DDA4210 Tutorial 1 beta

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1 DDA4210 Tutorial 1: Ensemble Learning

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2 Introduction to Ensemble Learning

The goal of ensemble methods is to combine the predictions of several base estimators built with a given learning algorithm in order to improve generalizability / robustness over a single estimator.

Two families of ensemble methods are usually distinguished:

• In averaging methods, the driving principle is to build several estimators independently and then to average their predictions. On average, the combined estimator is usually better than any of the single base estimator because its variance is reduced.

Examples: Bagging methods, Forests of randomized trees, ...

• By contrast, in boosting methods, base estimators are built sequentially and one tries to reduce the bias of the combined estimator. The motivation is to combine several weak models to produce a powerful ensemble.

Examples: AdaBoost, Gradient Tree Boosting, ...

3 Table of Contents

This assignment has 3 parts. You will learn some typical models of ensemble learning on sythetic and real-world datasets, which will help you understand the idea of ensemble learning better and prepare you for the mini-project. - 4 Bagging - 4.1 BaggingClassifier - 4.2 BaggingRegressor - 4.3 *Exercise* - 5 Random Forest - 5.1 RandomForestClassifier - 5.2 RandomForestRegressor - 5.3 *Exercise* - 6 Boosting - 6.1 AdaBoost - 6.2 Gradient Boosting - 6.3 *Exercise* - 7 Comparative Analysis (Optional)

4 Bagging Meta-Estimator

In ensemble algorithms, bagging methods form a class of algorithms which build several instances of a black-box estimator on random subsets of the original training set and then aggregate their individual predictions to form a final prediction. These methods are used as a way to reduce the variance of a base estimator (e.g., a decision tree).

In many cases, bagging methods constitute a very simple way to improve with respect to a single model, without making it necessary to adapt the underlying base algorithm.

Bagging methods come in many flavours but mostly differ from each other by the way they draw random subsets of the training set:

- When random subsets of the dataset are drawn as random subsets of the samples, then this algorithm is known as Pasting [B1999].
- When samples are drawn with replacement, then the method is known as Bagging [B1996].
- When random subsets of the dataset are drawn as random subsets of the features, then the method is known as Random Subspaces [H1998].
- Finally, when base estimators are built on subsets of both samples and features, then the method is known as Random Patches [LG2012].

In scikit-learn, bagging methods are offered as a unified BaggingClassifier meta-estimator (resp. BaggingRegressor), taking as input a user-specified estimator along with parameters specifying the strategy to draw random subsets. - In particular, max_samples and max_features control the size of the subsets (in terms of samples and features), - while bootstrap and bootstrap_features control whether samples and features are drawn with or without replacement. - When using a subset of the available samples the generalization accuracy can be estimated with the out-of-bag samples by setting oob_score=True.

4.1 BaggingClassifier

A Bagging classifier is an ensemble meta-estimator that fits base classifiers each on random subsets of the original dataset and then aggregate their individual predictions (either by voting or by averaging) to form a final prediction. Such a meta-estimator can typically be used as a way to reduce the variance of a black-box estimator (e.g., a decision tree), by introducing randomization into its construction procedure and then making an ensemble out of it.

4.2 BaggingRegressor

A Bagging regressor is an ensemble meta-estimator that fits base regressors each on random subsets of the original dataset and then aggregate their individual predictions (either by voting or by averaging) to form a final prediction. Such a meta-estimator can typically be used as a way to reduce the variance of a black-box estimator (e.g., a decision tree), by introducing randomization into its construction procedure and then making an ensemble out of it.

