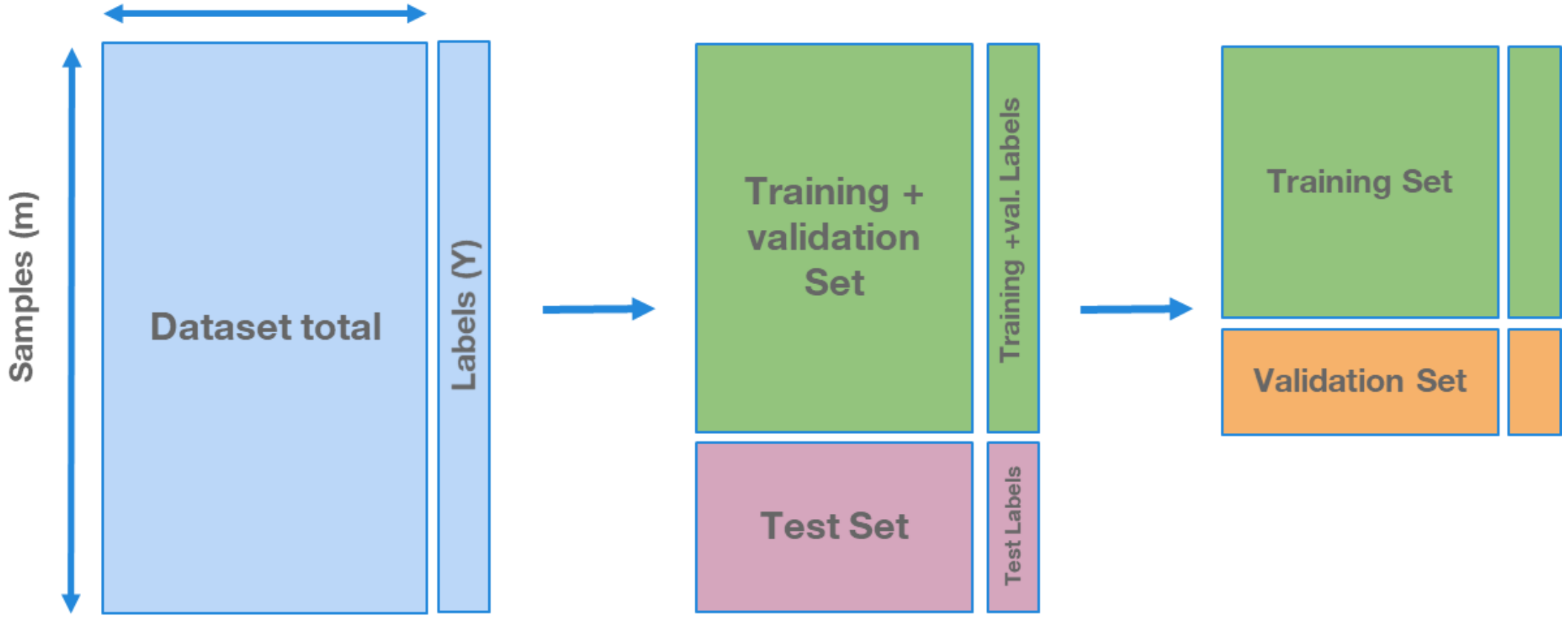
DATA SCIENCE

Modelos de Aprendizaje Supervisado

Construcción de la Base

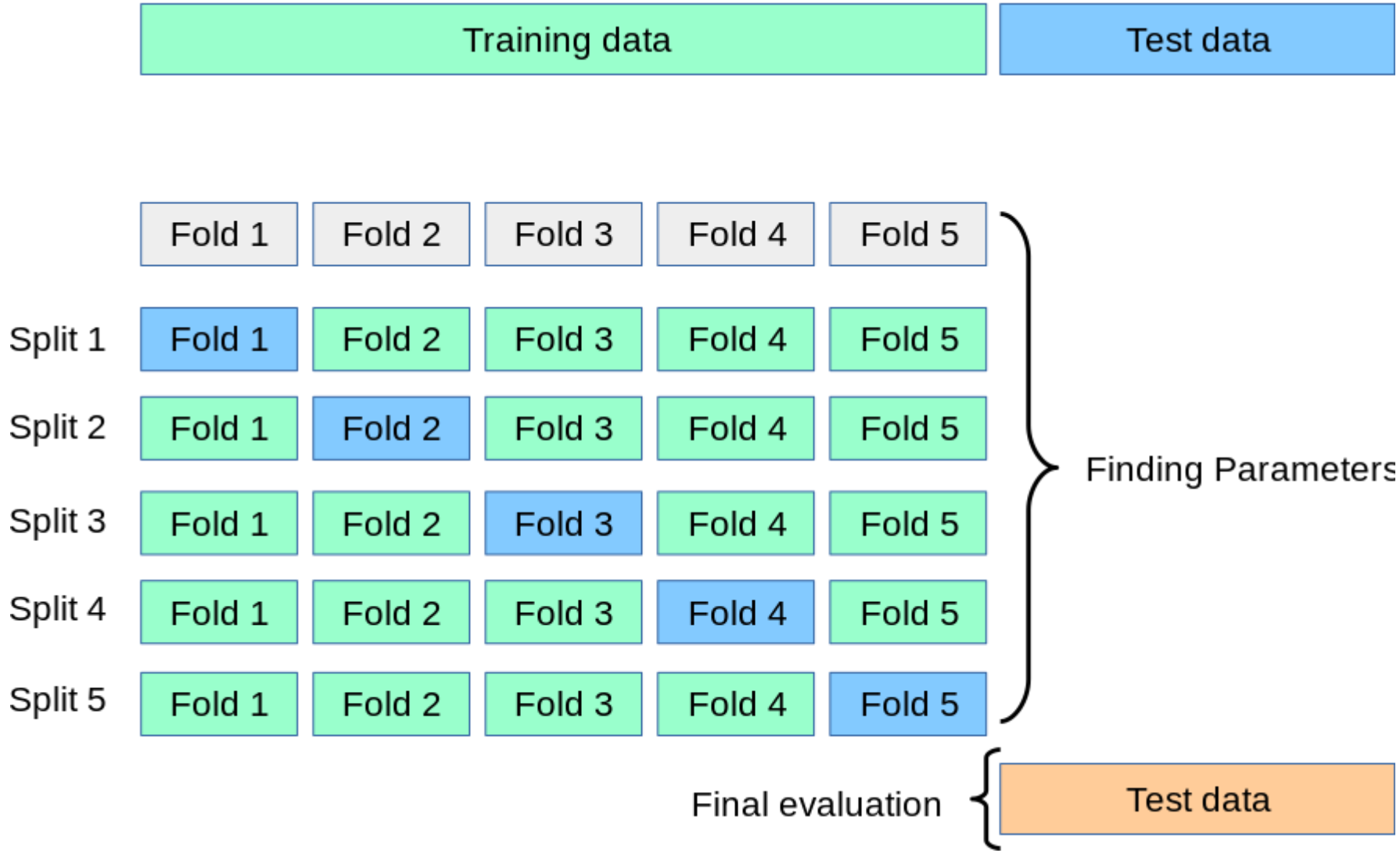
Construcción de la Base



El clasificador aprenderá la regla de decisión utilizando el train set (samples + labels). Luego clasificará las muestras de test (sin mirar las labels de test) y se medirá la exactitud de clasificación en testeo.

Cross Validation

Cross Validation



Optimización de Hiperparámetros

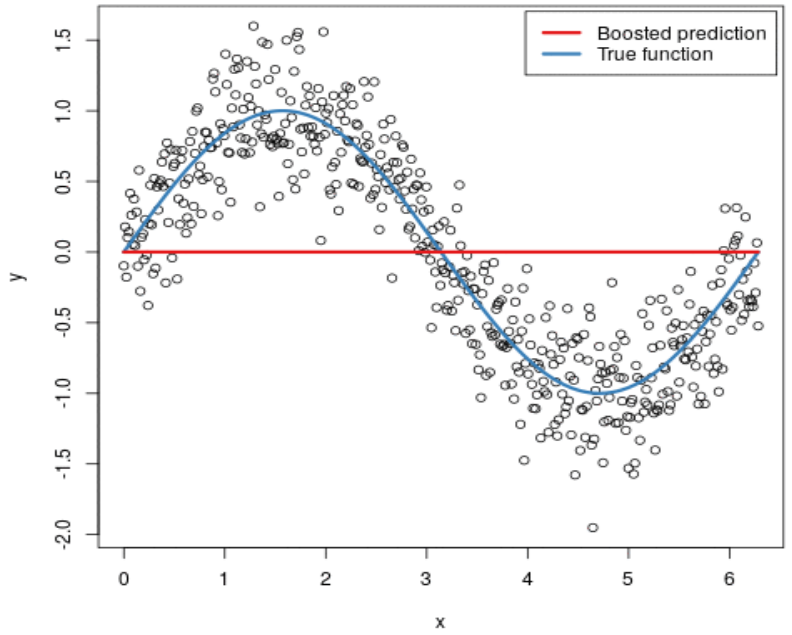
Grid Search

Random Search

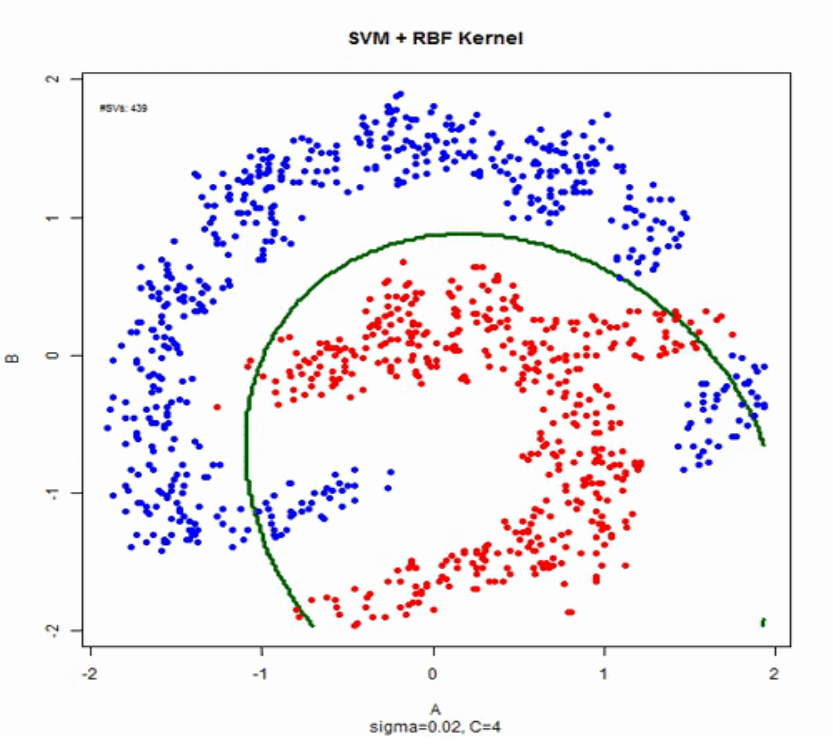
Bayesian Optimization

Modelado

Tipos de Modelos



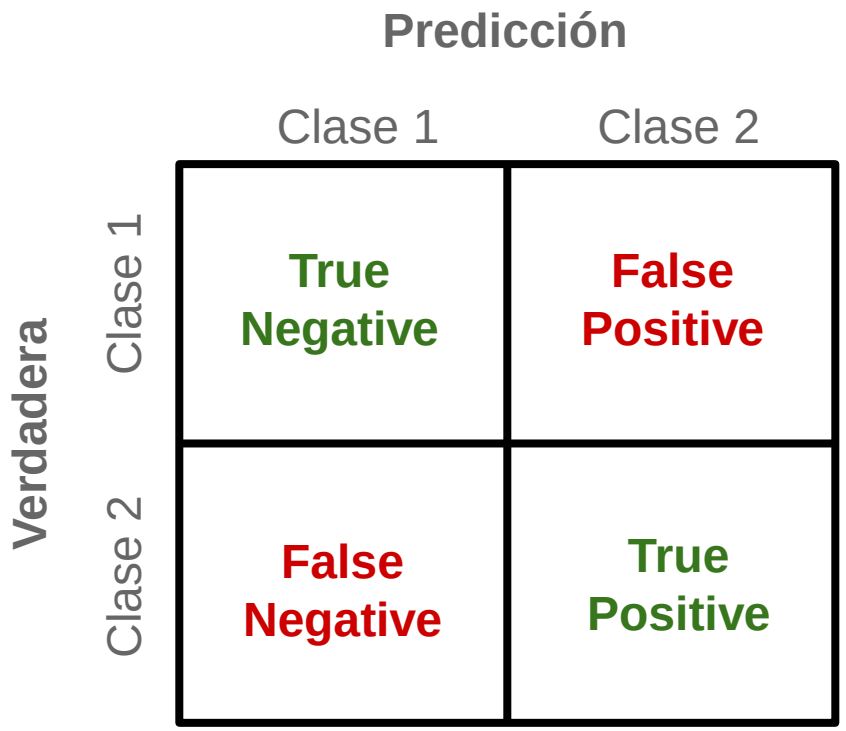
Regresión



Clasificación

Medición de Resultados

Para Clasificación: Matriz de Confusión



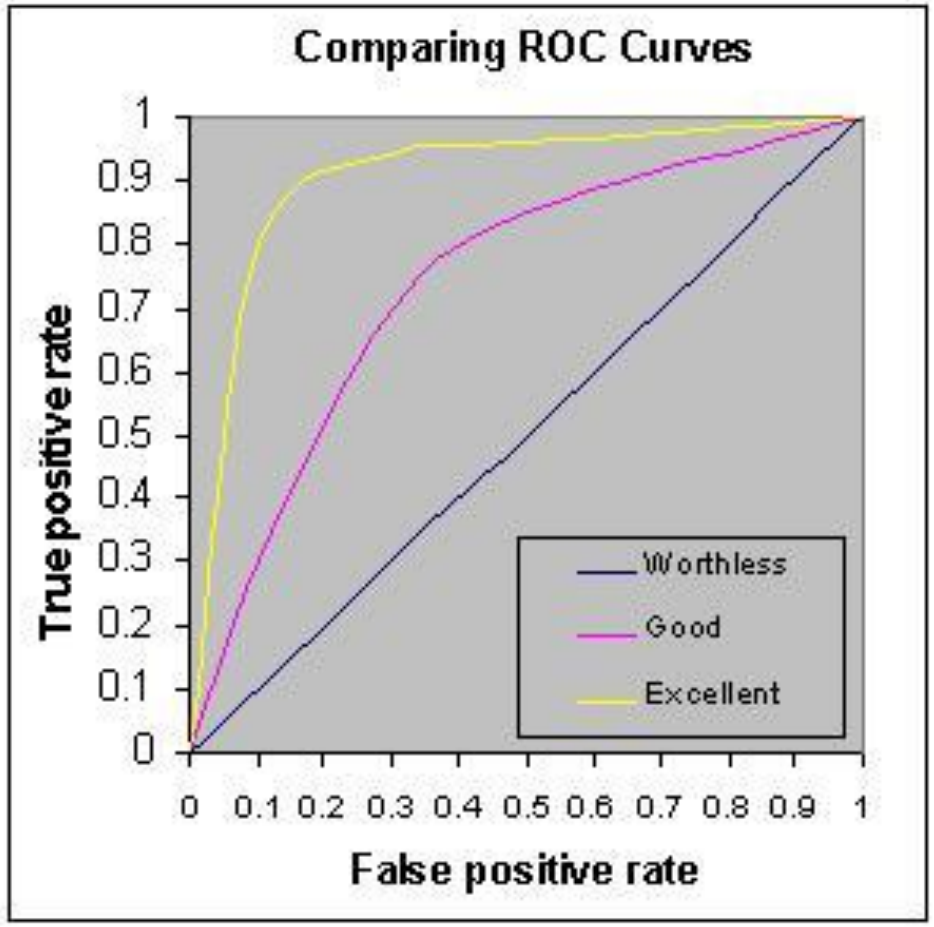
Accuracy = (TN+TP) / Total

Error = (FP+FN) / Total

Recall = TP / (FP+TP)

