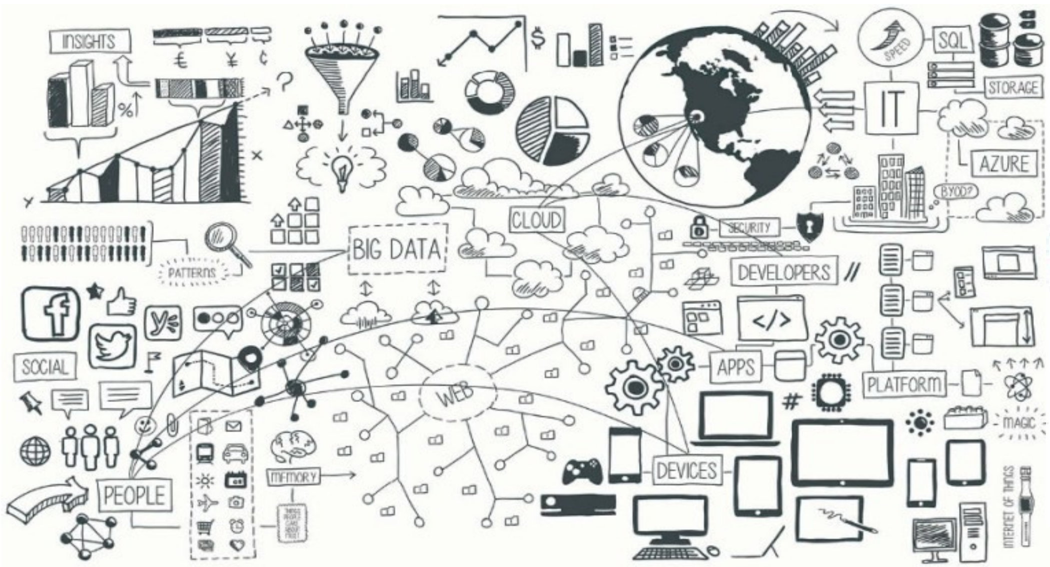
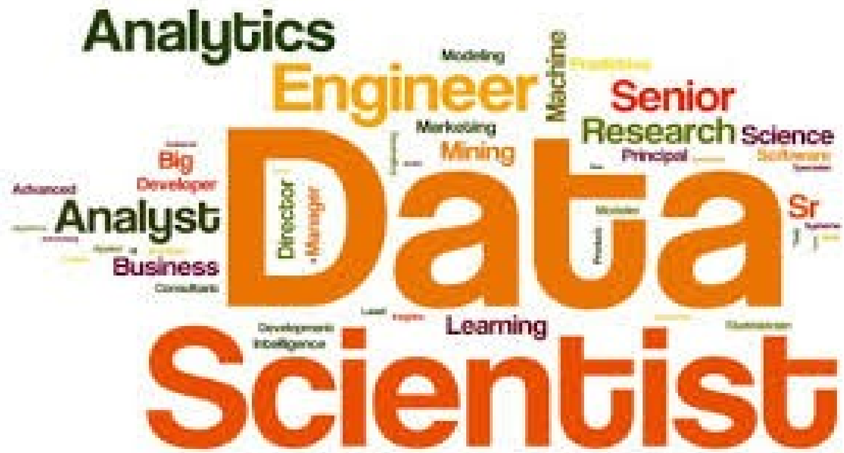
Data Mining (Minería de Datos)

Ensembles: Gradient Boosting





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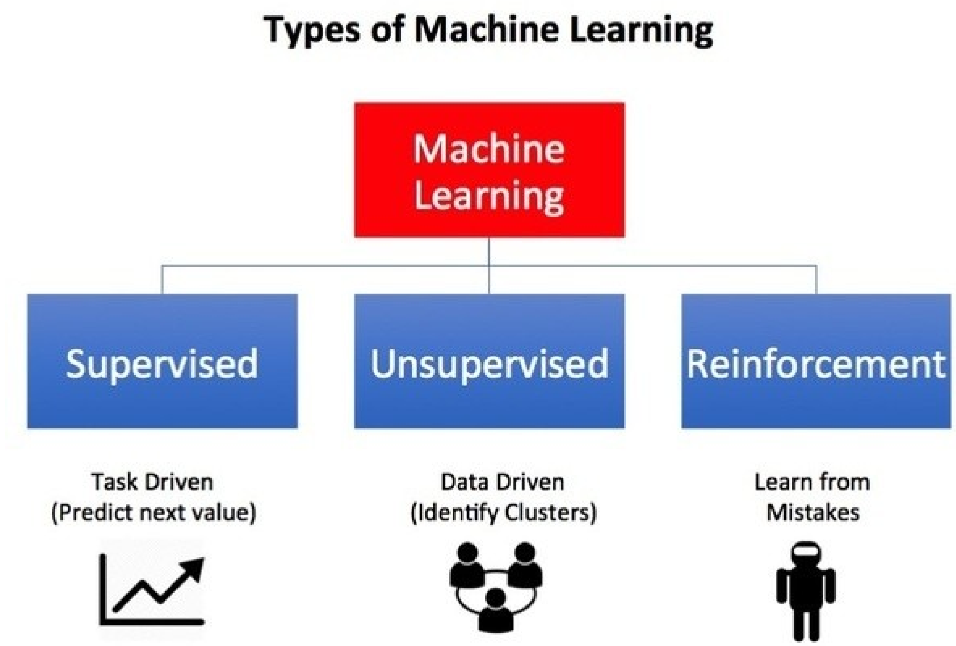
MACC / IFCA

UNIVERSIDAD DE CANTABRIA
CSIC



Oct	29	Aplazada (sesión de refuezo)
	31	Presentación, introducción y perspectiva histórica
Nov	5	Paradigmas, problemas canonicos y data challenges
	7	Reglas de asociación
	12	Práctica: Reglas de asociación
	14	Evaluación, sobrejuste y crossvalidacion
	19	Práctica: Cross-validación
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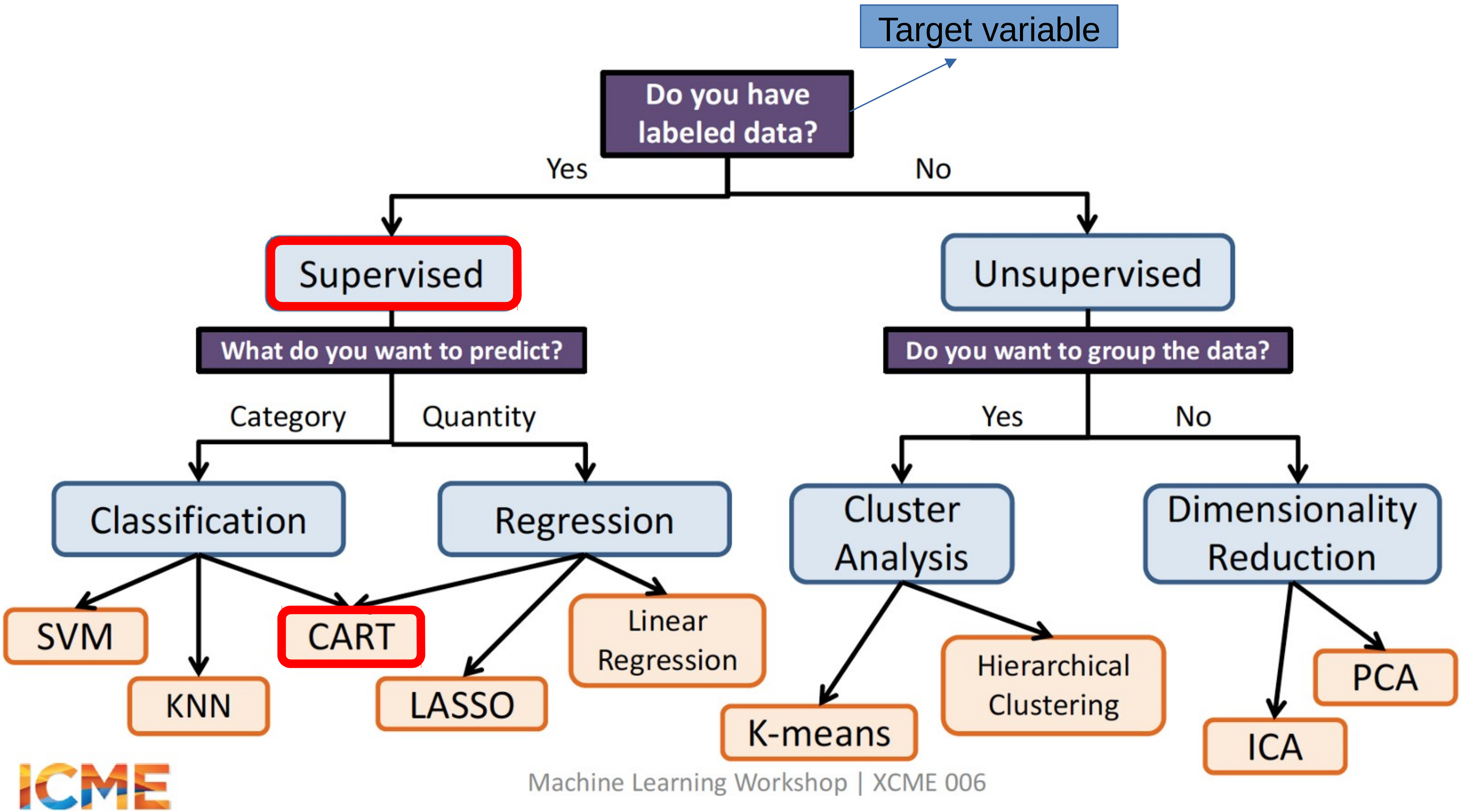
	21a	Practica: El paquete CARET
	21b	Examen

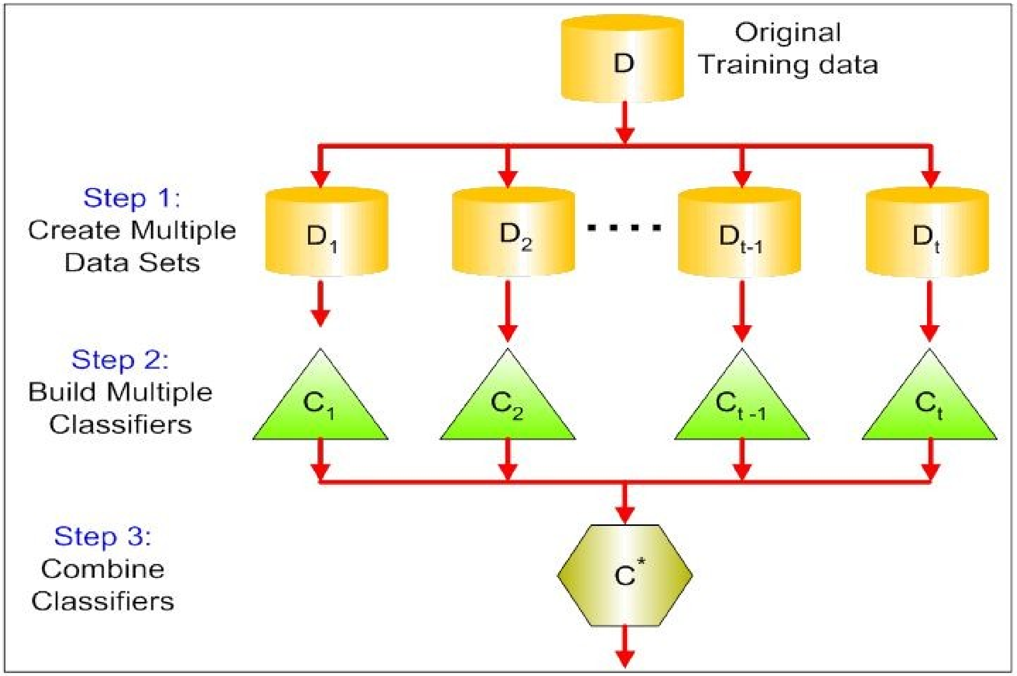
NOTA: Las líneas de código de R en esta presentación se muestran sobre un fondo gris

Calendar

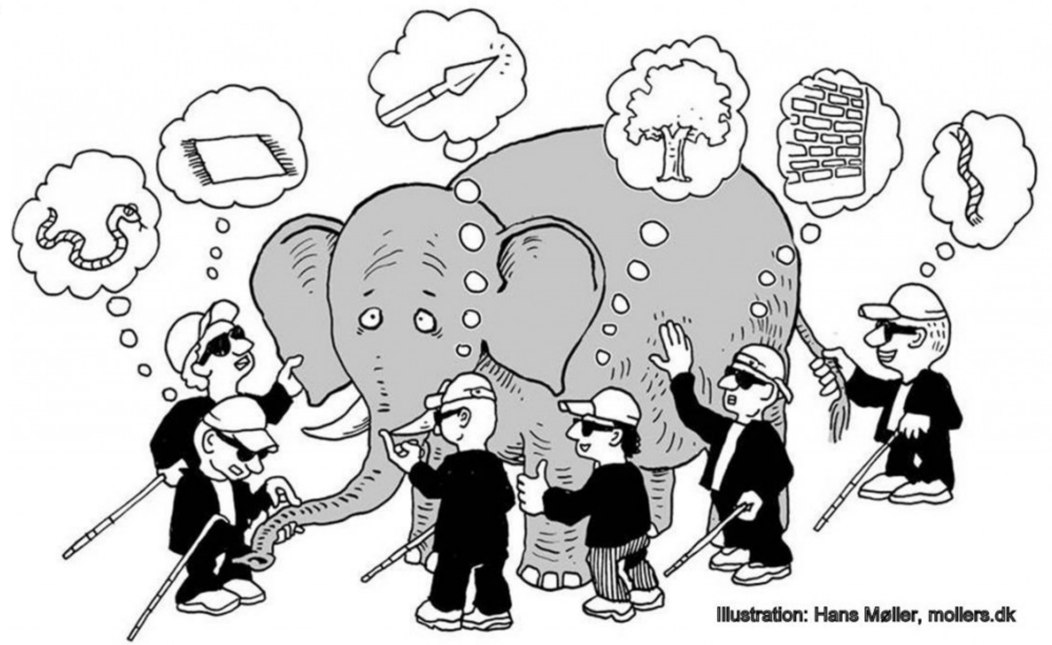

Target variable
Do you have labeled data?
Yes
No
Supervised
Unsupervised
What do you want to predict?
Do you want to group the data?
Category
Quantity
Yes
No
Classification
Regression
Cluster Analysis
Dimensionality Reduction
SVM
KNN
CART
LASSO
Linear Regression
K-means
Hierarchical Clustering
PCA
ICA
ICME
Machine Learning Workshop | XCME 006