4.3 Exercise

```
# Baggging decision trees in 2d
# Based on https://github.com/ageron/handson-ml2/blob/master/06_decision_trees.
import numpy as np
import matplotlib.pyplot as plt
import os

try:
    from sklearn.metrics import accuracy_score
except ModuleNotFoundError:
    %pip install -qq scikit-learn
    from sklearn.metrics import accuracy_score
```

```
# TODO: Import BaggingClassifier and meta-estimator
pass
End of your code.
from matplotlib.colors import ListedColormap
from sklearn.model selection import train test split
from sklearn.datasets import make moons
X, y = make_moons(n_samples=500, noise=0.30, random_state=42)
X train, X test, y train, y test = train test_split(X, y, random_state=42)
def plot_decision_boundary(clf, X, y, axes=[-1.5, 2.45, -1, 1.5], alpha=0.5, u
⇔contour=True):
  x1s = np.linspace(axes[0], axes[1], 100)
  x2s = np.linspace(axes[2], axes[3], 100)
  x1, x2 = np.meshgrid(x1s, x2s)
  X_{new} = np.c_{x1.ravel(), x2.ravel()]
  y_pred = clf.predict(X_new).reshape(x1.shape)
  custom_cmap = ListedColormap(["#fafab0", "#9898ff", "#a0faa0"])
  plt.contourf(x1, x2, y_pred, alpha=0.3, cmap=custom_cmap)
  if contour:
     custom_cmap2 = ListedColormap(["#7d7d58", "#4c4c7f", "#507d50"])
     plt.contour(x1, x2, y_pred, cmap=custom_cmap2, alpha=0.8)
  plt.plot(X[:, 0][y == 0], X[:, 1][y == 0], "yo", alpha=alpha)
  plt.plot(X[:, 0][y == 1], X[:, 1][y == 1], "bs", alpha=alpha)
  plt.axis(axes)
  plt.xlabel(r"", fontsize=18)
  plt.ylabel(r"", fontsize=18, rotation=0)
# TODO: Instantiate DecisionTreeClassifier
pass
End of your code.
y_pred_tree = tree_clf.predict(X_test)
```

```
dtree_acc = accuracy_score(y_test, y_pred_tree)
# plt.figure()
plt.figure(figsize=(11,11)) # modified by me
plt.subplot(221) # modified by me
plot_decision_boundary(tree_clf, X, y)
plt.title("Decision Tree, test accuracy={:0.2f}".format(dtree_acc))
# plt.savefig("figures/dtree_bag_size0.pdf", dpi=300)
# plt.show()
bag_sizes = [10, 50, 100]
for i, bag_size in enumerate(bag_sizes): # modified by me
   bag_clf = BaggingClassifier(
      DecisionTreeClassifier(random_state=42),
      # TODO: Specify the number of meta estimators
      End of your code.
      ,max samples=100, bootstrap=True, random state=42
   )
   bag_clf.fit(X_train, y_train)
   y_pred = bag_clf.predict(X_test)
   bag_acc = accuracy_score(y_test, y_pred)
   # plt.figure()
   plt.subplot(222 + i) # modified by me
   plot_decision_boundary(bag_clf, X, y)
   plt.title("Bag of {} decision trees, test accuracy={:0.2f}".
 →format(bag_size, bag_acc))
   # plt.savefig("figures/dtree_bag_size{}.pdf".format(bag_size), dpi=300)
   # plt.show()
plt.show()
```

5 Random Forests

In random forests (see RandomForestClassifier and RandomForestRegressor classes), each tree in the ensemble is built from a sample drawn with replacement (i.e., a bootstrap sample) from the training set.

Furthermore, when splitting each node during the construction of a tree, the best split is found either from all input features or a random subset of size max_features. (See the parameter tuning guidelines for more details).

The purpose of these two sources of randomness is to decrease the variance of the forest estimator. Indeed, individual decision trees typically exhibit high variance and tend to overfit. The injected randomness in forests yield decision trees with somewhat decoupled prediction errors. By taking an average of those predictions, some errors can cancel out. Random forests achieve a reduced variance by combining diverse trees, sometimes at the cost of a slight increase in bias. In practice the variance reduction is often significant hence yielding an overall better model.

5.1 RandomForestClassifier

A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is controlled with the max_samples parameter if bootstrap=True (default), otherwise the whole dataset is used to build each tree.

5.2 RandomForestRegressor

A random forest is a meta estimator that fits a number of classifying decision trees on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is controlled with the max_samples parameter if bootstrap=True (default), otherwise the whole dataset is used to build each tree.