Precision = = TP / (FN+TP)

Área bajo la curva ROC



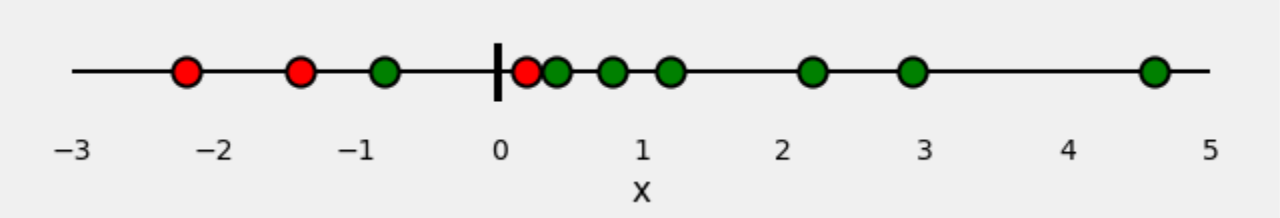
Y	Prob
1	0,9
1	0,88
1	0,84
0	0,83
1	0,8
1	0,77
1	0,75
0	0,75

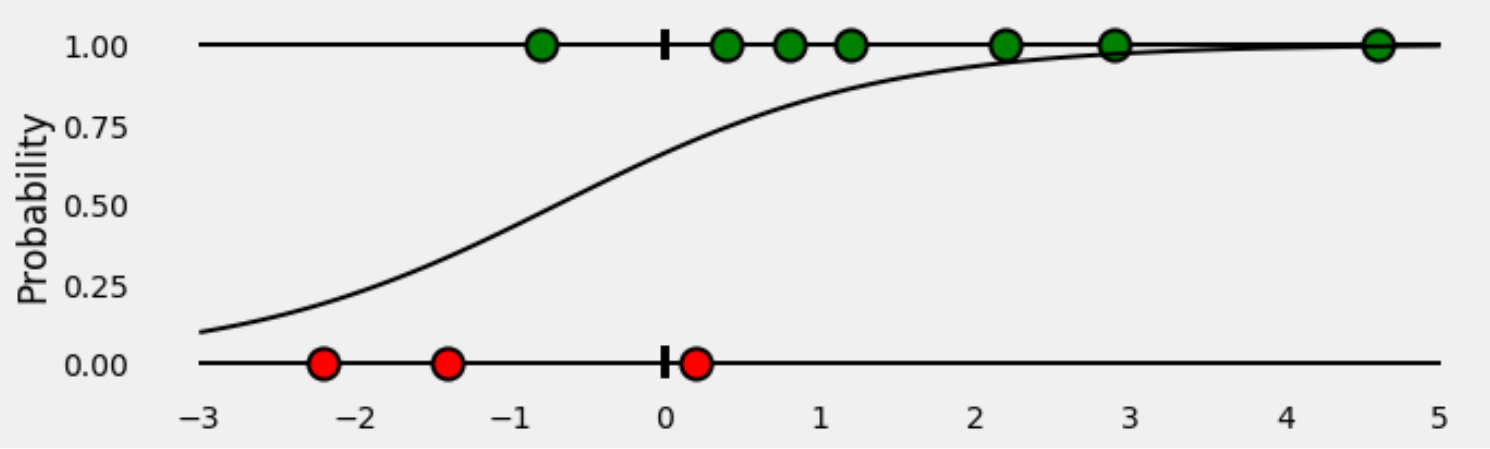
Ejemplo Visual: http://www.navan.name/roc/

Log Loss - Entropía Cruzada Binaria

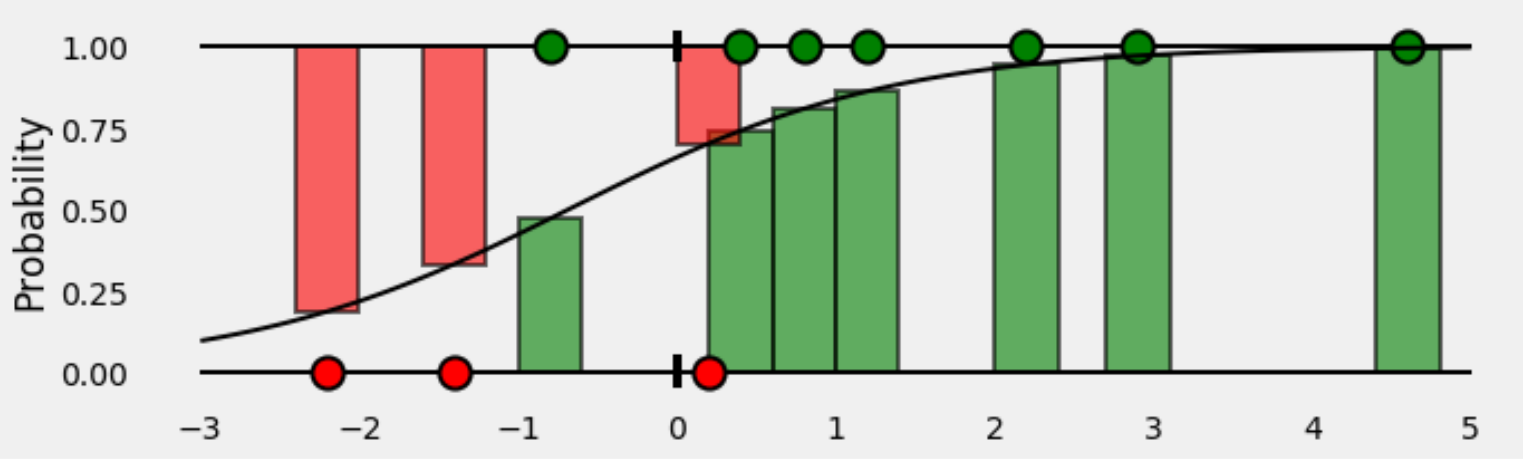
Binary Cross-Entropy

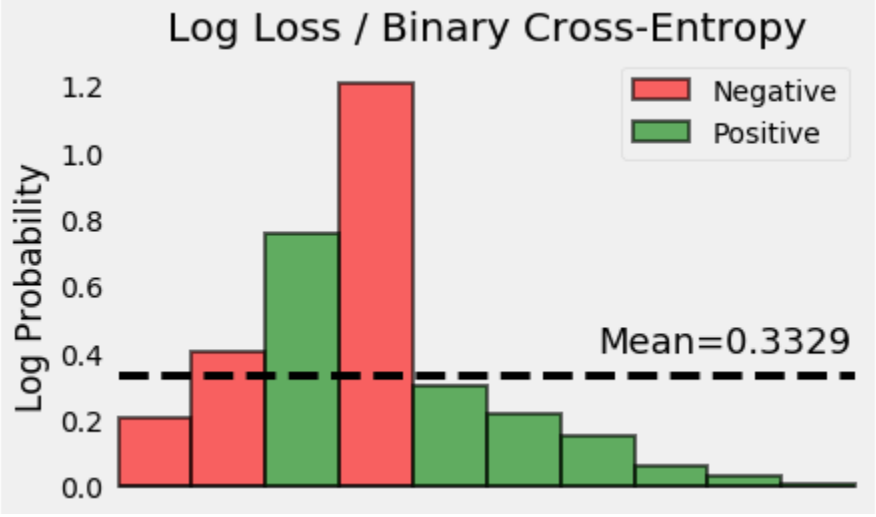
$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$





Log Loss - Entropía Cruzada Binaria

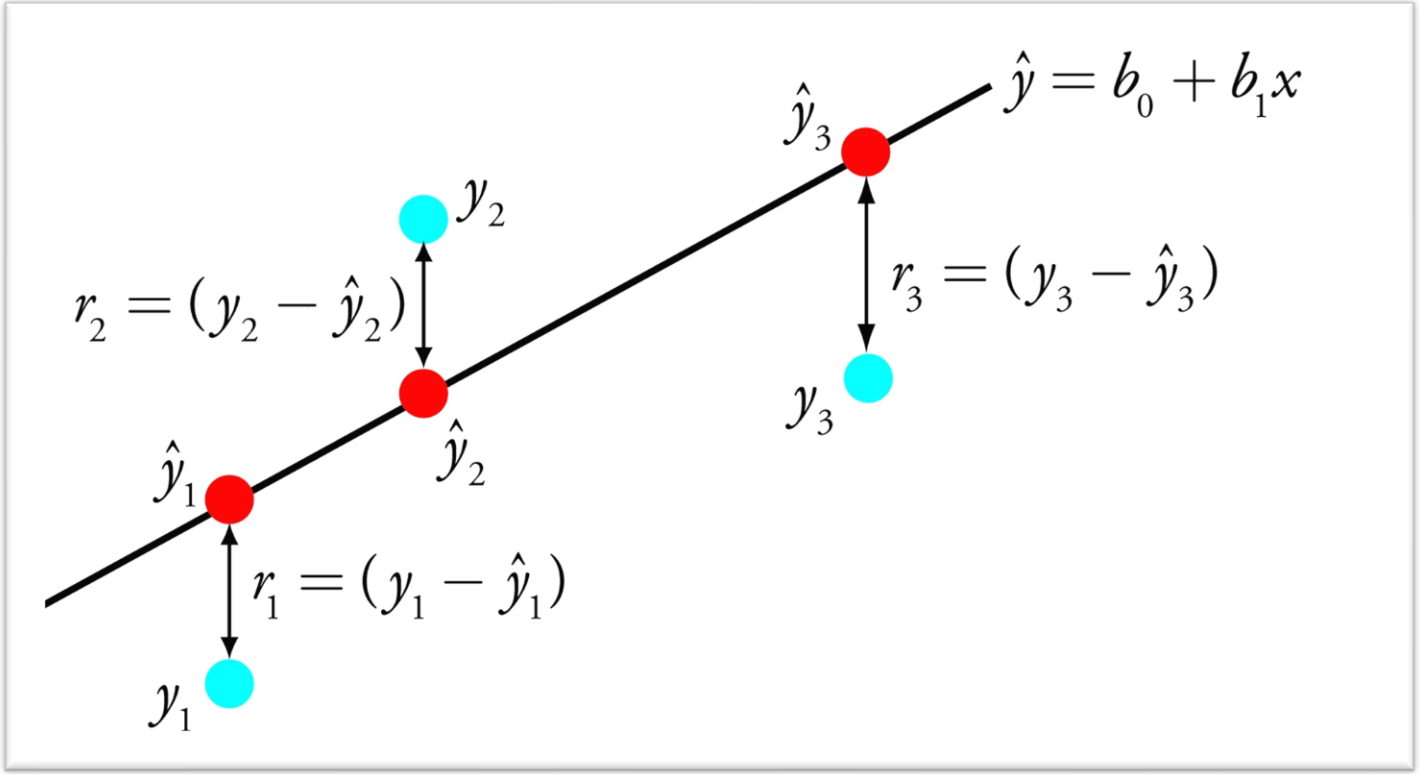




Para Regresión: Error Medio Cuadrático o Absoluto

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

$$MAE = \frac{\sum_{i=1}^{n} |y_i - y_i^p|}{n}$$



Regularización

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 + \lambda f(\beta)$$

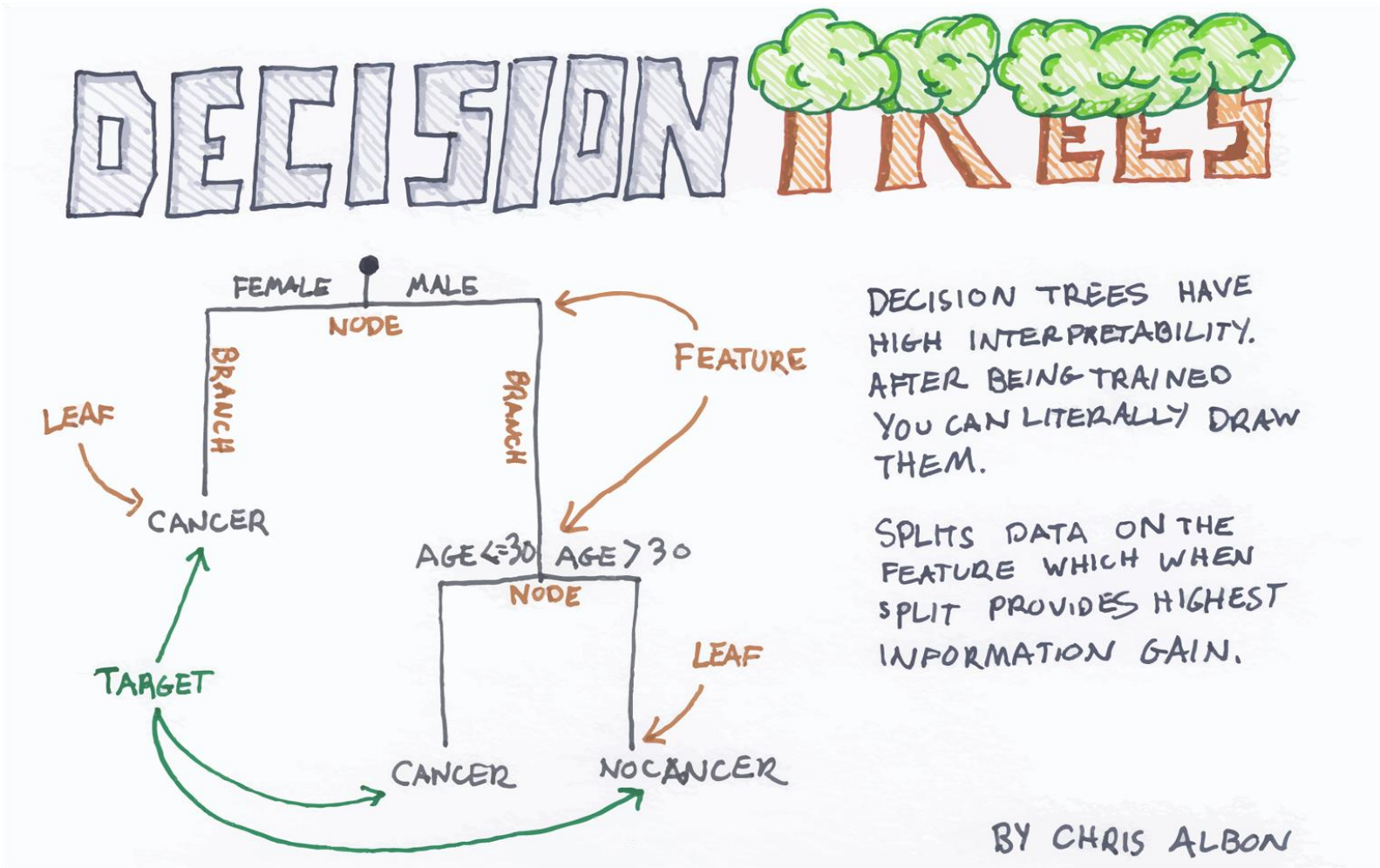
L1 (Lasso) $+ \lambda \sum_{i=1}^{N} |w_i|$

