BCMF

[1]:
```
if 'google.colab' in str(get_ipython()):
    print("Running on Google Colab")
    from google.colab import drive
    drive.mount('/content/drive')

    #===== FIX THIS PATH =====
    %cd "/content/drive/My Drive/[PATH TO PROJECT FOLDER ON GDRIVE]"
    #===== FIX THIS PATH =====

    %pip install imblearn # Used for resampling dataset (not pre-installed on Colab)
else:
    print("Not running on Google Colab")
```

```
Not running on Google Colab
```

1 Utility code

[2]:
```
import pandas as pd
import seaborn as sns
import os.path
import pickle
from sklearn.model_selection import StratifiedKFold, GridSearchCV
from sklearn.metrics import classification_report, confusion_matrix, ConfusionMatrixDisplay
from IPython.display import display, Image
```

```python
import sklearn
import matplotlib.pyplot as plt
import numpy as np

print(f'The scikit-learn version is {sklearn.__version__}')
```

```
The scikit-learn version is 1.2.2
```

[3]:

```python
RANDOM_STATE = 69420

sns.set_theme(font_scale=.7)
pd.set_option("display.precision", 4)

CACHE_DIR = "cache"

# Create cache directory if not already present
if not os.path.isdir(CACHE_DIR):
    os.makedirs(CACHE_DIR)

def load_pickle(p):
    with open(p, "rb") as f:
        return pickle.load(f)

def dump_pickle(obj, p):
    with open(p, "wb") as f:
        pickle.dump(obj, f)

def grid_search(params, scores, base_model, Xtr, ytr, Xte, yte,
                n_splits=3, n_jobs=None, random_state=RANDOM_STATE,
                pickle_file="", overwrite_pickle=False, verbose=1):
    """
    Perform a grid search on a given model using the given parameters and scores

    Parameters
```

```
    ----------
    params : dict
        A dictionary containing the parameters to be tested in the grid search
    scores : list or string
        A list of strings containing the scores to be used in the grid search
    base_model : sklearn estimator
        The estimator object to optimize
    Xtr : np.array
        The training data
    ytr : np.array
        The training labels
    Xte : np.array
        The testing data
    yte : np.array
        The testing labels
    n_splits : int (default: 3)
        The number of splits to be used in the cross validation
    n_jobs : int or None (default: None)
        Number of threads to use. None means 1 and -1 means using all available
    random_state : int
        The random seed to be used in the cross validation
    pickle_file : str
        The path to the pickle file to be used to cache the grid search results
    overwrite_pickle : bool
        Whether to overwrite the pickle file if it already exists

    Returns
    -------
    dict
        A dictionary containing the results of the grid search
    """

    # If no pickle file is given, use the model's name as the pickle file
    if pickle_file.strip() == "":
```

```python
        pickle_file = base_model.__class__.__name__ + "__gridsearch.pickle"

    pickle_file = os.path.join(CACHE_DIR, pickle_file)

    # If the pickle file already exists and we don't want to overwrite it, load the results from it and return
    if os.path.isfile(pickle_file) and not overwrite_pickle:
        print(f"Grid search already cached in {pickle_file} - loading...")
        return load_pickle(pickle_file)

    # Create a stratified k-fold object
    skf = StratifiedKFold(n_splits=n_splits, random_state=random_state, shuffle=True)
    results = {}

    # If passed a single score as a string, wrap it in a list
    if type(scores) == str:
        scores = [scores]

    # GridSearchCV expects a list of dictionaries,
    # so if passed a single dictionary, wrap it in a list
    if not type(params) is list:
        params = [params]

    for score in scores:
        print(f"Tuning hyperparameters for: {score}...")

        clf = GridSearchCV(estimator=base_model,#sklearn.base.clone(base_model),
                           param_grid=params,
                           scoring=score,
                           return_train_score=False,
                           n_jobs=n_jobs,
                           cv=skf, verbose=verbose)

        clf.fit(Xtr, ytr)
```

```
        # Retrieve the best model from the grid search
        best_model = clf.best_estimator_
        classes = best_model.classes_

        y_pred = best_model.predict(Xte)

        # Generate classification report and confusion matrix
        report = classification_report(yte,y_pred, zero_division=0)
        cm = confusion_matrix(yte, y_pred, labels=classes, normalize="true")

        results[score] = {
            "model": best_model,
            "report": report,
            "matrix": cm
        }

        print("done")

    # Cache the results in a pickle file
    with open(pickle_file, "wb") as f:
        print(f"Caching grid search result in {pickle_file}...")
        pickle.dump(results, f)

    return results

def fit_and_predict(model, X_train, y_train, X_test, y_test):
    """
    Fit a model and predict the test data

    Parameters
    ----------
    model : sklearn BaseEstimator
        The model to be used
    X_train : np.array
```

```
        The training data
    y_train : np.array
        The training labels
    X_test : np.array
        The testing data
    y_test : np.array
        The testing labels

    Returns
    -------
    y_pred, rep, cm
        predicted labels, the classification report and the confusion matrix
    """

    print("Fitting model...", end="")
    model.fit(X_train, y_train)
    print("done")

    print("Testing...", end="")
    y_pred = model.predict(X_test)
    print("done")

    rep = classification_report(y_test, y_pred)
    cm = confusion_matrix(y_test, y_pred, labels=model.classes_, normalize="true")

    return y_pred, rep, cm

def print_model_results(model, report, conf_matrix, conf_matrix_title = ""):
    """

    Print the results of a model

    Parameters
    ----------
```

```
    model : sklearn BaseEstimator
        The model of which to print the parameters
    report : str
        The classification report
    conf_matrix : np.array
        The confusion matrix
    conf_matrix_title : str (default: "")
        The title of the confusion matrix plot. If empty, defaults to the class name of the model
    """

    print("Classification report:")
    print(report)

    print(f"Best parameters:")
    print(*[f"\t{n}: {v}" for n, v in model.get_params().items()], sep="\n")

    print()

    # If the model has feature importances, print them
    # (applies for tree-based models)
    if hasattr(model, "feature_importances_"):
        names = model.feature_names_in_
        print("Feature importances:")
        for name, imp in zip(names, model.feature_importances_):
            print(f"\t{name}: {imp:.3f}")

    disp = ConfusionMatrixDisplay(conf_matrix, display_labels=model.classes_)
    disp.plot()
    disp.ax_.get_images()[0].set_clim(0, 1)

    if conf_matrix_title == "":
        conf_matrix_title = model.__class__.__name__

    disp.ax_.set_title(conf_matrix_title)
```

```python
    disp.ax_.grid(False)

def print_gridsearch_results(results, cm_model_name=""):
    """
    Print information about the best model for each score in the grid search results

    Parameters
    ----------
    results : dict
        The results of calling grid_search
    features : list
        The features used in the model
    """

    for score, res in results.items():
        print("-" * 20)
        print(f"Score: {score}")

        if cm_model_name == "":
            cm_title = res['model'].__class__.__name__

        cm_title = f"{cm_model_name} - Tuned for {score}"

        print_model_results(res["model"], res["report"], res["matrix"], conf_matrix_title=cm_title)

def pairplot_or_image(data, img_path, target, overwrite=False, diag_kind="auto", height=1.5, legend=True):
    """
    Display a pairplot of the data. If the cached image already exists, display it instead

    Parameters
    ----------
    data : pd.DataFrame
        The data to plot
    img_path : str
```

```
        The path to save the image
    target : str
        The target variable
    overwrite : bool (default: False)
        Whether to overwrite the image if it already exists
    diag_kind : str (default: "auto")
        The kind of plot to use on the diagonal
    height : float (default: 1.5)
        The height of the plot
    legend : bool (default: True)
        Whether to display the legend
    """

    img_path = os.path.join(CACHE_DIR, img_path)

    if os.path.isfile(img_path) and not overwrite:
        display(Image(filename=img_path))
    else:
        pplot = sns.pairplot(data, hue=target, diag_kind=diag_kind, height=height)

        if not legend:
            pplot._legend.remove()

        pplot.figure.savefig(img_path)

# Forgot to store the classification report as a dictionary
# so we need to parse the report string
def report_str_to_dict(rep, n_classes=2):
    """
    Convert a classification report string to a dictionary

    Parameters
    ----------
    rep : str
```

```
        The classification report string
    n_classes : int (default: 2)
        The number of classes in the report

    Returns
    -------
    dict
        A dictionary containing the classification report, formatted as follows:
        ```
        {
            "class1": {
                "precision": float,
                "recall": float,
                "f1-score": float,
                "support": float
            },
            "class2": {...},
            ...
            "classN": {...},
            "accuracy": float,
            "macro_avg": {
                "precision": float,
                "recall": float,
                "f1-score": float
            },
            "weighted_avg": {
                "precision": float,
                "recall": float,
                "f1-score": float
            },
            "support": float
        }
        ```
    """
```

```
    rep = rep.strip()
    lines = rep.split("\n")

    class_lines = [l.split() for l in rep.split("\n")[2:2+n_classes]]
    classes_dict = {l[0]: {k: float(v) for k, v in zip(["precision", "recall", "f1-score", "support"], l[1:])}␣
↪for l in class_lines}

    global_lines = [l.replace(" avg", "_avg").split() for l in lines[-3:]]
    total_support = float(global_lines[0][-1])
    global_dict = {l[0]: l[1:-1] for l in global_lines}

    global_dict["accuracy"] = float(global_dict["accuracy"][0])

    averages = ["macro_avg", "weighted_avg"]

    for avg in averages:
        global_dict[avg] = {k: float(v) for k, v in zip(["precision", "recall", "f1-score"], global_dict[avg])}

    global_dict["support"] = total_support

    # merge the two dictionaries
    rep_dict = {**classes_dict, **global_dict}

    return rep_dict

def plot_old_to_new(old_dict, new_dict,
                    xlabel="", ylabel="", title="",
                    show_values=True, x_padding=.05, ax=None,
                    color_direction=True, x_range=None, yticks=True):
    """
    Plot a comparison between two dictionaries, assumed to have the same keys

    Parameters
```

```
    ----------
    old_dict : dict
        Dictionary with the old values
    new_dict : dict
        Dictionary with the new values
    xlabel : str (default: "")
        The x-axis label
    ylabel : str (default: "")
        The y-axis label
    title : str (default: "")
        The title of the plot
    show_values : bool (default: True)
        Whether to label each point with its value
    x_padding : float (default: .05)
        The padding to add to the x-axis limits
    ax : plt.Axes (default: None)
        The axes object to plot on. If None, a new figure is created
    color_direction : bool (default: True)
        Whether to color the arrows based on the direction of change
    x_range : tuple (default: None)
        The range of the x-axis. If None, the range is determined from the values
    yticks : bool (default: True)
        Whether to show the y-ticks labels
    """

    names = list(old_dict.keys())
    names.reverse()

    old_values = [old_dict[n] for n in names]
    new_values = [new_dict[n] for n in names]

    # Number of objects
    n = len(names)
```

```
    # Positions for the objects on the y-axis
    y_positions = np.arange(n)

    # The changes in value
    delta_values = np.array(new_values) - np.array(old_values)

    # Create the plot
    if ax is None:
        _, ax = plt.subplots()

    ax.title.set_text(title)

    went_up = [delta > 0 for delta in delta_values]

    # Determine the colors based on the direction of change
    colors = ["black" for _ in names] if not color_direction else ['green' if went_up[i] else 'red' for i, _ in␣
↪enumerate(names)]

    # Plot the arrows with colors
    for i in range(n):
        ax.quiver(old_values[i], y_positions[i], delta_values[i], 0,
                  angles='xy', scale_units='xy', scale=1, color=colors[i],
                  width=.005, headwidth=3, headlength=3)

    if show_values:
        # Label the points
        for i, _ in enumerate(names):
            ax.text(old_values[i], y_positions[i], f'{old_values[i]}', ha='right' if went_up[i] else "left",␣
↪va='center')
            ax.text(new_values[i], y_positions[i], f'{new_values[i]}', ha='left' if went_up[i] else "right",␣
↪va='center')

    # Set the y-ticks to the object names
```

```python
    ax.set_yticks(y_positions)
    if yticks:
        ax.set_yticklabels(names)
    else:
        ax.set_yticklabels([])

    # Set labels
    if xlabel != "":
        ax.set_xlabel(xlabel)
    if ylabel != "":
        ax.set_ylabel(ylabel)

    # Determine the x-axis limits

    if x_range is not None:
        min_value, max_value = x_range
    else:
        min_value = min(min(old_values), min(new_values))
        max_value = max(max(old_values), max(new_values))

    # Set the x-axis limits with padding
    ax.set_xlim(min_value - x_padding, max_value + x_padding)

    # Show grid
    ax.grid(True)

    if ax is None:
        # Display the plot
        plt.show()
```

2 Data preparation

The dataset contains the following attributes:

ATTRIBUTE	DATATYPE	DESCRIPTION
id	Int	Device identifier
Product Id	String	Unique Id, combination of the Type attribute and a number identifier
Type	String	Type of product/device (possible values: “L”,“M”,“H”)
Air Temperature	Float	Air temperature (Kelvin)
Process Temperature	Float	Production process temperature (Kelvin)
Rotational Speed	Int	Speed in RPM
Torque	Float	Torque in Nm (Newton Meter)
Tool Wear	Int	Time unit needed to wear down the product/tool
TWF	Int	Tool Wear Failure (binary)
HDF	Int	Heat Dissipation Failure (binary)
PWF	Int	Power Failure (binary)
OSF	Int	Overstrain Failure (binary)
RNF	Int	Random Failure (binary)
Machine Failure	Int	Failure binary feature (*class attribute*)

More domain knowledge details can be found here.

2.1 Preprocessing

[4]:
```
data = pd.read_csv("BCMF_data.csv")
data.set_index("id", inplace=True)

print(f"Total size: {len(data)}")
```

```
Total size: 136429
```

Here we see the main characteristic of this dataset, its *extreme imbalance*. This is dealt with in the following sections, first by oversampling the minority class, and by choosing the macro recall average as a metric for tuning.

[5]:
```
target = "Machine failure"

data[target] = data[target].astype("category")
```

```python
c0, c1 = data[target].value_counts()
ratio = c0 / c1

print(f"Class 0: {c0} ({c0 / len(data) * 100:.2f}%)")
print(f"Class 1: {c1} ({c1 / len(data) * 100:.2f}%)")
print(f"Ratio: {ratio:.2f}:1")
```

```
Class 0: 134281 (98.43%)
Class 1: 2148 (1.57%)
Ratio: 62.51:1
```

The "Product ID" attribute is irrelevant for this project

[6]:
```python
data.drop(columns=["Product ID"], inplace=True)
```

Converting the "type" attribute from categorical to numerical

[7]:
```python
data["Type"] = data["Type"].astype("category")
# We need to convert the type to an actual numerical value to perform
# resampling later
data["Type"] = data["Type"].cat.codes
```

This dataset was artificially generated from another one, so there are (very) few inconsistencies. Namely, the TWF,HDF,PWF,OSF and RNF columns indicate the type of failure (see here) but we can find a small number of rows that have failure indicators set to a value different from the class attribute.

These inconsistent rows are removed since their whole data isn't considered reliable. We then also remove these failure indicators since they become redundant.