Ensemble learning

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 learning

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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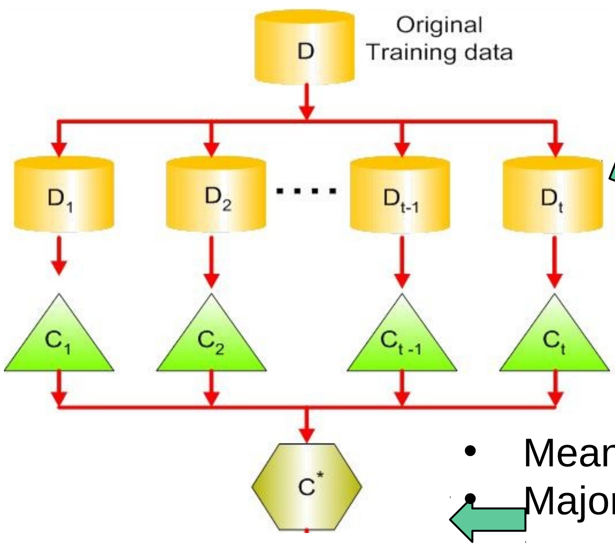

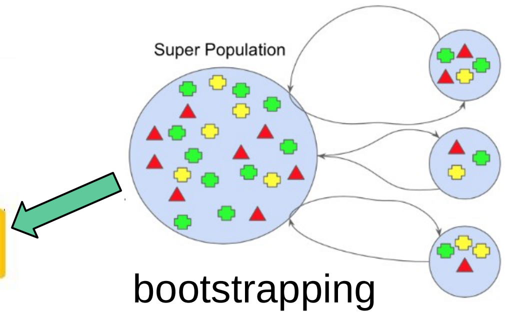

- Mean (prediction)
- Majority voting (classification)

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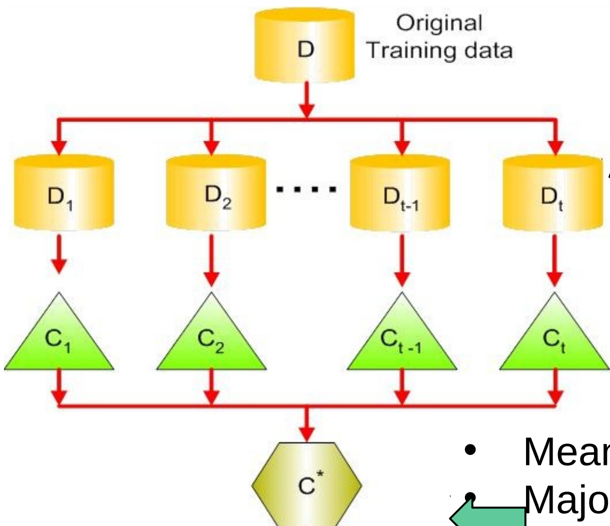

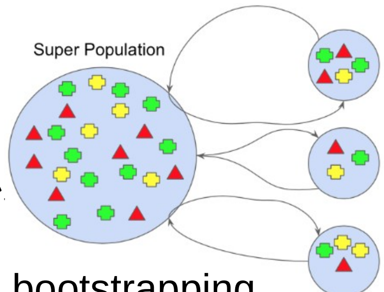

bootstrapping

- Mean (prediction)
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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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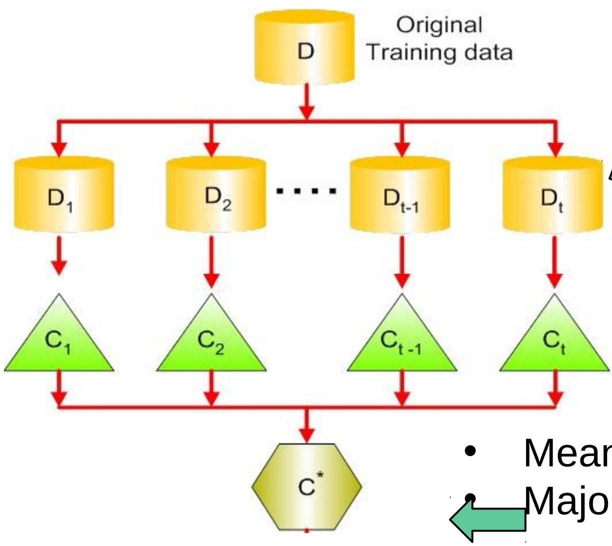

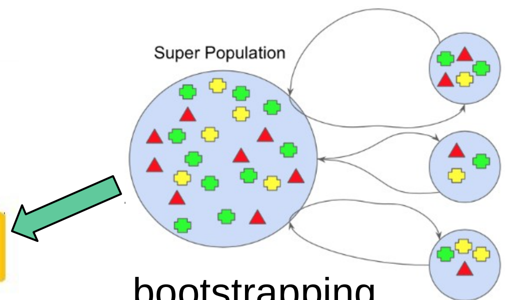

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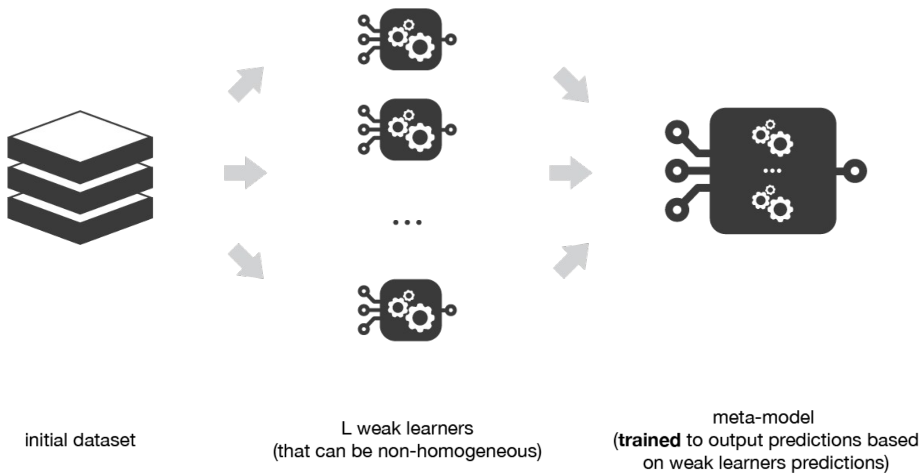

Heterogenous Weak Learners

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.

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

https://towardsdatascience.com/ensemble-methods-bagging-boosting-and-stacking-c9214a10a205

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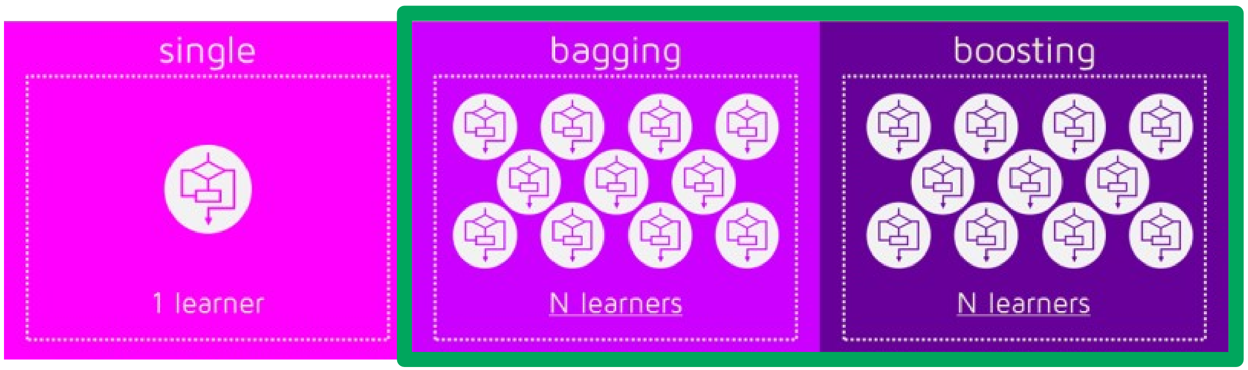
Homogenous Weak Learners

