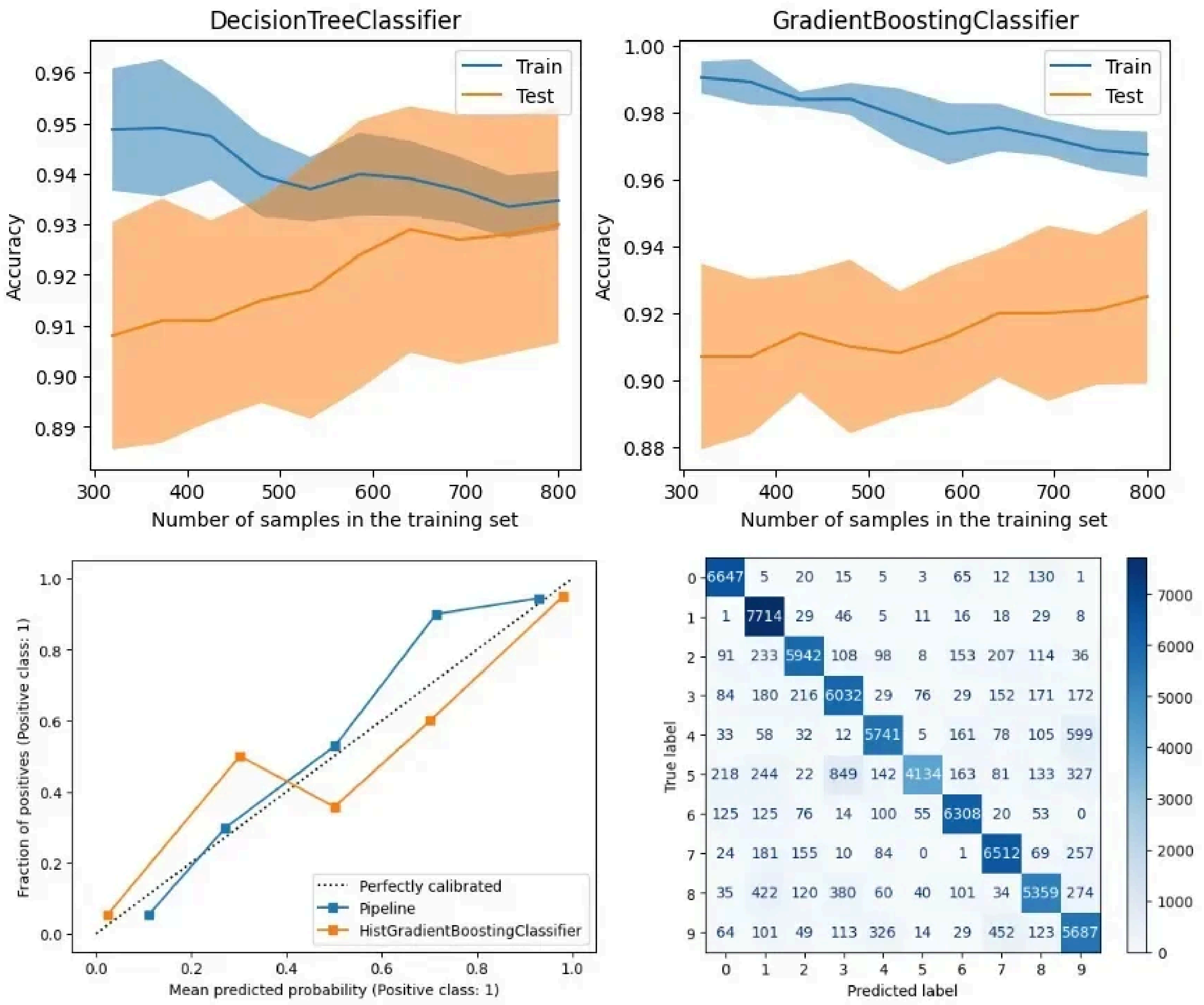
DS r/datascience • 1 day ago
qtalen

Scikit-learn Visualization Guide: Making Models Speak

ML

Use the Display API to replace complex Matplotlib code

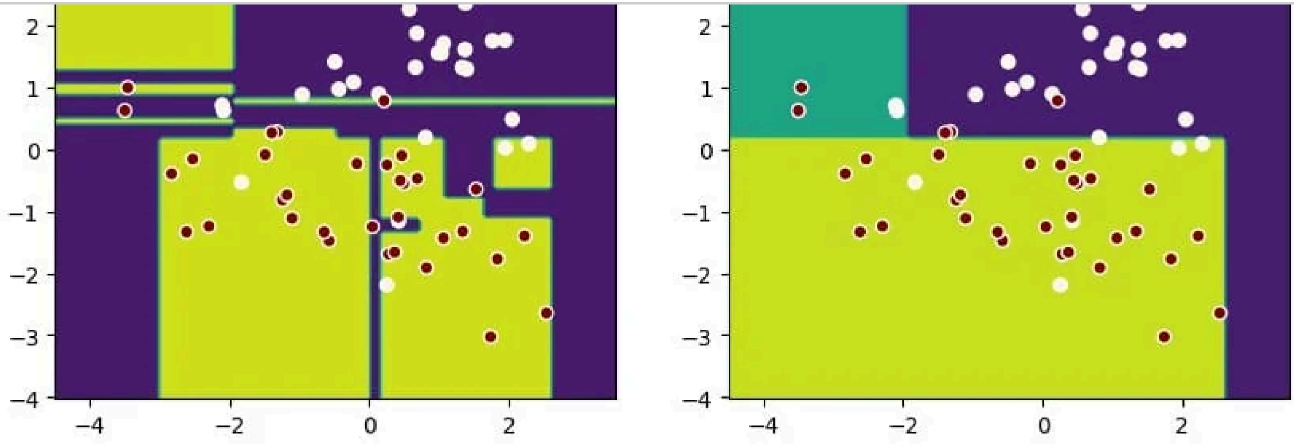


Scikit-learn Visualization Guide: Making Models Speak.

Introduction

In the journey of machine learning, explaining models with visualization is as important as training them.

A good chart can show us what a model is doing in an easy-to-understand way. Here's an example:



Decision boundaries of two different generalization performances.

This graph makes it clear that for the same dataset, the model on the right is better at generalizing.

Most machine learning books prefer to use raw Matplotlib code for visualization, which leads to issues:

1. You have to learn a lot about drawing with Matplotlib.
2. Plotting code fills up your notebook, making it hard to read.
3. Sometimes you need third-party libraries, which isn't ideal in business settings.

Good news! Scikit-learn now offers Display classes that let us use methods like from_estimator and from_predictions to make drawing graphs for different situations much easier.

Curious? Let me show you these cool APIs.

Scikit-learn Display API Introduction