[8]:
```python
# Rows where the target is 0 and TWF, HDF, PWF, OSF, RNF are 1 are invalid
# Rows where the target is 1 and TWF, HDF, PWF, OSF, RNF are all 0 are invalid
data['tmp'] = data[['TWF', 'HDF', 'PWF', 'OSF', 'RNF']].sum(axis=1)

invalid = data[(data[target] == 0) & (data["tmp"] != 0)].index
invalid = invalid.append(data[(data[target] == 1) & (data["tmp"] == 0)].index)
```

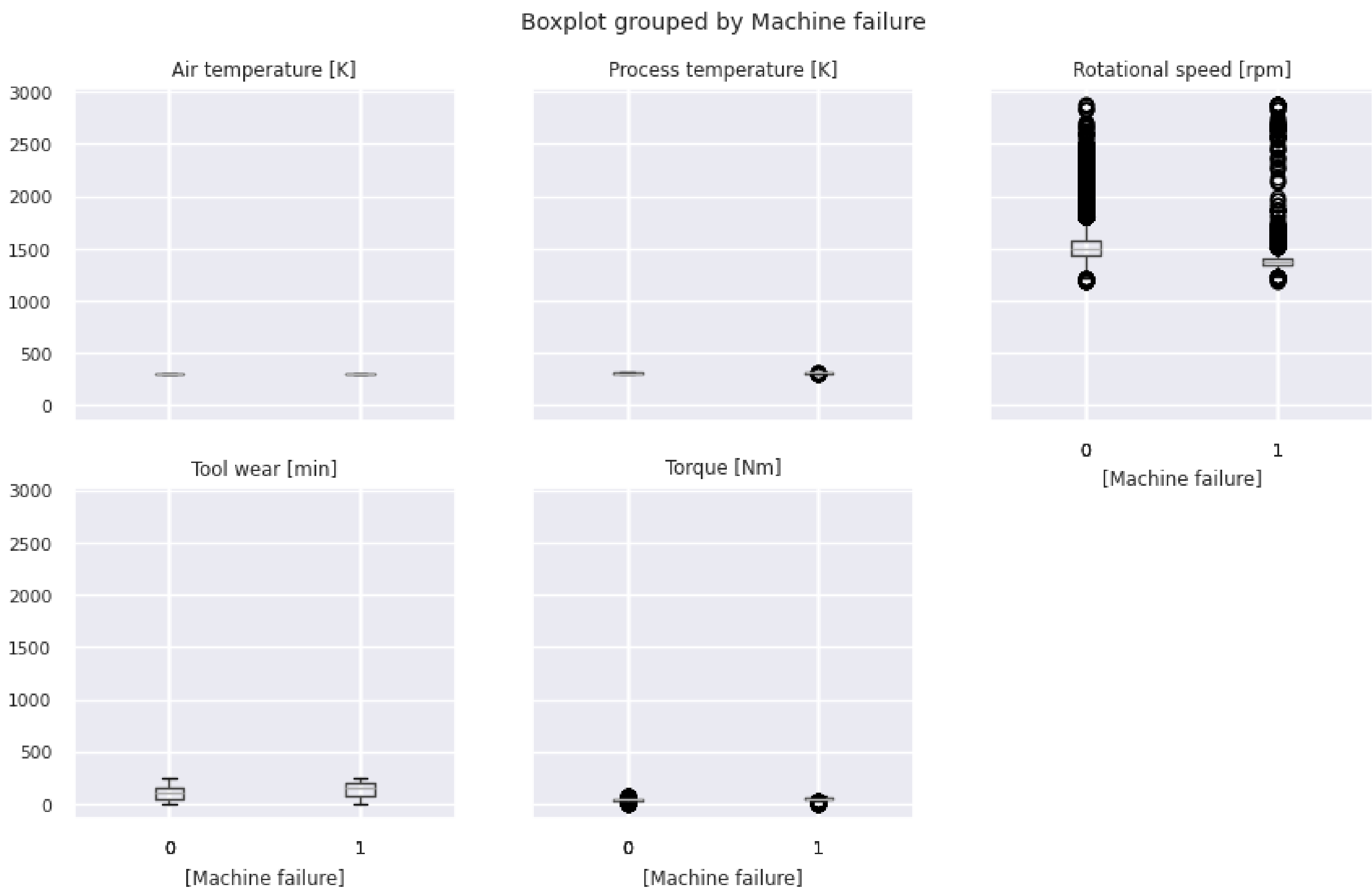
```
print(f"{len(invalid)} invalid rows")
# Remove rows
data.drop(invalid, inplace=True)

# Remove TWF, HDF, PWF, OSF, RNF columns
data.drop(columns=["tmp", "TWF", "HDF", "PWF", "OSF", "RNF"], inplace=True)
```

```
822 invalid rows
```

[9]:
```
# The describe() method doesn't apply to categorical columns (like Type)
data.drop(columns=["Type"]).describe()
```

[9]:
```
       Air temperature [K]  Process temperature [K]  Rotational speed [rpm]  \
count          135607.0000              135607.0000             135607.0000
mean              299.8605                 309.9402               1520.4675
std                 1.8613                   1.3851                137.8523
min               295.3000                 305.8000               1181.0000
25%               298.3000                 308.7000               1432.0000
50%               300.0000                 310.0000               1493.0000
75%               301.2000                 310.9000               1580.0000
max               304.4000                 313.8000               2886.0000

       Torque [Nm]  Tool wear [min]
count  135607.0000      135607.0000
mean       40.3192         104.3506
std         8.4648          63.9209
min         3.8000           0.0000
25%        34.6000          48.0000
50%        40.4000         106.0000
75%        46.0000         159.0000
max        76.6000         253.0000
```

[10]:
```
data.drop(columns=["Type"]).boxplot(figsize=(10, 6), by=target, layout=(2, 3));
```

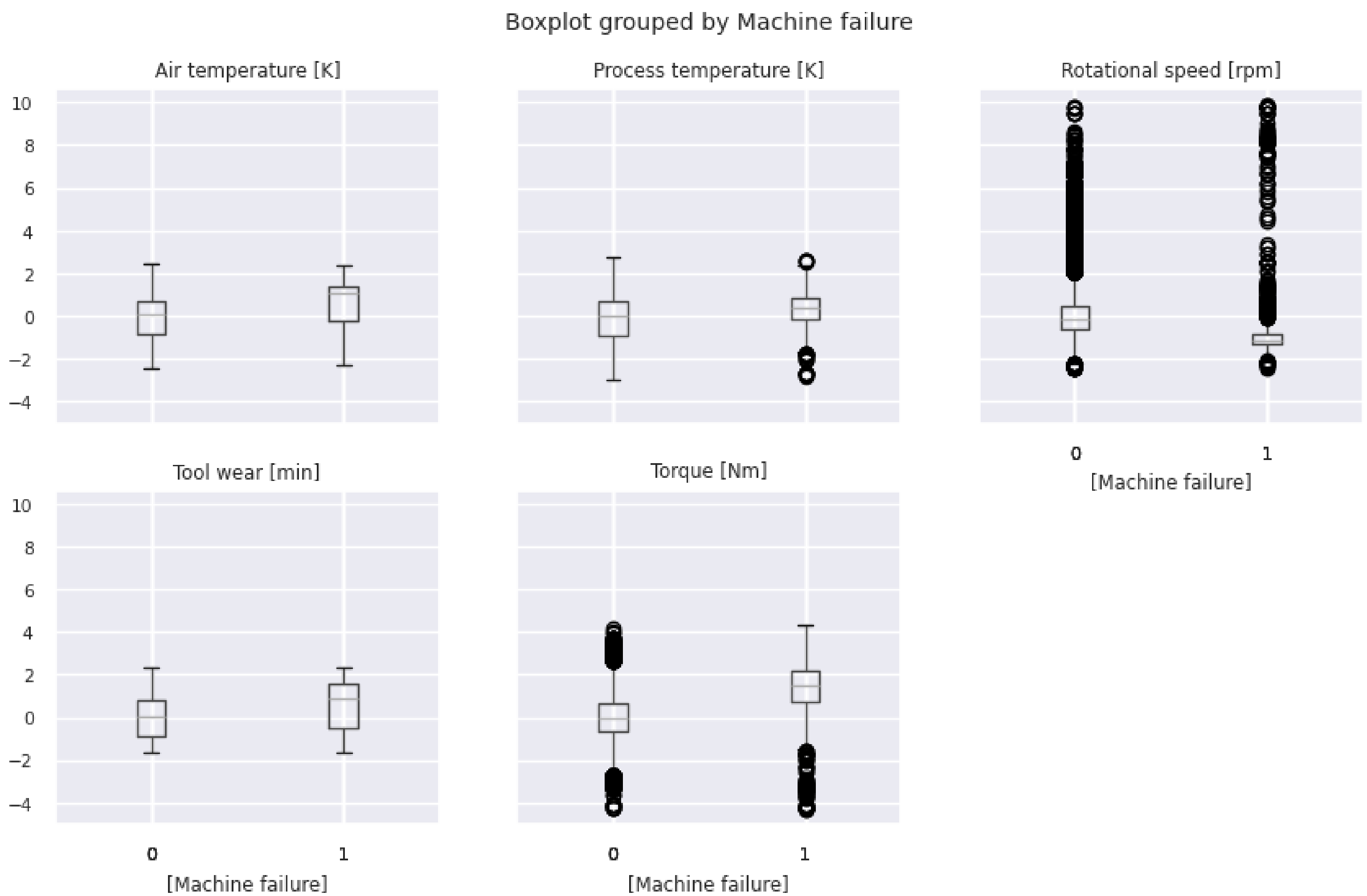


This boxplot (and the previous description) shows that the attributes have widely different scales, so we need to normalize them

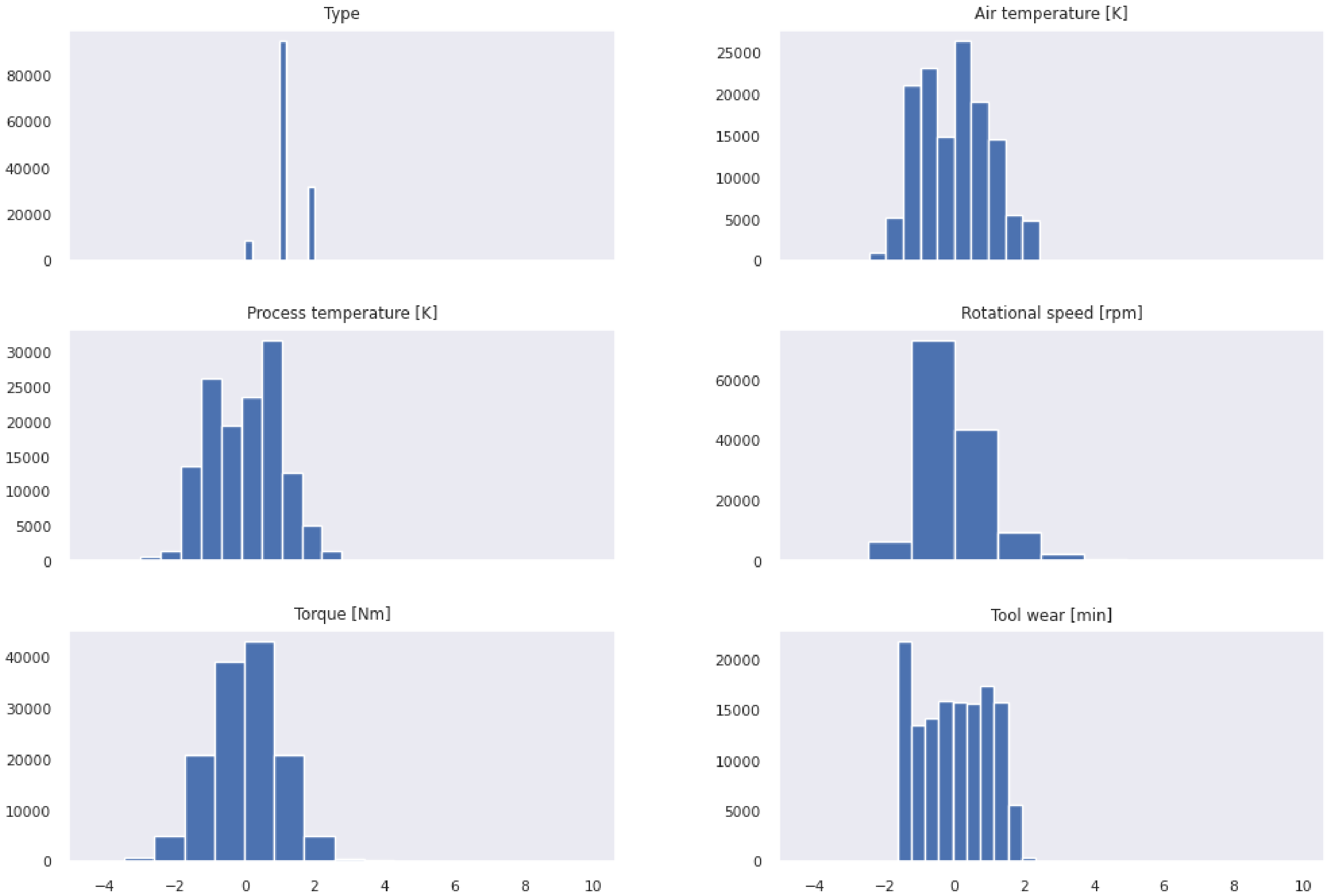
[11]:
```
for col in [c for c in data.columns if not c in [target, "Type"]]:
    data[col] = (data[col] - data[col].mean()) / data[col].std()
```

The following plots show the final distributions of the attributes. Due to the high imbalance, the pairplot had to be split between the classes so that the plots for the “Failed” class could be seen.

[12]:
```
data.drop(columns=["Type"]).boxplot(figsize=(10, 6), by=target, layout=(2, 3));
```

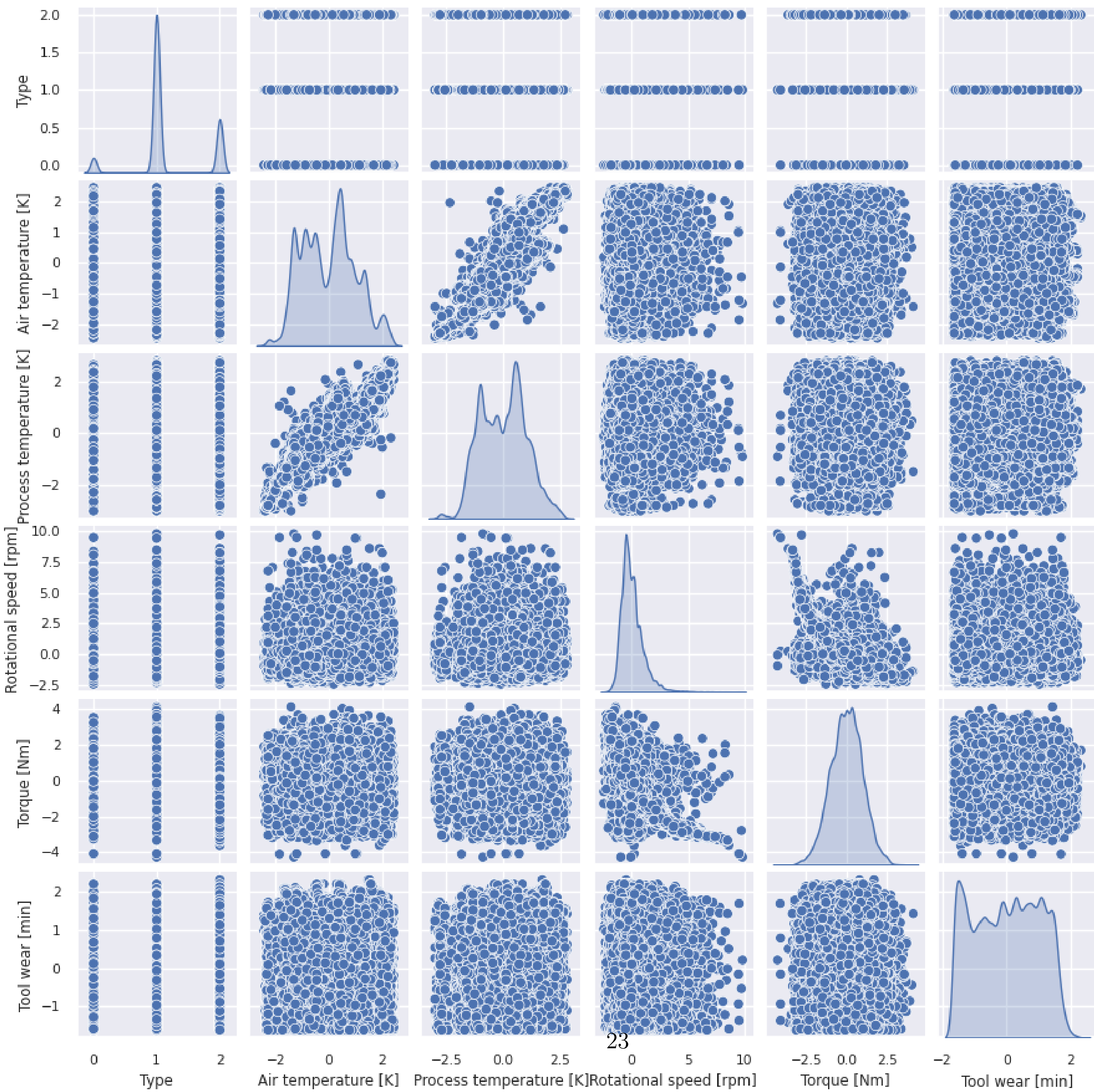



```
[13]: data.hist(grid=False, sharex=True, figsize=(12, 8));
```


Type
Air temperature [K]
Process temperature [K]
Rotational speed [rpm]
Torque [Nm]
Tool wear [min]
80000
60000
40000
20000
0
25000
20000
15000
10000
5000
0
30000
25000
20000
15000
10000
5000
0
60000
40000
20000
0
40000
30000
20000
10000
0
20000
15000
10000
5000
0
−4
−2
0
2
4
6
8
10

[14]:
```
# Due to the high imbalance, the minority class ends up being barely noticable in this plot,
# hence the separation
#pairplot_or_image(data, "full_pairplot.png", target)
```