Bagging and Boosting



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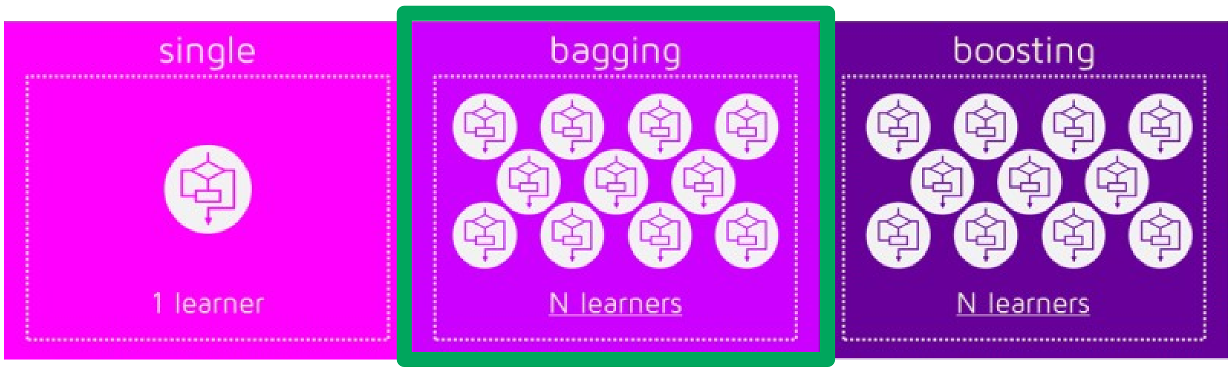

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Random Forests

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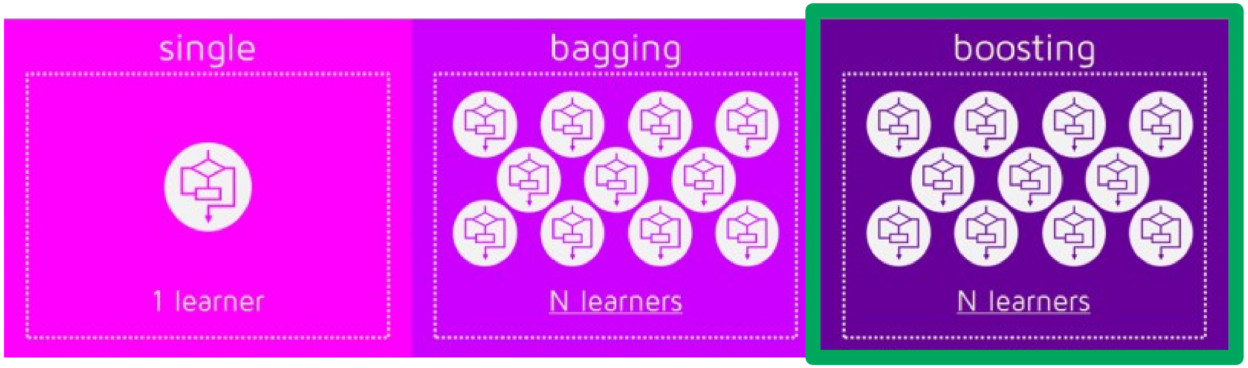

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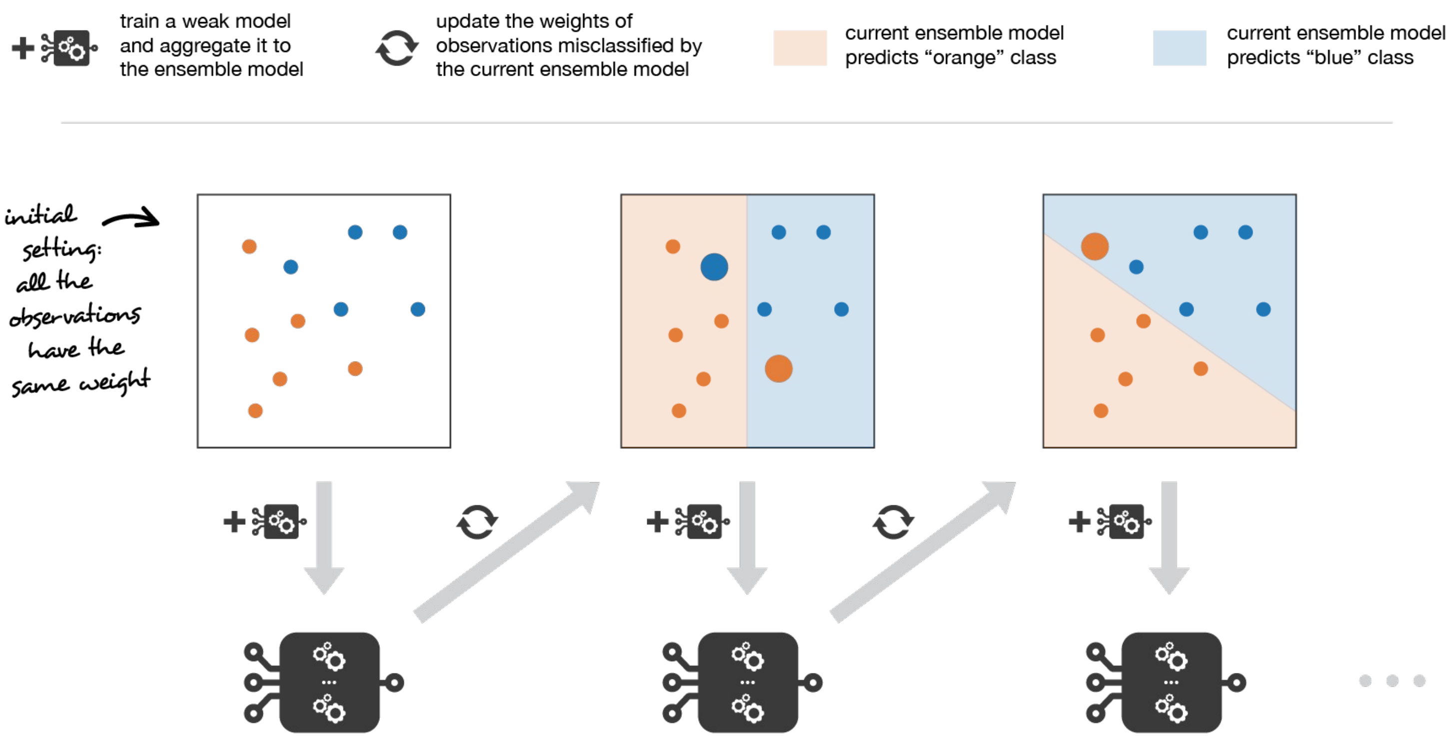
AdaBoost: Adaptive Boosting

Ensemble: Boosting Methods

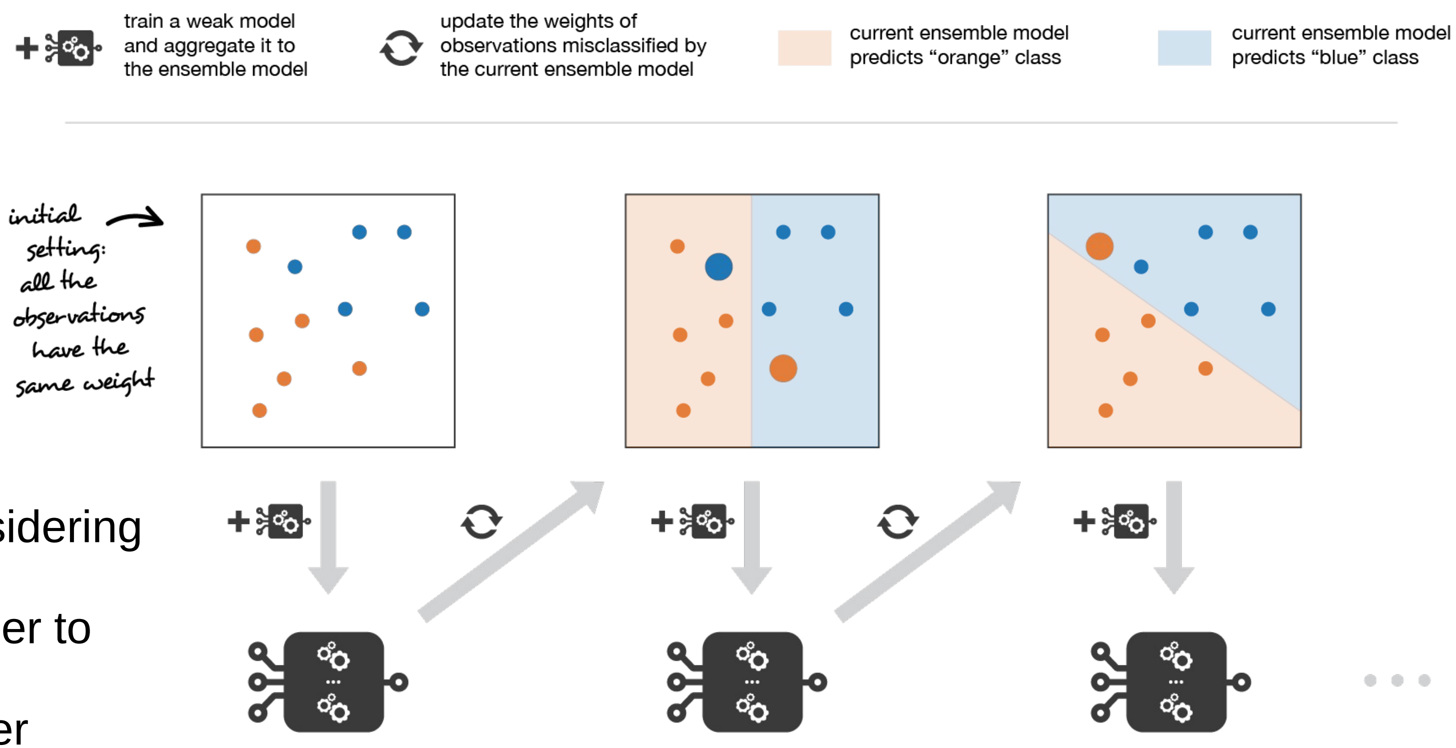
Adaptative Boosting (AdaBoost)



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

Ensemble: Boosting Methods

Adaptative Boosting (AdaBoost)

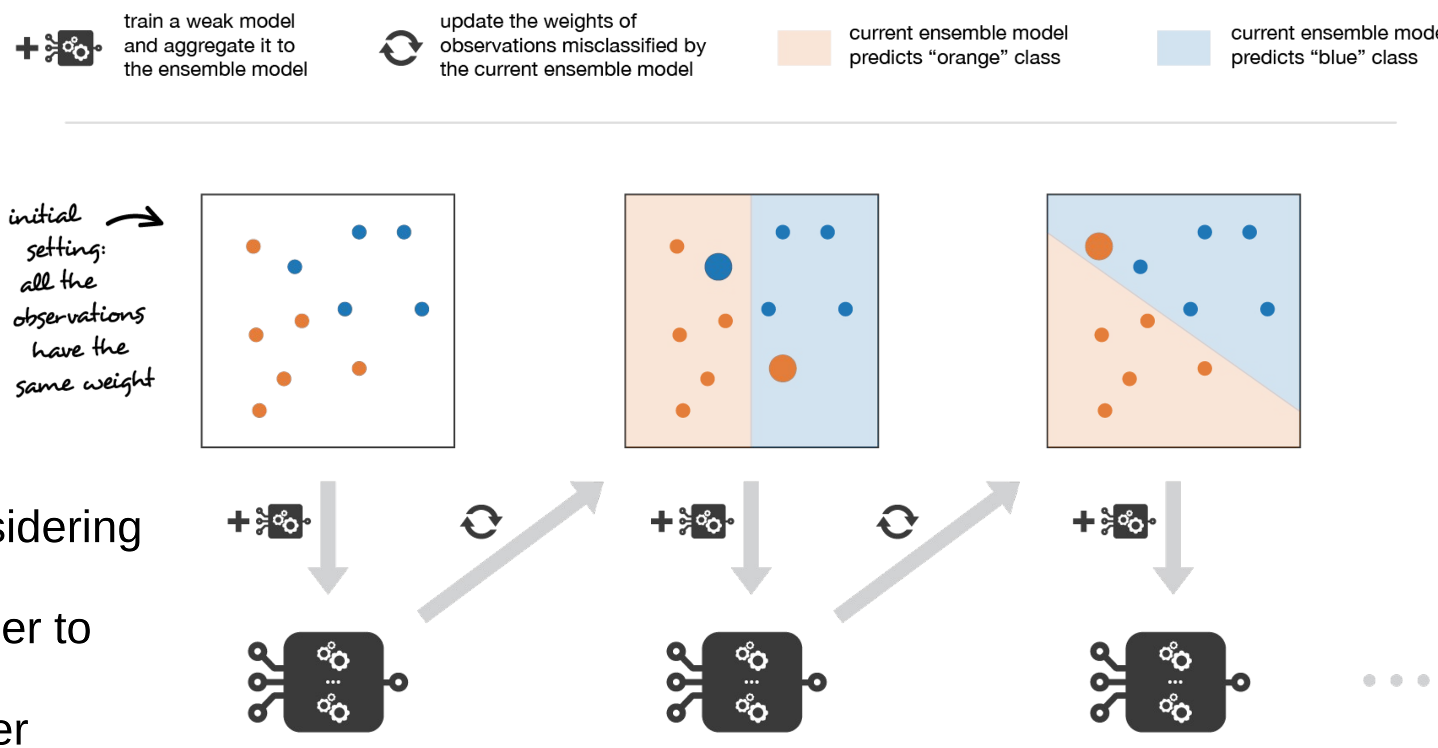


Step 1: All the observations have the **same weights**

a) Fit the weak model considering the observations weights.
b) Evaluate the weak learner to obtain its coefficient.
c) Update the strong learner adding the weak learner.
d) Update the obervations weights

Ensemble: Boosting Methods

Adaptative Boosting (AdaBoost)



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

Repeat (1:L):
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).

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

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

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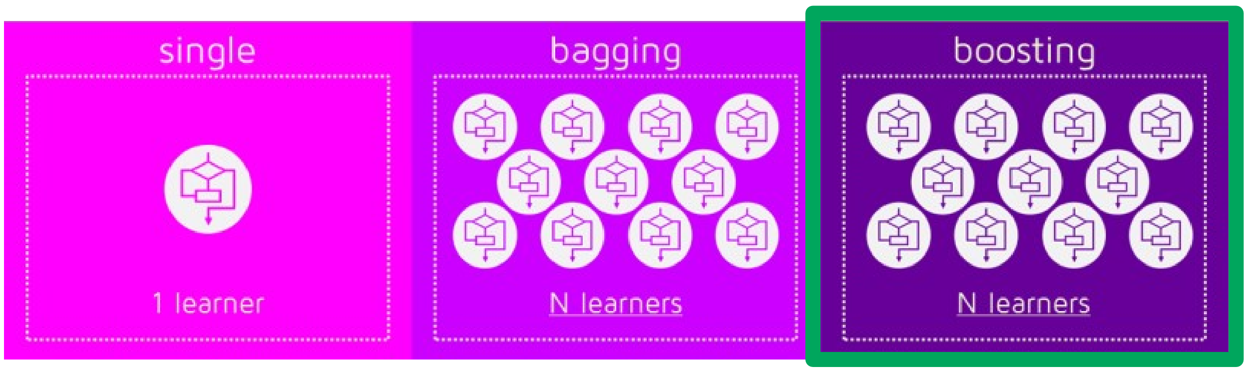


Homogenous Weak Learners

High bias and low variance

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

Gradient Descent Boosting

Gradient Boosting

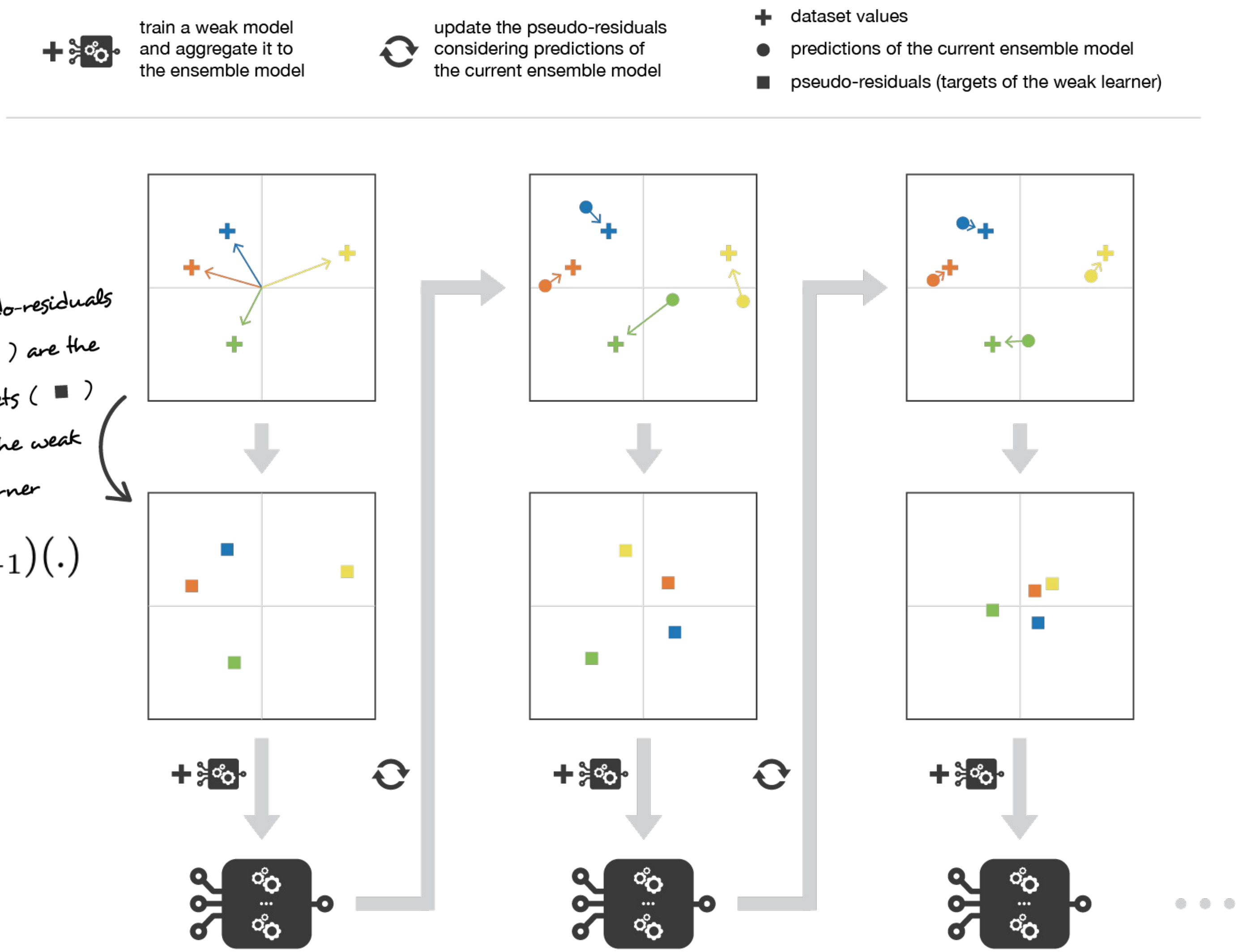
Gradient boosting casts the problem into a gradient descent one: at each iteration we fit a weak learner to the opposite of the gradient of the current fitting error with respect to the current ensemble model.

pseudo-residuals (↗) are the targets (■) of the weak learner

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

Pseudo-residuals:

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



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

Ensemble: Boosting Methods

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Pseudo-residuals:

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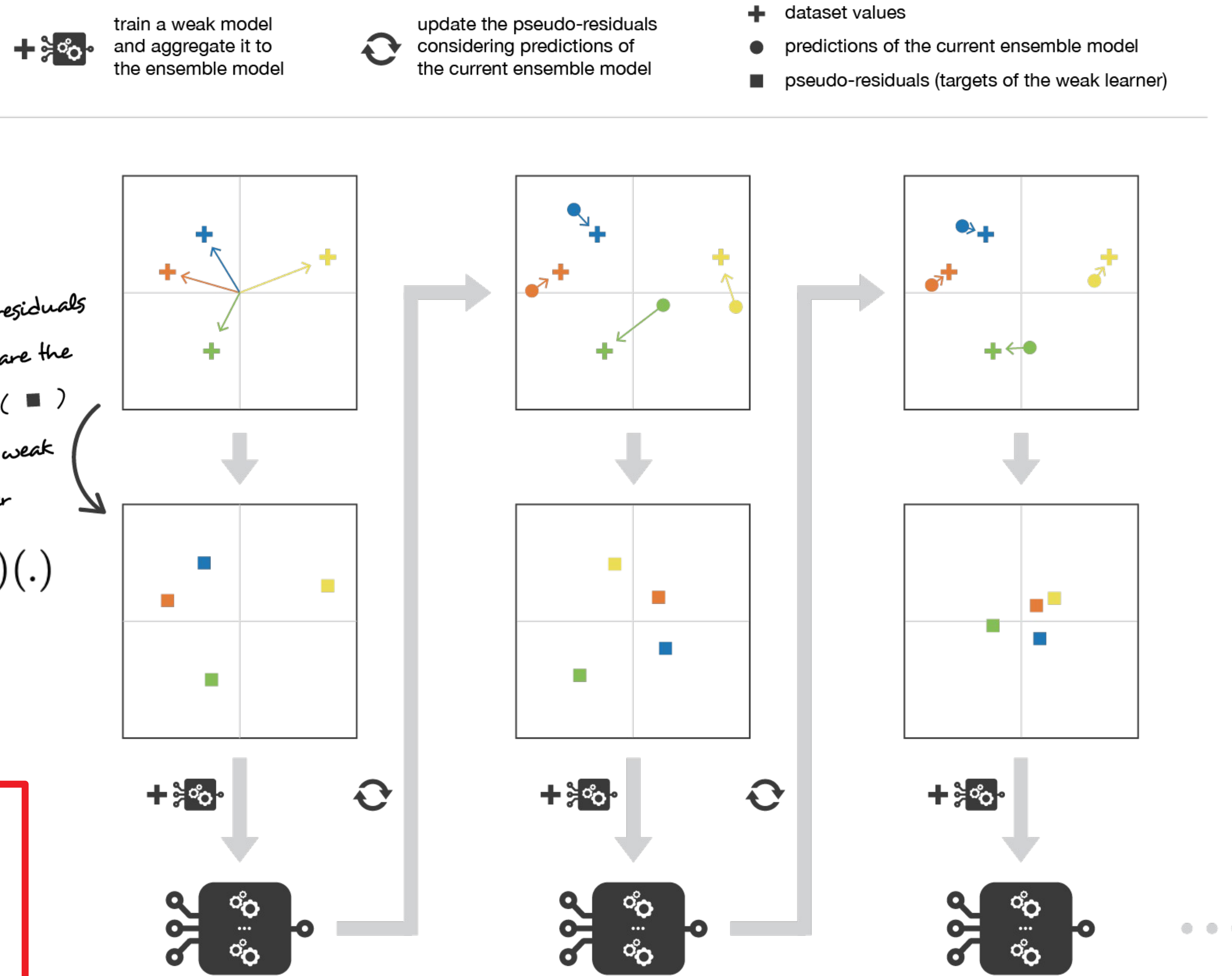
Step size: how much we update the ensemble model in the direction of the new weak learner



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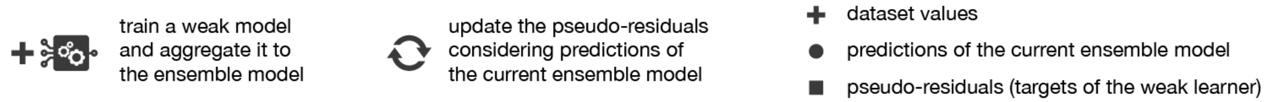
Gradient Boosting



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

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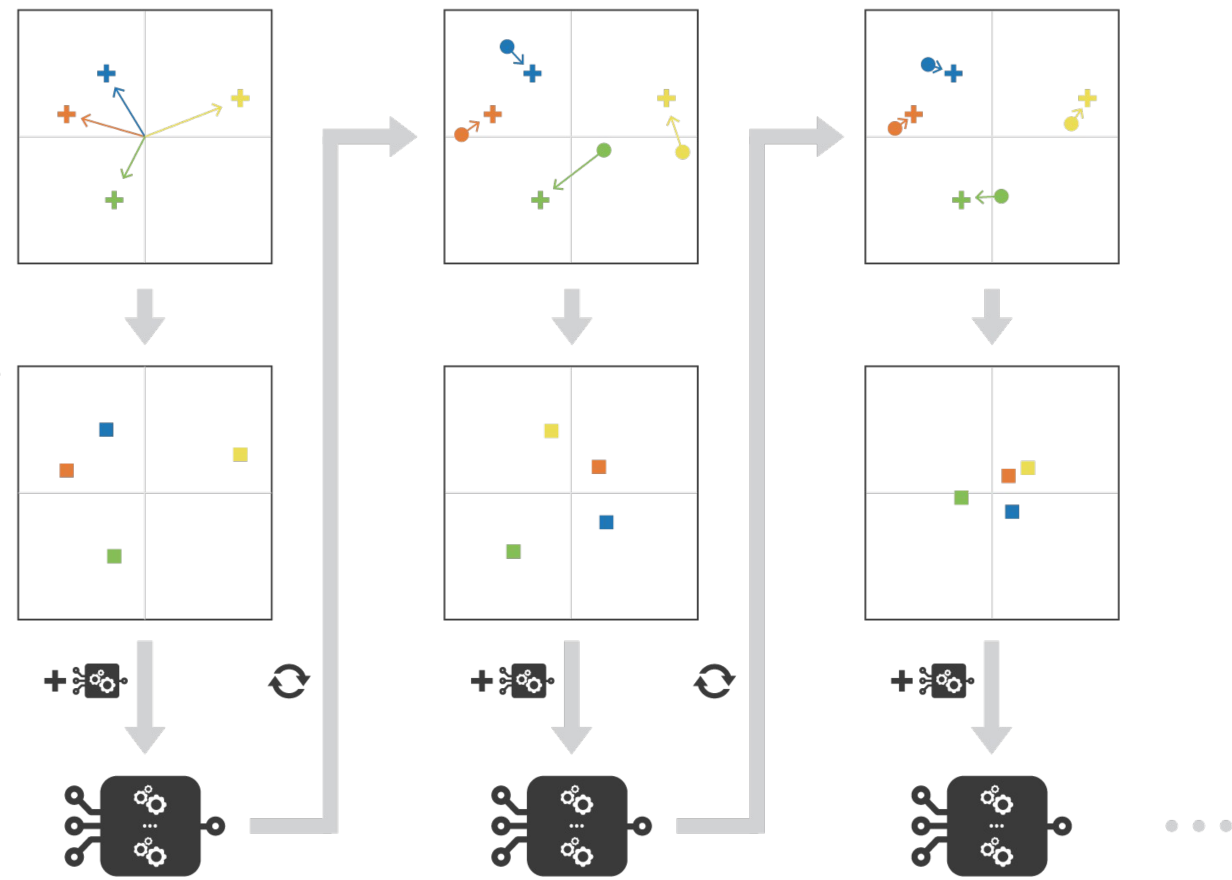

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Ensemble: Boosting Methods

Gradient Boosting

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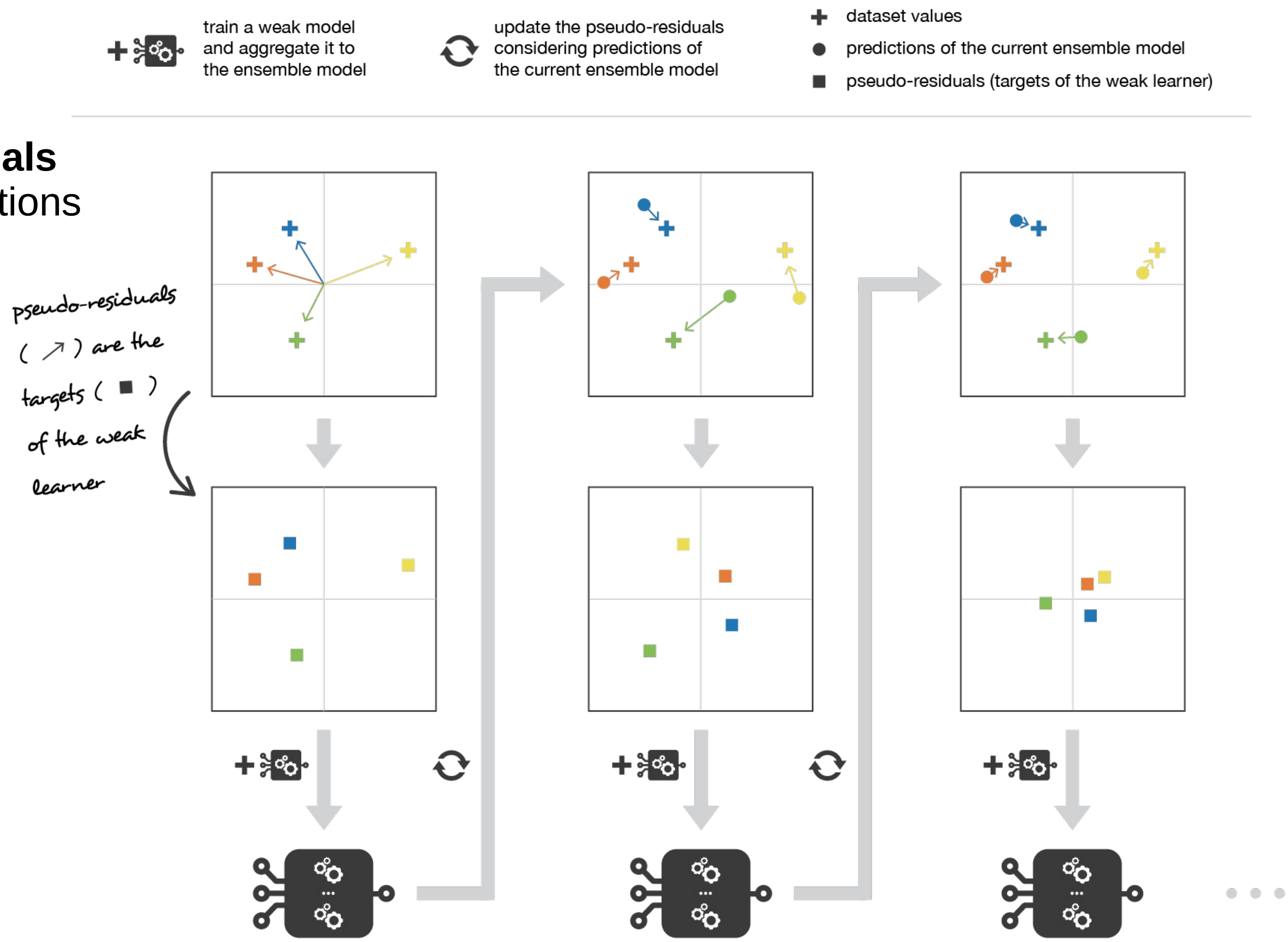