Use utils.discovery.all_displays to find available APIs

Scikit-learn (sklearn) always adds Display APIs in new releases, so it's key to know what's available in your version.

Sklearn's utils.discovery.all_displays lets you see which classes you can use.

```
from sklearn.utils.discovery import all_displays

displays = all_displays()
displays
```

For example, in my Scikit-learn 1.4.0, these classes are available:

```
[('CalibrationDisplay', sklearn.calibration.CalibrationDisplay),
 ('ConfusionMatrixDisplay',
  sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay),
 ('DecisionBoundaryDisplay',
  sklearn.inspection._plot.decision_boundary.DecisionBoundaryDisplay),
```

```
  sklearn.inspection._plot.partial_dependence.PartialDependenceDisplay),
 ('PrecisionRecallDisplay',
  sklearn.metrics._plot.precision_recall_curve.PrecisionRecallDisplay),
 ('PredictionErrorDisplay',
  sklearn.metrics._plot.regression.PredictionErrorDisplay),
 ('RocCurveDisplay', sklearn.metrics._plot.roc_curve.RocCurveDisplay),
 ('ValidationCurveDisplay',
  sklearn.model_selection._plot.ValidationCurveDisplay)]
```

Using inspection.DecisionBoundaryDisplay for decision boundaries

Since we mentioned it, let's start with decision boundaries.