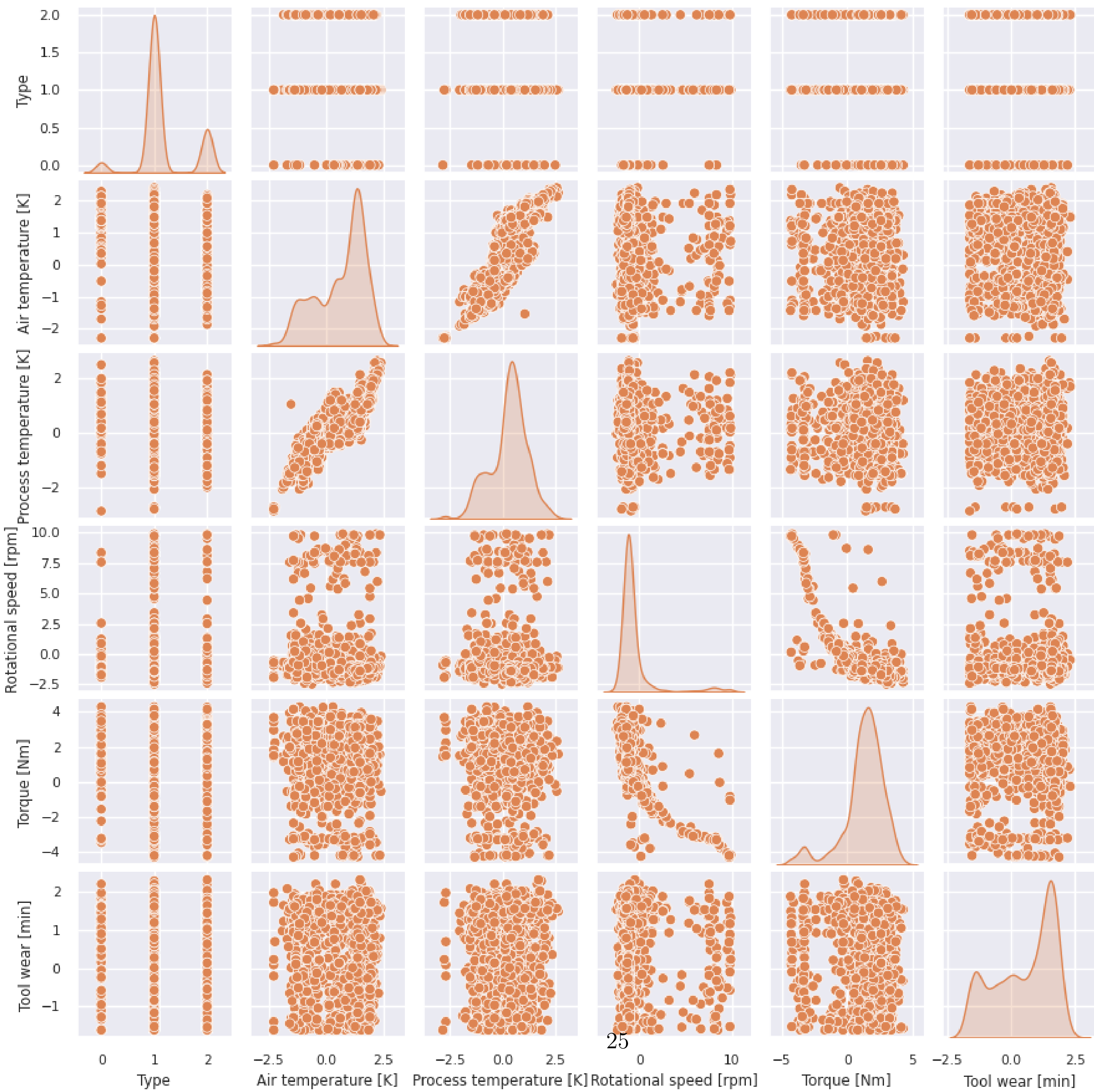
[15]:
```
pairplot_or_image(data[data[target] == 0], "not_failed.png", target, overwrite=False, legend=False)
```



Type
Air temperature [K]
Process temperature [K]
Rotational speed [rpm]
Torque [Nm]
Tool wear [min]

[16]:

```
pairplot_or_image(data[data[target] == 1], "failed.png", target, overwrite=False, legend=False)
```


Type
Air temperature [K]
Process temperature [K]
Rotational speed [rpm]
Torque [Nm]
Tool wear [min]

2.2 Resampling & train/test split

[17]:
```
# Basic paramters
test_size = 0.2

X = data.drop(columns=[target], axis=1)
y = data[target]
```

Resampling allows us to change the minority-majority class ratio. This can be done by either: - *over*-sampling the minority, i.e. duplicating minority datapoints - *under*-sampling the majority, i.e. removing majority datapoints

The first option could lead to overfitting but doesn't remove any data. The second option, however, to achieve the desired ratio would have to remove a lot of data, *for this particular dataset*. We therefore choose the over-sampling method.

With the imblearn library, this is done using the SMOTE method.

[18]:
```
from sklearn.model_selection import train_test_split
from imblearn.over_sampling import SMOTE

Xtr_orig, Xte, ytr_orig, yte = train_test_split(X, y, test_size=test_size, random_state=RANDOM_STATE)

print(f"Test set size: {len(Xte)}")

# Resample to get a different ratio between minority and majority
resampler = SMOTE(random_state=RANDOM_STATE, sampling_strategy=(1. / 10.))

Xtr, ytr = Xtr_orig, ytr_orig

if resampler is not None:
    Xtr, ytr = resampler.fit_resample(Xtr_orig, ytr_orig)

    print(f"Initial train size: {len(Xtr_orig)}")
```

```
    print(f"Resampled train size: {len(Xtr)}")
else:
    print(f"Train size: {len(Xtr)}")
```

```
Test set size: 27122
Initial train size: 108485
Resampled train size: 117901
```

3 Models

We test the following estimators, from the scikit-learn library: - Decision Tree - Random Forest - AdaBoost - k-Nearest Neighbors - Gaussian Naive Bayes - Perceptron - Support Vector Machine - SGD

For each model, we compute a baseline first and then we tune the hyperparameters using a grid search. The estimators are presented in the order in which they've been tested and (almost) all discussion of the results has been left for the "Conclusion" section at the end.

3.1 Decision Tree

[19]:
```
from sklearn.tree import DecisionTreeClassifier
```

This model will be tested on both the original and resampled datasets.

3.1.1 Baseline

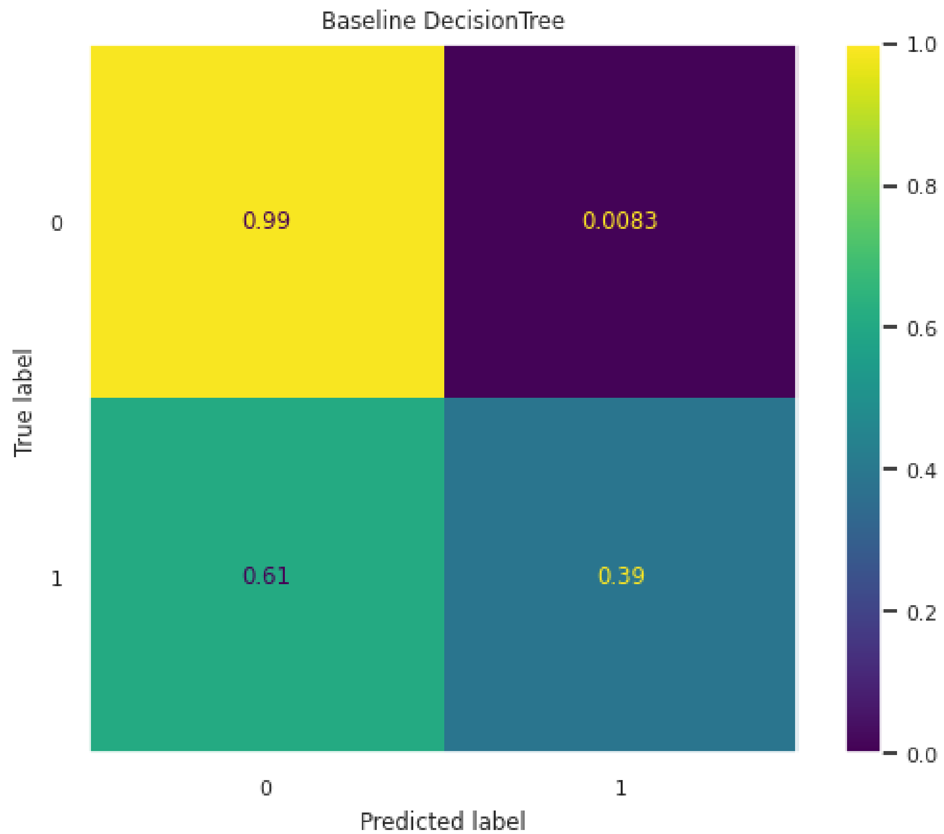
Original dataset

[20]:
```
base_dt_orig = DecisionTreeClassifier(random_state=RANDOM_STATE)

y_pred, rep, cm = fit_and_predict(base_dt_orig, Xtr_orig, ytr_orig, Xte, yte)
```

```
Fitting model...done
Testing...done
```

[21]:
```
print_model_results(base_dt_orig, rep, cm, "Baseline DecisionTree")
```

```
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.99      0.99     26783
           1       0.37      0.39      0.38       339

    accuracy                           0.98     27122
   macro avg       0.68      0.69      0.69     27122
weighted avg       0.98      0.98      0.98     27122

Best parameters:
        ccp_alpha: 0.0
        class_weight: None
        criterion: gini
        max_depth: None
        max_features: None
        max_leaf_nodes: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        random_state: 69420
        splitter: best

Feature importances:
        Type: 0.031
        Air temperature [K]: 0.179
        Process temperature [K]: 0.146
        Rotational speed [rpm]: 0.181
        Torque [Nm]: 0.288
        Tool wear [min]: 0.175
```



[22]:
```
print(f"Tree depth: {base_dt_orig.get_depth()}")
```

```
Tree depth: 30
```

[23]:
```
base_dt_orig.tree_.node_count
```

[23]: 3139

Oversampled dataset

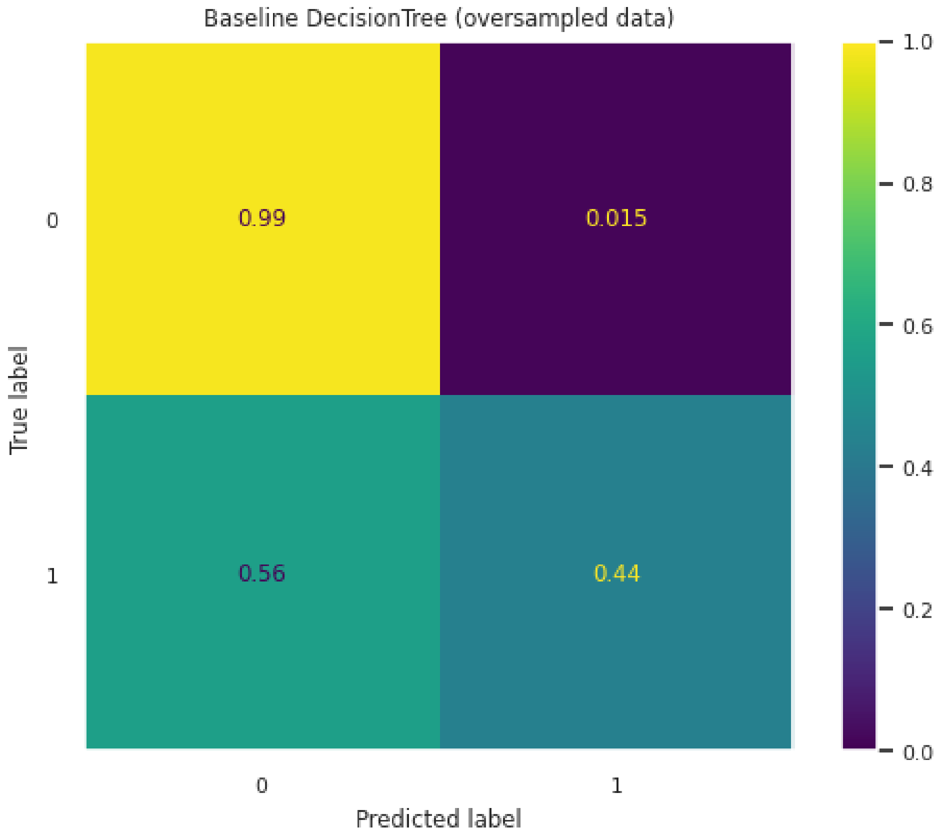
[24]:
```
base_dt_os = DecisionTreeClassifier(random_state=RANDOM_STATE)

y_pred, rep, cm = fit_and_predict(base_dt_os, Xtr, ytr, Xte, yte)
```

```
Fitting model...

done
Testing...done
```

[25]:
```
print_model_results(base_dt_os, rep, cm, "Baseline DecisionTree (oversampled data)")
```

```
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.99      0.99     26783
           1       0.27      0.44      0.34       339

    accuracy                           0.98     27122
   macro avg       0.63      0.71      0.66     27122
weighted avg       0.98      0.98      0.98     27122

Best parameters:
        ccp_alpha: 0.0
        class_weight: None
        criterion: gini
        max_depth: None
        max_features: None
        max_leaf_nodes: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        random_state: 69420
        splitter: best
```

```
Feature importances:
        Type: 0.013
        Air temperature [K]: 0.219
        Process temperature [K]: 0.109
        Rotational speed [rpm]: 0.292
        Torque [Nm]: 0.223
        Tool wear [min]: 0.144
```



[26]:
```
print(f"Tree depth: {base_dt_os.get_depth()}")
```

```
Tree depth: 35
```

[27]:
```
base_dt_os.tree_.node_count
```

[27]:
```
5865
```

As will be the case for all following models, the baseline(s) show an "alleged" accuracy around 98%, actually due to the high imbalance. The following gridsearch will show which alternative metric was chosen to optimize each estimator.

Finally, though the effect isn't too pronounced, the model performs better on the resampled dataset. This is expected, as the model is able to learn more from the minority class, and such data will be used for the following models.

[28]:
```
base_rep_dt = rep
```

3.1.2 Grid search

[29]:
```
max_depth = base_dt_os.get_depth()+1

results_dt = grid_search({'max_depth': [*range(4,max_depth)],
                        'criterion' : ['entropy', 'gini'],
                        "class_weight": [None, "balanced"]},
                       # Searching over all metrics will take around 30 minutes using Colab
                       ["precision_macro", "recall_macro", "f1_macro", "accuracy"],
                       base_dt_os, Xtr, ytr, Xte, yte)
```

```
Grid search already cached in cache/DecisionTreeClassifier__gridsearch.pickle -
loading...
```

[30]:
```
print_gridsearch_results(results_dt)
```

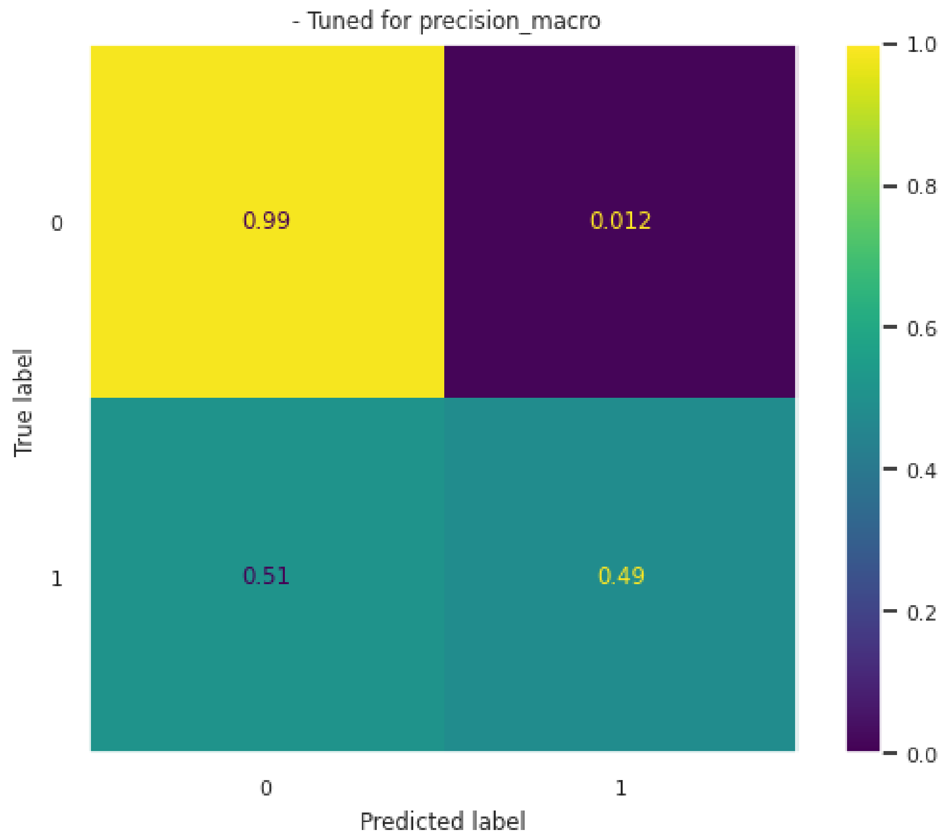
```
--------------------
Score: precision_macro
Classification report:
```

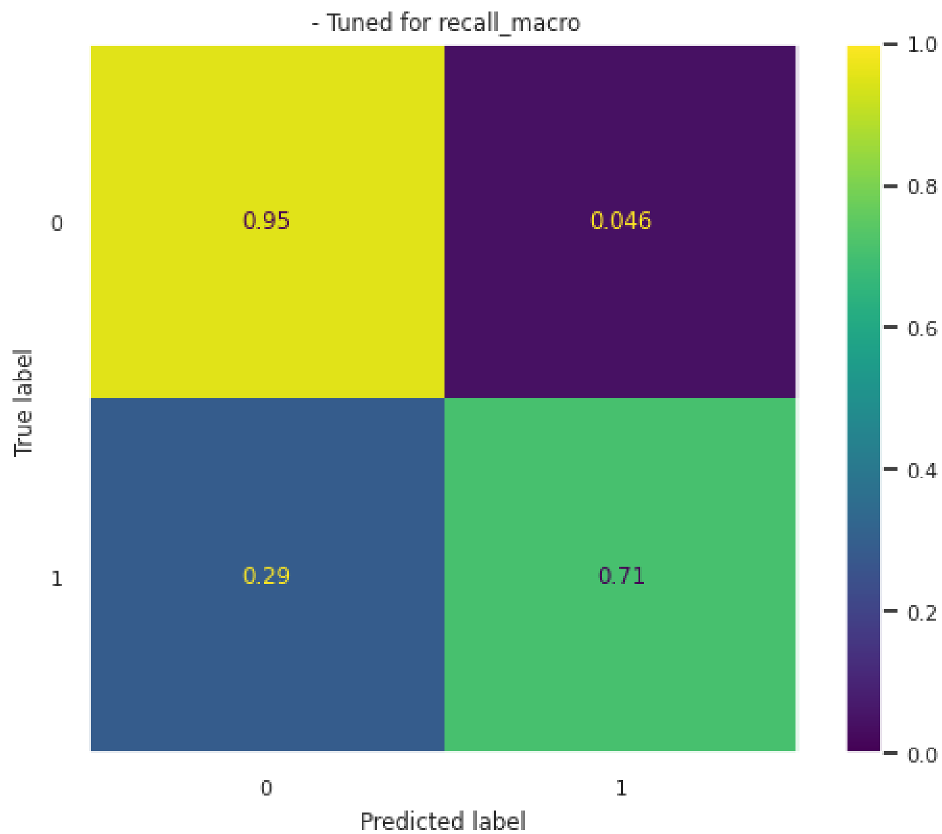
```
              precision    recall  f1-score   support

           0       0.99      0.99      0.99     26783
           1       0.34      0.49      0.40       339

    accuracy                           0.98     27122
   macro avg       0.67      0.74      0.70     27122
weighted avg       0.99      0.98      0.98     27122

Best parameters:
        ccp_alpha: 0.0
        class_weight: None
        criterion: gini
        max_depth: 14
        max_features: None
        max_leaf_nodes: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        random_state: 69420
        splitter: best

Feature importances:
        Type: 0.012
        Air temperature [K]: 0.218
        Process temperature [K]: 0.091
        Rotational speed [rpm]: 0.308
        Torque [Nm]: 0.235
        Tool wear [min]: 0.137
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support
```

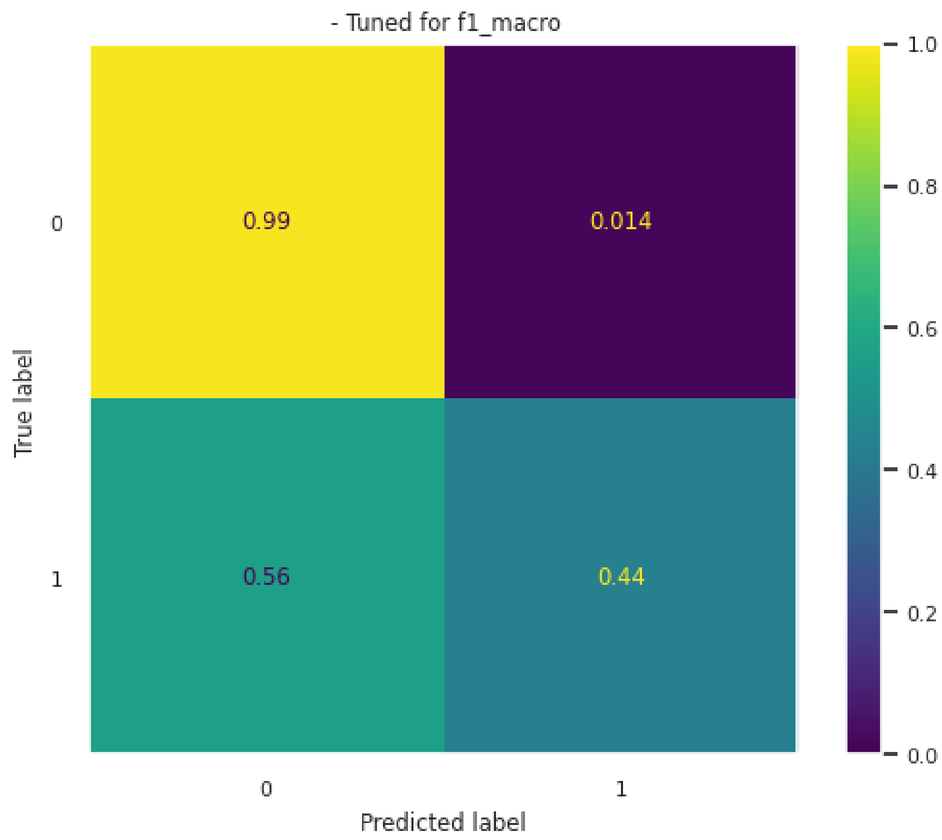
```
           0       1.00      0.95      0.97     26783
           1       0.16      0.71      0.27       339

    accuracy                           0.95     27122
   macro avg       0.58      0.83      0.62     27122
weighted avg       0.99      0.95      0.97     27122

Best parameters:
        ccp_alpha: 0.0
        class_weight: balanced
        criterion: gini
        max_depth: 13
        max_features: None
        max_leaf_nodes: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        random_state: 69420
        splitter: best

Feature importances:
        Type: 0.009
        Air temperature [K]: 0.074
        Process temperature [K]: 0.039
        Rotational speed [rpm]: 0.464
        Torque [Nm]: 0.229
        Tool wear [min]: 0.184
--------------------
Score: f1_macro
Classification report:
              precision    recall  f1-score   support
```

```
           0       0.99      0.99      0.99     26783
           1       0.28      0.44      0.34       339

    accuracy                           0.98     27122
   macro avg       0.64      0.71      0.67     27122
weighted avg       0.98      0.98      0.98     27122

Best parameters:
        ccp_alpha: 0.0
        class_weight: None
        criterion: entropy
        max_depth: 30
        max_features: None
        max_leaf_nodes: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        random_state: 69420
        splitter: best

Feature importances:
        Type: 0.013
        Air temperature [K]: 0.168
        Process temperature [K]: 0.098
        Rotational speed [rpm]: 0.333
        Torque [Nm]: 0.226
        Tool wear [min]: 0.162

--------------------
Score: accuracy
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.99      0.99     26783
```

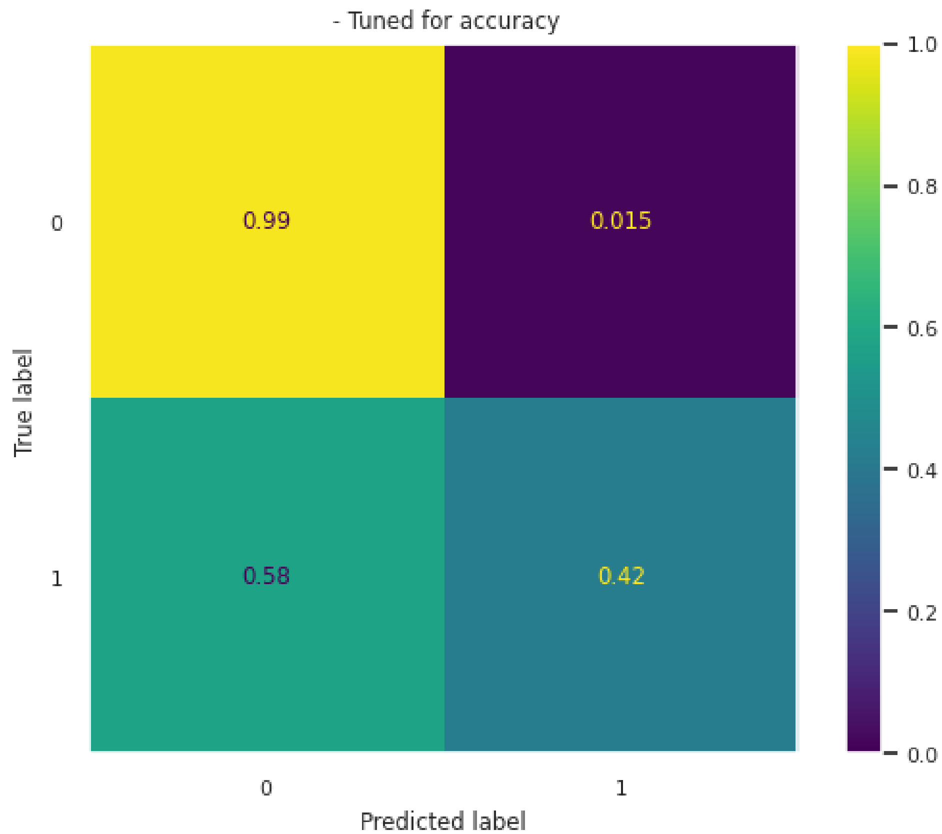
```
           1       0.26      0.42      0.32       339

    accuracy                           0.98     27122
   macro avg       0.63      0.70      0.66     27122
weighted avg       0.98      0.98      0.98     27122

Best parameters:
        ccp_alpha: 0.0
        class_weight: balanced
        criterion: entropy
        max_depth: 32
        max_features: None
        max_leaf_nodes: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        random_state: 69420
        splitter: best

Feature importances:
        Type: 0.013
        Air temperature [K]: 0.116
        Process temperature [K]: 0.078
        Rotational speed [rpm]: 0.365
        Torque [Nm]: 0.243
        Tool wear [min]: 0.185
```


- Tuned for precision_macro
0.99
0.012
0.51
0.49
True label
Predicted label
0
1
0
1
1.0
0.8
0.6
0.4
0.2
0.0


- Tuned for recall_macro
0.95
0.046
0.29
0.71
True label
Predicted label
0
1
0
1
1.0
0.8
0.6
0.4
0.2
0.0



- Tuned for f1_macro
0.99
0.014
0.56
0.44
True label
0
1
Predicted label
1.0
0.8
0.6
0.4
0.2
0.0



We clearly see that targeting the `recall_macro` metric produces a far better estimator compared to those obtained for the other metrics, whose performance remains close to the baseline. This is expected, since it requires the model to classify correctly a higher percentage of datapoints *for both classes*. Due to this outstanding result, for all following models this will be the only metric used in the grid searches.

The optimized model uses the following hyperparameters (among those used for the grid search): - `class_weight`: `"balanced"` - `criterion`: `"gini"` - `max_depth`: 13

A balanced class weighting is a logical better choice since it *"uses the values of y to automatically adjust weights inversely proportional to* *class frequencies in the input data"* (see the sklearn documentation) - this is another response to the imbalanced nature of the dataset.

3.2 Random Forest

[31]:
```
from sklearn.ensemble import RandomForestClassifier
```

3.2.1 Baseline

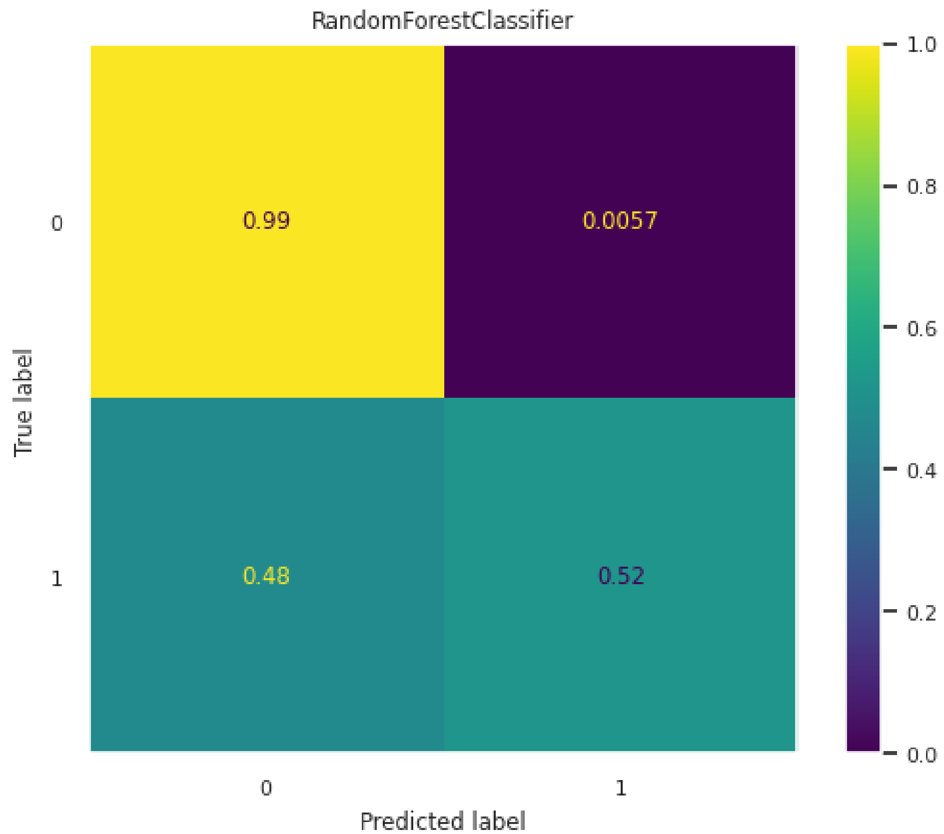
[32]:
```
base_rf = RandomForestClassifier(random_state=RANDOM_STATE)

y_pred, base_rep_rf, cm = fit_and_predict(base_rf, Xtr, ytr, Xte, yte)
```

```
Fitting model...done
Testing...done
```

[33]:
```
print_model_results(base_rf, base_rep_rf, cm)
```

```
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.99      0.99     26783
           1       0.53      0.52      0.53       339

    accuracy                           0.99     27122
   macro avg       0.76      0.76      0.76     27122
weighted avg       0.99      0.99      0.99     27122

Best parameters:
        bootstrap: True
        ccp_alpha: 0.0
        class_weight: None
        criterion: gini
        max_depth: None
        max_features: sqrt
        max_leaf_nodes: None
```

```
        max_samples: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        n_estimators: 100
        n_jobs: None
        oob_score: False
        random_state: 69420
        verbose: 0
        warm_start: False

Feature importances:
        Type: 0.014
        Air temperature [K]: 0.180
        Process temperature [K]: 0.117
        Rotational speed [rpm]: 0.260
        Torque [Nm]: 0.283
        Tool wear [min]: 0.146
```



[34]:
```
max_rf_depth = max([estimator.get_depth() for estimator in base_rf.estimators_])
print(f"Deepest tree: {max_rf_depth}")
```

```
Deepest tree: 41
```

[35]:
```
max_rf_estimators = base_rf.n_estimators
print(f"# of estimators: {max_rf_estimators}")
```

```
# of estimators: 100
```

3.2.2 Grid Search

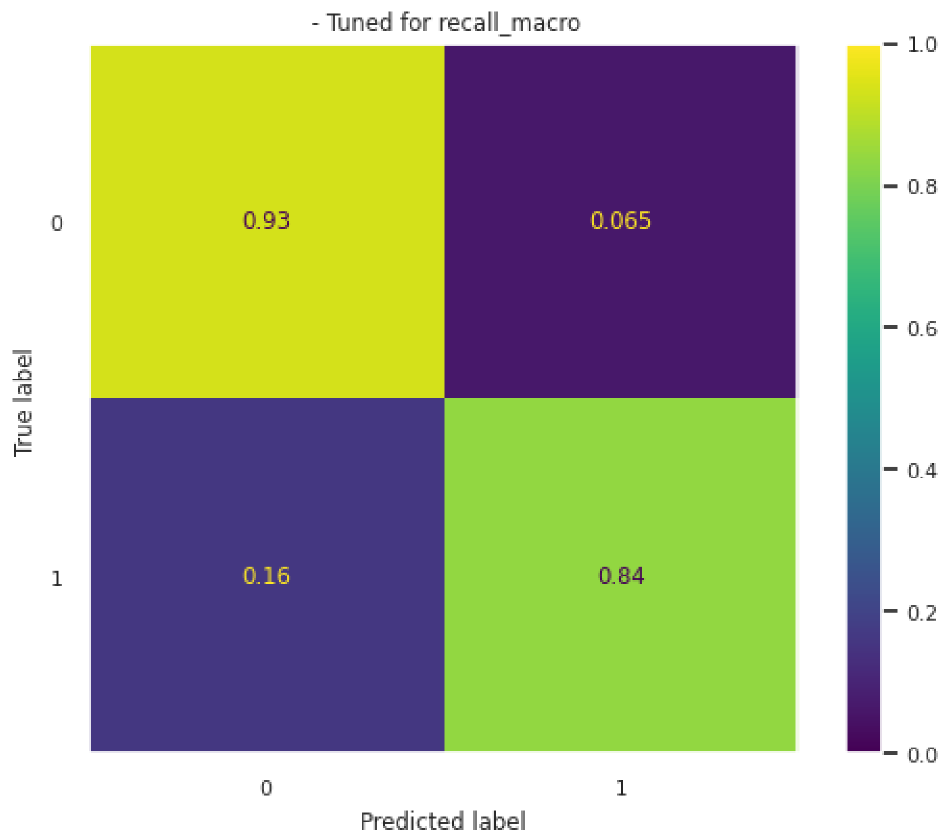
[36]:
```python
params = {'max_depth': [*range(4,10), None],
          "criterion": ["entropy", "gini"],
           "class_weight": [None, "balanced"],
          'n_estimators':list(range(10,max_rf_estimators+1,10))
          }

results_rf = grid_search(params, ["recall_macro"], base_rf, Xtr, ytr, Xte, yte, n_jobs=9,␣
 ↪overwrite_pickle=False, verbose=3)
```

```
Grid search already cached in cache/RandomForestClassifier__gridsearch.pickle -
loading...
```

[37]:
```python
print_gridsearch_results(results_rf)
```

```
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.93      0.97     26783
           1       0.14      0.84      0.24       339

    accuracy                           0.93     27122
   macro avg       0.57      0.89      0.60     27122
weighted avg       0.99      0.93      0.96     27122

Best parameters:
        bootstrap: True
        ccp_alpha: 0.0
        class_weight: balanced
        criterion: gini
```

```
        max_depth: 9
        max_features: sqrt
        max_leaf_nodes: None
        max_samples: None
        min_impurity_decrease: 0.0
        min_samples_leaf: 1
        min_samples_split: 2
        min_weight_fraction_leaf: 0.0
        n_estimators: 100
        n_jobs: None
        oob_score: False
        random_state: 69420
        verbose: 0
        warm_start: False

Feature importances:
        Type: 0.008
        Air temperature [K]: 0.120
        Process temperature [K]: 0.035
        Rotational speed [rpm]: 0.344
        Torque [Nm]: 0.326
        Tool wear [min]: 0.166
```



3.3 AdaBoost

3.3.1 Baseline

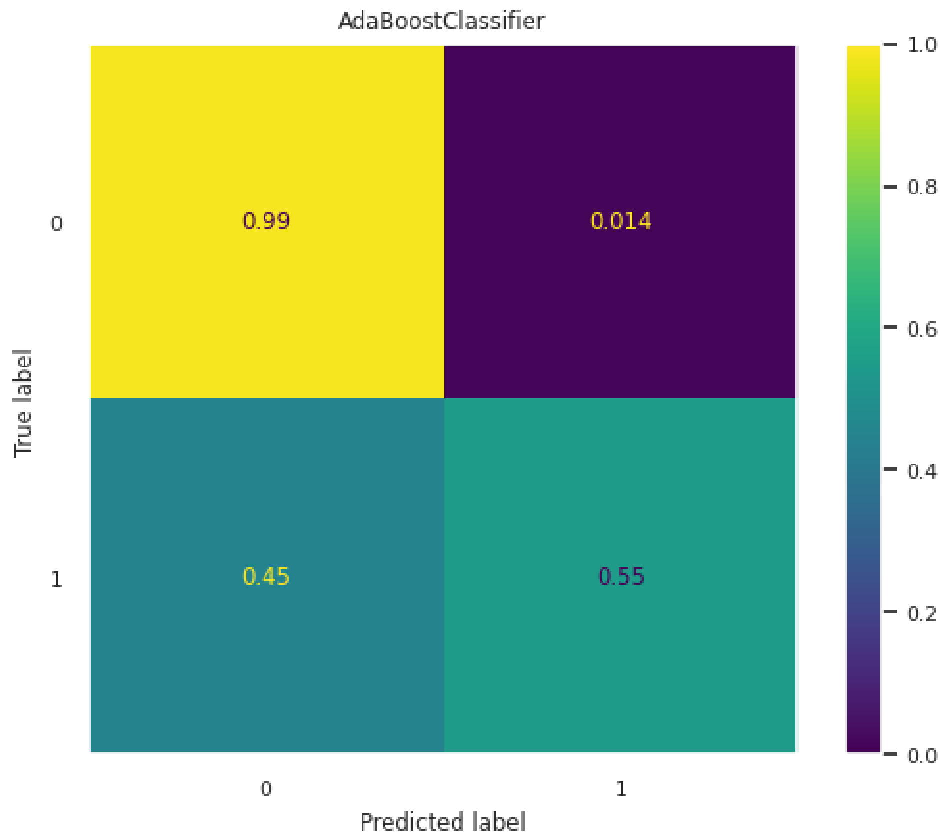
[38]:
```
from sklearn.ensemble import AdaBoostClassifier
```

[39]:
```
ada = AdaBoostClassifier(random_state=RANDOM_STATE)

ypred, base_rep_ada, cm = fit_and_predict(ada, Xtr, ytr, Xte, yte)
```

```
Fitting model...done
Testing...done
```

[40]:
```
print_model_results(ada, base_rep_ada, cm)
```

```
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.99      0.99     26783
           1       0.33      0.55      0.42       339

    accuracy                           0.98     27122
   macro avg       0.66      0.77      0.70     27122
weighted avg       0.99      0.98      0.98     27122

Best parameters:
        algorithm: SAMME.R
        base_estimator: deprecated
        estimator: None
        learning_rate: 1.0
        n_estimators: 50
        random_state: 69420

Feature importances:
        Type: 0.040
        Air temperature [K]: 0.120
        Process temperature [K]: 0.140
        Rotational speed [rpm]: 0.240
        Torque [Nm]: 0.240
        Tool wear [min]: 0.220
```



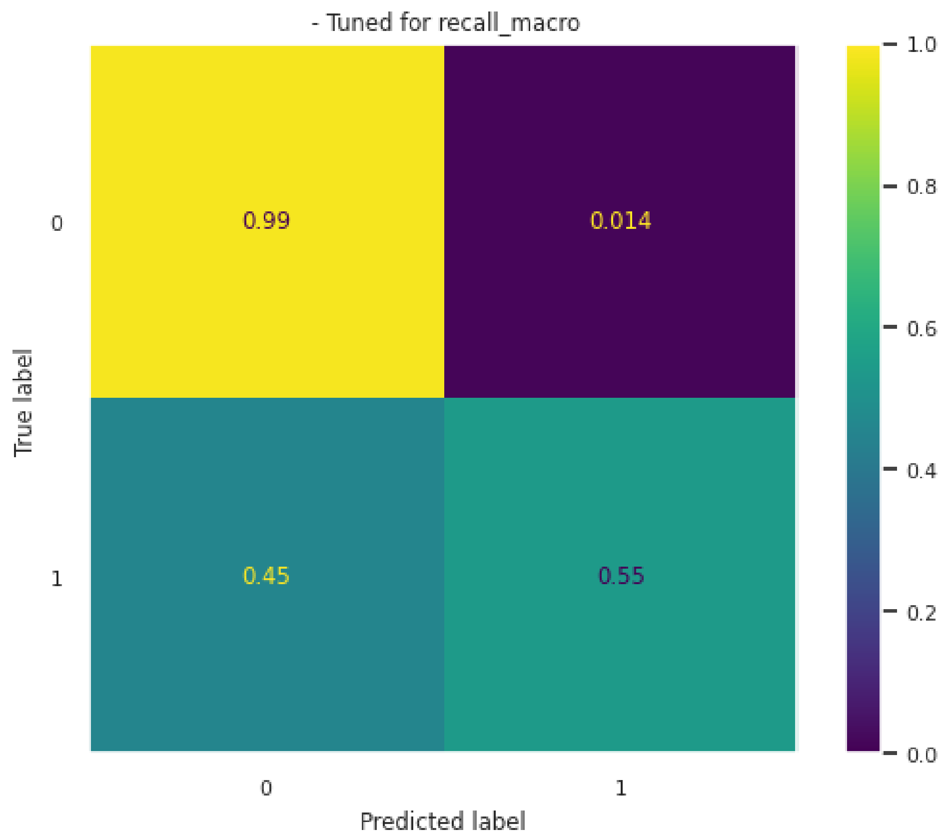
3.3.2 Grid search

[41]:
```
results_ada = grid_search({'n_estimators':range(10, 100+1, 10),
                           'learning_rate':[0.2 * i for i in range(1, 8)],
                           }, ["recall_macro"], ada, Xtr, ytr, Xte, yte, overwrite_pickle=False, verbose=3,␣
 ↪n_jobs=8)
```

```
Grid search already cached in cache/AdaBoostClassifier__gridsearch.pickle -
loading...
```

[42]:
```
print_gridsearch_results(results_ada)
```

```
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.99      0.99     26783
           1       0.34      0.55      0.42       339

    accuracy                           0.98     27122
   macro avg       0.67      0.77      0.70     27122
weighted avg       0.99      0.98      0.98     27122

Best parameters:
        algorithm: SAMME.R
        base_estimator: deprecated
        estimator: None
        learning_rate: 1.4000000000000001
        n_estimators: 100
        random_state: 69420

Feature importances:
        Type: 0.020
        Air temperature [K]: 0.210
        Process temperature [K]: 0.290
        Rotational speed [rpm]: 0.170
        Torque [Nm]: 0.210
        Tool wear [min]: 0.100
```



3.4 K-Nearest Neighbor

3.4.1 Baseline

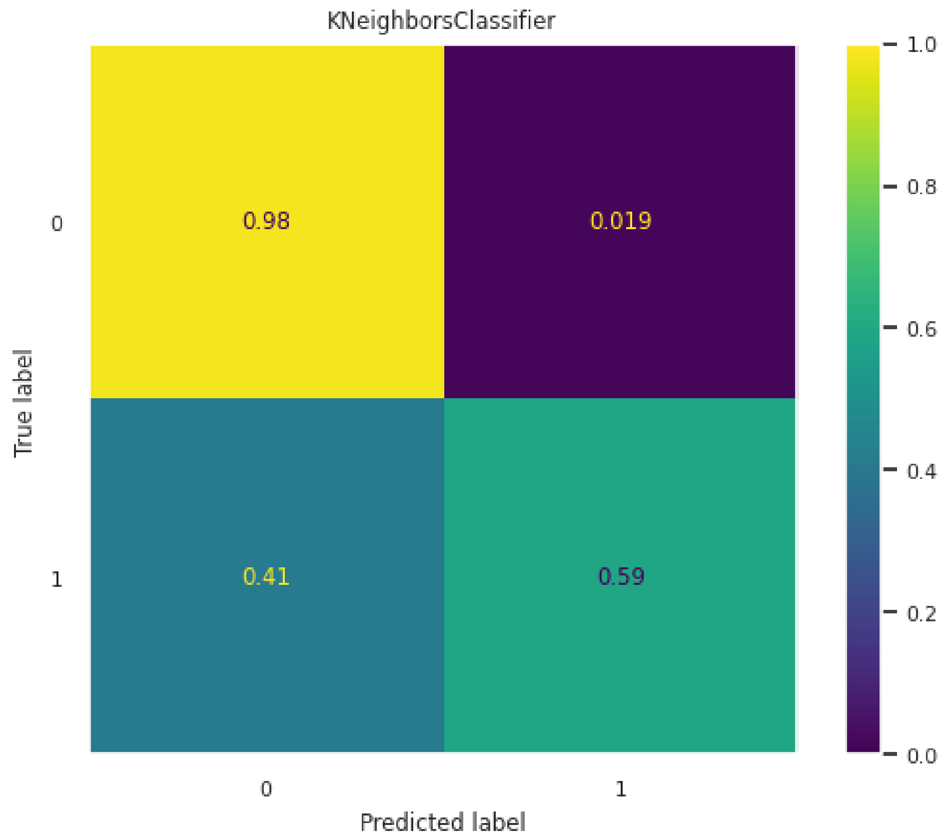
[43]:
```
from sklearn.neighbors import KNeighborsClassifier
```

[79]:
```
kn = KNeighborsClassifier()

ypred, base_rep_knn, cm = fit_and_predict(kn, Xtr, ytr, Xte, yte)
```

```
Fitting model...done
Testing...done
```

[80]:
```
print_model_results(kn, base_rep_knn, cm)
```

```
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.98      0.99     26783
           1       0.28      0.59      0.38       339

    accuracy                           0.98     27122
   macro avg       0.64      0.78      0.68     27122
weighted avg       0.99      0.98      0.98     27122

Best parameters:
        algorithm: auto
        leaf_size: 30
        metric: minkowski
        metric_params: None
        n_jobs: None
        n_neighbors: 5
        p: 2
        weights: uniform
```



3.4.2 Grid search

[89]:
```
base_params = {"n_neighbors": range(1, 30),
                "metric": ["euclidean", "manhattan"],
                "n_jobs": [2],
                }
```

```
btree_algo_params = {"algorithm": ["ball_tree", "kd_tree"],
                     "leaf_size": [10*i for i in range(1,10)],
                     **base_params}

other_algo_params = {"algorithm": ["auto", "brute"],
                     **base_params}

results_knn = grid_search([btree_algo_params, other_algo_params], ["recall_macro"],
                          kn, Xtr, ytr, Xte, yte, overwrite_pickle=False, n_jobs=6, verbose=3)
```

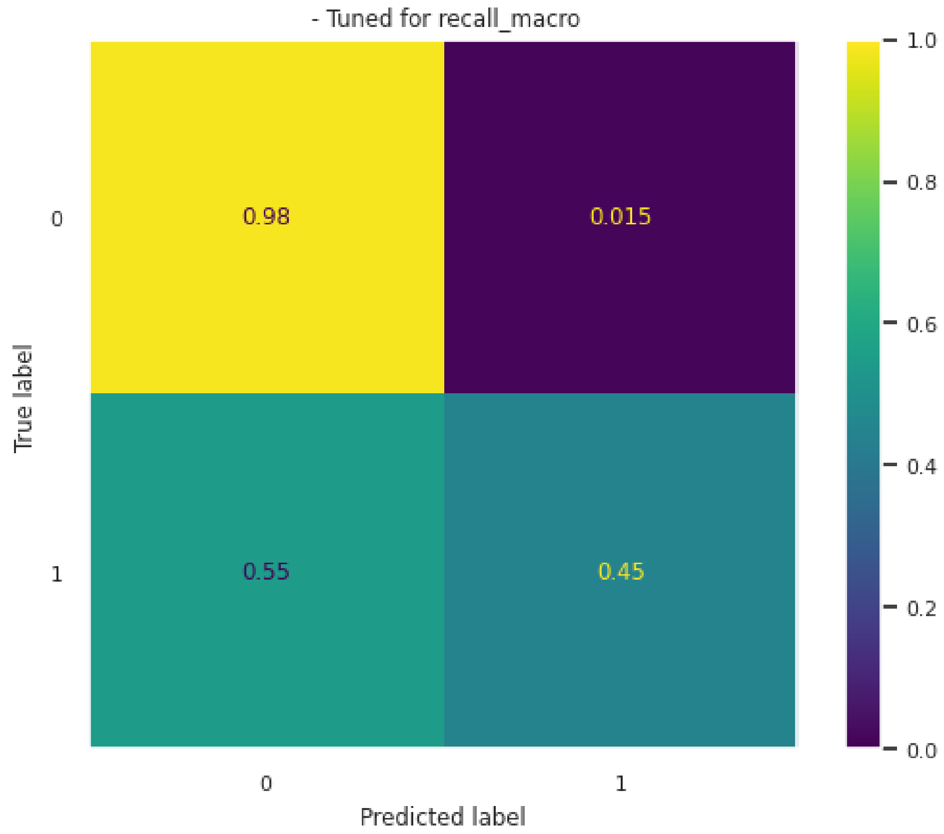
```
Grid search already cached in cache/KNeighborsClassifier__gridsearch.pickle -
loading...
```

[88]:

```
print_gridsearch_results(results_knn)
```

```
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.98      0.99     26783
           1       0.27      0.45      0.34       339

    accuracy                           0.98     27122
   macro avg       0.63      0.72      0.66     27122
weighted avg       0.98      0.98      0.98     27122

Best parameters:
        algorithm: kd_tree
        leaf_size: 40
        metric: manhattan
        metric_params: None
        n_jobs: 2
        n_neighbors: 1
        p: 2
```

```
weights: uniform
```



3.5 Gaussian Naive Bayes

3.5.1 Baseline

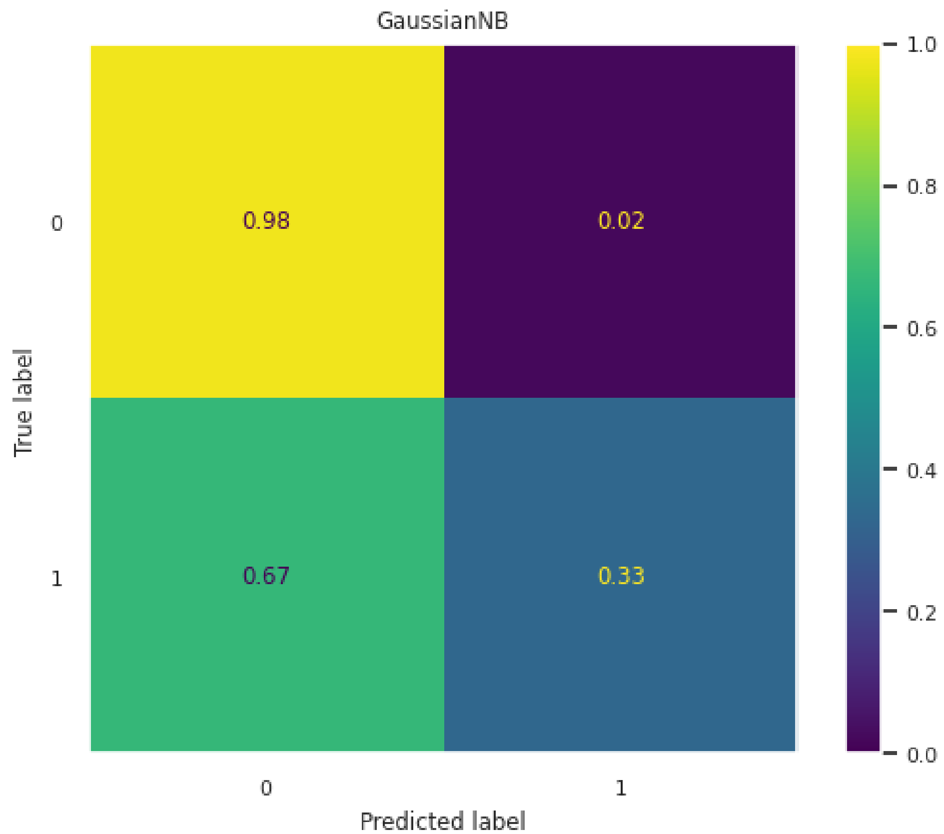
[48]:
```
from sklearn.naive_bayes import GaussianNB
```

[49]:
```
gnb = GaussianNB()

ypred, base_rep_gnb, cm = fit_and_predict(gnb, Xtr, ytr, Xte, yte)
```

```
Fitting model...done
Testing...done
```

[50]:
```
print_model_results(gnb, base_rep_gnb, cm)
```

```
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.98      0.99     26783
           1       0.18      0.33      0.23       339

    accuracy                           0.97     27122
   macro avg       0.58      0.66      0.61     27122
weighted avg       0.98      0.97      0.98     27122

Best parameters:
        priors: None
        var_smoothing: 1e-09
```



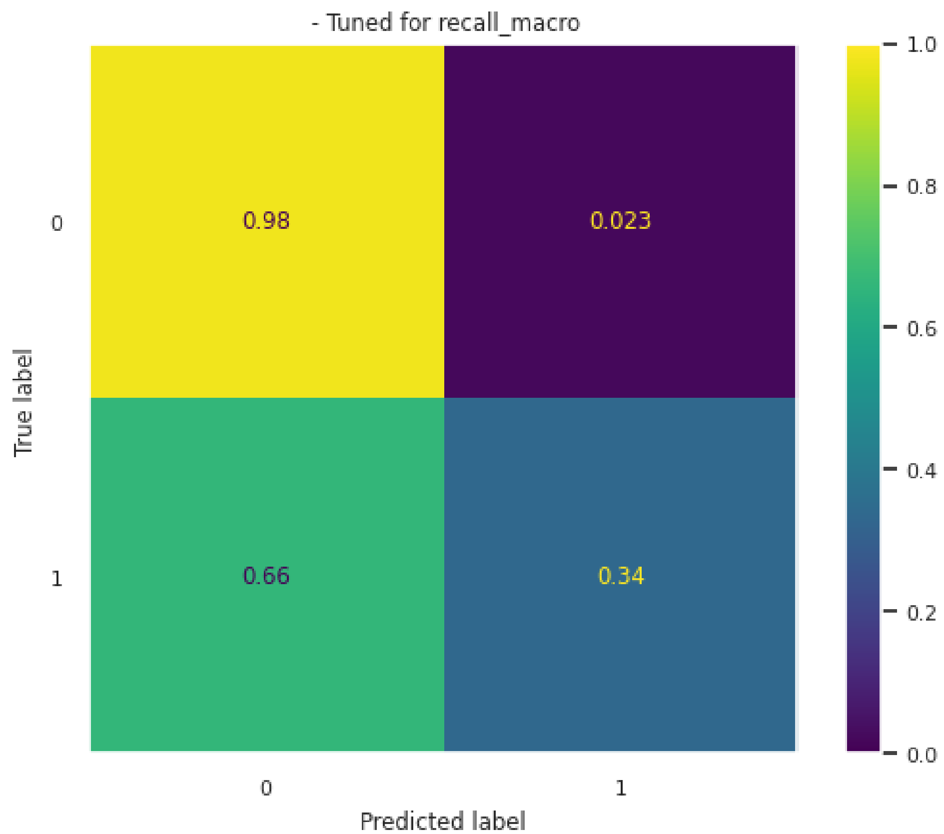
3.5.2 Grid search

[51]:
```
results_gnb = grid_search({'var_smoothing': [10**(-exp) for exp in range(1, 60)]},
                          ["recall_macro"], gnb, Xtr, ytr, Xte, yte)
```

```
Grid search already cached in cache/GaussianNB__gridsearch.pickle - loading...
```

[52]:
```
print_gridsearch_results(results_gnb)
```

```
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       0.99      0.98      0.98     26841
           1       0.17      0.34      0.23       382

    accuracy                           0.97     27223
   macro avg       0.58      0.66      0.61     27223
weighted avg       0.98      0.97      0.97     27223

Best parameters:
        priors: None
        var_smoothing: 1e-08
```



3.6 Perceptron

3.6.1 Baseline

[53]:
```
from sklearn.linear_model import Perceptron
```

[54]:

```
lp = Perceptron(random_state=RANDOM_STATE)

ypred, base_rep_lp, cm = fit_and_predict(lp, Xtr, ytr, Xte, yte)
```

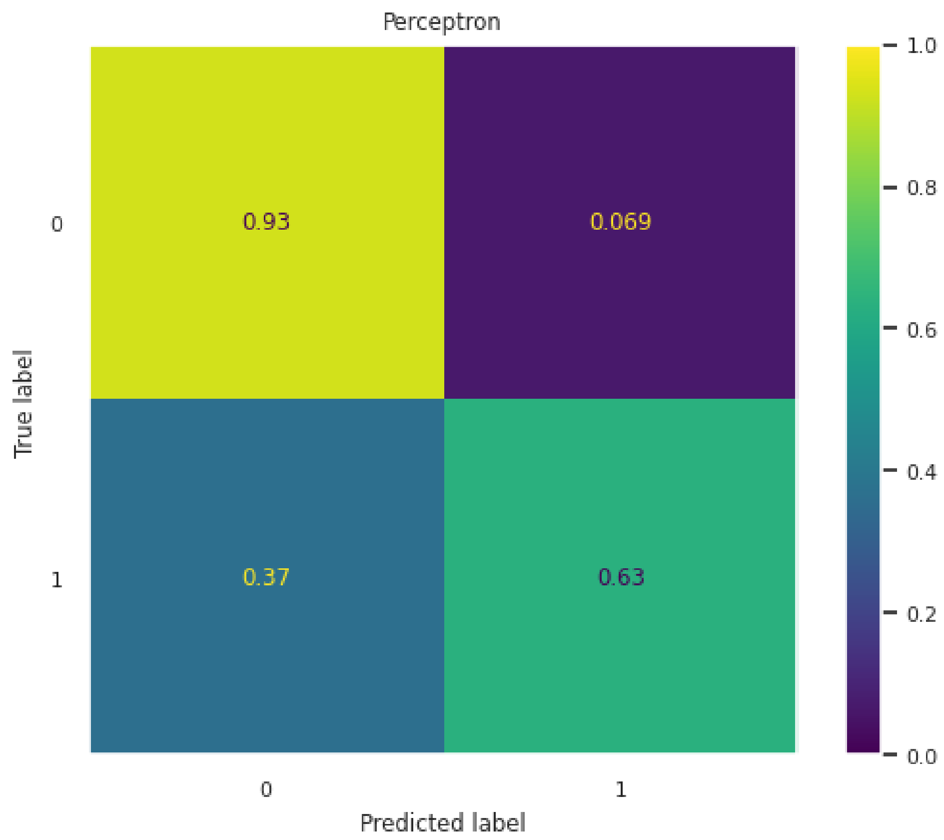
```
Fitting model...done
Testing...done
```

[55]:

```
print_model_results(lp, base_rep_lp, cm)
```

```
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.93      0.96     26783
           1       0.10      0.63      0.18       339

    accuracy                           0.93     27122
   macro avg       0.55      0.78      0.57     27122
weighted avg       0.98      0.93      0.95     27122

Best parameters:
        alpha: 0.0001
        class_weight: None
        early_stopping: False
        eta0: 1.0
        fit_intercept: True
        l1_ratio: 0.15
        max_iter: 1000
        n_iter_no_change: 5
        n_jobs: None
        penalty: None
        random_state: 69420
        shuffle: True
        tol: 0.001
        validation_fraction: 0.1
        verbose: 0
```

```
warm_start: False
```



3.6.2 Grid search

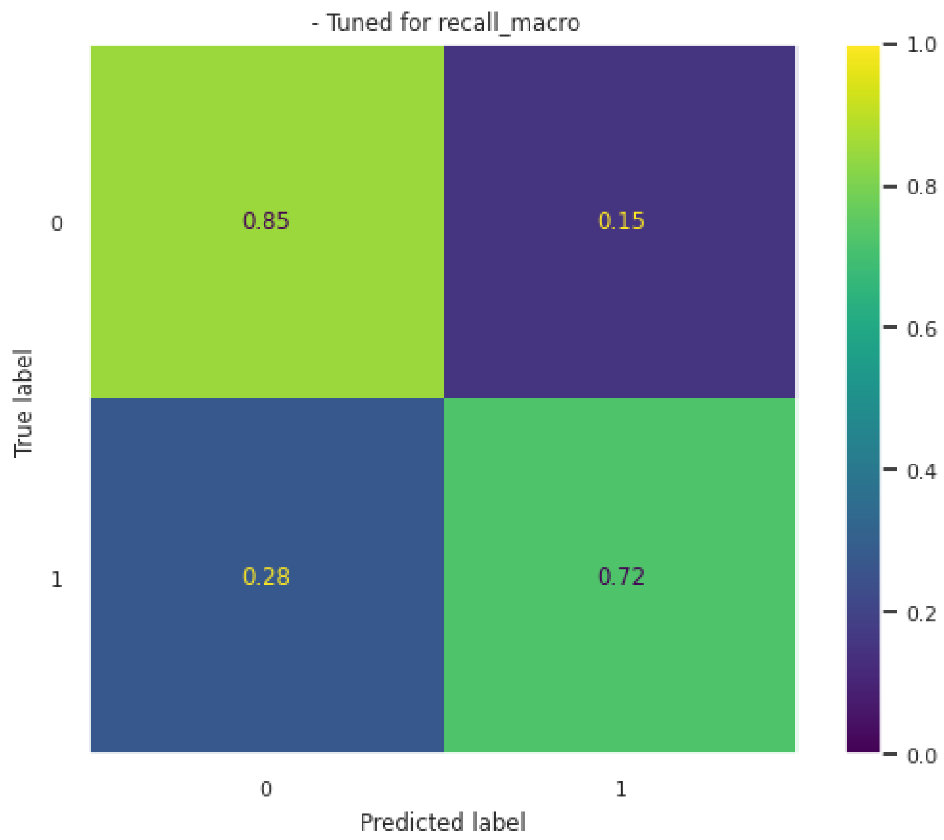
[56]:
```
base_params = {'early_stopping': [True,False],
               'class_weight':[None,'balanced'],
               "eta0": [10.0**i for i in range(-5, 2)],
               }

elasticnet_params = {'l1_ratio': [0.1, 0.15, 0.5, 0.9],
                     'penalty': ["elasticnet"],
                     **base_params
                     }

other_penalties_params = {'penalty': ["l1", "l2", None],
                          **base_params
                         }

results_perc = grid_search([elasticnet_params, other_penalties_params], ["recall_macro"], lp, Xtr, ytr, Xte, yte)
```

```
Grid search already cached in cache/Perceptron__gridsearch.pickle - loading...
```

[57]:
```
print_gridsearch_results(results_perc)
```

```
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.85      0.92     26783
           1       0.06      0.72      0.11       339

    accuracy                           0.85     27122
   macro avg       0.53      0.79      0.51     27122
weighted avg       0.98      0.85      0.91     27122

Best parameters:
```

```
alpha: 0.0001
class_weight: balanced
early_stopping: True
eta0: 1.0
fit_intercept: True
l1_ratio: 0.15
max_iter: 1000
n_iter_no_change: 5
n_jobs: None
penalty: None
random_state: 69420
shuffle: True
tol: 0.001
validation_fraction: 0.1
verbose: 0
warm_start: False
```



3.7 Support Vector Machine

3.7.1 Baseline

[58]:
```
from sklearn.svm import SVC
```

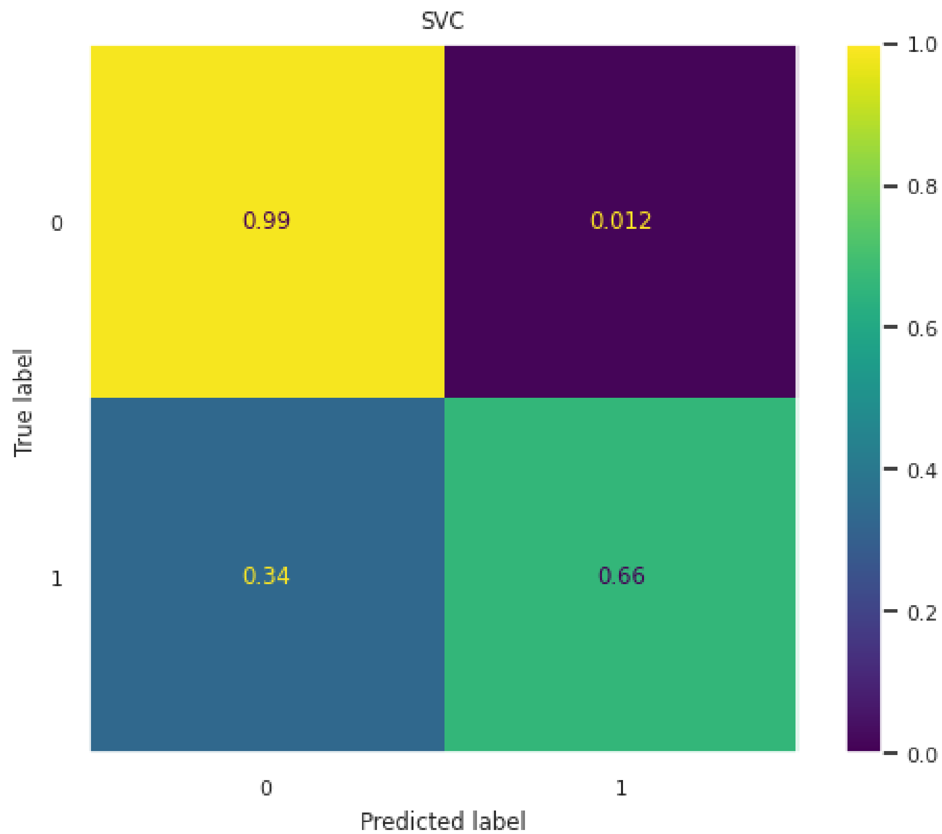
[59]:
```
svc = SVC(random_state=RANDOM_STATE)
overwrite = False
pickle_path = f"{CACHE_DIR}/SVC__baseline.pickle"
cached = os.path.isfile(pickle_path)

if cached and not overwrite:
    print(f"Baseline model already cached in {pickle_path} - loading...")
    tmp = load_pickle(pickle_path)
else:
    if cached and overwrite:
        print(f"Overwriting cached model...")

    tmp = [svc, fit_and_predict(svc, Xtr, ytr, Xte, yte)]
    dump_pickle(tmp, pickle_path)

svc = tmp[0]
y_pred, base_rep_svc, cm = tmp[1]
```

```
Baseline model already cached in cache/SVC__baseline.pickle - loading...
```

[60]:
```
print_model_results(svc, base_rep_svc, cm)
```

```
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.99      0.99     26783
           1       0.41      0.66      0.51       339

    accuracy                           0.98     27122
   macro avg       0.70      0.82      0.75     27122
weighted avg       0.99      0.98      0.99     27122

Best parameters:
        C: 1.0
        break_ties: False
```

```
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: 69420
shrinking: True
tol: 0.001
verbose: False
```



3.7.2 Grid search

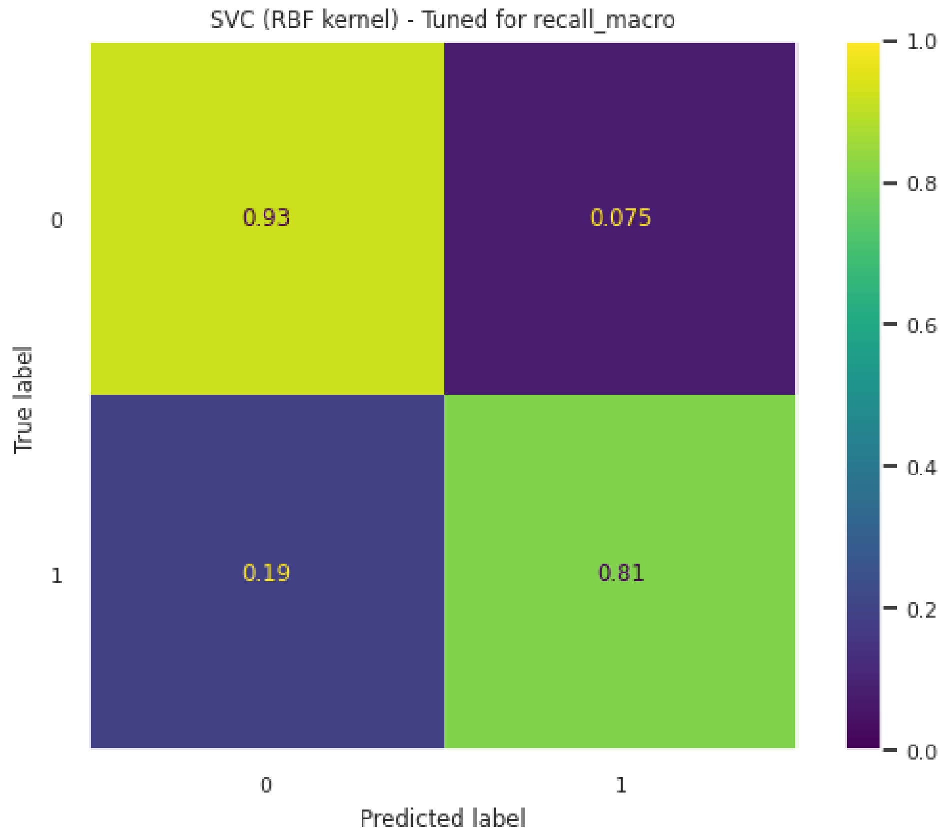
Due to the extremely long training time of this model, the tuning has been performed separately for the two kernels tested (`rbf` and `poly`).

[61]:
```
# WARNING: using Colab, this took more than 1 hr
results_svc_rbf = grid_search({'kernel': ['rbf'],
```

```python
                    'gamma': ["scale","auto",1e-3, 1e-4],
                    'C': [1, 10, 100],
                    "shrinking": [True, False],
                    'class_weight': [None, "balanced"]},
                    ["recall_macro"], svc, Xtr, ytr, Xte, yte,
                    n_splits=2, n_jobs=10, overwrite_pickle=False, verbose=3,
                    pickle_file="SVC__gridsearch_rbf.pickle")

print_gridsearch_results(results_svc_rbf, cm_model_name="SVC (RBF kernel)")
```

```
Grid search already cached in cache/SVC__gridsearch_rbf.pickle - loading...
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.93      0.96     26783
           1       0.12      0.81      0.21       339

    accuracy                           0.92     27122
   macro avg       0.56      0.87      0.59     27122
weighted avg       0.99      0.92      0.95     27122

Best parameters:
        C: 100
        break_ties: False
        cache_size: 200
        class_weight: balanced
        coef0: 0.0
        decision_function_shape: ovr
        degree: 3
        gamma: auto
        kernel: rbf
        max_iter: -1
```

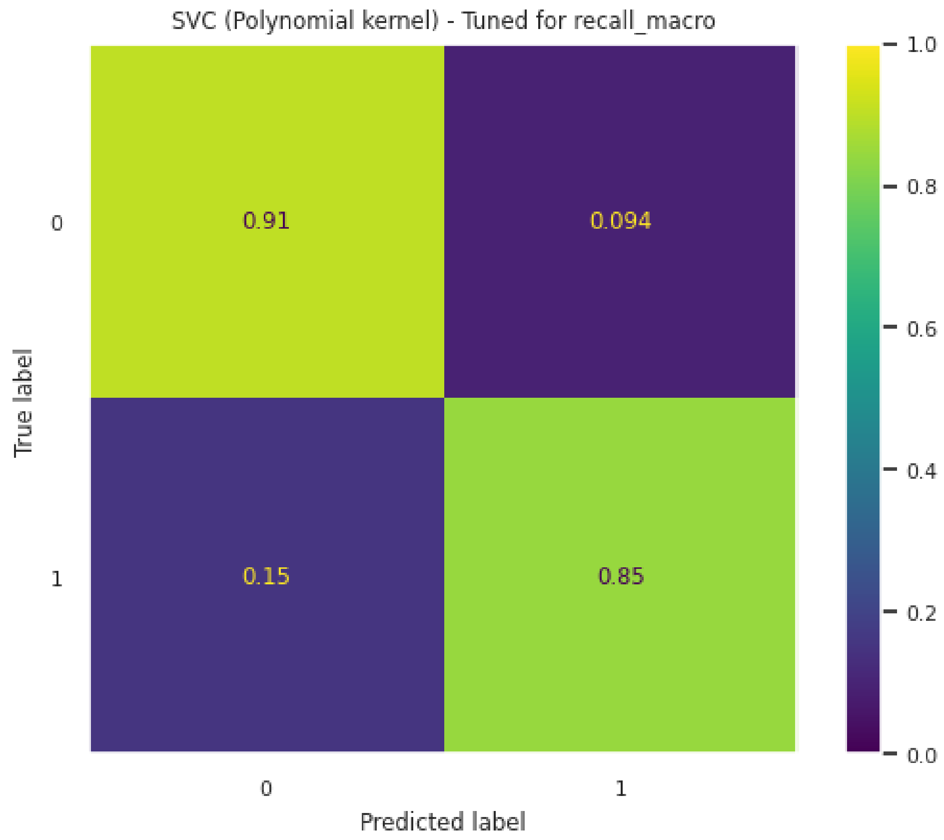
```
probability: False
random_state: 69420
shrinking: False
tol: 0.001
verbose: False
```



[62]:
```python
# WARNING: using Colab, this took more than 1 hr
results_svc_poly = grid_search({'kernel': ['poly'],
                    'gamma': ["scale","auto",1e-3, 1e-4],
                    'C': [1, 10, 100],
                    'class_weight': [None, "balanced"]},
                    ["recall_macro"], svc, Xtr, ytr, Xte, yte,
                    n_splits=2, n_jobs=10, overwrite_pickle=False, verbose=3,
                    pickle_file="SVC__gridsearch_poly.pickle")

print_gridsearch_results(results_svc_poly, cm_model_name="SVC (Polynomial kernel)")
```

```
Grid search already cached in cache/SVC__gridsearch_poly.pickle - loading...
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.91      0.95     26783
           1       0.10      0.85      0.18       339

    accuracy                           0.90     27122
   macro avg       0.55      0.88      0.57     27122
weighted avg       0.99      0.90      0.94     27122

Best parameters:
        C: 1.0
        break_ties: False
        cache_size: 200
        class_weight: balanced
        coef0: 0.0
        decision_function_shape: ovr
        degree: 3
        gamma: scale
        kernel: poly
```

```
max_iter: -1
probability: False
random_state: 69420
shrinking: True
tol: 0.001
verbose: False
```



[63]:
```
# We see that, although just slightly, the best model uses the poly kernel
results_svc = results_svc_poly
```

3.8 Gradient descent

3.8.1 Baseline

[64]:
```
from sklearn.linear_model import SGDClassifier
```

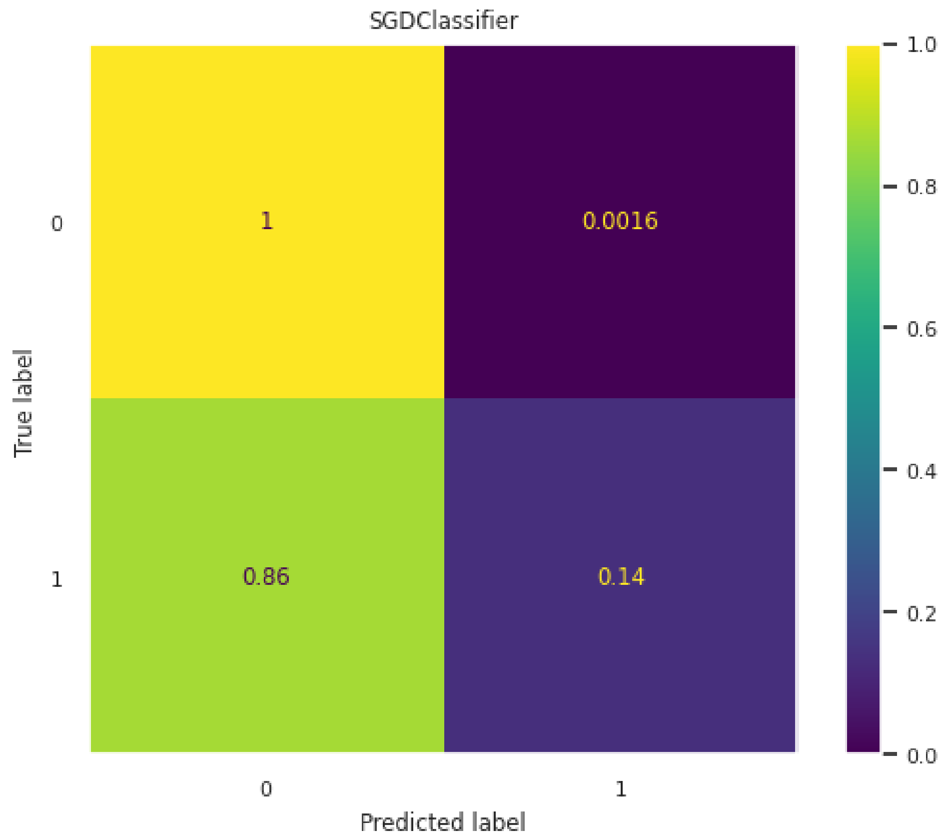
[65]:
```
sgd = SGDClassifier(random_state=RANDOM_STATE)

y_pred, base_rep_sgd, cm = fit_and_predict(sgd, Xtr, ytr, Xte, yte)
```

```
Fitting model...done
Testing...done
```

[66]:
```
print_model_results(sgd, base_rep_sgd, cm)
```

```
Classification report:
              precision    recall  f1-score   support

           0       0.99      1.00      0.99     26783
           1       0.52      0.14      0.21       339

    accuracy                           0.99     27122
   macro avg       0.75      0.57      0.60     27122
weighted avg       0.98      0.99      0.98     27122

Best parameters:
        alpha: 0.0001
        average: False
        class_weight: None
        early_stopping: False
        epsilon: 0.1
        eta0: 0.0
        fit_intercept: True
```

```
l1_ratio: 0.15
learning_rate: optimal
loss: hinge
max_iter: 1000
n_iter_no_change: 5
n_jobs: None
penalty: l2
power_t: 0.5
random_state: 69420
shuffle: True
tol: 0.001
validation_fraction: 0.1
verbose: 0
warm_start: False
```



3.8.2 Grid search

[67]:
```
base_params = {'class_weight': [None, "balanced"],
               "alpha": [10**e for e in range(-5, 2)],
               "penalty": ["l2", "l1", "elasticnet", None],
               "loss": ["hinge", "log_loss", "modified_huber", "perceptron"],
               }
```

```python
# The eta0 parameter is disregarded when learning_rate="optimal"
optimal_lr_params = {"learning_rate": ["optimal"],
                     **base_params}

other_lr_params = {"learning_rate": ["constant", "invscaling", "adaptive"],
                   "eta0": [0.01, 0.1, 1],
                   **base_params}

results_sgd = grid_search([optimal_lr_params, other_lr_params], ["recall_macro"], sgd, Xtr, ytr, Xte, yte,␣
↪overwrite_pickle=False, verbose=3, n_jobs=8)
```

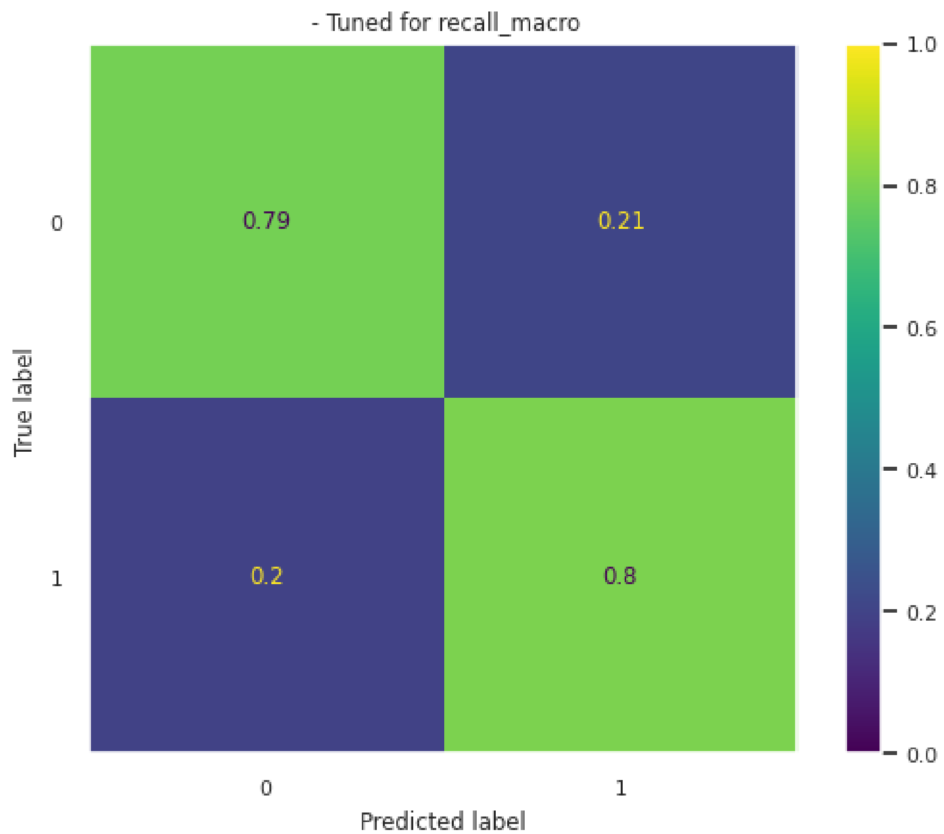
```
Grid search already cached in cache/SGDClassifier__gridsearch.pickle -
loading...
```

[68]:

```python
print_gridsearch_results(results_sgd)
```

```
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.79      0.88     26783
           1       0.05      0.80      0.09       339

    accuracy                           0.79     27122
   macro avg       0.52      0.80      0.48     27122
weighted avg       0.98      0.79      0.87     27122

Best parameters:
        alpha: 1
        average: False
        class_weight: balanced
        early_stopping: False
        epsilon: 0.1
```

```
eta0: 0.1
fit_intercept: True
l1_ratio: 0.15
learning_rate: invscaling
loss: hinge
max_iter: 1000
n_iter_no_change: 5
n_jobs: None
penalty: elasticnet
power_t: 0.5
random_state: 69420
shuffle: True
tol: 0.001
validation_fraction: 0.1
verbose: 0
warm_start: False
```



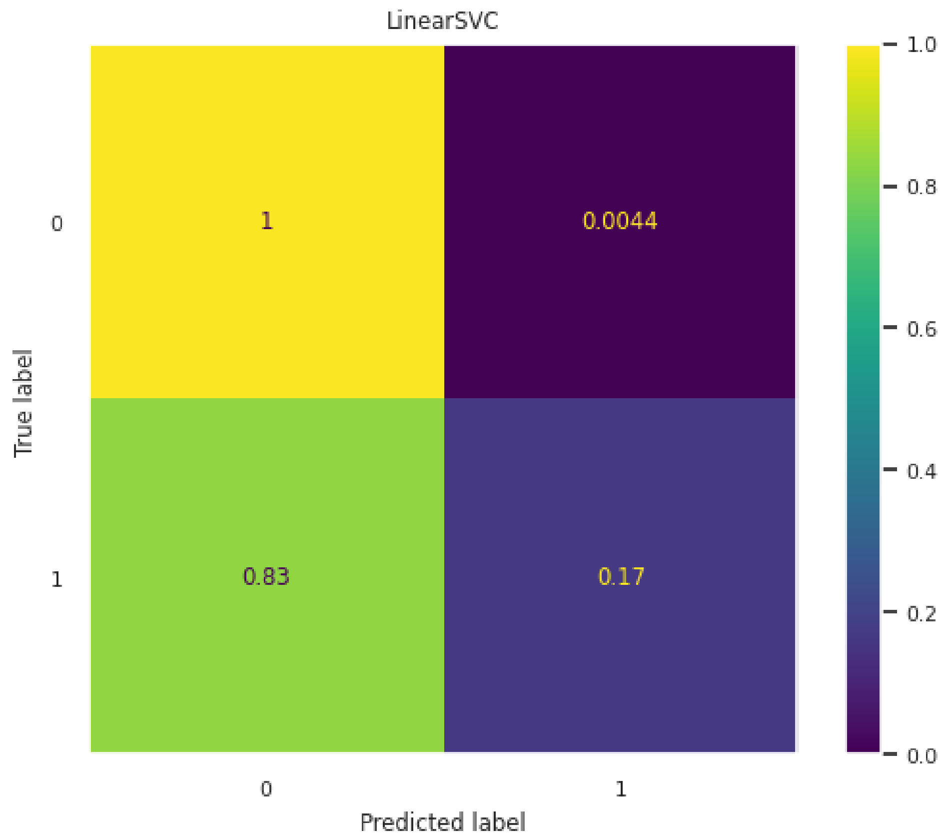
The value for the `loss` parameter was selected to be `"hinge"`. As stated in the documentation, this means that the model is actually fitting a *linear* support vector classifier. Indeed, using the `LinearSVC` class, which directly implements the same thing, we see basically the same results, both before and after tuning:

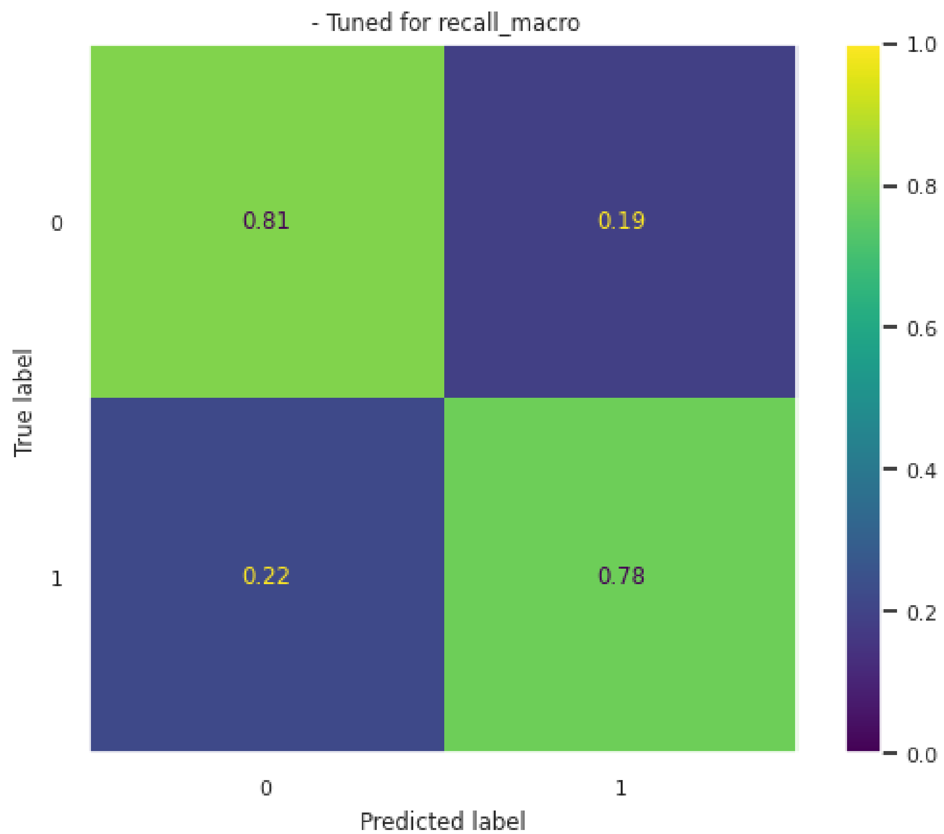
[69]:
```
from sklearn.svm import LinearSVC

lsvm = LinearSVC(random_state=RANDOM_STATE, max_iter=6000, dual=False)
```

```python
ypred, base_rep_lsvm, cm = fit_and_predict(lsvm, Xtr, ytr, Xte, yte)

print_model_results(lsvm, base_rep_lsvm, cm)

results_svc_linear = grid_search({'penalty': ["l1", "l2"],
                    'C': [1, 10, 100],
                    'class_weight': [None, "balanced"]},
                    ["recall_macro"], lsvm, Xtr, ytr, Xte, yte,
                    n_jobs=10, overwrite_pickle=False, verbose=3, pickle_file="SVC__linear.pickle")

print_gridsearch_results(results_svc_linear)
```

```
Fitting model...done
Testing...done
Classification report:
              precision    recall  f1-score   support

           0       0.99      1.00      0.99     26783
           1       0.32      0.17      0.22       339

    accuracy                           0.99     27122
   macro avg       0.66      0.58      0.61     27122
weighted avg       0.98      0.99      0.98     27122

Best parameters:
        C: 1.0
        class_weight: None
        dual: False
        fit_intercept: True
        intercept_scaling: 1
        loss: squared_hinge
        max_iter: 6000
        multi_class: ovr
```

```
        penalty: l2
        random_state: 69420
        tol: 0.0001
        verbose: 0

Grid search already cached in cache/SVC__linear.pickle - loading...
--------------------
Score: recall_macro
Classification report:
              precision    recall  f1-score   support

           0       1.00      0.81      0.89     26783
           1       0.05      0.78      0.09       339

    accuracy                           0.81     27122
   macro avg       0.52      0.79      0.49     27122
weighted avg       0.98      0.81      0.88     27122

Best parameters:
        C: 1
        class_weight: balanced
        dual: False
        fit_intercept: True
        intercept_scaling: 1
        loss: squared_hinge
        max_iter: 6000
        multi_class: ovr
        penalty: l2
        random_state: 69420
        tol: 0.0001
        verbose: 0
```


LinearSVC
True label
Predicted label
0
1
0
1
1
0.0044
0.83
0.17
1.0
0.8
0.6
0.4
0.2
0.0



4 Conclusions

[70]:
```
reports = {
    "DecisionTree": [base_rep_dt, results_dt],
    "RandomForest": [base_rep_rf, results_rf],
    "AdaBoost": [base_rep_ada, results_ada],
```

```
    "KNN": [base_rep_knn, results_knn],
    "GaussianNB": [base_rep_gnb, results_gnb],
    "Perceptron": [base_rep_lp, results_perc],
    "SVC": [base_rep_svc, results_svc],
    "SGD": [base_rep_sgd, results_sgd]
}

reports = {k : (report_str_to_dict(v0), report_str_to_dict(v1["recall_macro"]["report"])) for k, v in reports.
 ↪items() for v0, v1 in [v]}
```

[71]:
```
model_names = reports.keys()
reports_baseline = {k: v[0] for k, v in reports.items()}
reports_gscv = {k: v[1] for k, v in reports.items()}
```

[72]:
```
recalls_gscv = {model: rep["macro_avg"]["recall"] for model, rep in reports_gscv.items()}
recalls_baseline = {model: rep["macro_avg"]["recall"] for model, rep in reports_baseline.items()}
```

Firstly, this plot shows an overall comparison of each model's performance for each class before and after tuning, measured through the recall for each class. As already stated, this remains basically the only reliable metric to evalutate these models due to the extreme imbalance found in the dataset.

After tuning, the models are thus classified as follows:

	Class 1 recall	*Recall (macro) average*
Random Forest	84%	**89%**
SVM	**85%**	88%
SGD	80%	80%
Perceptron	72%	79%
Decision Tree	71%	83%
AdaBoost	55%	77%
KNN	45%	72%
Gaussian NB	34%	66%

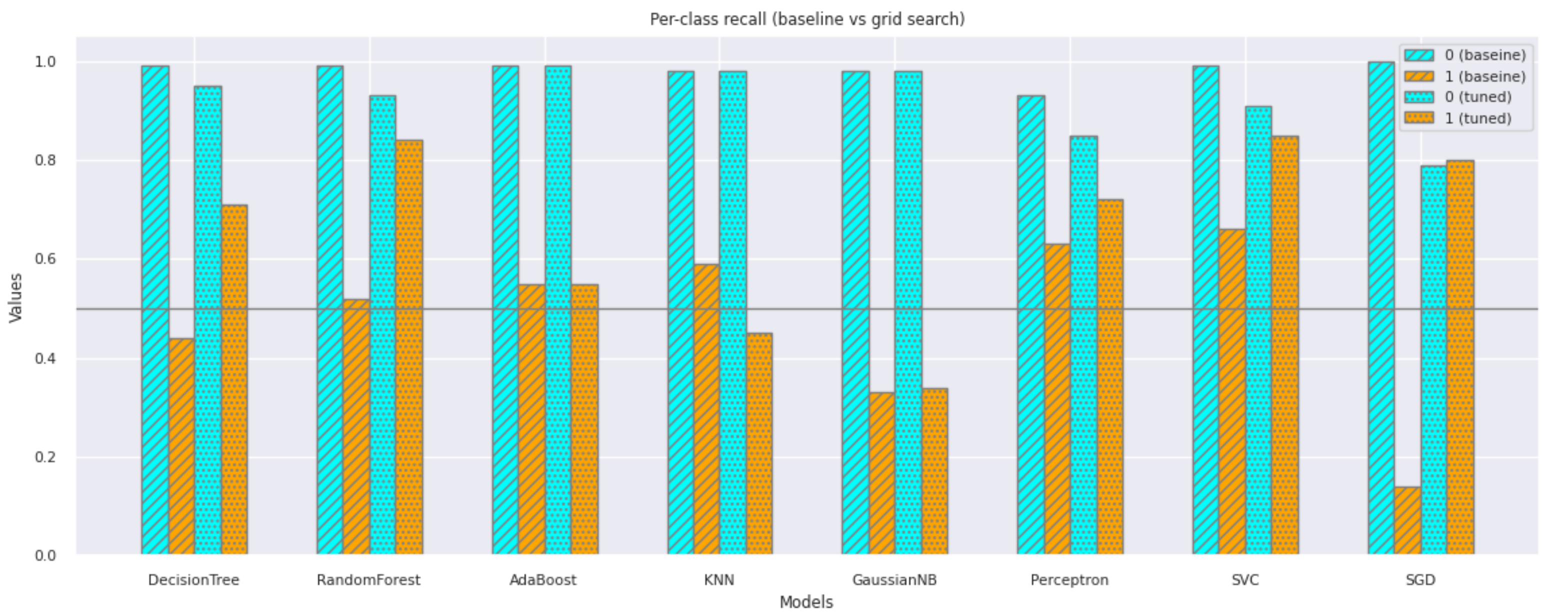
The tuned parameters of the two "winning" models are: - Random Forest - `max_depth`: 9 - `criterion`: `"gini"` - `class_weight`: `"balanced"`

- `n_estimators`: 100 - Support Vector Machine - `kernel`: `"poly"` - `class_weight`: `"balanced"` - `shrinking`: `False` - `gamma`: `"auto"` - `C`: 100 However, being a few orders of magnitude faster to train, the former may be considered more optimal.

The particularly bad performance of the KNN and Gaussian Naive Bayes classifiers was, to be fair, to be expected, though for different reasons: - For the KNN model, the pairplots at the beginning show that the two classes are mostly overlapping and to not form well distinct clusters - For the GNB model, its basic assumption of conditional independence between the attributes is clearly faulty in this context, since (for example) the rotational speed of a machine obviously influences its operating temperature

[73]:
```
# Bar plot properties
bar_width = 0.15  # Width of the bars

# Number of objects
n_objects = len(model_names)

# Create a figure and axis
_, ax = plt.subplots(figsize=(14, 5))

# Y positions for groups of bars
index = np.arange(n_objects)

tmp = [
    [reports_baseline[m]["0"]["recall"] for m in model_names],
    [reports_baseline[m]["1"]["recall"] for m in model_names],
    [reports_gscv[m]["0"]["recall"] for m in model_names],
    [reports_gscv[m]["1"]["recall"] for m in model_names],
]

for i, t in enumerate(tmp):
    ax.bar(index + bar_width*(i - 1.5), t, bar_width, edgecolor='grey',
           color="cyan" if (i%2) == 0 else "orange",
           label=f"{i%2} ({'baseine' if i < 2 else 'tuned'})",
           hatch="////" if i < 2 else "....")

ax.legend()
```

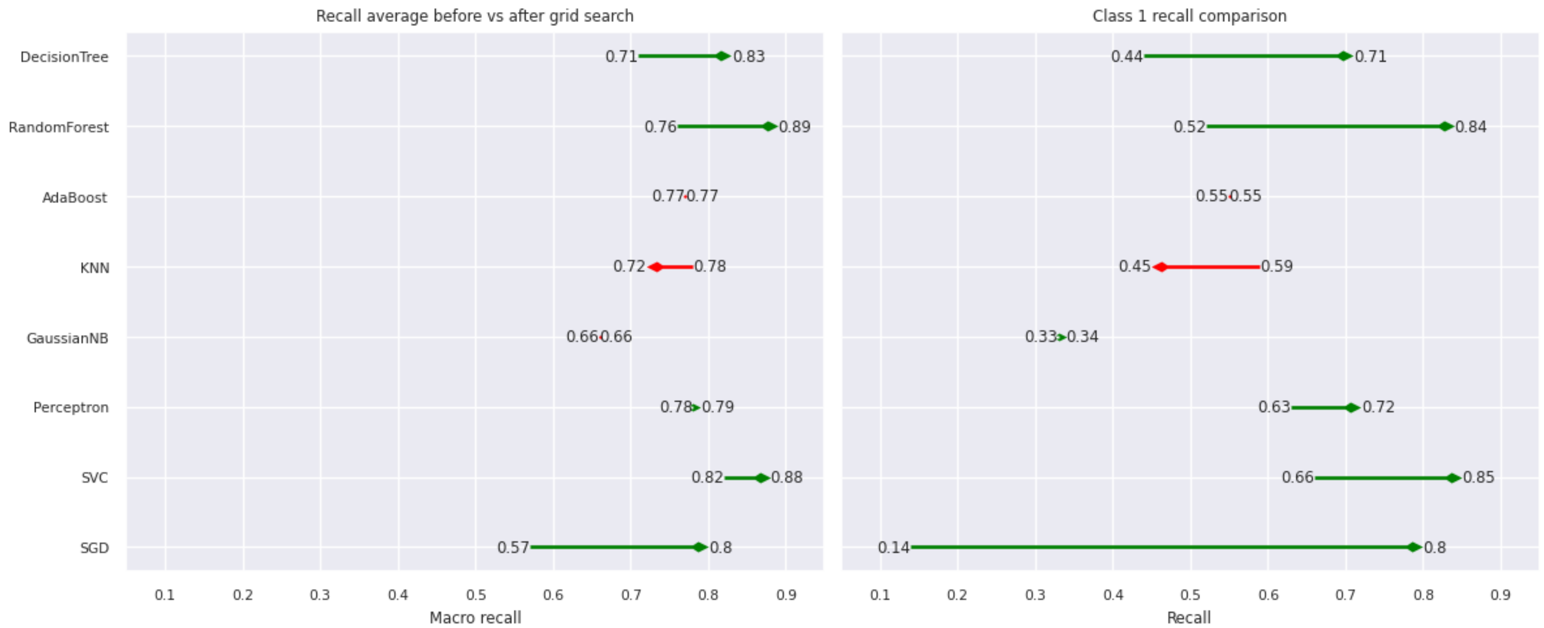
```
# Add labels and title
ax.set_xlabel('Models')
ax.set_ylabel('Values')
ax.set_xticks(index)
ax.set_xticklabels(model_names)
ax.set_title('Per-class recall (baseline vs grid search)')

# Horizontal line at y=.5
ax.axhline(.5, color='grey', lw=1)

# Show the plot
plt.show()
```



The following plots shows the *changes* in the recall metric, both for the macro average (left) and just for class 1 (right). It is noteworthy how the SGD model went from a baseline of 57% up to 80%, by far the largest improvement.

The worst performing models either didn't improve (AdaBoost and Gaussian Naive Bayes) or became worse (K-Nearest Neighbor). This may have two reasons: - none of these have a "class weight" parameter, unlike the other five, and thus couldn't be tuned to "pay more attention" to one class than the other - cross-validation is performed on a *slice* of the training set (unlike the default model, which used all of it). This is especially damning for the KNN classifier because it doesn't really perform any analysis of the training data, instead simply using it "as-is".

[74]:
```
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(12, 5))

plot_old_to_new(recalls_baseline, recalls_gscv,
                xlabel="Macro recall", ylabel="", x_range=(.1, .9), ax=ax1,
                title="Recall average before vs after grid search")

class1_recalls_gscv = {model: rep["1"]["recall"] for model, rep in reports_gscv.items()}
class1_recalls_baseline = {model: rep["1"]["recall"] for model, rep in reports_baseline.items()}

plot_old_to_new(class1_recalls_baseline, class1_recalls_gscv, ax=ax2, yticks=False,
                xlabel="Recall", ylabel="", x_range=(.1, .9), title="Class 1 recall comparison")

fig.tight_layout()
plt.show()
```



The main focus of this project ended up being *how to deal with severly imbalanced data*, more than the classification task itself. This, at least for the given dataset, was achieved in three main ways: 1. using a per-class weighing of the datapoints, when supported 2. performing dataset resampling during preprocessing to make the minority class easier to learn 3. targeting the `recall_macro` scoring metric when tuning instead of accuracy or precision - this metric is an *unweighted* average of the recalls for each class, making thus sure that the result doesn't de facto only account for the majority datapoints - the majority class being so dominant, it is acceptable to be slightly less accurate in classifying it if it means being way more sensitive to the minority