5.3 Exercise

```
[]: # This example shows the use of a forest of trees to evaluate the importance of \Box
    ⇔features on an artificial classification task.
    # The blue bars are the feature importances of the forest, along with their
     ⇔inter-trees variability represented by the error bars.
    # step 1: Data generation and model fitting
    # We generate a synthetic dataset with only 3 informative features.
    # We will explicitly not shuffle the dataset to ensure that the informative
     \hookrightarrow features will correspond to the three first columns of X.
    # In addition, we will split our dataset into training and testing subsets.
    import matplotlib.pyplot as plt
    from sklearn.datasets import make_classification
    from sklearn.model_selection import train_test_split
    X, y = make_classification(
       n samples=1000,
       n features=10,
       n informative=3,
       n redundant=0,
       n repeated=0,
       n_classes=2,
       random_state=0,
       shuffle=False,
    X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y,_
     →random_state=42)
    # TODO: Import RandomForestClassifier
    # A random forest classifier will be fitted to compute the feature importances.
    End of your code.
```

```
feature_names = [f"feature {i}" for i in range(X.shape[1])]
# TODO: Instantiate RandomForestClassifier
pass
End of your code.
forest.fit(X_train, y_train)
# step 2: Feature importance based on mean decrease in impurity
# Feature importances are provided by the fitted attribute feature importances
# and they are computed as the mean and standard deviation of accumulation of \Box
→ the impurity decrease within each tree.
import time
import numpy as np
start time = time.time()
# TODO: acquire the importance of features
pass
End of your code.
std = np.std([tree.feature_importances_ for tree in forest.estimators_], axis=0)
elapsed_time = time.time() - start_time
print(f"Elapsed time to compute the importances: {elapsed_time:.3f} seconds")
# Let's plot the impurity-based importance.
import pandas as pd
forest_importances = pd.Series(importances, index=feature_names)
fig, ax = plt.subplots()
forest_importances.plot.bar(yerr=std, ax=ax)
ax.set_title("Feature importances using MDI")
ax.set_ylabel("Mean decrease in impurity")
fig.tight_layout()
```

6 Boosting

The module sklearn ensemble includes the popular boosting algorithm AdaBoost, introduced in 1995 by Freund and Schapire [FS1995].

The core principle of AdaBoost is to fit a sequence of weak learners (i.e., models that are only slightly better than random guessing, such as small decision trees) on repeatedly modified versions of the data. The predictions from all of them are then combined through a weighted majority vote (or sum) to produce the final prediction. The data modifications at each so-called boosting iteration consist of applying weights $w_1, w_2, ..., w_N$ to each of the training samples. Initially, those weights are all set to $w_i = 1/N$, so that the first step simply trains a weak learner on the original data. For each successive iteration, the sample weights are individually modified and the learning algorithm is reapplied to the reweighted data. At a given step, those training examples that were incorrectly predicted by the boosted model induced at the previous step have their weights increased, whereas the weights are decreased for those that were predicted correctly. As iterations proceed, examples that are difficult to predict receive ever-increasing influence. Each subsequent weak learner is thereby forced to concentrate on the examples that are missed by the previous ones in the sequence [HTF].

6.1 AdaBoost

The following example shows how to fit an AdaBoost classifier with 100 weak learners:

Explanation of hyparameters: - The number of weak learners is controlled by the parameter n_estimators. - The learning_rate parameter controls the contribution of the weak learners in the final combination. - By default, weak learners are decision stumps. Different weak learners can be specified through the estimator parameter. - The main parameters to tune to obtain good results are n_estimators and the complexity of the base estimators (e.g., its depth max_depth or minimum required number of samples to consider a split min_samples_split).

6.2 Gradient Tree Boosting

Gradient Tree Boosting or Gradient Boosted Decision Trees (GBDT) is a generalization of boosting to arbitrary differentiable loss functions, see the seminal work of [Friedman2001]. GBDT is an accurate and effective off-the-shelf procedure that can be used for both regression and classification problems in a variety of areas including Web search ranking and ecology.