If you use Matplotlib to draw them, it's a hassle:

- Use np.linspace to set coordinate ranges;
- Use plt.meshgrid to calculate the grid;
- Use plt.contourf to draw the decision boundary fill;
- Then use plt.scatter to plot data points.

Now, with inspection.DecisionBoundaryDispla, you can simplify this process:

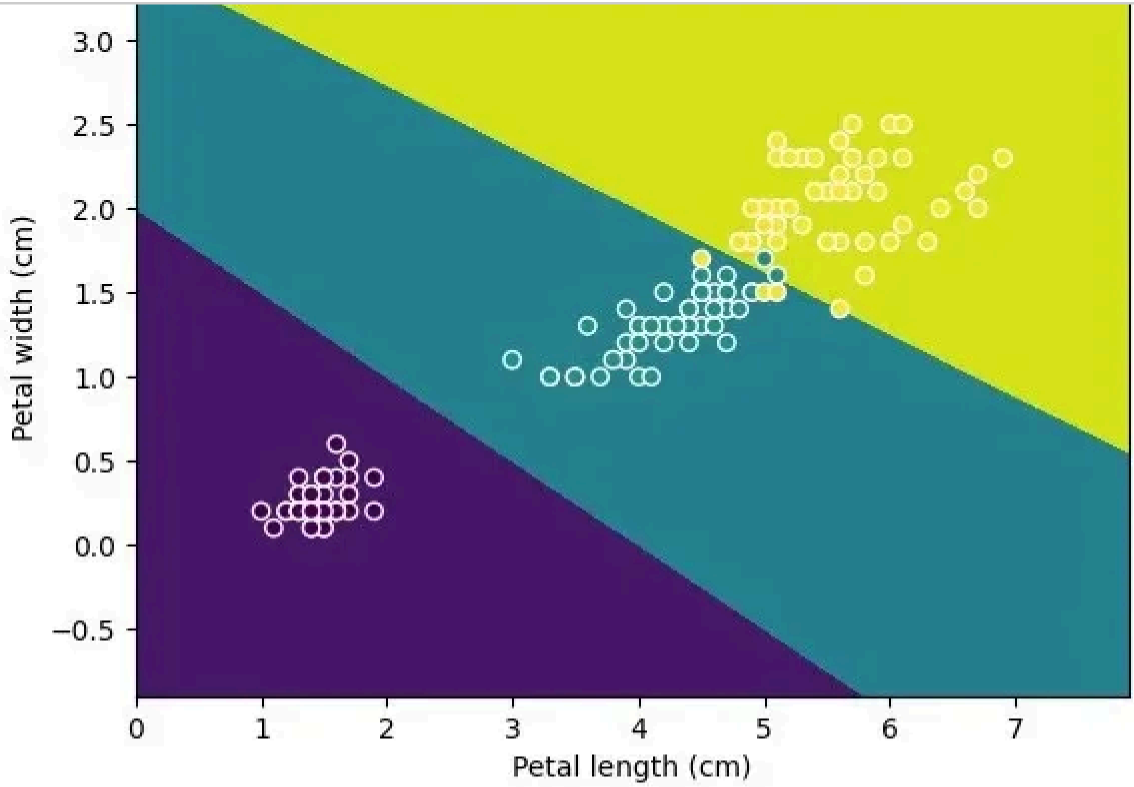
```
from sklearn.inspection import DecisionBoundaryDisplay
from sklearn.datasets import load_iris
from sklearn.svm import SVC
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
import matplotlib.pyplot as plt

iris = load_iris(as_frame=True)
X = iris.data[['petal length (cm)', 'petal width (cm)']]
y = iris.target


svc_clf = make_pipeline(StandardScaler(),
                        SVC(kernel='linear', C=1))
svc_clf.fit(X, y)

display = DecisionBoundaryDisplay.from_estimator(svc_clf, X,
                                                 grid_resolution=1000,
                                                 xlabel="Petal length (cm)",
                                                 ylabel="Petal width (cm)")
plt.scatter(X.iloc[:, 0], X.iloc[:, 1], c=y, edgecolors='w')
plt.title("Decision Boundary")
plt.show()
```

