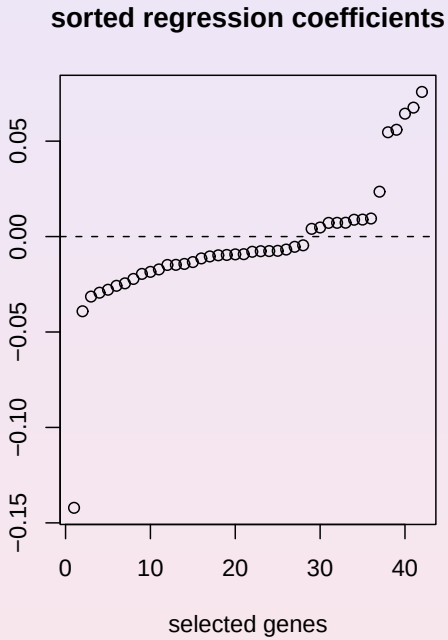
cross-validated misclassification error (2/3 training; 1/3 test)

Lasso	L_2Boosting	FPLR	Pelora	1-NN	DLDA	SVM
21.1%	17.7%	35.25%	27.8%	43.25%	36.12%	36.88%

multivariate gene selection

best 200 genes (Wilcoxon test)
no additional gene selection

42 (out of 7129) selected genes ($n = 49$) and gene importance



identifiability problem: strong correlations among some genes

$\rightsquigarrow$ consider groups of highly correlated genes
biological categories (e.g. GO ontology), ...

Connections to Lasso (for linear models):
Efron, Hastie, Johnstone, Tibshirani (2004): for special design matrices,

iterations of L_2Boosting with "infinitesimally" small ν
yield all Lasso solutions when varying λ

Zhao and Yu (2005): for general design matrices,
when adding some backward steps
the solutions from Lasso and modified Boosting "coincide"

greedy (plus backward steps) and convex optimization are surprisingly similar

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Consistency for high dimensions: an analysis of an algorithm

$$Y_i = \beta_0 + \sum_{j=1}^{p} \beta_j X_i^{(j)} + \epsilon_i \ (i = 1, \ldots, n), \quad p \gg n$$

Theorem (PB, 2006)

L_2Boosting with comp. linear LS is consistent (with suitable number of boosting iterations) if:

- $p_n = O(\exp(Cn^{1-\xi}))$ $(0 < \xi < 1)$ (high-dimensional)
  essentially exponentially many variables relative to n
- $\sup_n \sum_{j=1}^{p_n} |\beta_{j,n}| < \infty$ ℓ^1-sparseness of true function

i.e. for suitable, slowly growing $m = m_n$:

$$\mathbb{E}_X |\hat{f}_{m_n,n}(X) - f_n(X)|^2 = o_P(1) \ (n \to \infty)$$

"no" assumptions about the predictor variables/design matrix

(similar result for Lasso: Greenshtein & Ritov (2004))

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population version: $\langle f, g \rangle = \int f(x) g(x) dP(x)$

$g_j(x) = x^{(j)}, \quad \|g_j\| = 1$

$R_0 f = f$

$R_m f = R_{m-1} f - \langle R_{m-1} f, g_{\hat{S}_m} \rangle g_{\hat{S}_m}, \quad m = 1, 2, \ldots$

$\hat{S}_m = \text{argmax}_j |\langle R_{m-1} f, g_j \rangle|$

$$\begin{aligned} \|R_m f\|^2 &= \|f - \sum_{k=1}^{m} \gamma_k g_{\hat{S}_k}\|^2 \\ &= \|R_{m-1} f\|^2 - |\langle R_{m-1} f, g_{\hat{S}_m} \rangle|^2 \quad \searrow \end{aligned}$$

- $\searrow 0$?
- uniform bound ?

Temlyakov (2000):
$\leq \|\beta\|_1 m^{-1/6}$

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linear model $\rightsquigarrow$ “prototype”-result

the methodology (and some of theory) is much more general

Other loss functions for boosting: beyond regression

for binary classification with $Y \in \{0, 1\}$:
$\rho(y, f) = \log_2(1 + \exp(-(2 \cdot y - 1)f))$
negative binomial log-likelihood
population minimizer: $f^*(x) = \frac{1}{2} \log(\frac{p(x)}{1-p(x)})$
$\rightsquigarrow$ can estimate probabilities $p(\cdot)$ from estimate $\hat{f}(\cdot)$

this is LogitBoost (Friedman, Hastie and Tibshirani, 2000)

for count data with $Y \in \{0, 1, 2, \ldots\}$:
$\rho(y, f) = \exp(f) - yf$
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for survival data with $Y \in \mathbb{R}^+$:
$\rho(y, f)$ from Cox's partial likelihood

etc...

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Computation

computation for general loss functions involves a
trivial extension only!
very different for LARS-type path-following algorithms for Lasso

instead of residuals in L_2Boosting

$$U_i = Y_i - \hat{f}_{m-1}(X_i),\ i = 1, \ldots, n$$

we use "generalized residuals"

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

since there is (usually) a closed form, simple expression of the partial derivative
$\rightsquigarrow$ same computational cost as for L_2Boosting

The mboost package in R (Hothorn & PB, 2006)

for various boosting algorithms and corresponding model fitting

- easy to use and coherent implementation for
  - regression
  - classification
  - Poisson regression
  - survival analysis with Cox's partial likelihood
  - your own loss function
- allows for various base procedures
  - componentwise linear least squares
  - componentwise smoothing splines
  - trees
- computationally very fast for high-dimensional generalized linear models

CPU time

Binary lymph node classification example: $p = 7129$, $n = 49$
with L_2Boosting or BinomialBoosting (LogitBoost)
for large range of solutions

it's less than a second!

0.906 seconds using `mboost` in `R` (Hothorn & PB, 2006)

in comparison:
for linear models, computing Lasso solutions for all λ's

2.603 seconds using `lars` in `R` (with `use.gram=F`)

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because it is so fast

$\rightsquigarrow$ local modeling over different inhomogeneous but related sub-populations ("borrowing strength from neighborhood")

$$\beta(t) \approx \beta(\text{neighb.}(t))$$

Motif detection using DNA sequence and gene expression data

(Meier, Liu, Liu & PB; work in progress)

$p = 4'312$, $n = 79'974$ from 18 sub-populations

Can we easily improve?

maybe (?) not that much with respect to prediction but often substantially with respect to variable/feature selection

approach for variable selection with Boosting:
variables which have been selected by the base procedure in the process of boosting

e.g. in a (generalized) linear model fit:
variables with corresponding regression coefficient $\neq 0$

$\rightsquigarrow$ no significance testing involved

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Building on the analogy with the Lasso

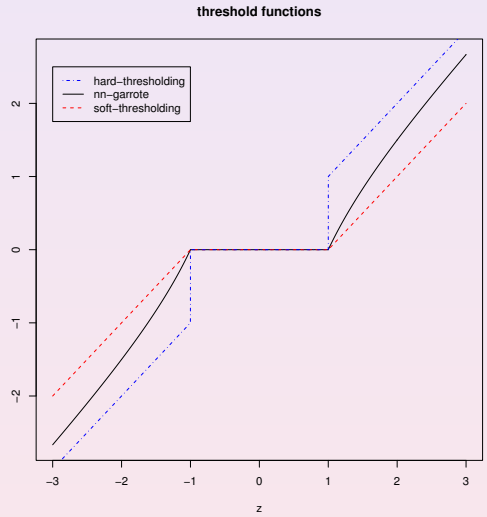
Meinshausen & PB (2006):
for linear models