The module sklearn ensemble provides methods for both classification and regression via gradient boosted decision trees.

The usage and the parameters of GradientBoostingClassifier and GradientBoostingRegressor are described below. The 2 most important parameters of these estimators are n_estimators and learning_rate.

6.2.1 Classification

GradientBoostingClassifier supports both binary and multi-class classification. The following example shows how to fit a gradient boosting classifier with 100 decision stumps as weak learners:

Explanation of hyparameters: - The number of weak learners (i.e. regression trees) is controlled by the parameter n_estimators; - The size of each tree can be controlled either by setting the tree depth via max_depth or by setting the number of leaf nodes via max_leaf_nodes. - The learning_rate is a hyper-parameter in the range (0.0, 1.0] that controls overfitting via shrinkage

6.2.2 Regression

GradientBoostingRegressor supports a number of different loss functions for regression which can be specified via the argument loss; the default loss function for regression is squared error ('squared_error').

```
[]: import numpy as np from sklearn.metrics import mean_squared_error
```

6.3 Exercise

```
[]:  # feature importance using random forests on ,mnist
   # Based on https://qithub.com/ageron/handson-ml2/blob/master/06 decision trees.
    \hookrightarrow ipynb
   import numpy as np
   import matplotlib.pyplot as plt
   import matplotlib as mpl
   np.random.seed(42)
   X = np.random.rand(100, 1) - 0.5
   y = 3*X[:, 0]**2 + 0.05 * np.random.randn(100)
   try:
      from sklearn.tree import DecisionTreeRegressor
   except ModuleNotFoundError:
      %pip install -qq scikit-learn
      from sklearn.tree import DecisionTreeRegressor
   # TODO: Instantiate DecisionTreeRegressor
   pass
   End of your code.
```

```
tree_reg2 = DecisionTreeRegressor(max_depth=2, random_state=42)
# TODO: Intermediate step for boosting.
pass
End of your code.
tree reg3 = DecisionTreeRegressor(max depth=2, random state=42)
# TODO: Intermediate step for boosting.
End of your code.
def plot_predictions(regressors, X, y, axes, label=None, style="r-", __

data_style="b.", data_label=None):
  x1 = np.linspace(axes[0], axes[1], 500)
  y pred = sum(regressor.predict(x1.reshape(-1, 1)) for regressor in_
⇔regressors)
  plt.plot(X[:, 0], y, data_style, label=data_label)
  plt.plot(x1, y pred, style, linewidth=2, label=label)
  if label or data label:
     plt.legend(loc="upper center", fontsize=16)
  plt.axis(axes)
plt.figure(figsize=(11,11))
plt.subplot(321)
plot_predictions([tree_reg1], X, y, axes=[-0.5, 0.5, -0.1, 0.8], label="",__
⇔style="g-", data_label="Training set")
plt.ylabel("", fontsize=16, rotation=0)
plt.title("Residuals and tree predictions", fontsize=16)
plt.subplot(322)
plot_predictions([tree_reg1], X, y, axes=[-0.5, 0.5, -0.1, 0.8],
           label="", data_label="Training set")
plt.ylabel("", fontsize=16, rotation=0)
plt.title("Ensemble predictions", fontsize=16)
plt.subplot(323)
plot_predictions([tree_reg2], X, y2, axes=[-0.5, 0.5, -0.5, 0.5],
```

```
label="", style="g-", data_style="k+", data_label="Residuals")
plt.ylabel("", fontsize=16)
plt.subplot(324)
plot_predictions([tree_reg1, tree_reg2], X, y, axes=[-0.5, 0.5, -0.1, 0.8],
                 label="")
plt.ylabel("", fontsize=16, rotation=0)
plt.subplot(325)
plot_predictions([tree_reg3], X, y3, axes=[-0.5, 0.5, -0.5, 0.5],
                 label="", style="g-", data_style="k+")
plt.ylabel("", fontsize=16)
plt.xlabel("", fontsize=16)
plt.subplot(326)
plot_predictions([tree_reg1, tree_reg2, tree_reg3], X, y,
                 axes=[-0.5, 0.5, -0.1, 0.8],
                 label="")
plt.xlabel("", fontsize=16)
plt.ylabel("", fontsize=16, rotation=0)
# plt.savefig("figures/boosted_regr_trees.pdf", dpi=300)
plt.show()
```