See the final effect in the figure:



Use DecisionBoundaryDisplay to draw a triple classification model.

Remember, Display can only draw 2D, so make sure your data has only two features or reduced dimensions.

Using calibration.CalibrationDisplay for probability calibration

To compare classification models, probability calibration curves show how confident models are in their predictions.

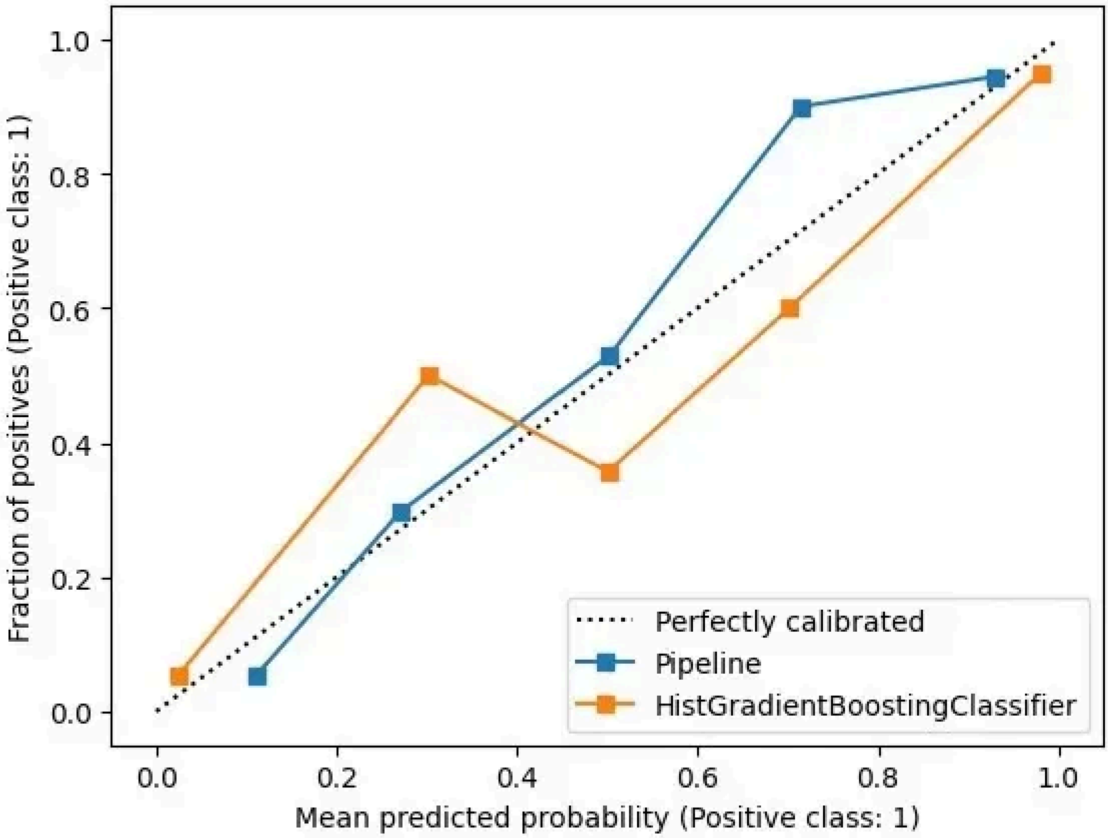
Note that CalibrationDisplay uses the model's predict_proba. If you use a support vector machine, set probability to True:

```
from sklearn.calibration import CalibrationDisplay
from sklearn.model_selection import train_test_split
from sklearn.datasets import make_classification
from sklearn.ensemble import HistGradientBoostingClassifier

X, y = make_classification(n_samples=1000,
                           n_classes=2, n_features=5,
                           random_state=42)
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.3, random_state=42)
proba_clf = make_pipeline(StandardScaler(),
                          SVC(kernel="rbf", gamma="auto",
                              C=10, probability=True))
proba_clf.fit(X_train, y_train)
```

```
hist_clf = HistGradientBoostingClassifier()
hist_clf.fit(X_train, y_train)

ax = plt.gca()
CalibrationDisplay.from_estimator(hist_clf,
                                  X_test, y_test,
                                  ax=ax)
plt.show()
```