- Lasso is consistent for variable selection, even for $p \gg n$, if the design matrix is not "too correlated"
  $P[\text{selected model} = \text{ true model}] \underbrace{\to 0}_{\text{quickly}} \quad (n \to \infty)$
- if the design is "too correlated"
  $\rightsquigarrow$ Lasso is inconsistent for variable selection

see also Zou (2006), Zhao and Yu (2006)

The “reason”

too much bias (or shrinkage), even for large values



Bias in soft-thresholding
is disturbing (at least sometimes)

better:
Nonnegative Garrote (Breiman, 1995)
and similar proposals

Twin Boosting (PB, 2006): Boosting-type answer addressing the problem of bias

is different from Sparse Boosting (PB & Yu, 2006)
but much more general and computationally much faster

Rough idea of Twin Boosting

- first round of boosting as usual: first twin
- second round of boosting which is forced to resemble the first round: second twin
- final estimate from the second round

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Rough idea of Twin Boosting

- first round of boosting as usual: first twin
- second round of boosting which is forced to resemble the first round: second twin
- final estimate from the second round

Twin L_2Boosting for linear models

recap: L_2Boosting with componentwise linear least squares

chooses variable j which reduces RSS most

$$\Leftrightarrow \quad |n^{-1}\sum_{i=1}^{n} U_i X_i^{(j)}| = |\widehat{\mathrm{Cor}}(U, X^{(j)})| \text{ maximal w.r.t. } j$$

if predictor variables are standardized

first round: boosting estimate $\hat{\beta}_{init}$ from L_2Boosting

second round: as L_2Boosting but selecting variable using

$$|n^{-1}\sum_{i=1}^{n} U_i X_i^{(j)}| \cdot |\hat{\beta}_{init,j}| \text{ maximal w.r.t. } j$$

final estimate from second round, "pulled toward" initial estim.

$\rightsquigarrow$ very easy and computationally efficient modification

Twin Boosting = iterated regularization

(we first tune round 1;
and fixing the tuning from round 1, we then tune round 2)

PB (2006):
for orthogonal linear models, as step-size factor $\nu \to 0$

Twin L_2Boosting and Adaptive Lasso coincide
(with β_{init} = estimate from first round of boosting)

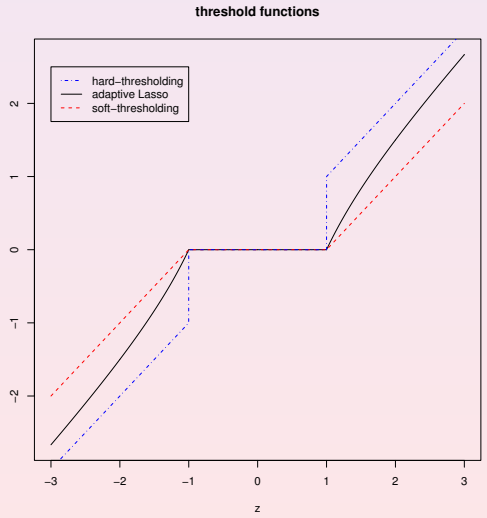
and Twin Boosting extends to very general settings

Adaptive Lasso (Zou, 2006)

$$\hat{\beta} = \text{argmin}_\beta \sum_{i=1}^{n} (Y_i - (X\beta)_i)^2 + \lambda \sum_{j=1}^{p} \frac{|\beta_j|}{\underbrace{|\beta_{init,j}|}_{\text{e.g. OLS if } p < n}}$$