L2 (Ridge) $+ \lambda \sum_{i=1}^{N} w_i^2$

Modelos Básicos

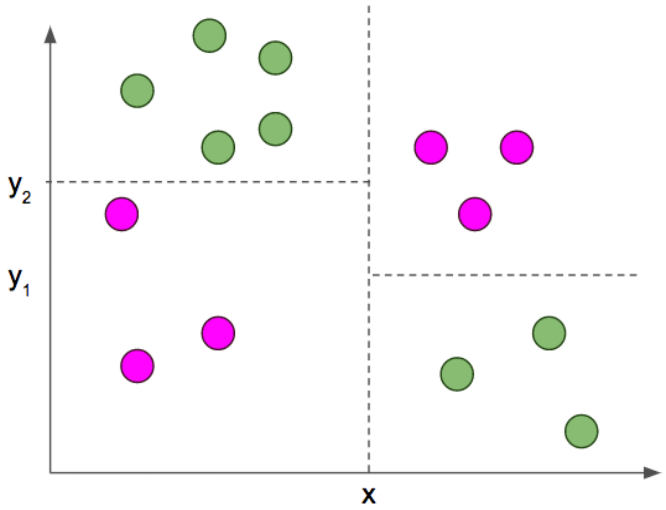
Arbol de Decisión

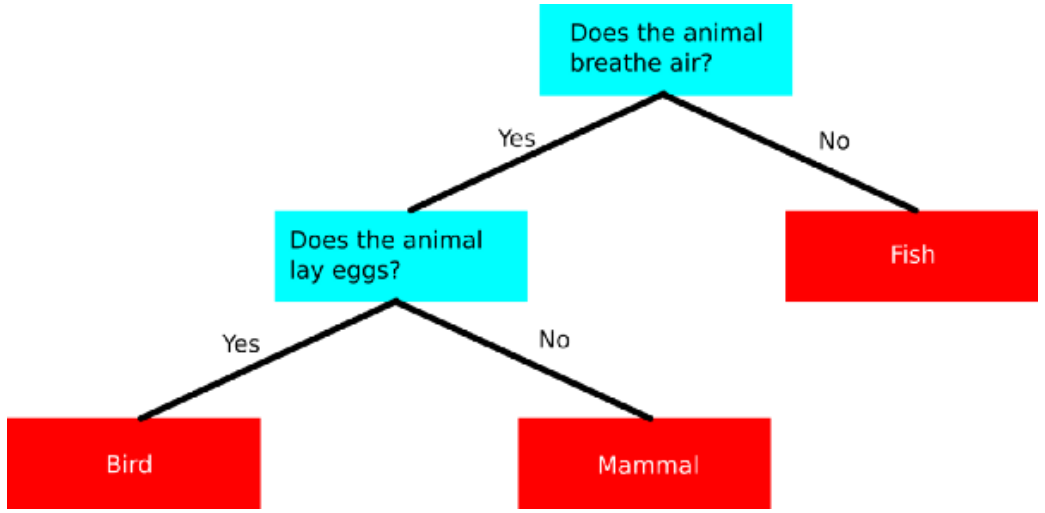
Arboles de Decisión



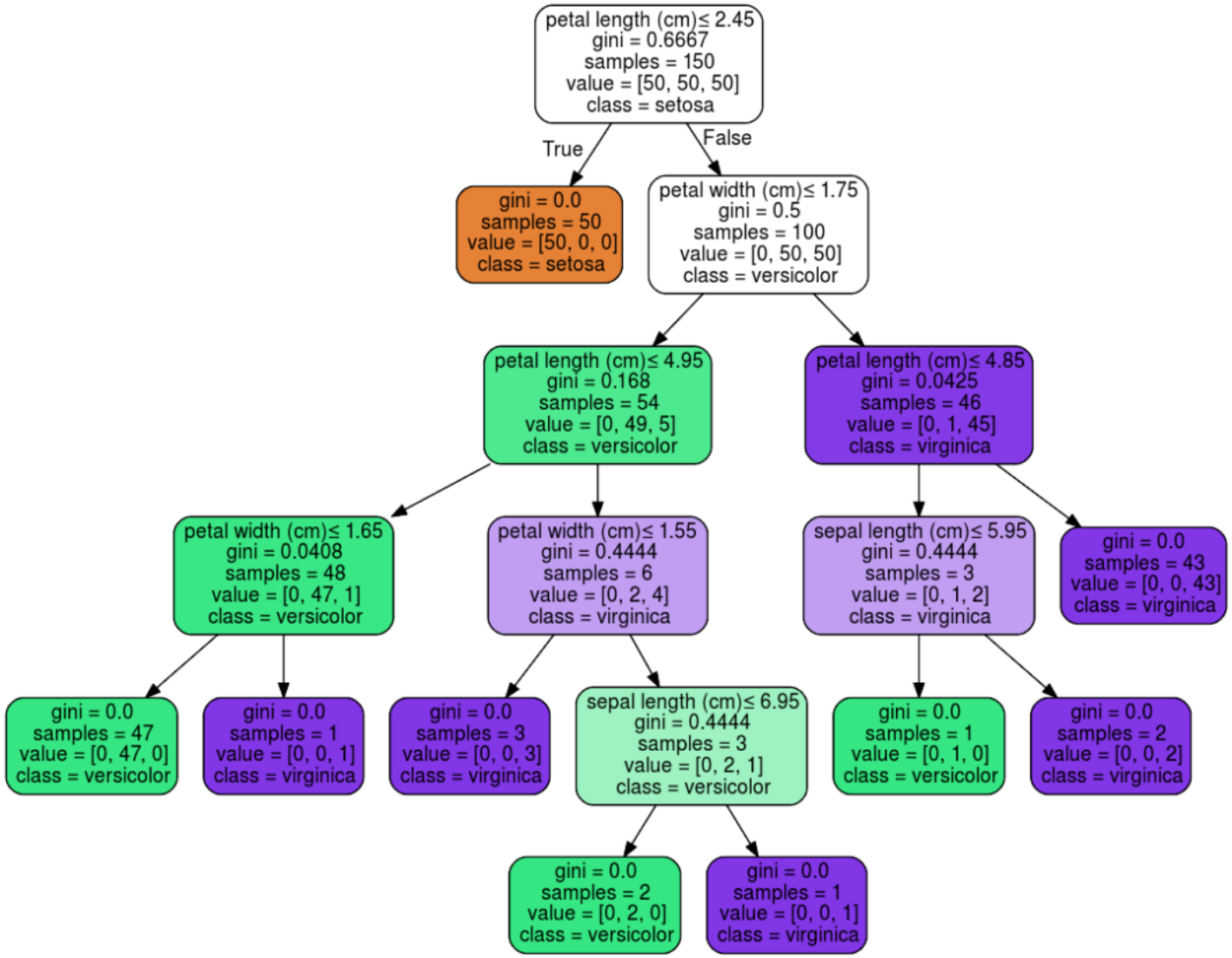
Arboles de Decisión

En función de los datos de entrenamiento, el modelo construye los niveles jerárquicos y las preguntas a realizar. Estas preguntas son determinadas en función de las “features” de nuestro dataset. El modelo de decision trees classification soporta problemas “multi-clase”.

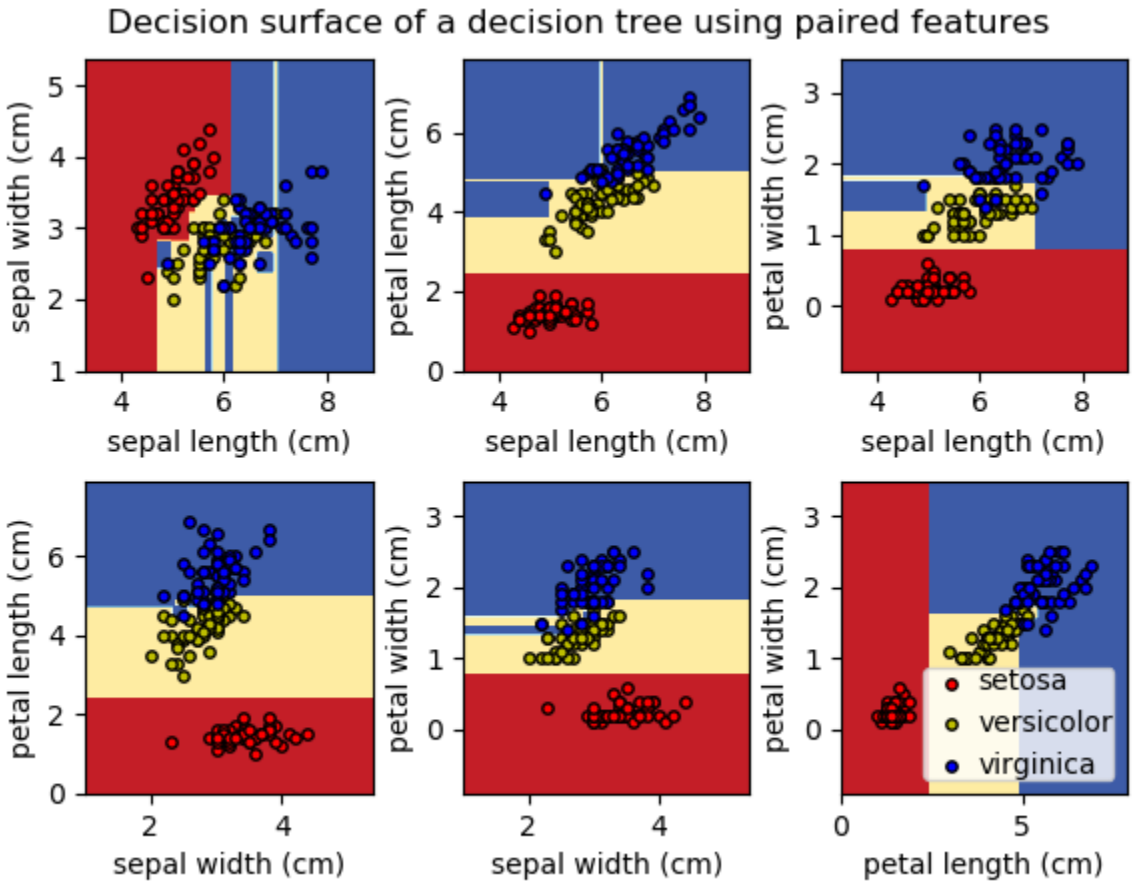




Arboles de Decisión - Iris



Arboles de Decisión - Iris



Arboles de Decisión

sklearn.tree.DecisionTreeClassifier

class sklearn.tree. **DecisionTreeClassifier** (*criterion='gini', splitter='best', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None, random_state=None, max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, class_weight=None, presort=False*)

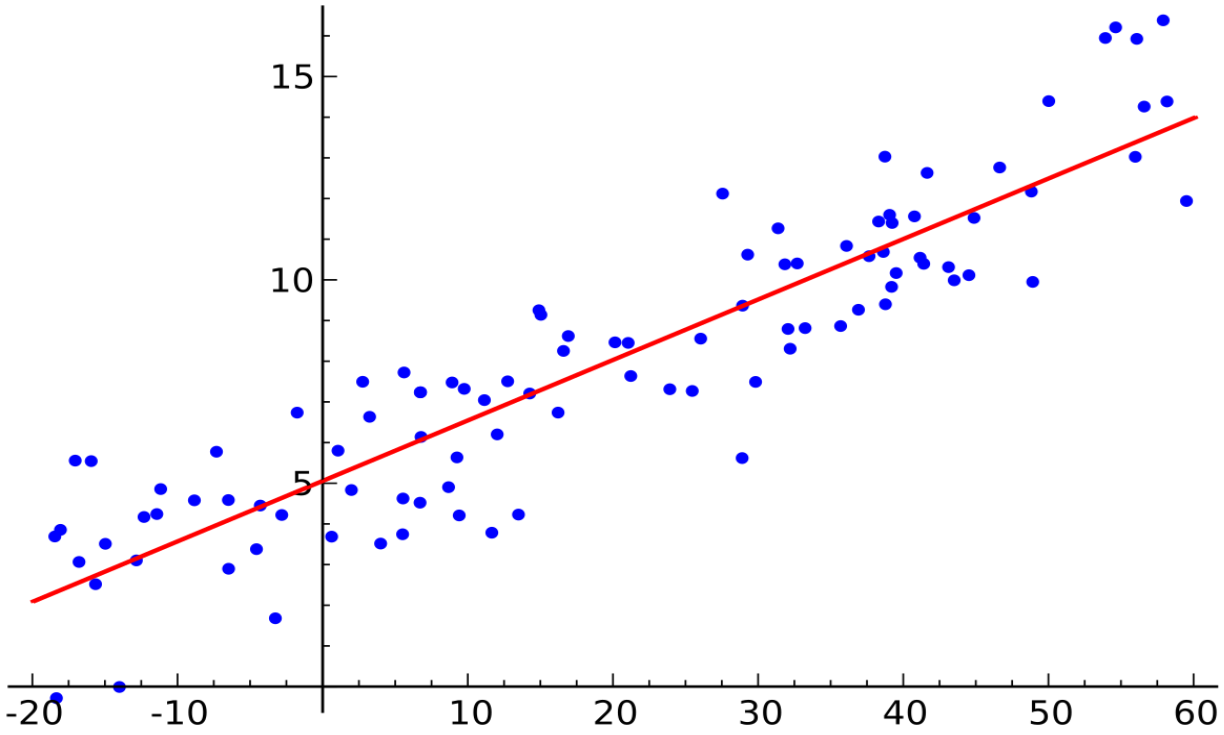
[source]

```
>>> from sklearn import tree
>>> X = [[0, 0], [1, 1]]
>>> Y = [0, 1]
>>> clf = tree.DecisionTreeClassifier()
>>> clf = clf.fit(X, Y)
```

Regresión lineal

Regresión lineal

Se utiliza principalmente para Modelos de **Regresión**
Donde la Variable objetivo es **Continua** (numero real)
Se busca una dependencia de este objetivo en relación a las otras variables



Regresión lineal

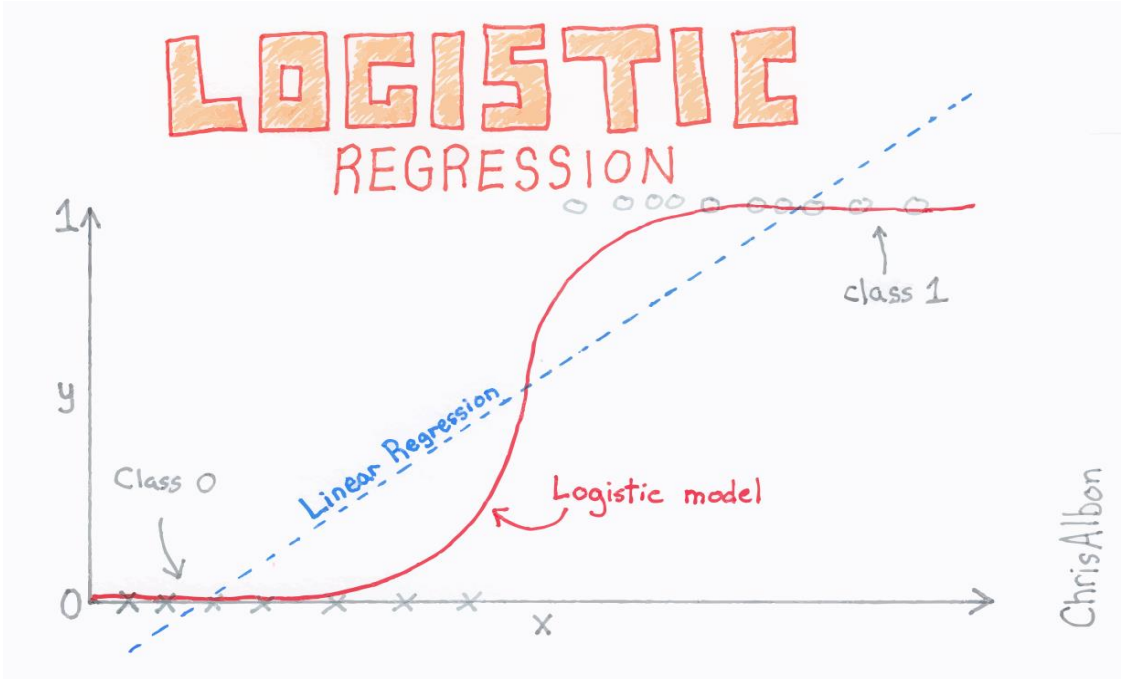
sklearn.linear_model.LinearRegression

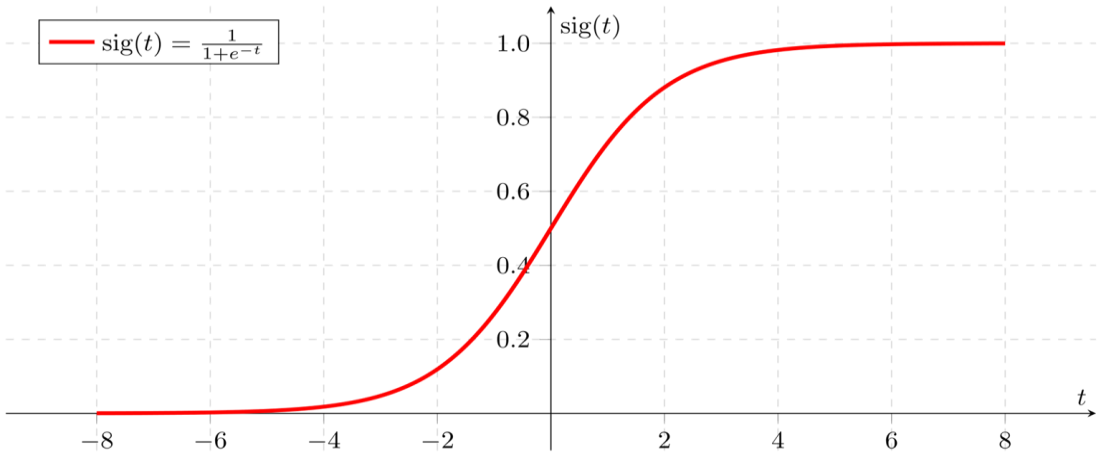
class sklearn.linear_model. **LinearRegression** (*fit_intercept=True, normalize=False, copy_X=True, n_jobs=None*)

[source]

```
>>> import numpy as np
>>> from sklearn.linear_model import LinearRegression
>>> X = np.array([[1, 1], [1, 2], [2, 2], [2, 3]])
>>> # y = 1 * x_0 + 2 * x_1 + 3
>>> y = np.dot(X, np.array([1, 2])) + 3
>>> reg = LinearRegression().fit(X, y)
>>> reg.score(X, y)
1.0
>>> reg.coef_
array([1., 2.])
>>> reg.intercept_
3.0000...
>>> reg.predict(np.array([[3, 5]]))
array([16.])
```

Regresión Logística





Función de activación "sigmoid": mapea cualquier valor de X a un valor entre 0 y 1 pero nunca llega a estos extremos.

$$f\left(x\right) = \frac{1}{1 - e^{-x}}$$

Regresión Logística

sklearn.linear_model.LogisticRegression

class sklearn.linear_model.**LogisticRegression**(*penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None*) [source]

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.linear_model import LogisticRegression
>>> X, y = load_iris(return_X_y=True)
>>> clf = LogisticRegression(random_state=0).fit(X, y)
>>> clf.predict(X[:2, :])
array([0, 0])
>>> clf.predict_proba(X[:2, :])
array([[9.8...e-01, 1.8...e-02, 1.4...e-08],
       [9.7...e-01, 2.8...e-02, ...e-08]])
>>> clf.score(X, y)
0.97...
```

Vecinos más Cercanos (KNN)

KNN – K Vecinos más Cercanos

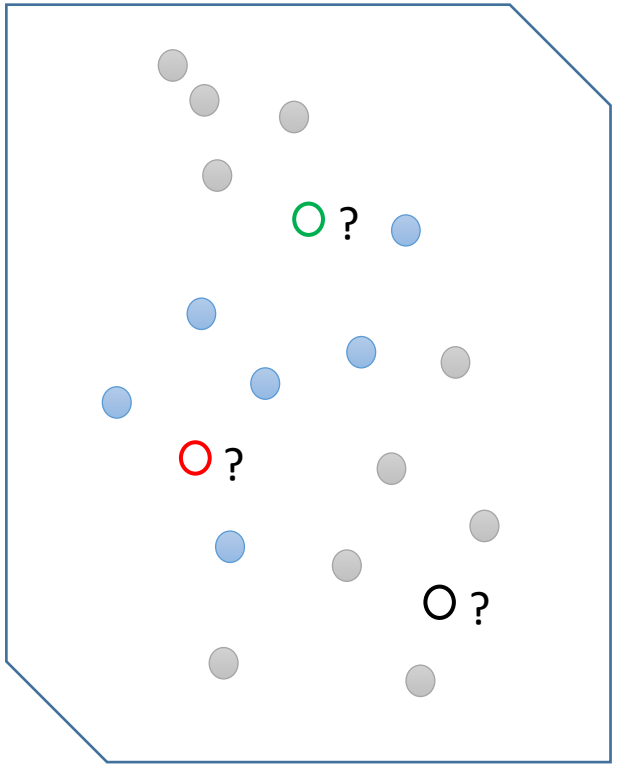
Requiere datos numéricos

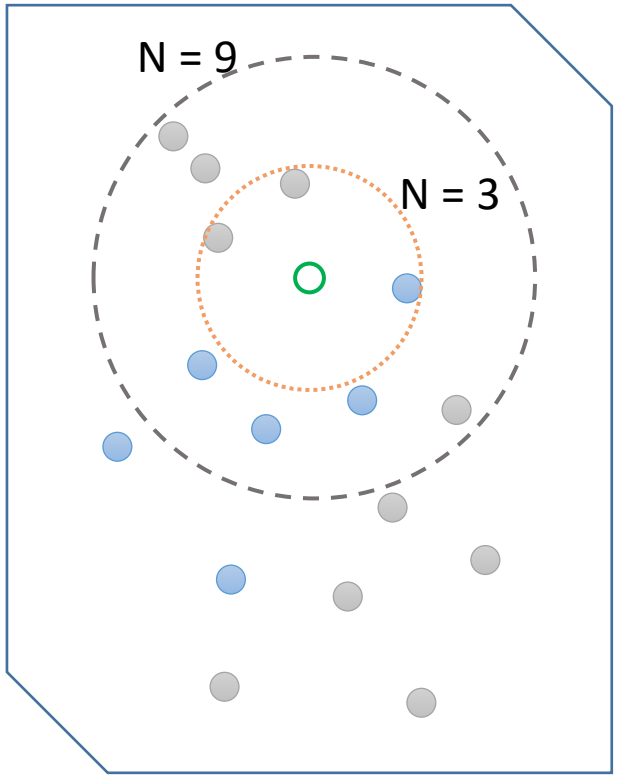
Los datos deben estar normalizados

Medida de distancia (Euclideana)

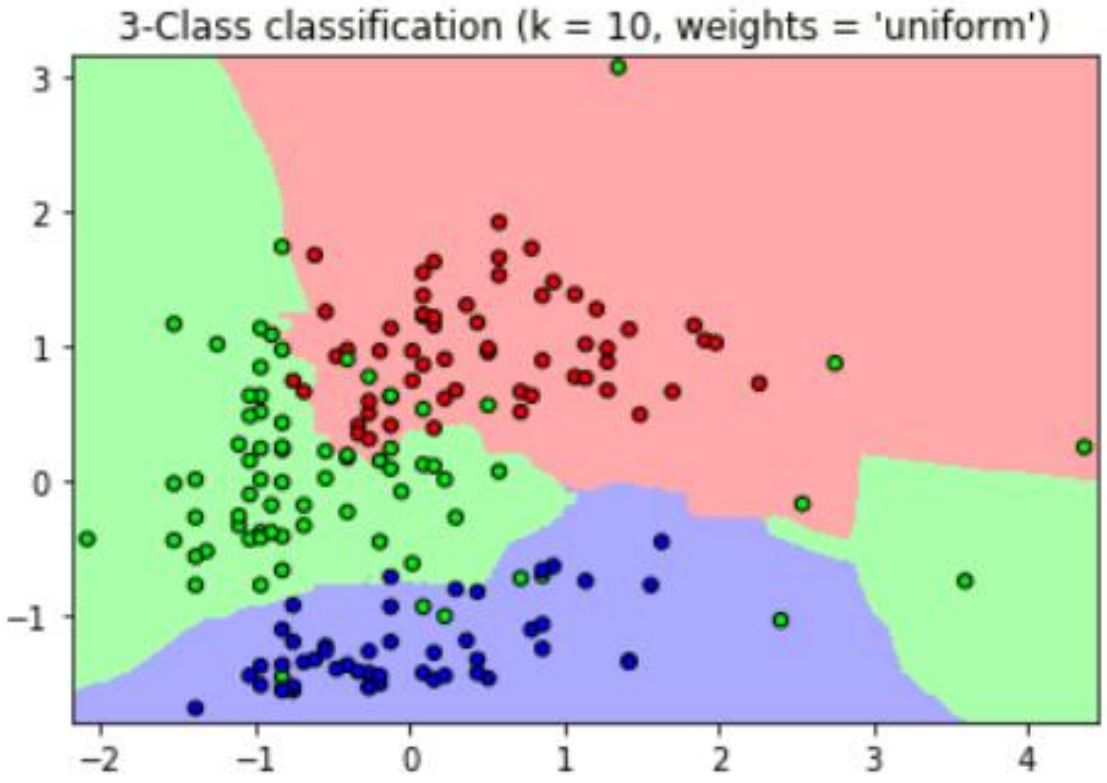
Se define la Cantidad de Vecinos

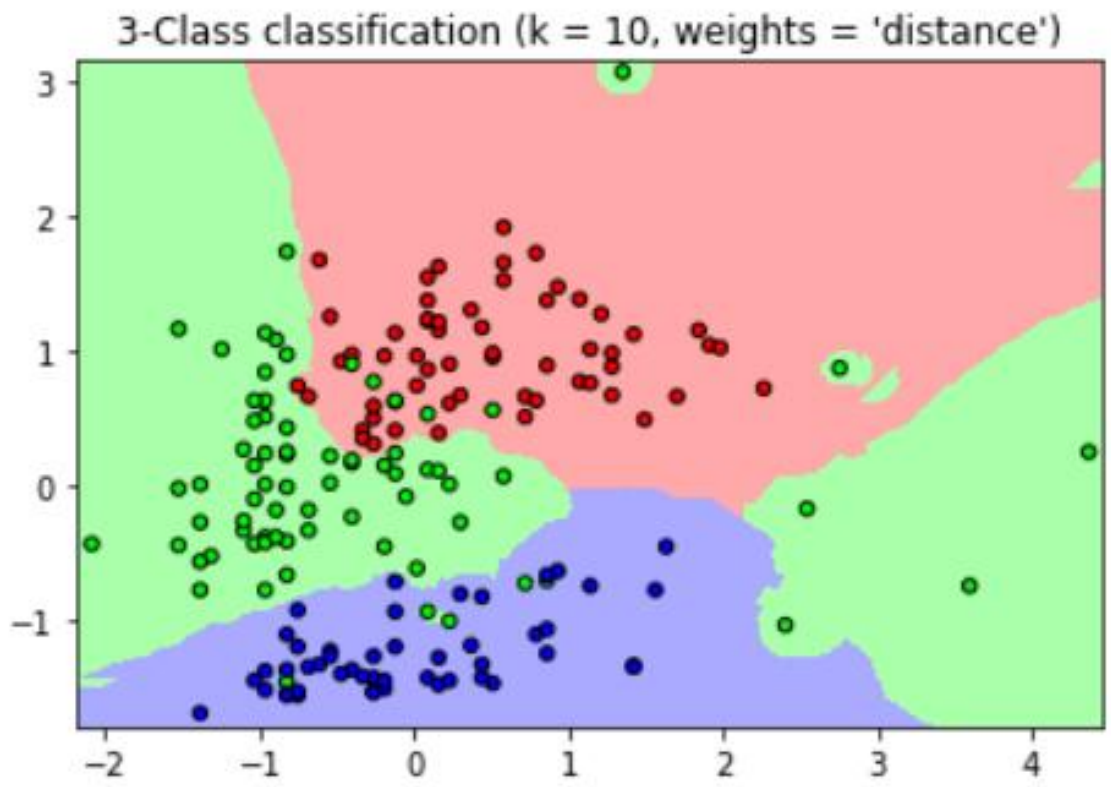
Se pueden dar “pesos” a los puntos



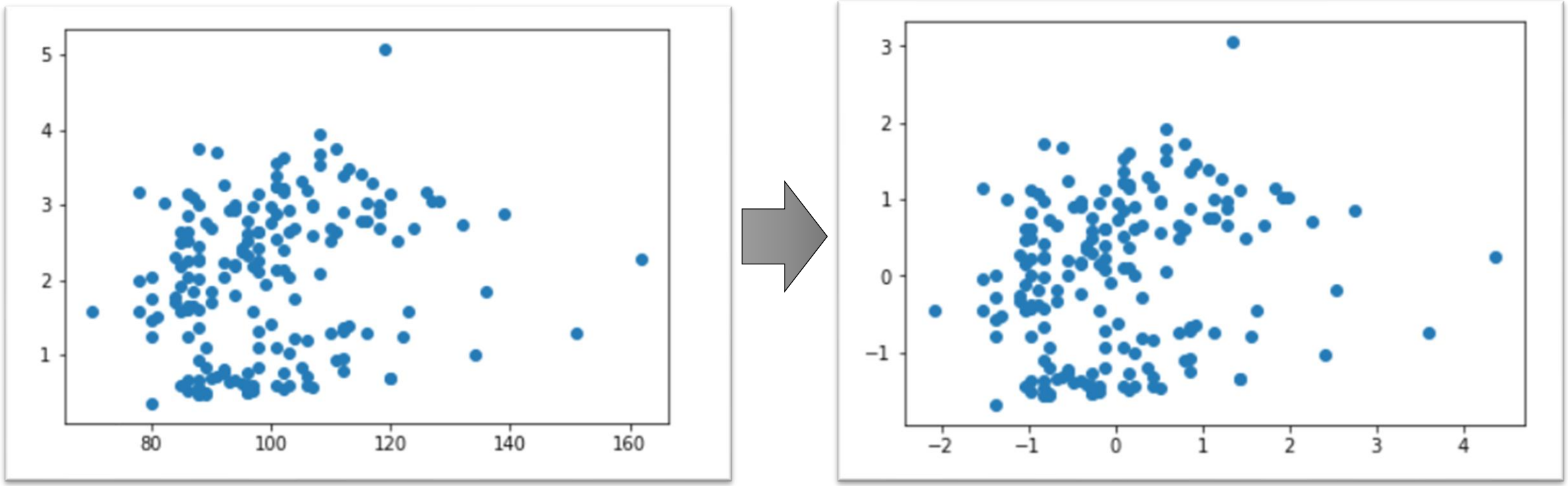


KNN – K Vecinos más Cercanos





KNN – K Vecinos más Cercanos



KNN – K Vecinos más Cercanos

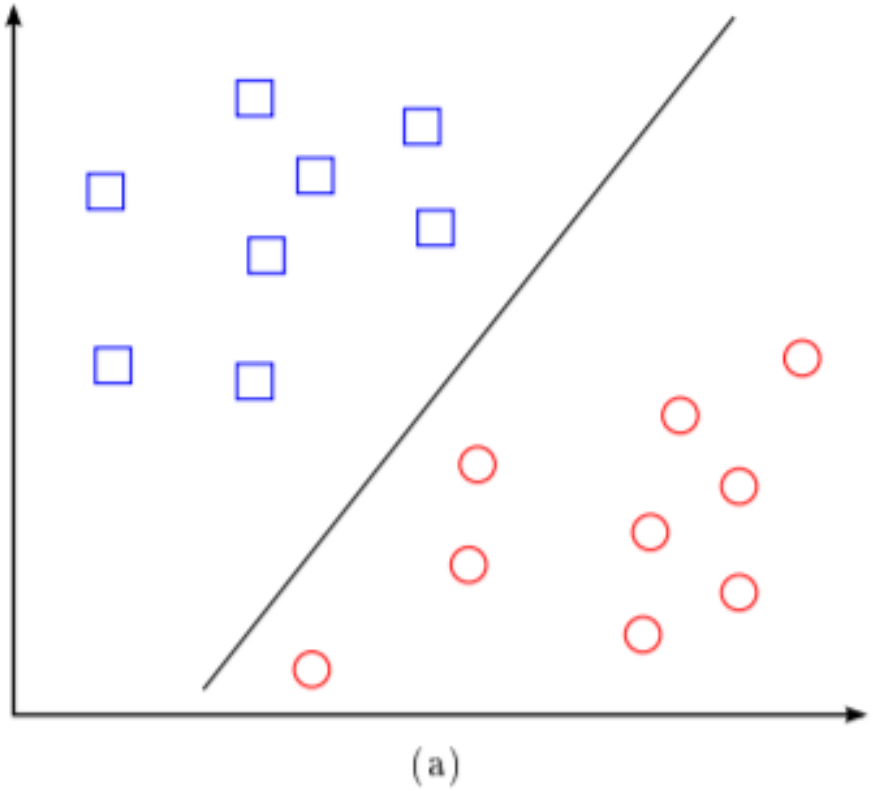
sklearn.neighbors.KNeighborsClassifier¶

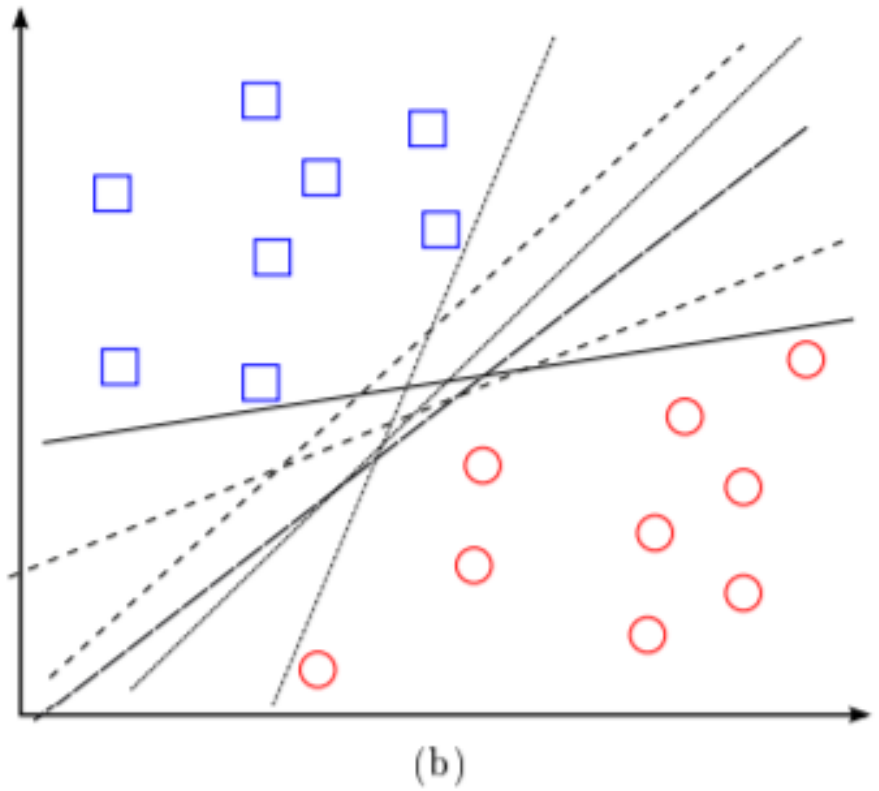
class sklearn.neighbors. **KNeighborsClassifier** (*n_neighbors=5, weights='uniform', algorithm='auto', leaf_size=30, p=2, metric='minkowski', metric_params=None, n_jobs=None, **kwargs*) [source]

```
>>> X = [[0], [1], [2], [3]]
>>> y = [0, 0, 1, 1]
>>> from sklearn.neighbors import KNeighborsClassifier
>>> neigh = KNeighborsClassifier(n_neighbors=3)
>>> neigh.fit(X, y)
KNeighborsClassifier(...)
>>> print(neigh.predict([[1.1]]))
[0]
>>> print(neigh.predict_proba([[0.9]]))
[[0.66666667 0.33333333]]
```

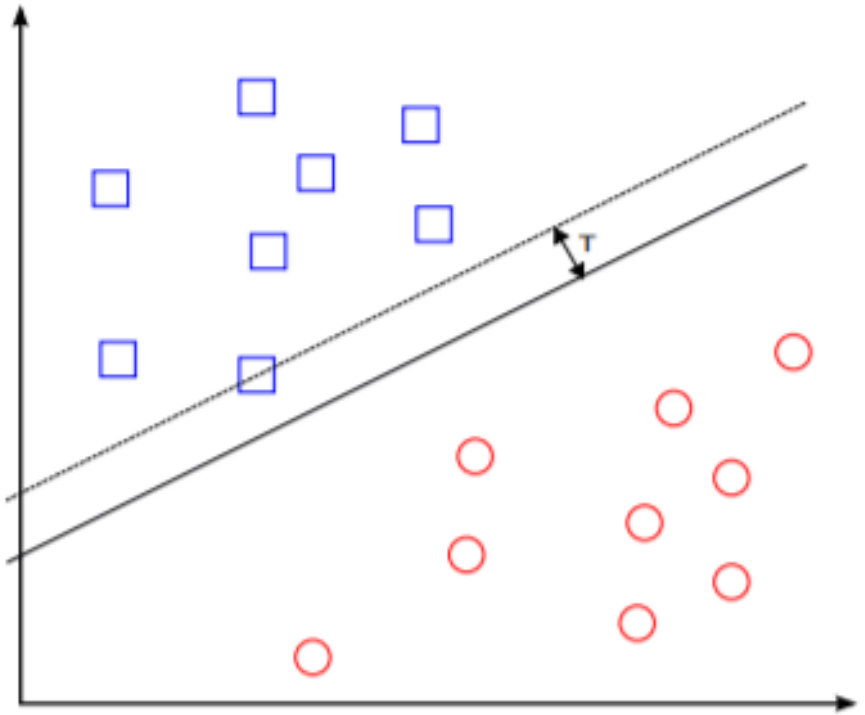
Support Vector Machine

Support Vector Machine

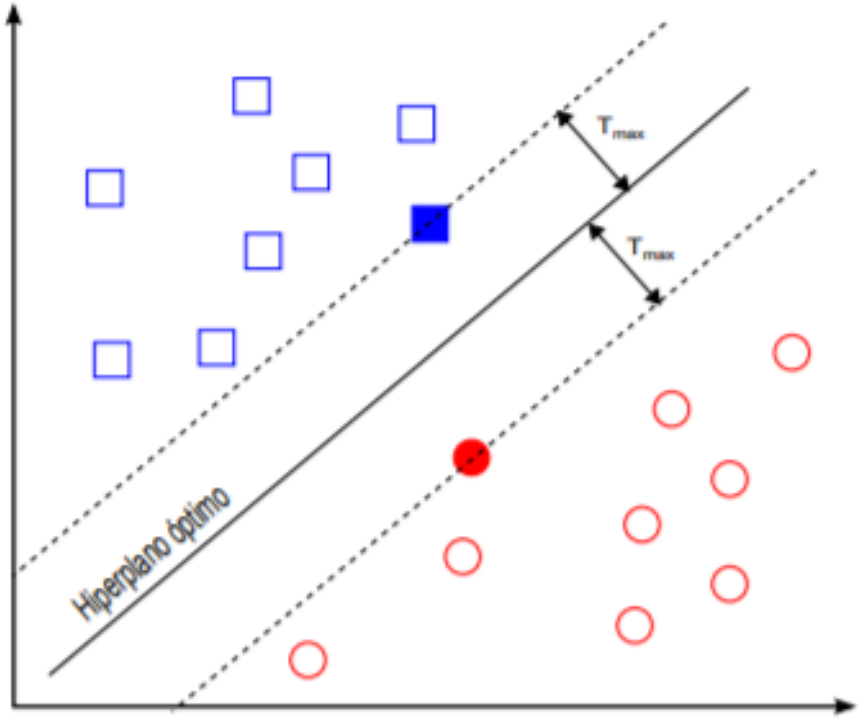




Support Vector Machine

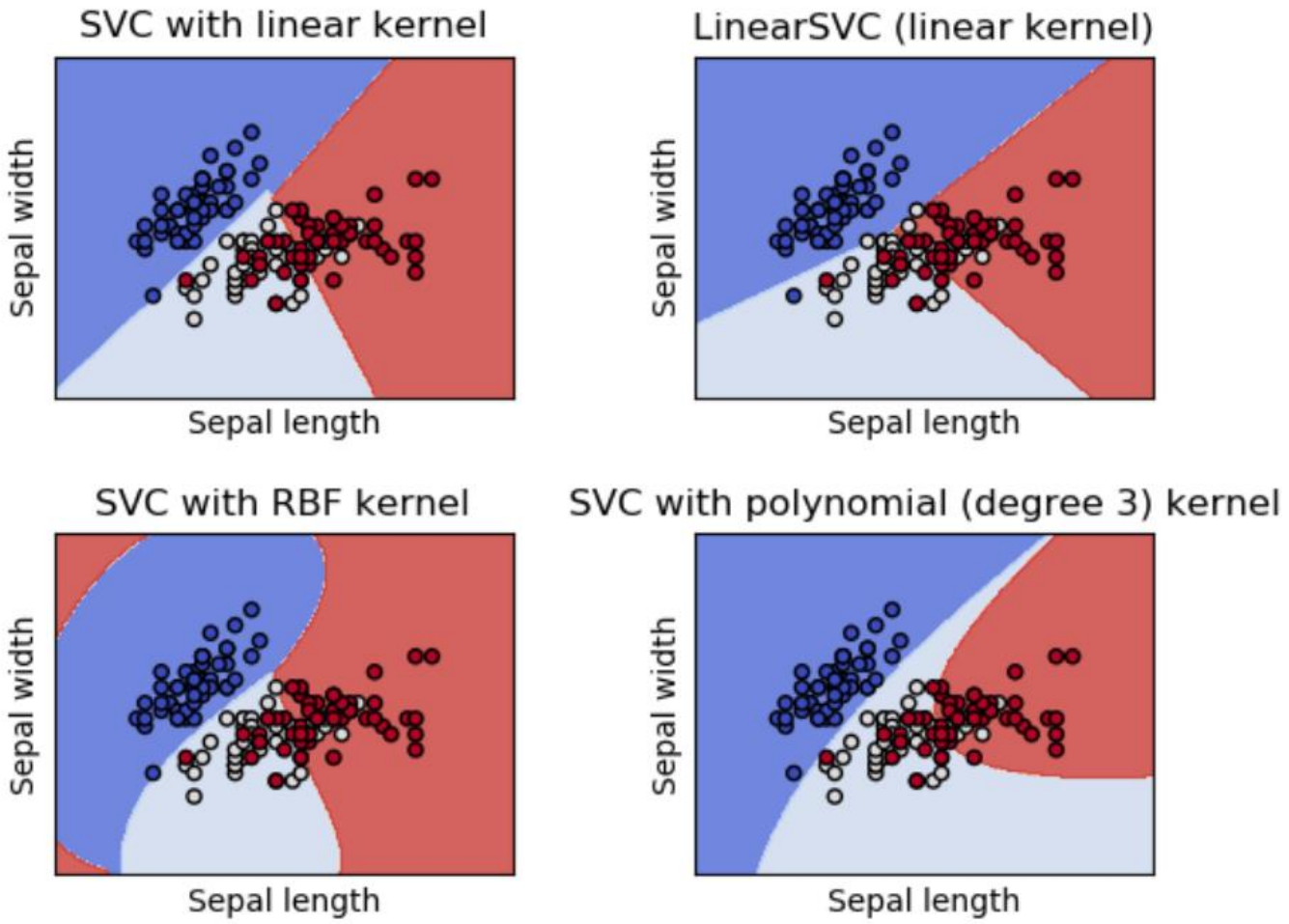


(a)



(b)

Support Vector Machine



Support Vector Machine

sklearn.svm.SVC

class sklearn.svm. **SVC** (*C=1.0, kernel='rbf', degree=3, gamma='auto_deprecated', coef0=0.0, shrinking=True, probability=False, tol=0.001, cache_size=200, class_weight=None, verbose=False, max_iter=-1, decision_function_shape='ovr', random_state=None*)

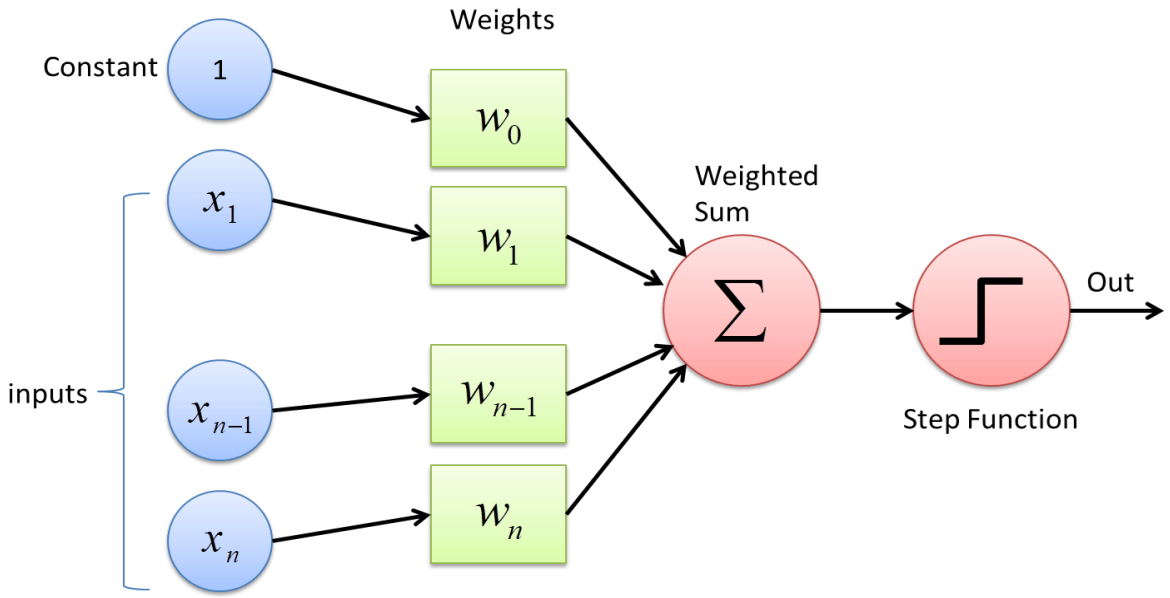
```
>>> from sklearn import svm
>>> X = [[0, 0], [1, 1]]
>>> y = [0, 1]
>>> clf = svm.SVC(gamma='scale')
>>> clf.fit(X, y)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='scale', kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
```

Modelos Avanzados

Redes Neuronales

Perceptrón

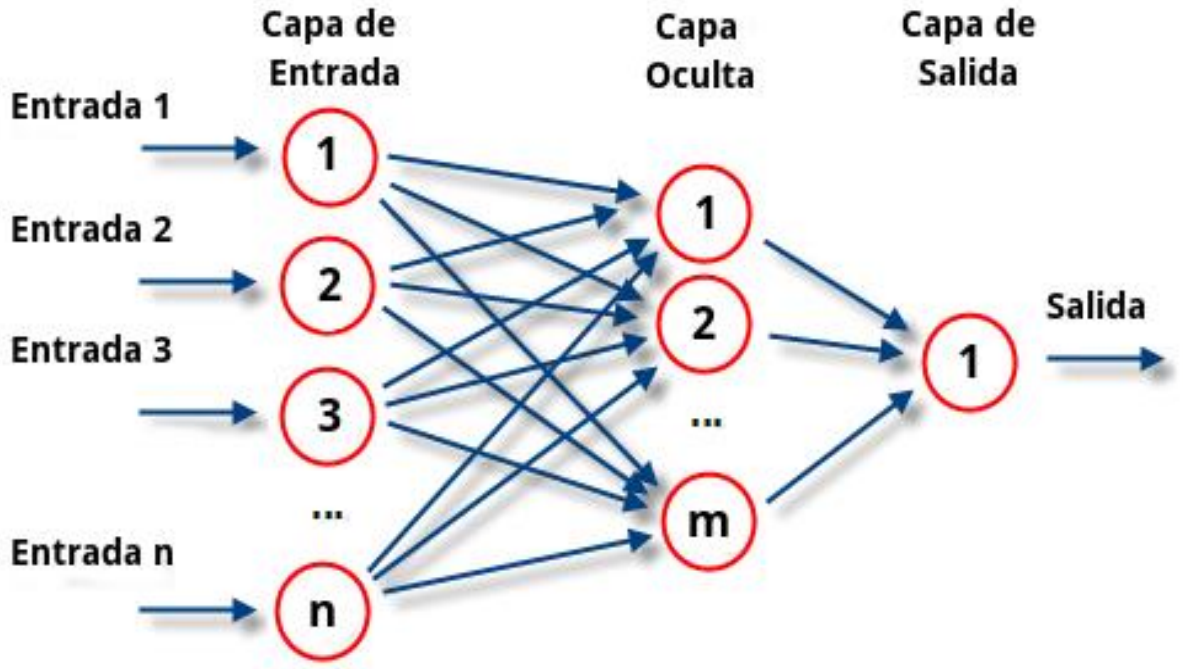
Es un algoritmo de Clasificación Lineal originado en los años 50s. Por cada “feature” tendremos una entrada al modelo y cada entrada se le asignará un “peso”. Una vez asignados los pesos se deberá sumar todas las entradas con sus pesos y determinar el valor de salida **(w*x+b).** El resultado se determina por la función de activación, que en el caso de ser binario resultará como 0 o 1 (en otros casos -1 o 1).



Perceptrón Multicapa (Multilayer Perceptron)

Si al modelo perceptrón le incorporamos capas intermedias entre la entrada y la salida obtenemos lo que comúnmente se llama “red neuronal con capas ocultas”.

El hecho de tener capas ocultas en el medio implica procesar la entrada con otro perceptrón lineal. Esta arquitectura permite poder captar patrones **no lineales.**



Perceptrón Multicapa (Multilayer Perceptron)

sklearn.neural_network.MLPClassifier

class sklearn.neural_network.**MLPClassifier**(*hidden_layer_sizes=(100,), activation='relu', *, solver='adam', alpha=0.0001, batch_size='auto', learning_rate='constant', learning_rate_init=0.001, power_t=0.5, max_iter=200, shuffle=True, random_state=None, tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True, early_stopping=False, validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08, n_iter_no_change=10, max_fun=15000*)

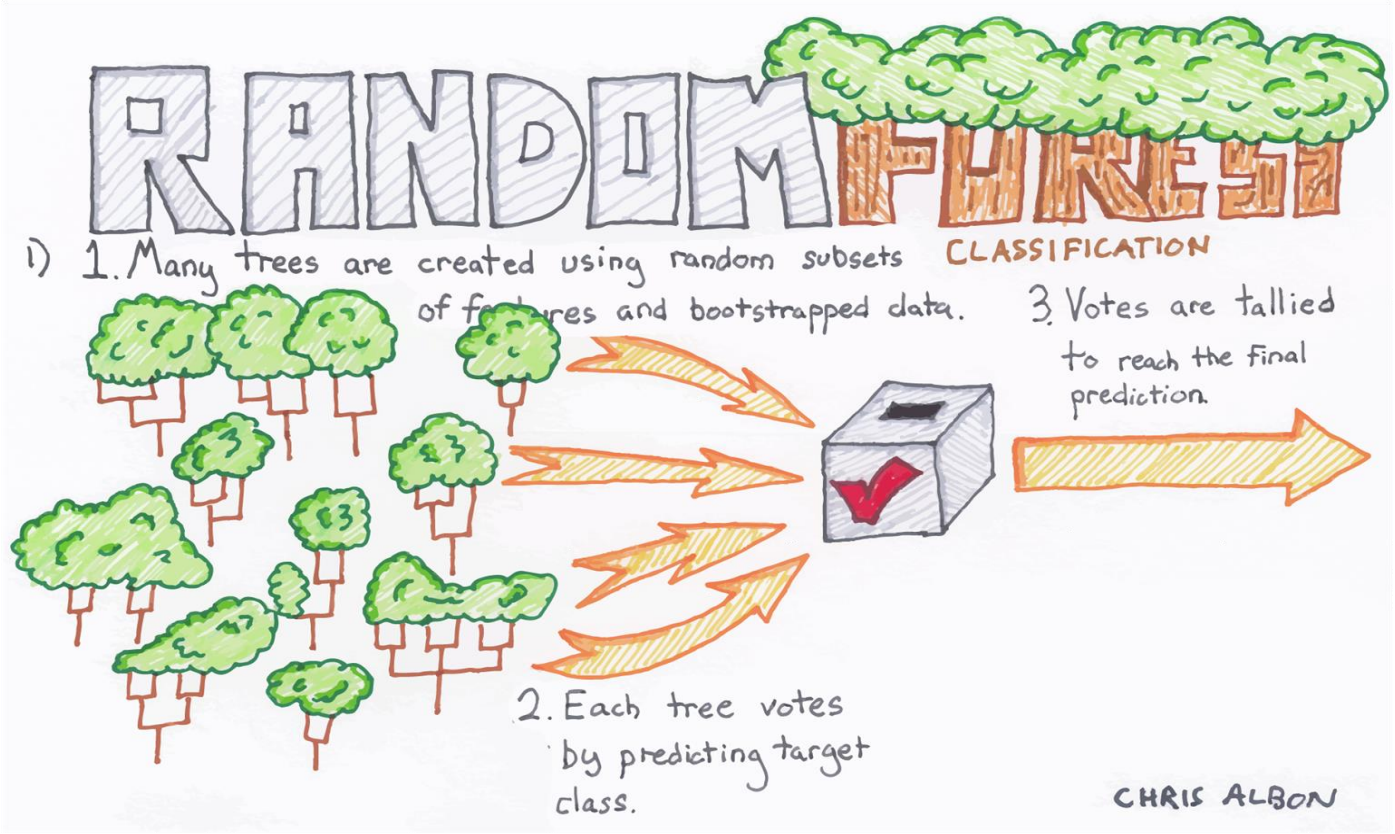
[source]

```
>>> from sklearn.neural_network import MLPClassifier
>>> from sklearn.datasets import make_classification
>>> from sklearn.model_selection import train_test_split
>>> X, y = make_classification(n_samples=100, random_state=1)
>>> X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y,
...                                                     random_state=1)
>>> clf = MLPClassifier(random_state=1, max_iter=300).fit(X_train, y_train)
>>> clf.predict_proba(X_test[:1])
array([[0.038..., 0.961...]])
>>> clf.predict(X_test[:5, :])
array([1, 0, 1, 0, 1])
>>> clf.score(X_test, y_test)
0.8...
```

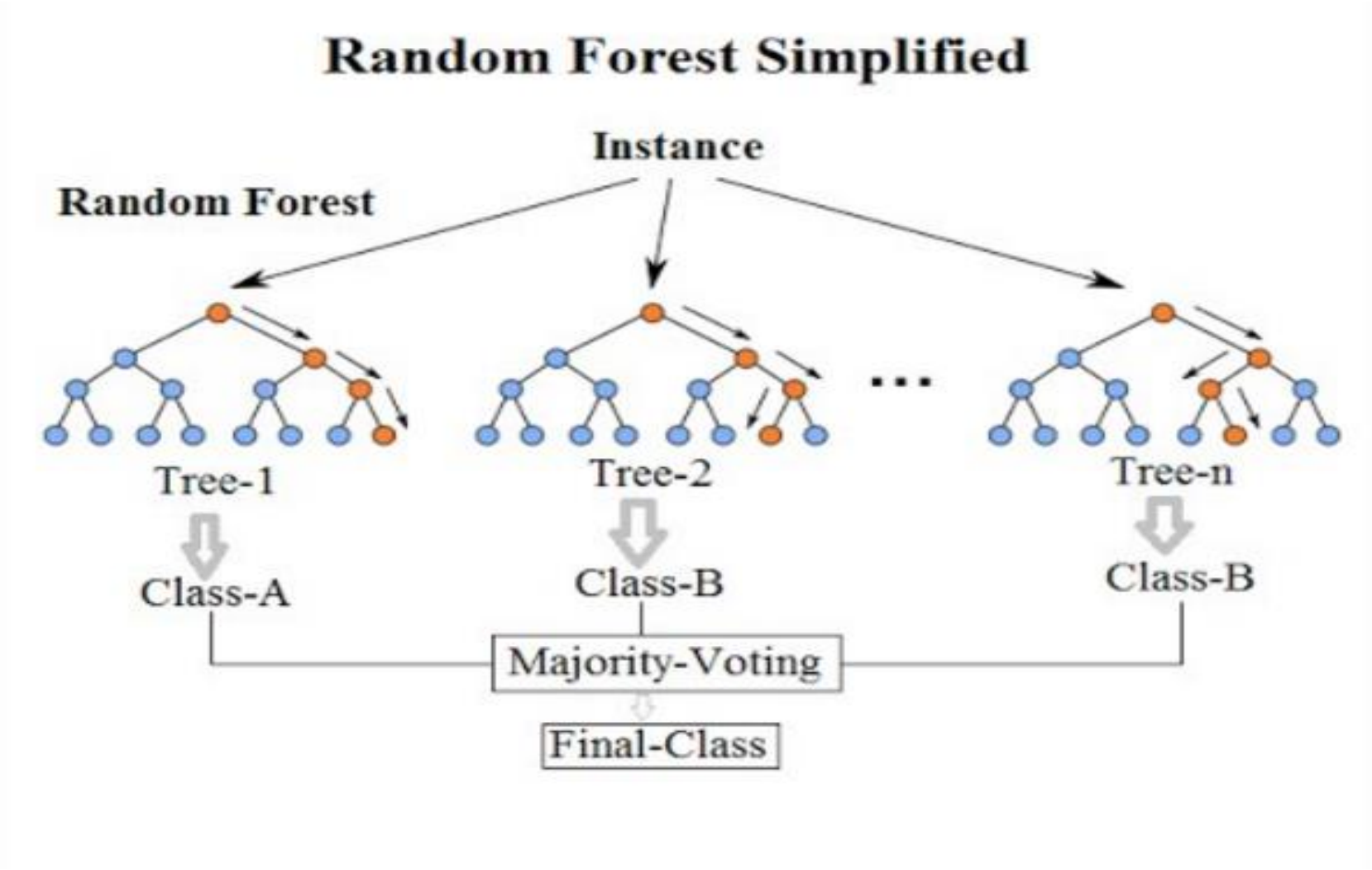
Bagging

Random Forest

Consiste en un conjunto de varios modelos de Decision Trees, todos realizan una predicciòn sobre un mismo dataset. La respuesta final contempla el resultado de todos los modelos, generando una respuesta mucho más robusta que un solo clasificador.



Random Forest



Random Forest

3.2.4.3.1. sklearn.ensemble.RandomForestClassifier

class sklearn.ensemble.**RandomForestClassifier**(*n_estimators=100, *, criterion='gini', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, bootstrap=True, oob_score=False, n_jobs=None, random_state=None, verbose=0, warm_start=False, class_weight=None, ccp_alpha=0.0, max_samples=None*) [source]

```
>>> from sklearn.ensemble import RandomForestClassifier
>>> from sklearn.datasets import make_classification
>>> X, y = make_classification(n_samples=1000, n_features=4,
...                            n_informative=2, n_redundant=0,
...                            random_state=0, shuffle=False)
>>> clf = RandomForestClassifier(max_depth=2, random_state=0)
>>> clf.fit(X, y)
RandomForestClassifier(...)
>>> print(clf.predict([[0, 0, 0, 0]]))
[1]
```

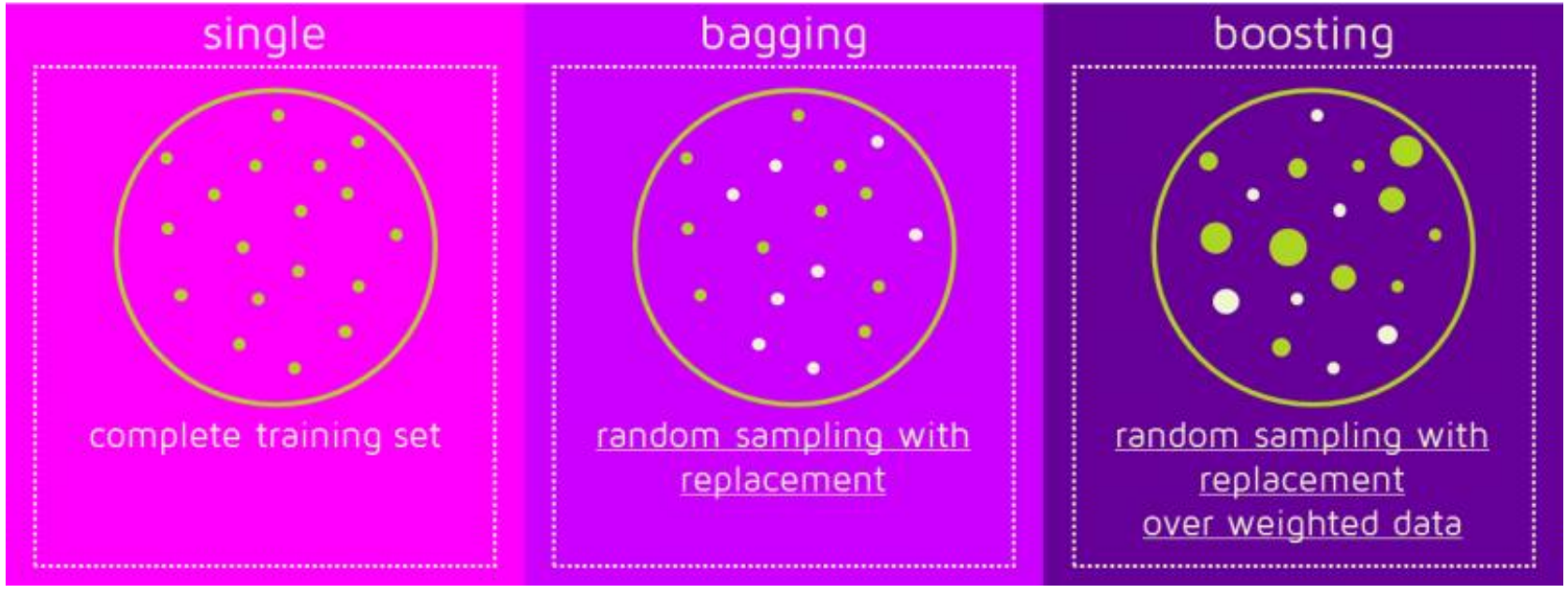
Boosting

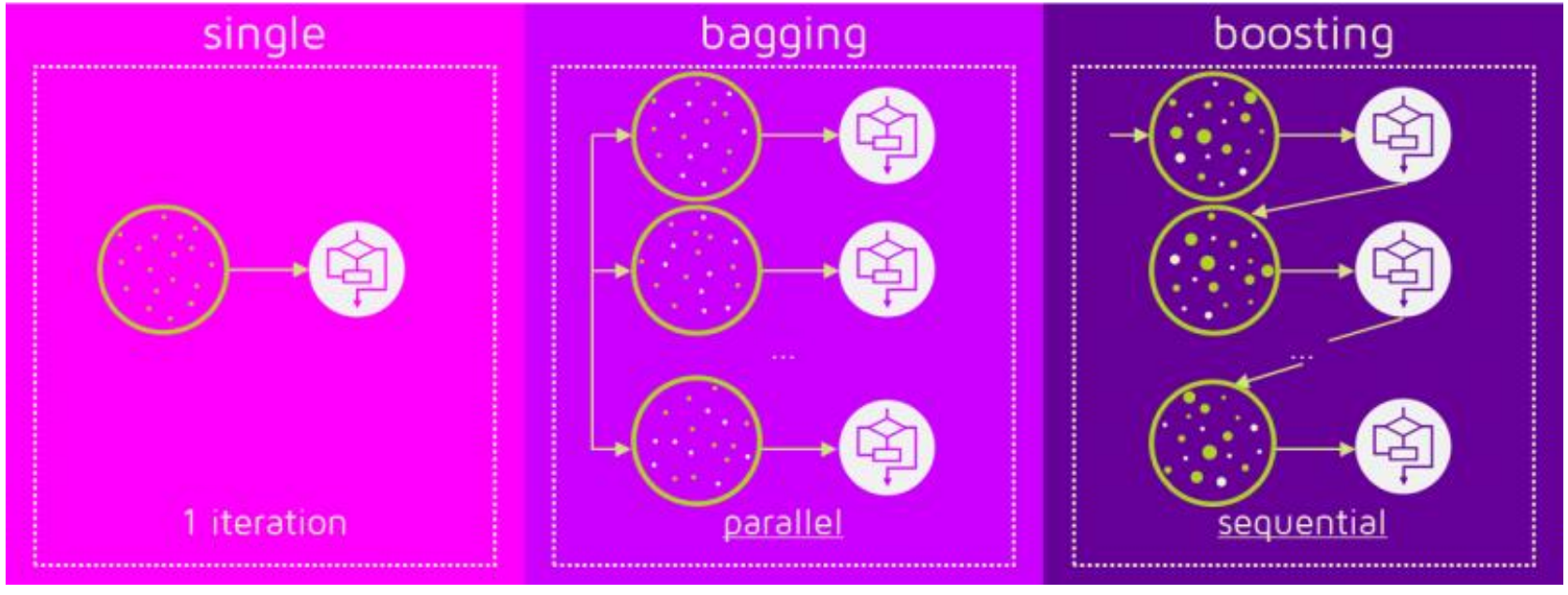
En qué consiste el Boosting?

El boosting consiste en combinar los resultados de varios clasificadores débiles para obtener un clasificador robusto.

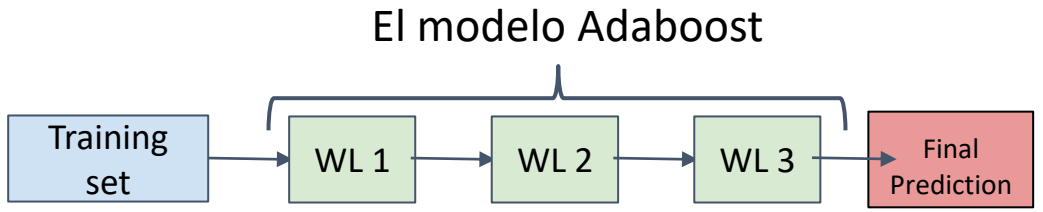
Cuando se añaden estos clasificadores débiles, se lo hace de modo que estos tengan diferente peso en función de la exactitud de sus predicciones.

Luego de que se añade un clasificador débil, los datos cambian su estructura de pesos: los casos que son mal clasificados ganan peso y los que son clasificados correctamente pierden peso.


single
bagging
boosting
complete training set
random sampling with replacement
random sampling with replacement over weighted data


single
bagging
boosting
1 iteration
parallel
sequential

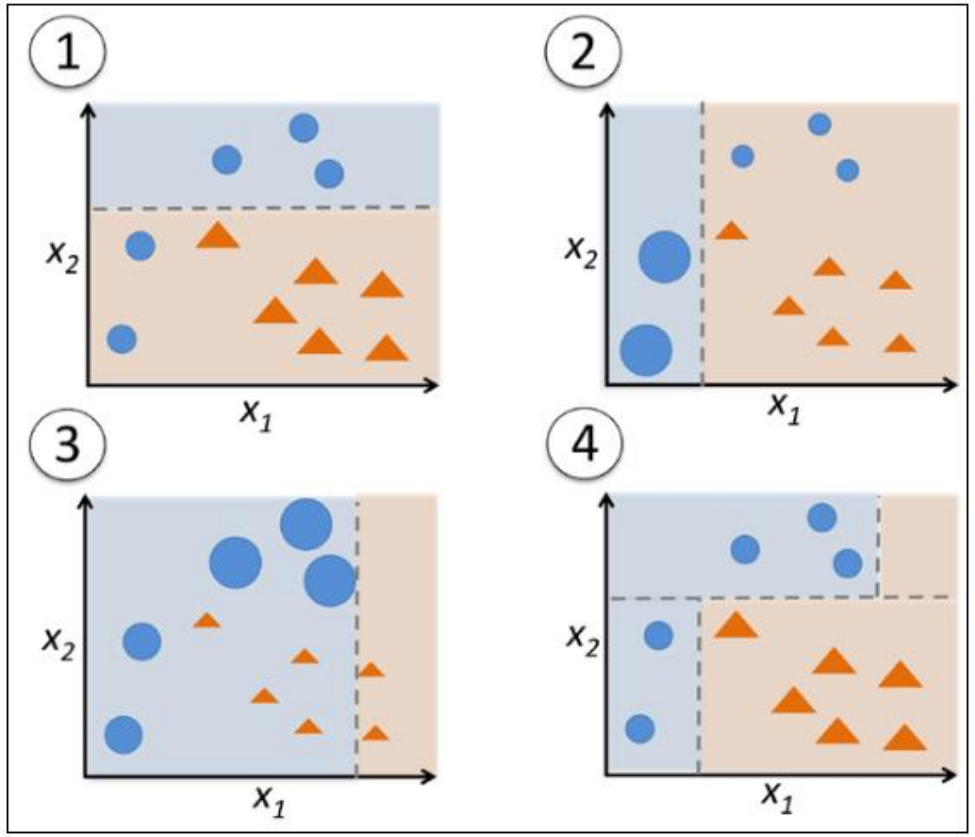
Adaboost



Construcción del algoritmo:

1. Elegir un “weak-learner”(árboles de bajo nivel)
2. Entrenarlo con todo el Training set
3. Identificar en qué instancias de entrenamiento la clasificación falla
4. Aprender de los errores: entrenar el siguiente “weak-learner” haciendo énfasis en las instancia de entrenamiento mal clasificadas
5. Repetir hasta conseguir el score deseado.

Modelo final: secuencia de “weak-learners “.



Adaboost

sklearn.ensemble.AdaBoostClassifier

class sklearn.ensemble.**AdaBoostClassifier**(*base_estimator=None, *, n_estimators=50, learning_rate=1.0, algorithm='SAMME.R', random_state=None*) ¶ [source]