Charts drawn by CalibrationDisplay.

Using metrics.ConfusionMatrixDisplay for confusion matrices

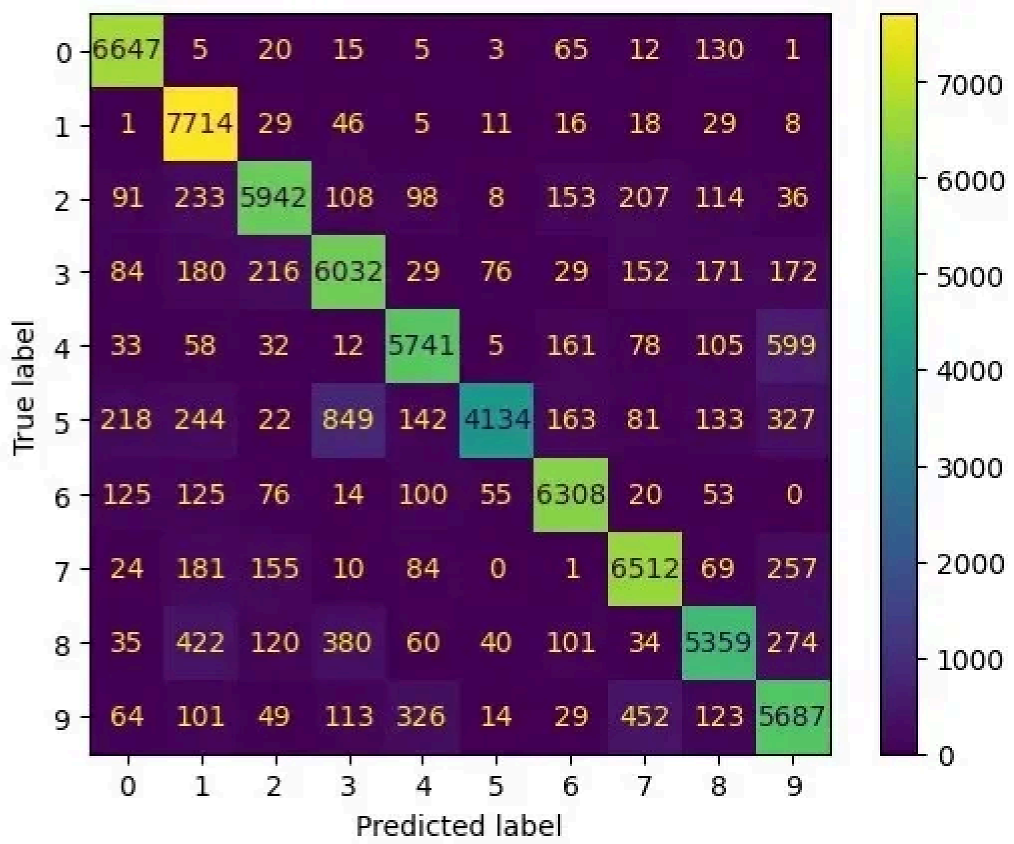
When assessing classification models and dealing with imbalanced data, we look at precision and recall.