7 Comparative analysis (Optional)

```
except ModuleNotFoundError:
    %pip install -qq scikit-learn
    from sklearn.metrics import accuracy_score
# omit numpy warnings (don't do it in real work)
np.seterr(divide="ignore", invalid="ignore")
np.warnings.filterwarnings("ignore")
# %matplotlib inline
# define plots common properties and color constants
plt.rcParams["font.family"] = "Arial"
plt.rcParams["axes.linewidth"] = 0.5
ORANGE, BLUE, PURPLE = "#FF8C00", "#0000FF", "#A020F0"
GRAY1, GRAY4, GRAY7 = "#231F20", "#646369", "#929497"
# we will calculate train and test error rates for all models
def error_rate(y_true, y_pred):
   return 1 - accuracy_score(y_true, y_pred)
"""Get. data"""
df = pd.read csv(
    "https://github.com/empathy87/
-The-Elements-of-Statistical-Learning-Python-Notebooks/blob/master/data/Spam.
⇔txt?raw=True"
)
df.head()
# PAGE 301. We coded spam as 1 and email as zero. A test set of size 1536 was
            randomly chosen, leaving 3065 observations in the training set.
target = "spam"
columns = [
    "word_freq_make",
    "word_freq_address",
    "word_freq_all",
    "word_freq_3d",
    "word_freq_our",
    "word_freq_over",
    "word_freq_remove",
    "word_freq_internet",
    "word_freq_order",
    "word_freq_mail",
    "word_freq_receive",
    "word_freq_will",
    "word_freq_people",
```

```
"word_freq_report",
    "word_freq_addresses",
    "word_freq_free",
    "word_freq_business",
    "word_freq_email",
    "word_freq_you",
    "word_freq_credit",
    "word_freq_your",
    "word_freq_font",
    "word_freq_000",
    "word_freq_money",
    "word_freq_hp",
    "word_freq_hpl",
    "word_freq_george",
    "word_freq_650",
    "word_freq_lab",
    "word_freq_labs",
    "word_freq_telnet",
    "word_freq_857",
    "word_freq_data",
    "word_freq_415",
    "word_freq_85",
    "word_freq_technology",
    "word freq 1999",
    "word_freq_parts",
    "word_freq_pm",
    "word_freq_direct",
    "word_freq_cs",
    "word_freq_meeting",
    "word_freq_original",
    "word_freq_project",
    "word_freq_re",
    "word_freq_edu",
    "word_freq_table",
    "word_freq_conference",
    "char_freq_;",
    "char_freq_(",
    "char_freq_[",
    "char freq !",
    "char_freq_$",
    "char_freq_#",
    "capital_run_length_average",
    "capital_run_length_longest",
    "capital_run_length_total",
# let's give columns more compact names
features = [
```

```
"make",
"address",
"all",
"3d",
"our",
"over",
"remove",
"internet",
"order",
"mail",
"receive",
"will",
"people",
"report",
"addresses",
"free",
"business",
"email",
"you",
"credit",
"your",
"font",
"000",
"money",
"hp",
"hpl",
"george",
"650",
"lab",
"labs",
"telnet",
"857",
"data",
"415",
"85",
"technology",
"1999",
"parts",
"pm",
"direct",
"cs",
"meeting",
"original",
"project",
"re",
"edu",
"table",
```

```
"conference",
   "ch_;",
   "ch(",
   "ch[",
   "ch!",
   "ch$",
   "ch#",
   "CAPAVE",
   "CAPMAX",
   "CAPTOT",
]
X, y = df[columns].values, df[target].values
# split by test column value
is_test = df.test.values
X_train, X_test = X[is_test == 0], X[is_test == 1]
y_train, y_test = y[is_test == 0], y[is_test == 1]
""" Logistic regression
As a sanity check, we try to match p301 test error rate of 7.6%.
11 11 11
try:
   import statsmodels.api as sm
except ModuleNotFoundError:
   %pip install -qq statsmodels
   import statsmodels.api as sm
from sklearn.metrics import accuracy_score
lr_clf = sm.Logit(y_train, sm.add_constant(X_train)).fit(disp=False)