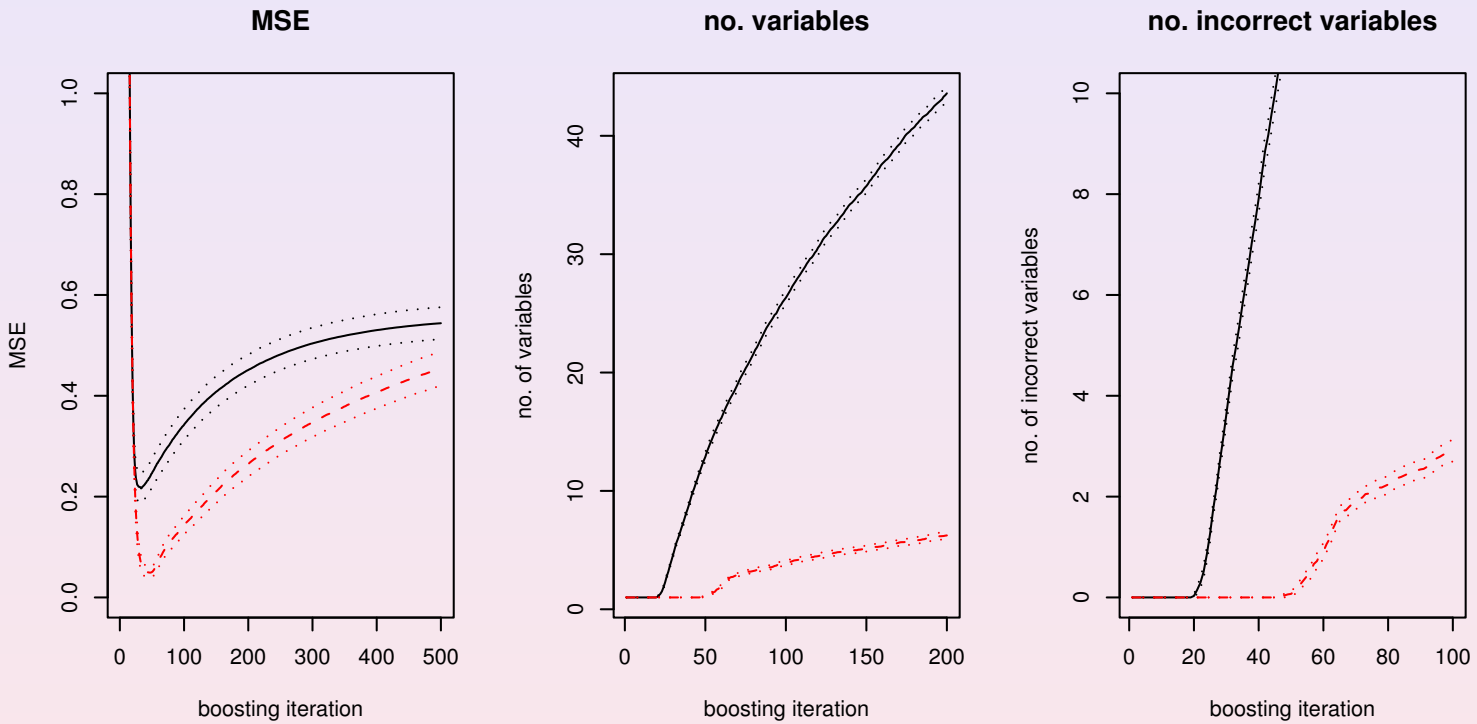
nice result (Zou, 2006):
adaptive Lasso is consistent for variable selection "in general"
(proof for low-dimensional problems only)

for orthogonal design
if β_{init} = OLS,
Adaptive Lasso = NN-garrote



Simulated example: n = 50, p=500

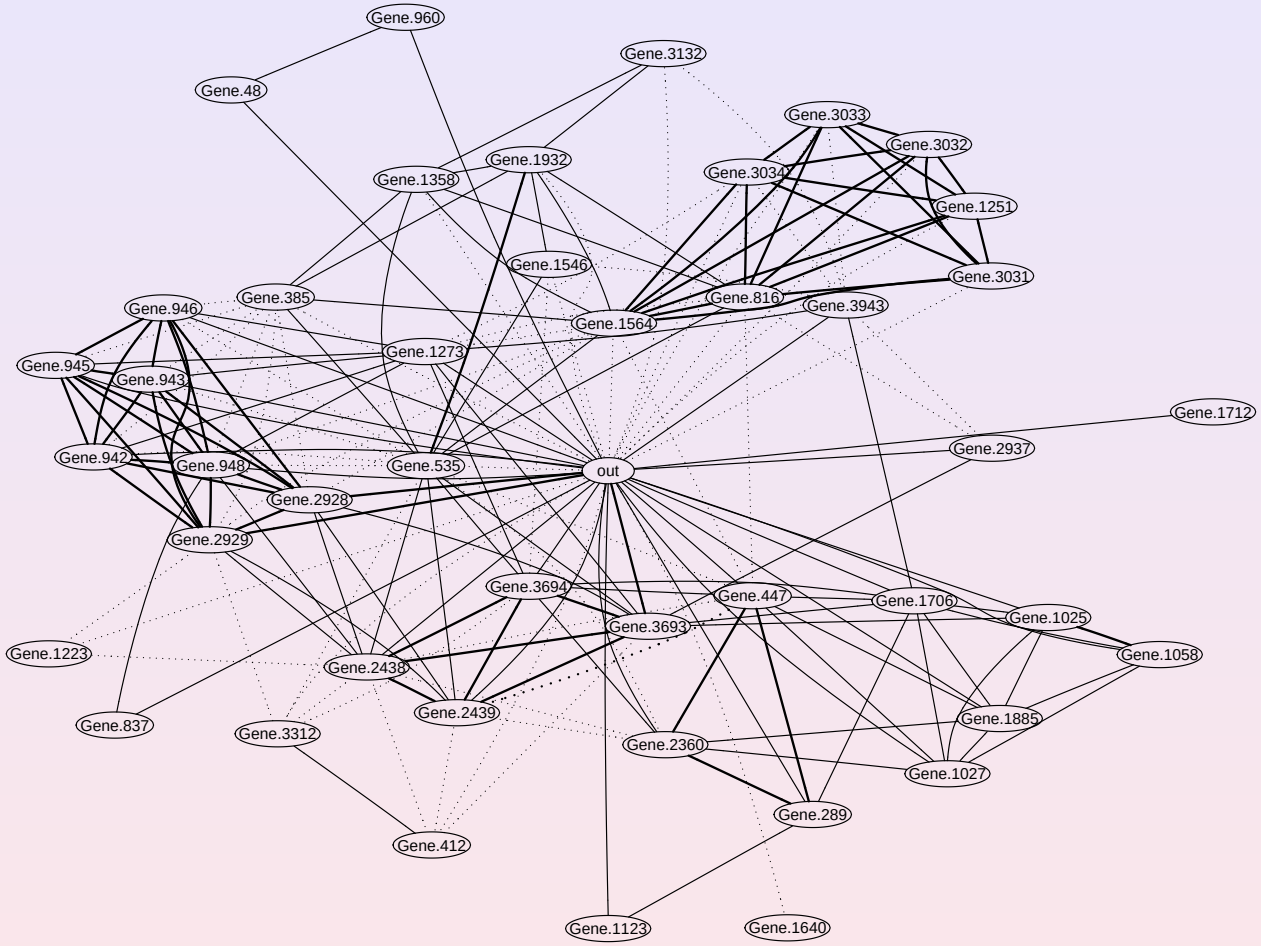
$$Y = \sum_{j=1}^{500} \beta_j X^{(j)} + \varepsilon, \ \beta_1 = 5, \beta_j = 0 \ (j = 2, \ldots, 500)$$



black: L_2Boosting red: Twin L_2Boosting

Twin L_2Boosting: more sparse and better variable selection than boosting

Response Y versus $p = 4088$ gene expressions in Bacillus Subtilis



neighbours of Y (selected genes) and their conditional dependencies n=115, p=4088

Boosting with regression tree base procedure
very popular in machine learning

trees can be very useful because:

- they can easily handle missing data
- they can easily deal with mixed categorical, ordinal, continuous data
- they are invariant under monotone covariate-transformations

Twin L_2Boosting for trees

first round: boosting estimate $\hat{f}_{init}$

second round: as boosting but select in each iteration the best tree $\hat{g}(\cdot)$ which reduces RSS and "resembles" $\hat{f}_{init}$

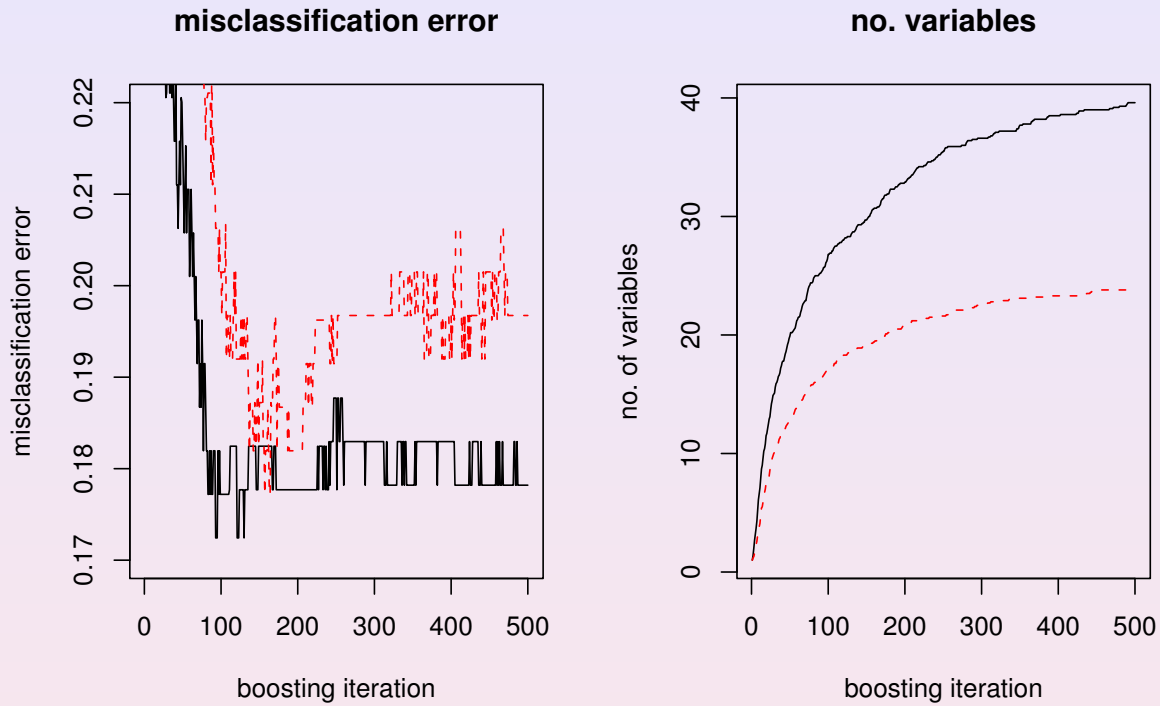
$$\underbrace{C^2(\hat{g})}_{\widehat{Cor}^2(\hat{g},\hat{f}_{init})} \cdot \underbrace{\left(2\sum_{i=1}^{n} U_i \hat{g}(X_i) - \sum_{i=1}^{n} \hat{g}(X_i)^2\right)}_{\text{"penalized correlation"}} \text{ is maximized w.r.t. } \hat{g}$$

in case of componentwise least squares and uncorrelated design

$$\propto |\hat{\beta}_{init,j}|^2 \cdot |\widehat{Cor}(U, X^{(j)})|^2$$

$\rightsquigarrow$ concept easily extends to other loss functions (e.g. classification)

Sonar data: binary classification with n=208, p = 60

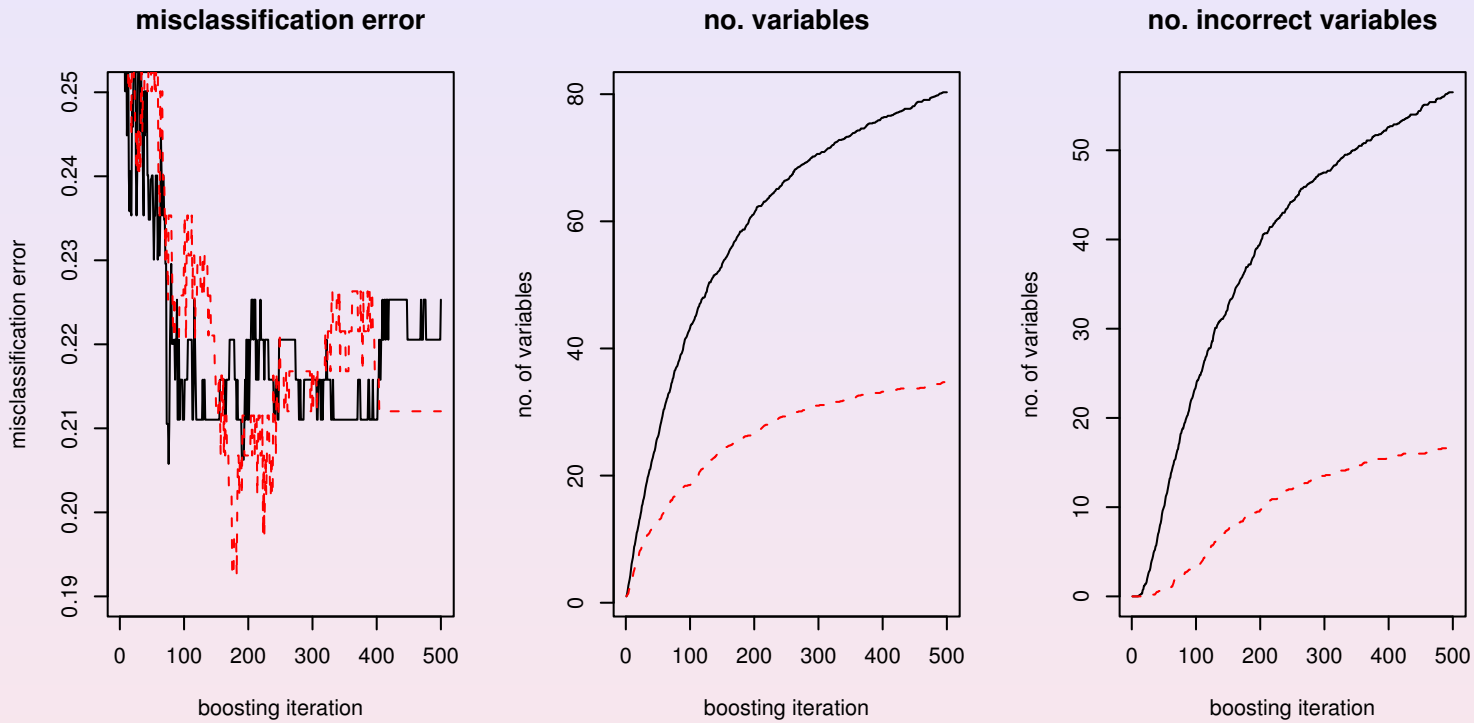


black: BinomialBoosting red: Twin BinomialBoosting

Twin Boosting: more sparse than boosting

with synthetically enlarged predictor space

adding 500 $\mathcal{N}(0,1)$-distributed ineffective predictor variables



black: BinomialBoosting red: Twin BinomialBoosting

$\rightsquigarrow$ improved variable selection with Twin Boosting

Conclusions

Boosting

- is mainly useful for high-dimensional and/or large datasets
- is computationally very efficient
- is very competitive for prediction

- Twin Boosting (e.g. iterated regularization) improves upon
  - variable selection
  - assigning variable importance in structured models (linear, additive, interaction)