These break down into TP, FP, TN, and FN – a confusion matrix.

To draw one, use metrics.ConfusionMatrixDisplay. It's well-known, so I'll skip the details.

```
from sklearn.datasets import fetch_openml
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import ConfusionMatrixDisplay

digits = fetch_openml('mnist_784', version=1)
X, y = digits.data, digits.target
rf_clf = RandomForestClassifier(max_depth=5, random_state=42)
rf_clf.fit(X, y)
```



Charts drawn with ConfusionMatrixDisplay.

metrics.RocCurveDisplay and metrics.DetCurveDisplay

These two are together because they're often used to evaluate side by side.

RocCurveDisplay compares TPR and FPR for the model.

For binary classification, you want low FPR and high TPR, so the upper left corner is best. The Roc curve bends towards this corner.

Because the Roc curve stays near the upper left, leaving the lower right empty, it's hard to see model differences.

So, we also use DetCurveDisplay to draw a Det curve with FNR and FPR. It uses more space, making it clearer than the Roc curve.

The perfect point for a Det curve is the lower left corner.

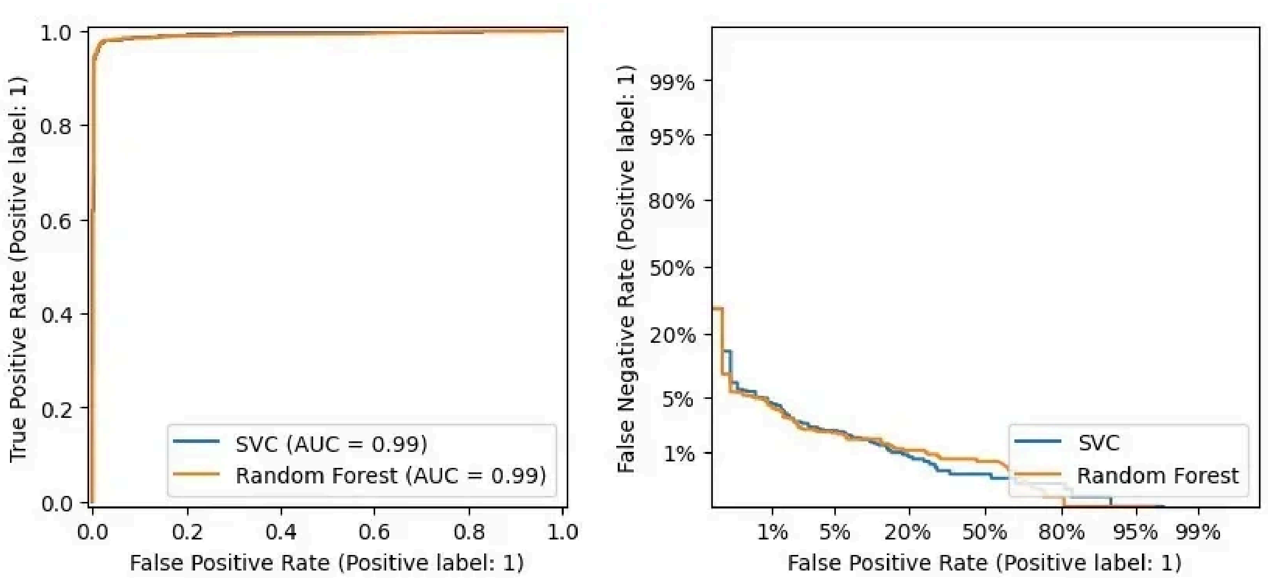
```
from sklearn.metrics import RocCurveDisplay
from sklearn.metrics import DetCurveDisplay

X, y = make_classification(n_samples=10_000, n_features=5,
                           n_classes=2, n_informative=2)
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                     test_size=0.3, random_state=42,
```

```
classifiers = {
    "SVC": make_pipeline(StandardScaler(), SVC(kernel="linear", C=0.1, random_state=42)
    "Random Forest": RandomForestClassifier(max_depth=5, random_state=42)
}

fig, [ax_roc, ax_det] = plt.subplots(1, 2, figsize=(10, 4))
for name, clf in classifiers.items():
    clf.fit(X_train, y_train)

    RocCurveDisplay.from_estimator(clf, X_test, y_test, ax=ax_roc, name=name)
    DetCurveDisplay.from_estimator(clf, X_test, y_test, ax=ax_det, name=name)
```