```
>>> from sklearn.ensemble import AdaBoostClassifier
>>> from sklearn.datasets import make_classification
>>> X, y = make_classification(n_samples=1000, n_features=4,
...                            n_informative=2, n_redundant=0,
...                            random_state=0, shuffle=False)
>>> clf = AdaBoostClassifier(n_estimators=100, random_state=0)
>>> clf.fit(X, y)
AdaBoostClassifier(n_estimators=100, random_state=0)
>>> clf.predict([[0, 0, 0, 0]])
array([1])
>>> clf.score(X, y)
0.983...
```

Gradient Boosting

Descenso del Gradiente

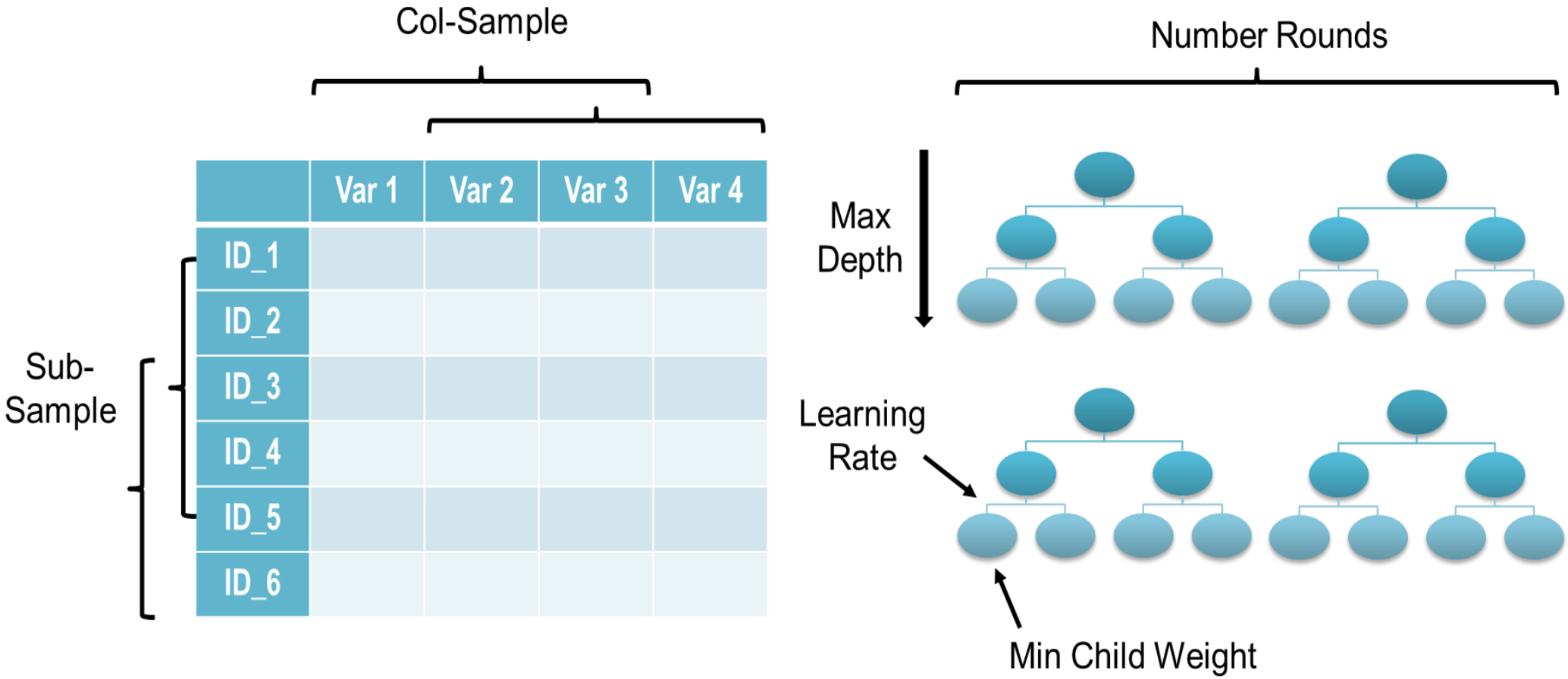
La idea de la potenciación del gradiente puede ser interpretado como un algoritmo de optimización en una función de coste adecuada.

Es decir, algoritmos que optimizan una función de coste sobre el espacio de función mediante la elección iterativa de una función (hipótesis débil) que apunta en la dirección del gradiente negativo.

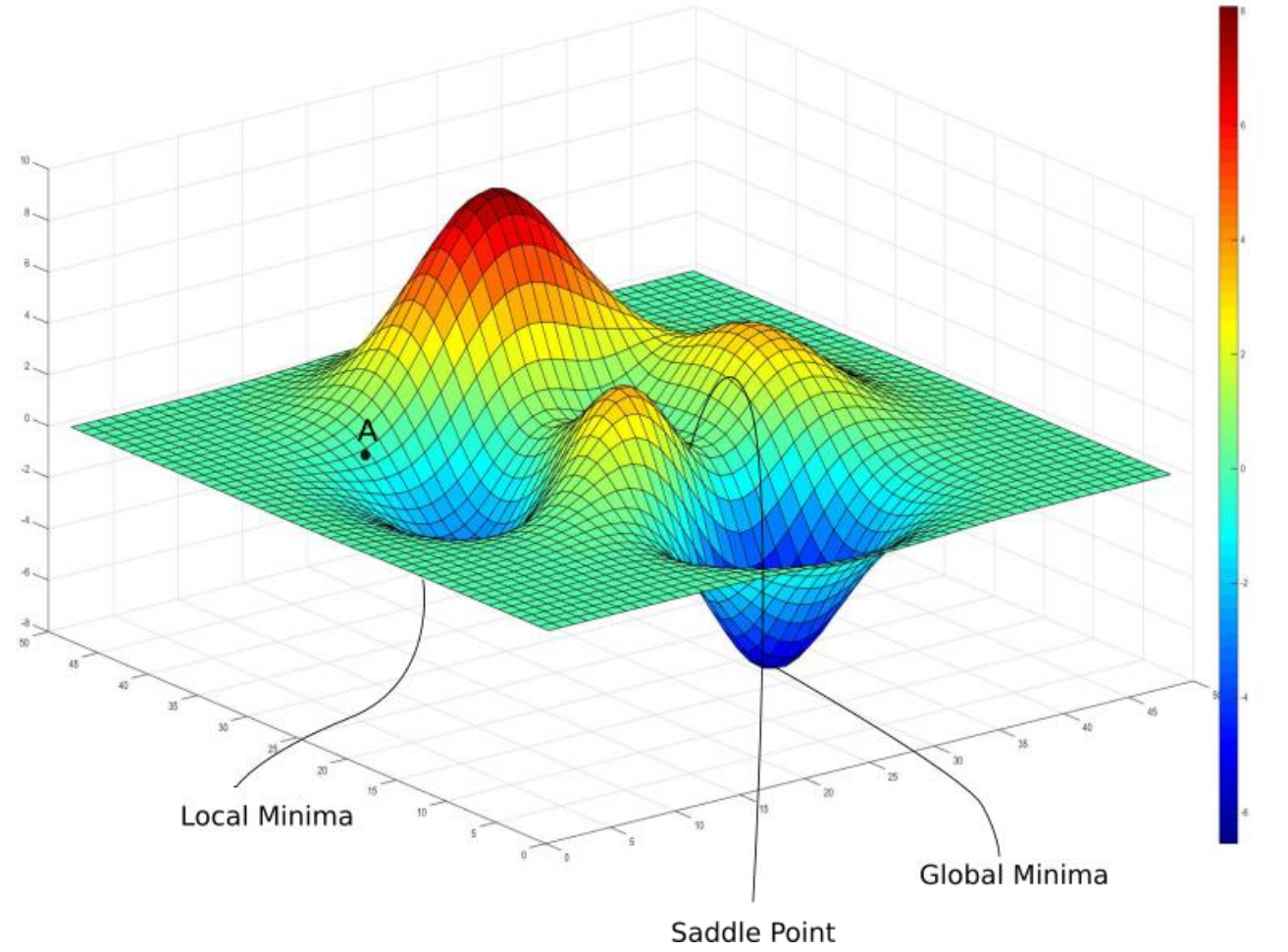
Imlementaciones Famosas:
XGBoost (DMLC)
LightGBM (Microsoft)

Ejemplo Visual: *http://arogozhnikov.github.io/2016/07/05/gradient_boosting_playground.html*

XGBoost – Definición de Parámetros



Graficar el Descenso del Gradiente



Gradient Boosting

sklearn.ensemble.HistGradientBoostingClassifier

class sklearn.ensemble.**HistGradientBoostingClassifier**(*loss='auto', *, learning_rate=0.1, max_iter=100, max_leaf_nodes=31, max_depth=None, min_samples_leaf=20, l2_regularization=0.0, max_bins=255, monotonic_cst=None, warm_start=False, early_stopping='auto', scoring='loss', validation_fraction=0.1, n_iter_no_change=10, tol=1e-07, verbose=0, random_state=None*) ¶

[source]

```
>>> # To use this experimental feature, we need to explicitly ask for it:
>>> from sklearn.experimental import enable_hist_gradient_boosting  # noqa
>>> from sklearn.ensemble import HistGradientBoostingClassifier
>>> from sklearn.datasets import load_iris
>>> X, y = load_iris(return_X_y=True)
>>> clf = HistGradientBoostingClassifier().fit(X, y)
>>> clf.score(X, y)
1.0
```

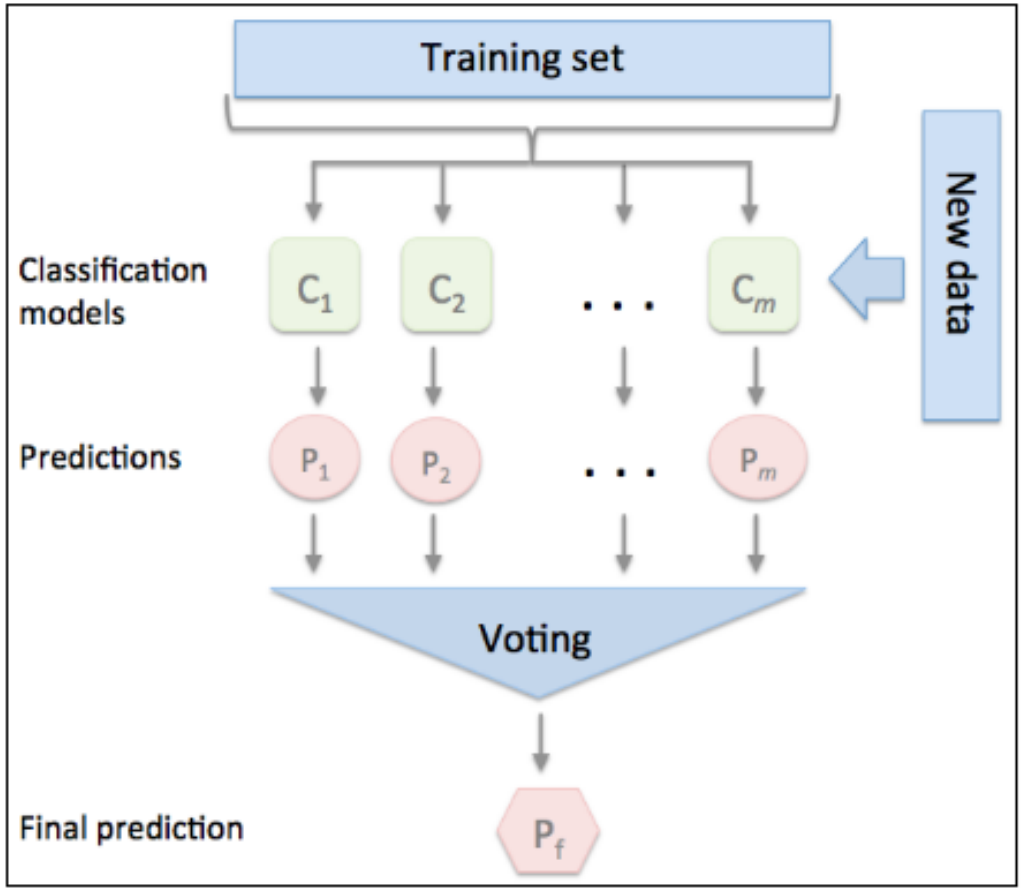
Ensembles de Modelos
Stacking

Stacking de modelos por votación

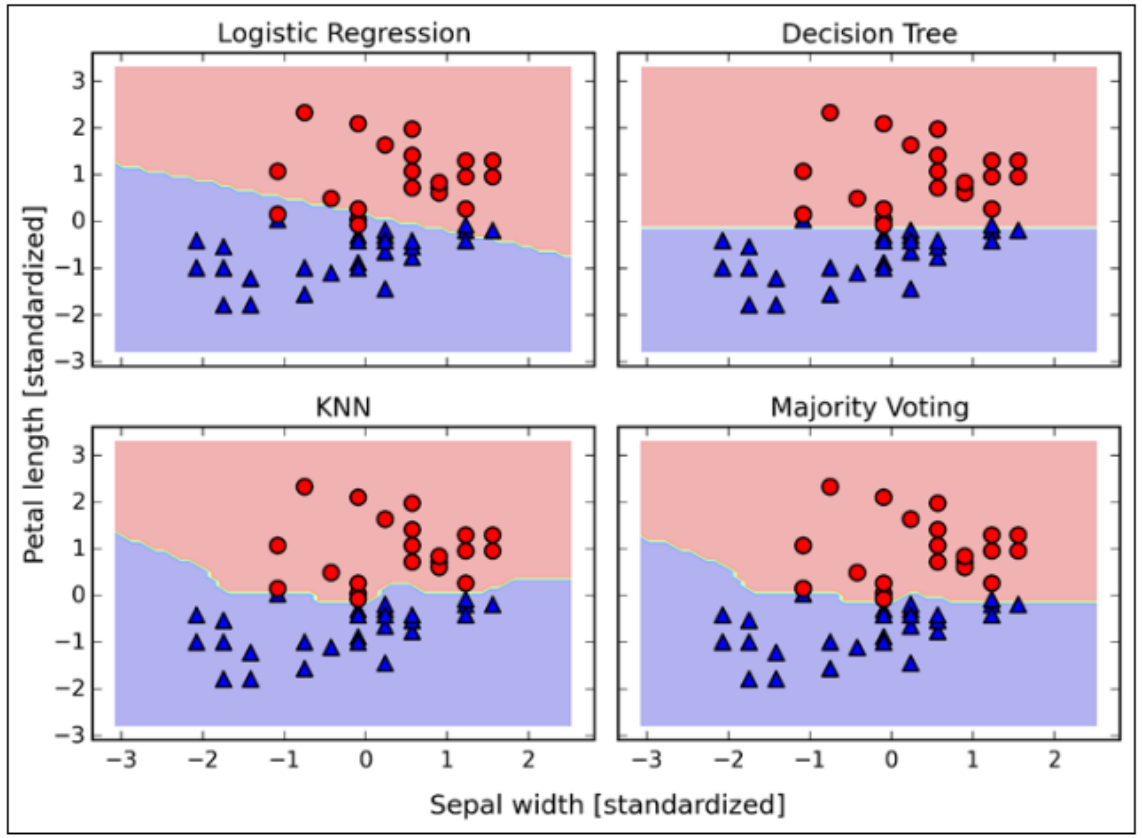
Construcción del algoritmo:

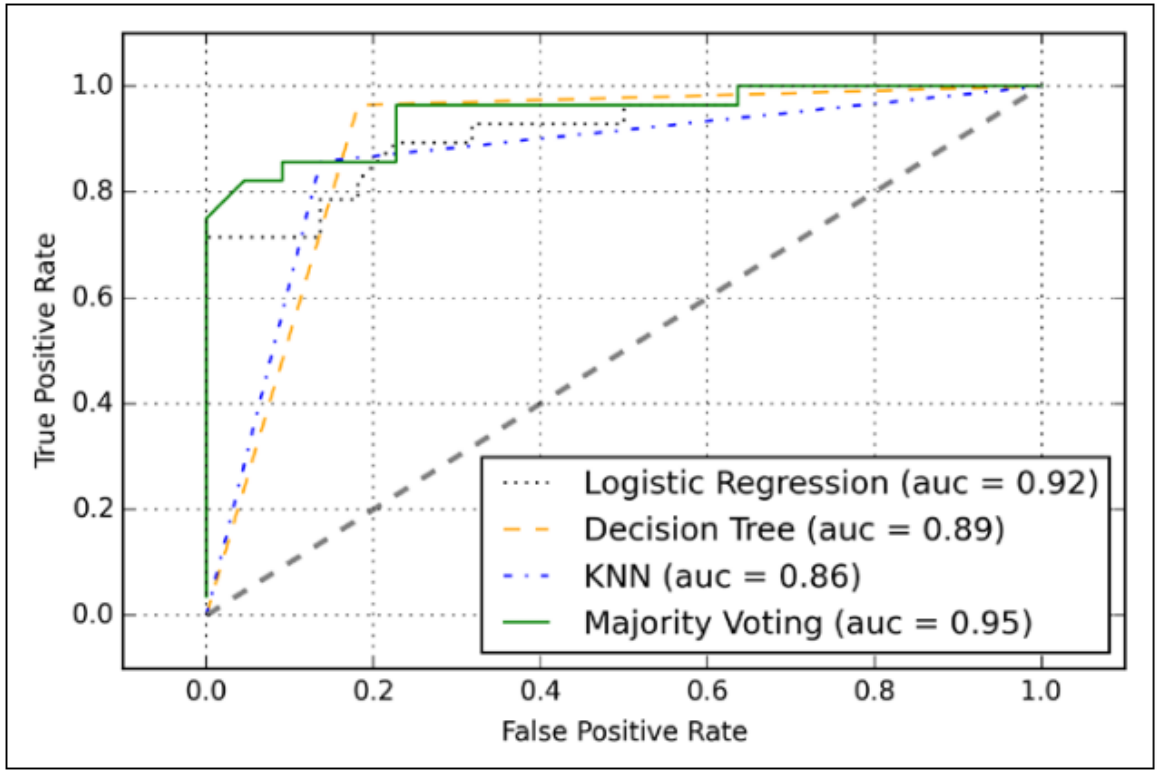
1. Elegir el número de clasificadores a combinar
2. Separar el Training set en m subconjuntos
3. Entrenar los m clasificadores, cada uno con un subconjunto del Training set

Predicción del ensemble: votación por mayoría



Ensemble de modelos por votación





Muchas Gracias!