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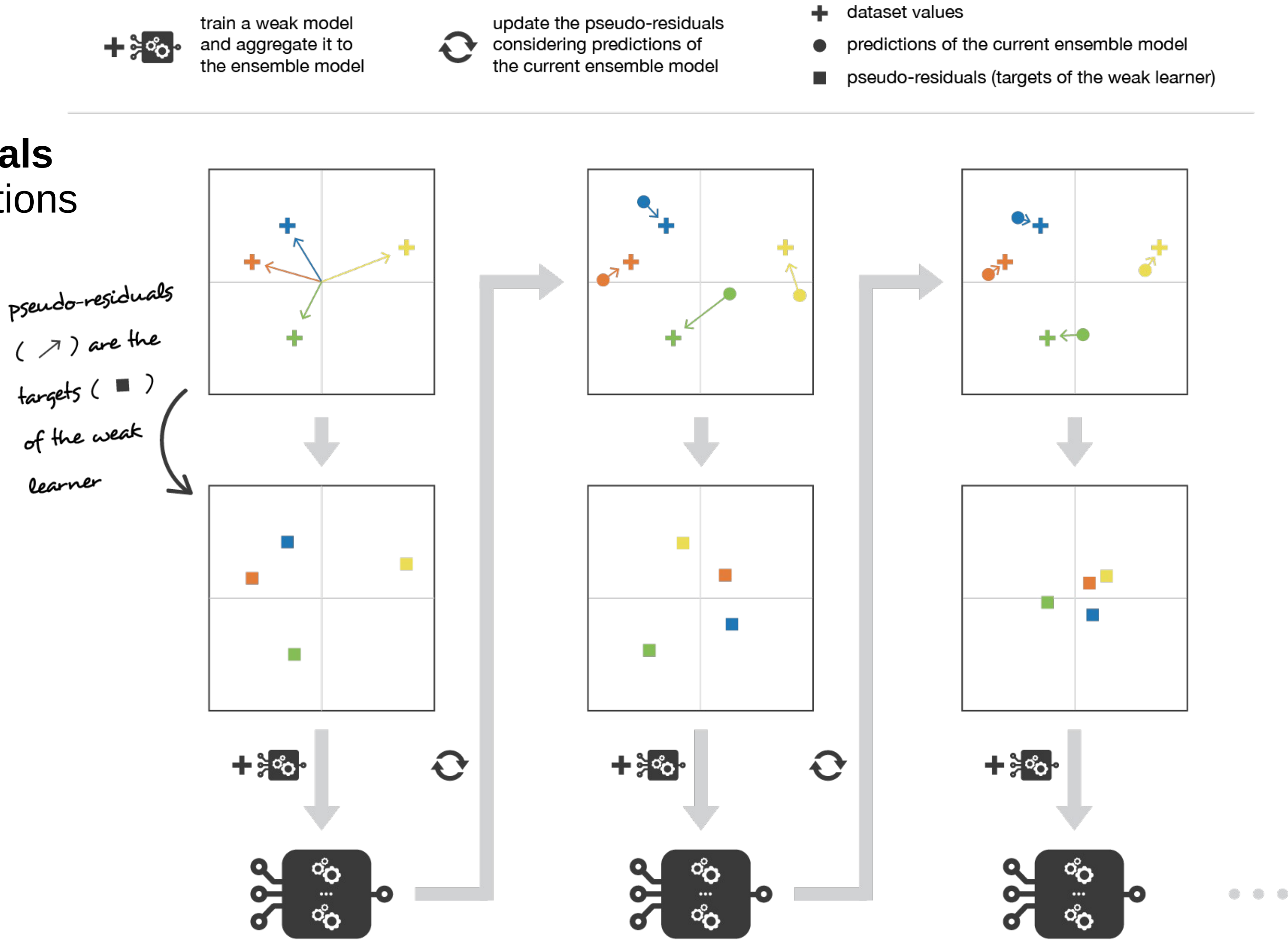

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https://www.kdnuggets.com/2018/07/intuitive-ensemble-learning-guide-gradient-boosting.html

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Ensemble: Boosting Methods

Adaptative vs Gradient Descent Boosting Approaches

Adaptative Boosting (AdaBoost)

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

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

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

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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.

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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.

Ensemble: Boosting Methods

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

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("gbm")`.

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`	A symbolic description of the model to be fit. The formula may include an offset term (e.g. y~offset(n)+x). If `keep.data = FALSE` in the initial call to `gbm` 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.

Extensions of Gradient Descent Boosting Approache

dmlc XGBoost

Extreme Gradient Boosting

XGBoost: A Scalable Tree Boosting System

Tianqi Chen
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Carlos Guestrin
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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

Ensemble: Boosting Methods

Extensions of Gradient Descent Boosting Approache

TensorFlow > Learn > TensorFlow Core > Tutorials

Boosted trees using Estimators

Contenido

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

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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.

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Ensemble Methods in R

Classification problem (iris)

```
## 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(gbm)
library(caret)
library(MASS)
```

```
## 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")
## Prediction for train
pred.t.train <- predict(t, iris[indtrain, ], type = "class")
```

```
## 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))
```

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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, ])
## Prediction for train
pred.rf.train <- predict(rf, iris[indtrain, ])
```

```
## 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))
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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, ])
## Prediction for train
pred.ab.train <- predict(ab, iris[indtrain, ])
```

```
## 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))
```

Ensemble Methods in R

Classification problem (iris)

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

```
## 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")
```

Ensemble Methods in R

Classification problem (iris)

```
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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 – 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))
```

Ensemble Methods in R

Classification problem (iris)

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

```
## 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=ntree_opt_cv,
          interaction.depth=20, shrinkage = 0.01)
print(gb)
summary(gb)
## Prediction for test
pred.gb.test <- predict(object = gb, newdata = iris[indtest, ], n.trees = ntree_opt_cv, type = "response")
## Prediction for train
pred.gb.train <- predict(object = gb, newdata = iris[indtrain, ], n.trees = ntree_opt_cv, type = "response")
```