# 0.5 is a threshold
y_test_hat = (lr_clf.predict(sm.add_constant(X_test)) > 0.5).astype(int)
lr_error_rate = error_rate(y_test, y_test_hat)
print(f"Logistic Regression Test Error Rate: {lr_error_rate*100:.1f}%")
# PAGE 590. A random forest classifier achieves 4.88% misclassification error
           on the spam test data, which compares well with all other methods,
           and is not significantly worse than gradient boosting at 4.5%.
ntrees list = [10, 50, 100, 200, 300, 400, 500]
# TODO: Import RandomForestClassifier
```

```
pass
End of your code.
rf_errors = []
for ntrees in ntrees list:
  # TODO: Instantiate RandomForestClassifier
  pass
  End of your code.
  y_test_hat = rf_clf.predict(X_test)
  rf_error_rate = error_rate(y_test, y_test_hat)
  rf_errors.append(rf_error_rate)
  print(f"RF {ntrees} trees, test error {rf_error_rate*100:.1f}%")
try:
  from catboost import CatBoostClassifier, Pool, cv
except ModuleNotFoundError:
  %pip install -qq catboost
  from catboost import CatBoostClassifier, Pool, cv
boost_errors = []
for ntrees in ntrees list:
  # TODO: Instantiate CatBoostClassifier
  End of your code.
  y_test_hat = boost_clf.predict(X_test)
  boost_error_rate = error_rate(y_test, y_test_hat)
  boost errors.append(boost error rate)
  print(f"Boosting {ntrees} trees, test error {boost_error_rate*100:.1f}%")
from sklearn.ensemble import BaggingClassifier
bag_errors = []
for ntrees in ntrees_list:
  # TODO: Instantiate BaggingClassifier
```

```
pass
   End of your code.
   y_test_hat = bag_clf.predict(X_test)
  bag_error_rate = error_rate(y_test, y_test_hat)
  bag errors.append(bag error rate)
  print(f"Bagged {ntrees} trees, test error {bag_error_rate*100:.1f}%")
plt.figure()
plt.plot(ntrees_list, rf_errors, "o-", color="blue", label="RF")
plt.plot(ntrees_list, boost_errors, "x-", color="green", label="Boosting")
plt.plot(ntrees_list, bag_errors, "^-", color="orange", label="Bagging")
plt.legend()
plt.xlabel("Number of trees")
plt.ylabel("Test error")
plt.tight_layout()
# plt.savefig("figures/spam_tree_ensemble_compare.pdf", dpi=300)
plt.show()
```

8 Recommended Materials

8.1 Gradient Boosting regression

A tutorial on gradient boosting regression can help you roughly understand a relatively complete process of ensemble learning.

8.2 Categorical Feature Support in Gradient Boosting

This tutorial compares the training times and prediction performances of HistGradientBoostingRegressor with different encoding strategies for categorical features.

8.3 Histogram-Based Gradient Boosting

Scikit-learn 0.21 introduced two new implementations of gradient boosting trees, namely HistGradientBoostingClassifier and HistGradientBoostingRegressor, inspired by LightGBM (See [Light-GBM]).

These histogram-based estimators can be **orders of magnitude faster** than GradientBoosting-Classifier and GradientBoostingRegressor when the number of samples is larger than tens of thousands of samples.

They also have built-in support for missing values, which avoids the need for an imputer.

The API of these estimators is slightly different, and some of the features from GradientBoosting-Classifier and GradientBoostingRegressor are not yet supported, for instance some loss functions.

9 References

- 1. Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., ... & Duchesnay, E. (2011). Scikit-learn: Machine learning in Python. the Journal of machine Learning research, 12, 2825-2830.
- 2. Murphy, K. P. (2022). Probabilistic machine learning: an introduction. MIT press.

[]: