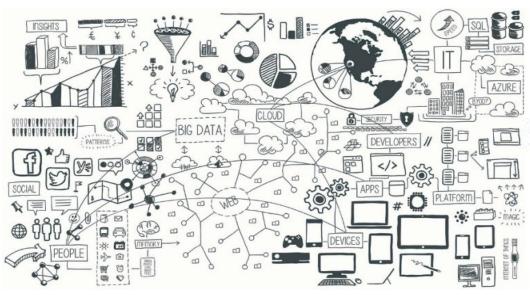
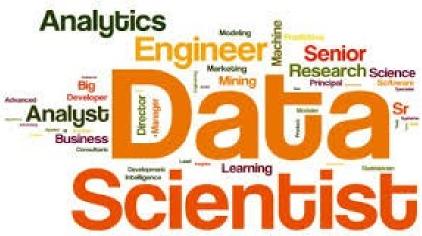
Data Mining (Minería de Datos)

Ensembles: Gradient Boosting





Sixto Herrera

Grupo de Meteorología

Univ. de Cantabria – CSIC MACC / IFCA



Master Universitario Oficial Data Science

con el apoyo del

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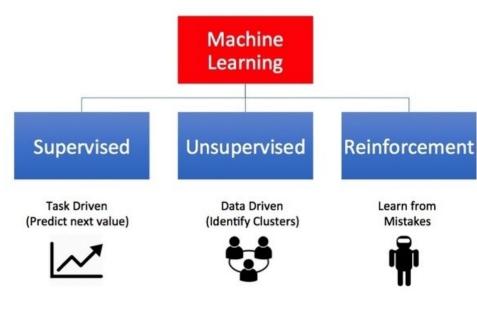
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Ensembles: Gradient Boosting

Types of Machine Learning



NOTA: Las líneas de código de R en esta presentación se muestran sobre un fondo gris.

Master Universitario Oficial Data Science **Ensembles:** con el apoyo del **Gradient Boosting** CSIC

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Reglas de asociación

Practica: Reglas de asociación

Árboles de clasificacion y decision

Practica: Árboles de clasificación

Técnicas de vecinos cercano (k-NN)

Practica: Crossvalidacion

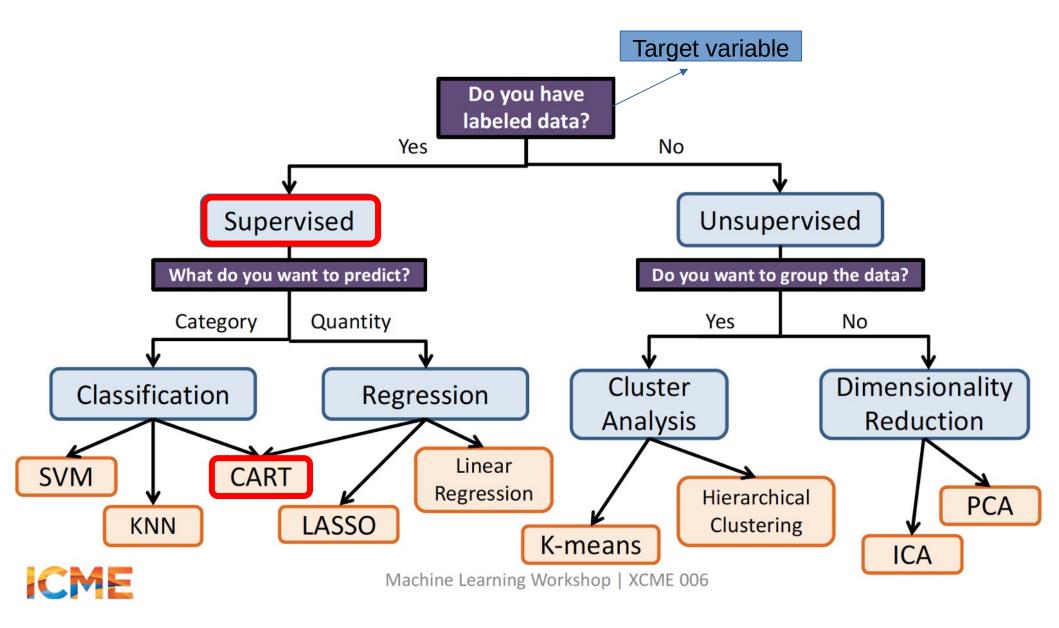
T01. Datos discretos

Evaluación, sobrejuste y crossvalidacion

	Práctica: Vecinos cercanos
	Comparación de Técnicas de Clasificación.
	Reducción de dimensión no lineal
	T02. Clasificación
	Árboles de clasificación y regresion (CART)
	Práctica: Árboles de clasificación y regresion (CART)
	Practica: El paquete CARET
	T03. Prediccion
Ī	Encombles, Pagging and Pageting
	Ensembles: Bagging and Boosting
	Random Forests y Gradient boosting
	Random Forests y Gradient boosting
	Random Forests y Gradient boosting Técnicas de agrupamiento
	Random Forests y Gradient boosting Técnicas de agrupamiento Técnicas de agrupamiento
	Random Forests y Gradient boosting Técnicas de agrupamiento Técnicas de agrupamiento Predicción Condicionada
	Random Forests y Gradient boosting Técnicas de agrupamiento Técnicas de agrupamiento Predicción Condicionada

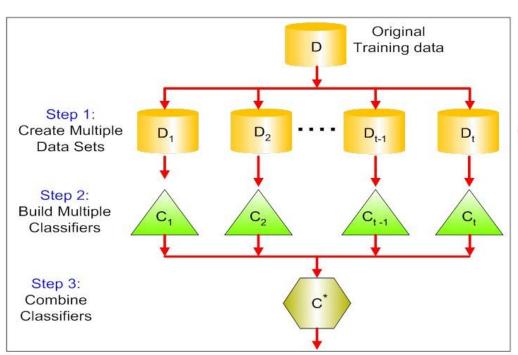
Presentación, introducción y perspectiva histórica

Paradigmas, problemas canonicos y data challenges

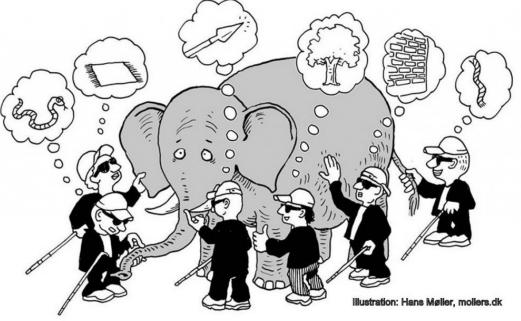




Ensemble learning is a supervised approach in which the basic idea is to generate multiple weak models on a training dataset and combining them to generate a strong model which improves the *stability* and the *performance* of the individual models.



The wisdom of the crowd



Fable of blind men and elephant
https://en.wikipedia.org/wiki/Blind men and an elephant







Ensemble approaches are typically used with CART.

Pros

Trees are very easy to explain (even easier than linear regression) Trees can be plotted graphically, and are easily interpreted Trees can easily handle qualitative predictors They work fine on both classification and regression problems

Cons

Poor prediction accuracy (compared with other approaches) Instability when changing the train/test partition (cross-validation is key)

By aggregating many trees, the instability of the trees can be reduced and their predictive performance substantially improved.





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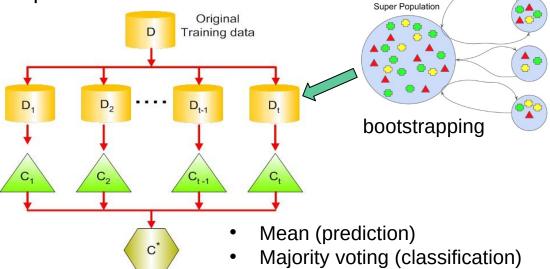
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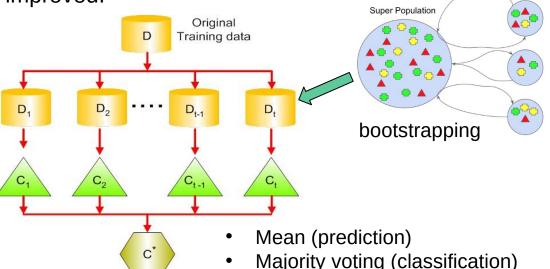
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Weak learners

Low bias and high variance



High degree of freedom models e.g. fully developed trees

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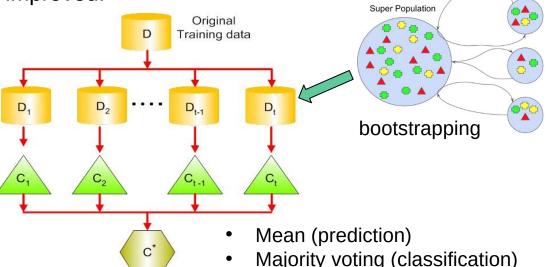
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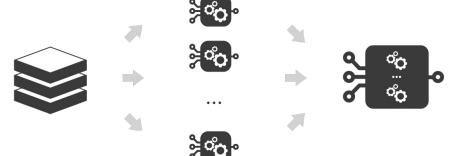
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Heterogenous Weak Learners

Stacking considers heterogeneous weak learners, learns them in parallel and combines them by training a meta-model to output a prediction based on the different weak models predictions.

initial dataset

L weak learners (that can be non-homogeneous)

meta-model
(trained to output predictions based on weak learners predictions)

https://stats.stackexchange.com/questions/290701/how-to-stack-machine-learning-models-ii

nttps://towardsdatascience.com/ensemble-methods-bagging-boosting-and-stackīng-c9214a10a20



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Bagging and Boosting

Homogenous Weak Learners



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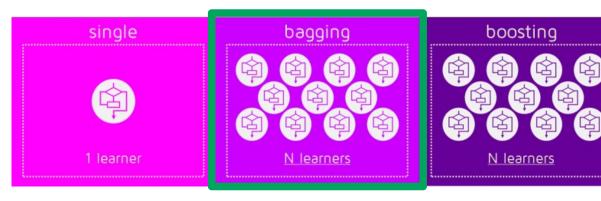
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High degree of freedom models e.g. fully developed trees



Random Forests

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VERSIDAD Universidad Internacion Menéndez Pelayo



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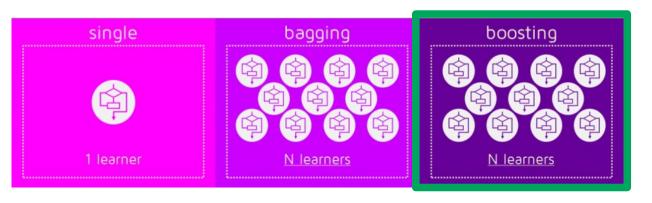
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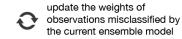
AdaBoost: Adaptive Boosting

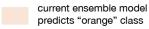


Adaptative Boosting (AdaBoost)



train a weak model and aggregate it to the ensemble model

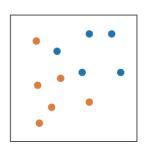


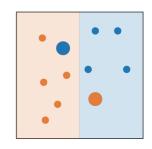


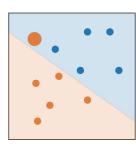
current ensemble model predicts "blue" class

Step 1: All the observations have the **same weights**























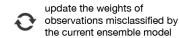


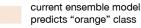


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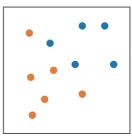


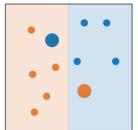


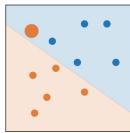
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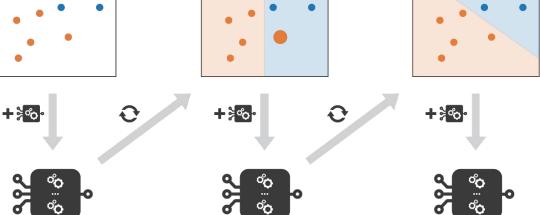








- a) Fit the weak model considering the observations weights.
- b) Evaluate the weak learner to obtain its coefficient.
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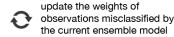


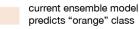


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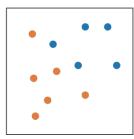


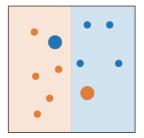


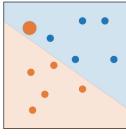
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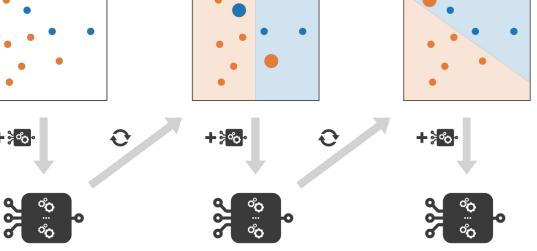








- a) Fit the weak model considering the observations weights.
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Result: A strong learner is obtained as a simple linear combination of weak learners weighted by coefficients expressing the performance of each learner. Variants of this algorithm could be obtained by modifying the loss function (e.g. logit for classification or L2 for regression).

$$s_L(.) = \sum_{l=1}^{L} c_l \times w_l(.) \qquad \text{where } c_l \text{'s are coefficients and } w_l \text{'s are weak learners}$$

$$(c_l, w_l(.)) = \underset{c, w(.)}{\operatorname{arg \, min}} E(s_{l-1}(.) + c \times w(.)) = \underset{c, w(.)}{\operatorname{arg \, min}} \sum_{n=1}^{N} e(y_n, s_{l-1}(x_n) + c \times w(x_n))$$







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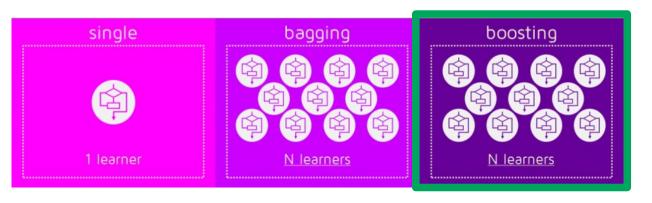
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Homogenous Weak Learners

High bias and low variance



Low degree if freedom models e.g. low depth trees



Gradient Descent Boosting





Gradient Boosting

train a weak model and aggregate it to

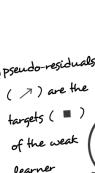


update the pseudo-residuals considering predictions of

- dataset values
- predictions of the current ensemble model
- pseudo-residuals (targets of the weak learner)

Gradient boosting casts the problem into a gradient descent one: at each iteration we fit a weak learner to the opposite of the pseudo-residuals gradient of the current fitting () are the error with respect to the

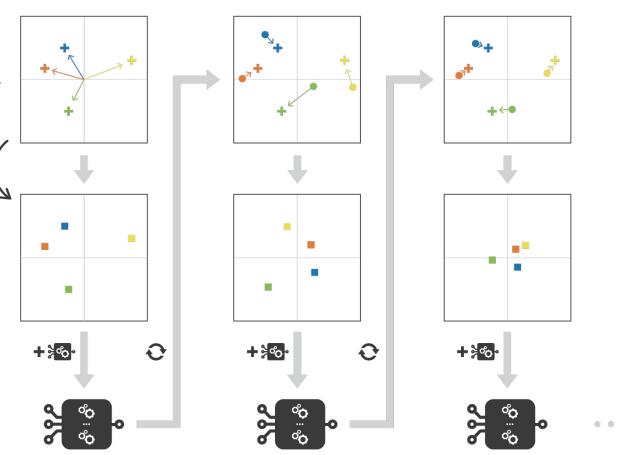
current ensemble model.



$$s_l(.) = s_{l-1}(.) - c_l \times \nabla_{s_{l-1}} E(s_{l-1})(.)$$

Pseudo-residuals:

$$-\nabla_{s_{l-1}}E(s_{l-1})(.)$$



$$s_L(.) = \sum_{l=1}^L c_l imes w_l(.)$$

where c_l 's are coefficients and w_l 's are weak learners

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Ensembles: Gradient Boosting

Introduction

Gradient Boosting



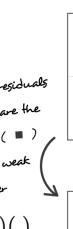
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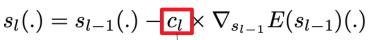


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Pseudo-residuals:

$$-\nabla_{s_{l-1}}E(s_{l-1})(.)$$

Step size: how much we update the ensemble model in the direction of the new weak learner

$$s_L(.) = \sum_{l=1}^{L} c_l \times w_l(.)$$

where c_l 's are coefficients and w_l 's are weak learners

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Ensembles: Gradient Boosting

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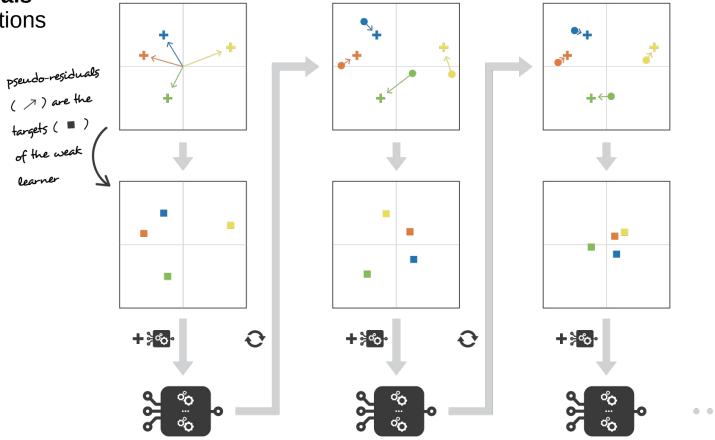
train a weak model and aggregate it to the ensemble mode

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update the pseudo-residuals considering predictions of the current ensemble model

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Step 1: The **pseudo-residuals** are set equal to the observations



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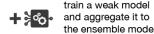
Master Universitario Oficial Data Science







Gradient Boosting



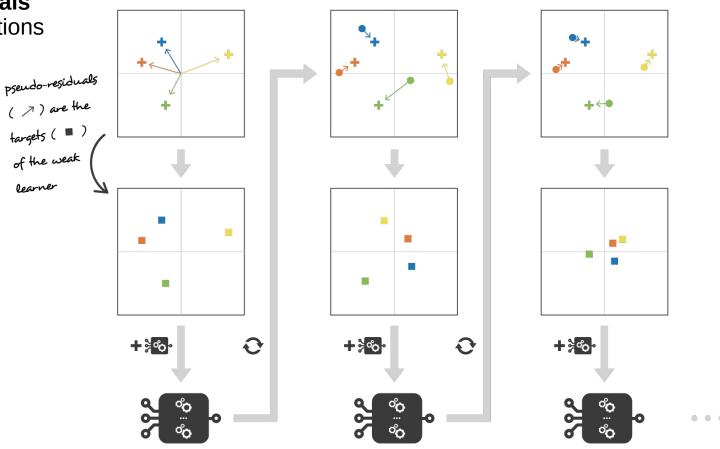


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- d) Update the pseudoresiduals



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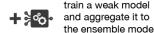
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Gradient Boosting



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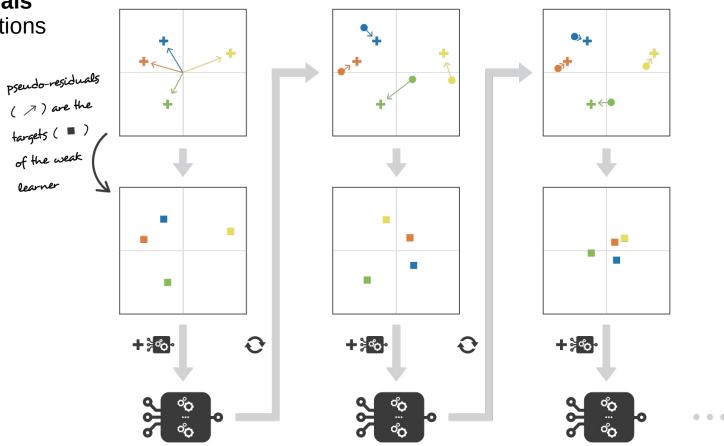
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Repeat (1:L):

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https://www.kdnuggets.com/2018/07/intuitive-ensemble-learning-guide-gradient-boosting.html

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Adaptative vs Gradient Descent Boosting Approaches

Adaptative Boosting (AdaBoost)

Step 1: All the observations have the **same** weights

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$$(c_l, w_l(.)) = \underset{c, w(.)}{\operatorname{arg\,min}} E(s_{l-1}(.) + c \times w(.))$$

$$\underset{c,w(.)}{\arg\min} \sum_{n=1}^{N} e(y_n, s_{l-1}(x_n) + c \times w(x_n))$$

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where c_l 's are coefficients and w_l 's are weak learners

Gradient Boosting

Gradient boosting casts the problem into a gradient descent one: at each iteration we fit a weak learner to the opposite of the gradient of the current fitting error with respect to the current ensemble model.

$$s_l(.) = s_{l-1}(.) - c_l \times \nabla_{s_{l-1}} E(s_{l-1})(.)$$

Pseudo-residuals: $-\nabla_{s_{l-1}}E(s_{l-1})(.)$

Step 1: The **pseudo-residuals** are set equal to the observations

Repeat (1:L):

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Adaptative vs Gradient Descent Boosting Approaches

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$$(c_l, w_l(.)) = \arg \min E(s_{l-1}(.) + c \times w(.))$$

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Gradient boosting casts the problem into a gradient descent one: at each iteration we fit a weak learner to the opposite of the gradient of the current fitting error with respect to the current ensemble model.

$$s_l(.) = s_{l-1}(.) - c_l \times \nabla_{s_{l-1}} E(s_{l-1})(.)$$

Pseudo-residuals: $-\nabla_{s_{l-1}}E(s_{l-1})(.)$

Step 1: The **pseudo-residuals** are set equal to the observations

Repeat (1:L):

- a) Fit the weak learner to pseudo-residuals.
- b) Compute the optimal step size of the weak learner.

Notice that, while adaptative boosting tries to solve at each iteration exactly the "local" optimisation problem (find the best weak learner and its coefficient to add to the strong model), gradient boosting uses instead a gradient descent approach and can more easily be adapted to large number of loss functions. Thus, gradient boosting can be considered as a generalization of adaboost to arbitrary differentiable loss functions.





Adaptative vs Gradient Descent Boosting Approaches

Adaptative Boosting

boosting {adabag}

R Documentation

Applies the AdaBoost.M1 and SAMME algorithms to a data set

Description

Fits the AdaBoost.M1 (Freund and Schapire, 1996) and SAMME (Zhu et al., 2009) algorithms using classification trees as single classifiers.

Usage

boosting(formula, data, boos = TRUE, mfinal = 100, coeflearn = 'Breiman', control....)

Arguments

formula a formula, as in the lm function.

data a data frame in which to interpret the variables named in formula.

boos if TRUE (by default), a bootstrap sample of the training set is drawn using the

weights for each observation on that iteration. If FALSE, every observation is

used with its weights.

mfinal an integer, the number of iterations for which boosting is run or the number of

trees to use. Defaults to mfinal=100 iterations.

if 'Breiman'(by default), alpha=1/2ln((1-err)/err) is used. If 'Freund' coeflearn

alpha=ln((1-err)/err) is used. In both cases the AdaBoost.M1 algorithm is used and alpha is the weight updating coefficient. On the other hand, if coeflearn is 'Zhu' the SAMME algorithm is implemented with alpha=ln((1-

err)/err)+ln(nclasses-1).

control options that control details of the rpart algorithm. See rpart.control for more

details.

further arguments passed to or from other methods.

Details

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Ensembles: Gradient Boosting

Gradient Boosting

R: Generalized Boosted Regression Modeling (GBM) • Find in Topic

gbm {gbm}

R Documentation

Generalized Boosted Regression Modeling (GBM)

Description

Fits generalized boosted regression models. For technical details, see the vignette: utils::browseVignettes("qbm").

Usage

gbm(formula = formula(data), distribution = "bernoulli", data = list(), weights, var.monotone = NULL, n.trees = 100, interaction.depth = 1, n.minobsinnode = 10, shrinkage = 0.1, bag.fraction = 0.5, train.fraction = 1, cv.folds = 0, keep.data = TRUE, verbose = FALSE, class.stratify.cv = NULL, n.cores = NULL)

Arguments

formula

*'*E

)(

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tiı

A symbolic description of the model to be fit. The formula may include an offset term (e.g. $y \sim offset(n) + x$). If keep.data = FALSE in the initial call to qbm then it is the user's responsibility to resupply the offset to gbm.more.

distribution

Either a character string specifying the name of the distribution to use or a list with a component name specifying the distribution and any additional parameters needed. If not specified, gbm will try to guess: if the response has only 2 unique values, bernoulli is assumed; otherwise, if the response is a factor, multinomial is assumed;

otherwise, if the response has class "Surv", coxph is assumed:

otherwise, gaussian is assumed.

Currently available options are "gaussian" (squared error), "laplace" (absolute loss), "tdist" (t-distribution loss), "bernoulli" (logistic regression for 0-1 outcomes), "huberized" (huberized hinge loss for 0-1 outcomes), classes), "adaboost" (the AdaBoost exponential loss for 0-1 outcomes), "poisson" (count outcomes), "coxph" (right censored observations), "quantile", or "pairwise" (ranking measure using the LambdaMart algorithm).

If quantile regression is specified, distribution must be a list of the form list(name = "quantile", alpha = 0.25) where alpha is the quantile to estimate. The current version's quantile regression method does not handle non-constant weights and will stop.

Introduction

Extensions of Gradient Descent Boosting Approache



Extreme Gradient Boosting

XGBoost: A Scalable Tree Boosting System

Tianqi Chen University of Washington tqchen@cs.washington.edu

Carlos Guestrin
University of Washington
guestrin@cs.washington.edu

https://arxiv.org/pdf/1603.02754.pdf https://github.com/dmlc/xgboost

https://xgboost.readthedocs.io/en/latest/parameter.html

Gradient Boosting

Gradient boosting casts the problem into a gradient descent one: at each iteration we fit a weak learner to the opposite of the gradient of the current fitting error with respect to the current ensemble model.

$$s_l(.) = s_{l-1}(.) - c_l \times \nabla_{s_{l-1}} E(s_{l-1})(.)$$

Pseudo-residuals: $-\nabla_{s_{l-1}}E(s_{l-1})(.)$

Step 1: The **pseudo-residuals** are set equal to the observations

Repeat (1:L):

- a) Fit the weak learner to pseudo-residuals.
- b) Compute the optimal step size of the weak learner.
- c) Update the strong learner adding the weak learner.
 - d) Update the pseudo-residuals

$$s_L(.) = \sum_{l=1}^{L} c_l \times w_l(.)$$

where c_l 's are coefficients and w_l 's are weak learners

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Ensembles: Gradient Boosting

Introduction

Extensions of Gradient Descent Boosting Approache

TensorFlow > Learn > TensorFlow Core > Tutorials

Boosted trees using Estimators

Contenido

Load the titanic dataset

Explore the data

Create feature columns and input functions

Train and evaluate the model

https://www.tensorflow.org/tutorials/estimator/boosted_trees

https://arxiv.org/pdf/1710.11555.pdf

TF Boosted Trees: A scalable TensorFlow based framework for gradient boosting

Natalia Ponomareva, Soroush Radpour, Gilbert Hendry, Salem Haykal, Thomas Colthurst, Petr Mitrichev, Alexander Grushetsky

> Google, Inc. tfbt-public@google.com

Abstract. TF Boosted Trees (TFBT) is a new open-sourced framework for the distributed training of gradient boosted trees. It is based on TensorFlow, and its distinguishing features include a novel architecture, automatic loss differentiation, layer-by-layer boosting that results in smaller ensembles and faster prediction, principled multi-class handling, and a number of regularization techniques to prevent overfitting.

Gradient Boosting

Gradient boosting casts the problem into a gradient descent one: at each iteration we fit a weak learner to the opposite of the gradient of the current fitting error with respect to the current ensemble model.

$$s_l(.) = s_{l-1}(.) - c_l \times \nabla_{s_{l-1}} E(s_{l-1})(.)$$

Pseudo-residuals: $-\nabla_{s_{l-1}}E(s_{l-1})(.)$

Step 1: The **pseudo-residuals** are set equal to the observations

Repeat (1:L):

- a) Fit the weak learner to pseudo-residuals.
- b) Compute the optimal step size of the weak learner.
- c) Update the strong learner adding the weak learner.
 - d) Update the pseudo-residuals







```
## R-Packages:
rm(list = ls())
install.packages("tree")
install.packages("randomForest")
install.packages("adabag")
install.packages("gbm")
## Loading R-Packages:
library(tree)
library(randomForest)
library(adabag)
library(qbm)
library(caret)
library(MASS)
```

```
## Accuracy (Trees):
print(sum(diag(table(pred.t.test, iris$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.t.train, iris$Species[indtrain]))) / length(indtrain))
```

```
## Train/Test partition:
set.seed(23)
n <- nrow(iris)
indtrain <- sample(1:n, round(0.75*n)) # indices for train
indtest <- setdiff(1:n, indtrain) # indices for test
```

```
## Single Tree:
t <- tree(Species ~., iris, subset = indtrain, control = tree.control(length(indtrain),
          mincut = 1, minsize = 2, mindev = 0)
## Prediction for test
pred.t.test <- predict(t, iris[indtest, ], type = "class")</pre>
## Prediction for train
pred.t.train <- predict(t, iris[indtrain, ], type = "class")</pre>
```





```
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```

```
## Accuracy (Trees):
print(sum(diag(table(pred.t.test, iris$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.t.train, iris$Species[indtrain]))) / length(indtrain))
```

Accuracy (Random Forests): print(sum(diag(table(pred.rf.test, iris\$Species[indtest]))) / length(indtest)) print(sum(diag(table(pred.rf.train, iris\$Species[indtrain]))) / length(indtrain))

```
## Train/Test partition:
set.seed(23)
n <- nrow(iris)
indtrain <- sample(1:n, round(0.75*n)) # indices for train
indtest <- setdiff(1:n, indtrain) # indices for test
```

```
## Bagging: Random Forests
rf <- randomForest(Species ~., iris, subset = indtrain, ntree = 500)
## Prediction for test
pred.rf.test <- predict(rf, iris[indtest, ])</pre>
## Prediction for train
pred.rf.train <- predict(rf, iris[indtrain, ])</pre>
```

library(MASS)





```
## R-Packages:
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## Accuracy (Trees):
print(sum(diag(table(pred.t.test, iris$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.t.train, iris$Species[indtrain]))) / length(indtrain))
```

Accuracy (Random Forests): print(sum(diag(table(pred.rf.test, iris\$Species[indtest]))) / length(indtest)) print(sum(diag(table(pred.rf.train, iris\$Species[indtrain]))) / length(indtrain))

Accuracy (AdaBoost): print(sum(diag(table(pred.ab.test\$class, iris\$Species[indtest])))/length(indtest)) print(sum(diag(table(pred.ab.train\$class, iris\$Species[indtrain])))/length(indtrain))

```
## Train/Test partition:
set.seed(23)
n <- nrow(iris)
indtrain <- sample(1:n, round(0.75*n)) # indices for train
indtest <- setdiff(1:n, indtrain) # indices for test
```

```
## Boosting: Adaptive Boosting (AdaBoost)
ab <- boosting(Species ~., iris[indtrain, ], mfinal = 20,
                control=rpart.control(minsplit = 2, minbucket = 1, cp = 0.01))
## Prediction for test
pred.ab.test <- predict(ab, iris[indtest, ])</pre>
## Prediction for train
pred.ab.train <- predict(ab, iris[indtrain, ])</pre>
```

library(MASS)





Ensembles: Gradient Boosting

Bagging: Random forest

```
## R-Packages:
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library(tree)
library(randomForest)
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library(gbm)
library(caret)
library(MASS)
```

```
## Accuracy (Trees):
```

print(sum(diag(table(pred.t.test, iris\$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.t.train, iris\$Species[indtrain]))) / length(indtrain))

Accuracy (Random Forests):

print(sum(diag(table(pred.rf.test, iris\$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.rf.train, iris\$Species[indtrain]))) / length(indtrain))

Accuracy (AdaBoost):

print(sum(diag(table(pred.ab.test\$class, iris\$Species[indtest])))/length(indtest)) print(sum(diag(table(pred.ab.train\$class, iris\$Species[indtrain])))/length(indtrain))

Accuracy (Gradient Boosting):

print(sum(diag(table(attributes(pred.gb.test)\$dimnames[[2]][apply(pred.gb.test, FUN = which.max, MARGIN = 1)], iris\$Species[indtest]))) / length(indtest)) print(sum(diag(table(attributes(pred.gb.test)\$dimnames[[2]][apply(pred.gb.train, FUN = which.max, MARGIN = 1)], iris\$Species[indtrain]))) / length(indtrain))

```
## Boosting: Gradient Boosting
```

gb <- gbm(Species~., data=iris[indtrain,], n.trees=1000, interaction.depth=20, shrinkage = 0.01)

Prediction for test

pred.gb.test <- predict(object = gb, newdata = iris[indtest,], n.trees = 1000, type = "response")

Prediction for train

pred.gb.train <- predict(object = gb, newdata = iris[indtrain,], n.trees = 1000, type = "response")

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Ensembles: Gradient Boosting

```
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library(MASS)
```

```
## Accuracy (Trees):
```

print(sum(diag(table(pred.t.test, iris\$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.t.train, iris\$Species[indtrain]))) / length(indtrain))

Accuracy (Random Forests):

print(sum(diag(table(pred.rf.test, iris\$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.rf.train, iris\$Species[indtrain]))) / length(indtrain))

Accuracy (AdaBoost):

print(sum(diag(table(pred.ab.test\$class, iris\$Species[indtest])))/length(indtest))
print(sum(diag(table(pred.ab.train\$class, iris\$Species[indtrain])))/length(indtrain))

Accuracy (Gradient Boosting):

print(sum(diag(table(attributes(pred.gb.test)\$dimnames[[2]][apply(pred.gb.test, FUN = which.max, MARGIN = 1)], iris\$Species[indtest]))) / length(indtest)) print(sum(diag(table(attributes(pred.gb.test)\$dimnames[[2]][apply(pred.gb.train, FUN = which.max, MARGIN = 1)], iris\$Species[indtrain]))) / length(indtrain))

```
## Boosting: Gradient Boosting – Tuning the parameters
```

```
gb.cv <- gbm(Species~., data=iris[indtrain, ], n.trees=1000, interaction.depth=20, shrinkage = 0.01, cv.folds = 4)
ntree_opt_cv <- gbm.perf(gb.cv, method = "cv")
ntree_opt_oob <- gbm.perf(gb.cv, method = "OOB")
print(c(ntree_opt_cv,ntree_opt_oob))
```





```
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```
## Accuracy (Trees):
print(sum(diag(table(pred.t.test, iris$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.t.train, iris$Species[indtrain]))) / length(indtrain))
```

Accuracy (Random Forests):
print(sum(diag(table(pred.rf.test, iris\$Species[indtest]))) / length(indtest))
print(sum(diag(table(pred.rf.train, iris\$Species[indtrain]))) / length(indtrain))

```
## Accuracy (AdaBoost):
print(sum(diag(table(pred.ab.test$class, iris$Species[indtest])))/length(indtest))
print(sum(diag(table(pred.ab.train$class, iris$Species[indtrain])))/length(indtrain))
```

Accuracy (Gradient Boosting):
print(sum(diag(table(attributes(pred.gb.test)\$dimnames[[2]][apply(pred.gb.test,
FUN = which.max, MARGIN = 1)], iris\$Species[indtest]))) / length(indtest))
print(sum(diag(table(attributes(pred.gb.test)\$dimnames[[2]][apply(pred.gb.train,
FUN = which.max, MARGIN = 1)], iris\$Species[indtrain]))) / length(indtrain))