Comparison Chart of RocCurveDisplay and DetCurveDisplay.

Using metrics.PrecisionRecallDisplay to adjust thresholds

With imbalanced data, you might want to shift recall and precision.

- For email fraud, you want high precision.
- For disease screening, you want high recall to catch more cases.

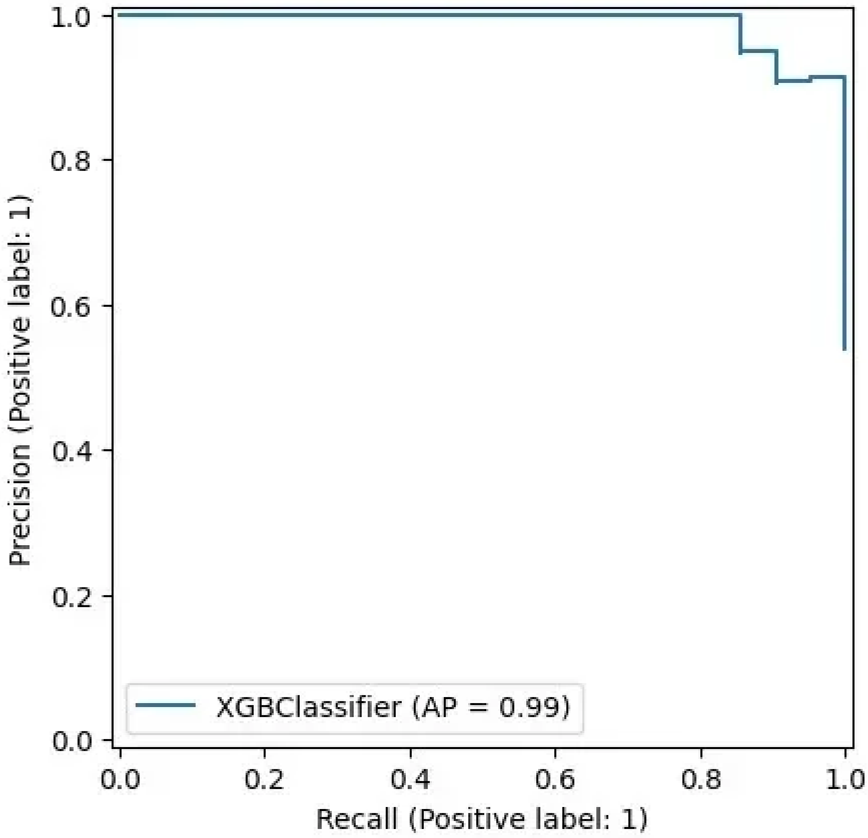
You can adjust the threshold, but what's the right amount?

Here, metrics.PrecisionRecallDisplay can help.

```
from xgboost import XGBClassifier
from sklearn.datasets import load_wine
from sklearn.metrics import PrecisionRecallDisplay

wine = load_wine()
X, y = wine.data[wine.target<=1], wine.target[wine.target<=1]
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
                                                    stratify=y, random_state=42)
```

```
PrecisionRecallDisplay.from_estimator(xgb_clf, X_test, y_test)
plt.show()
```



Charting xgboost model evaluation using PrecisionRecallDisplay.

This shows that models following Scikit-learn's design can be drawn, like xgboost here. Handy, right?

Using metrics.PredictionErrorDisplay for regression models

We've talked about classification, now let's talk about regression.

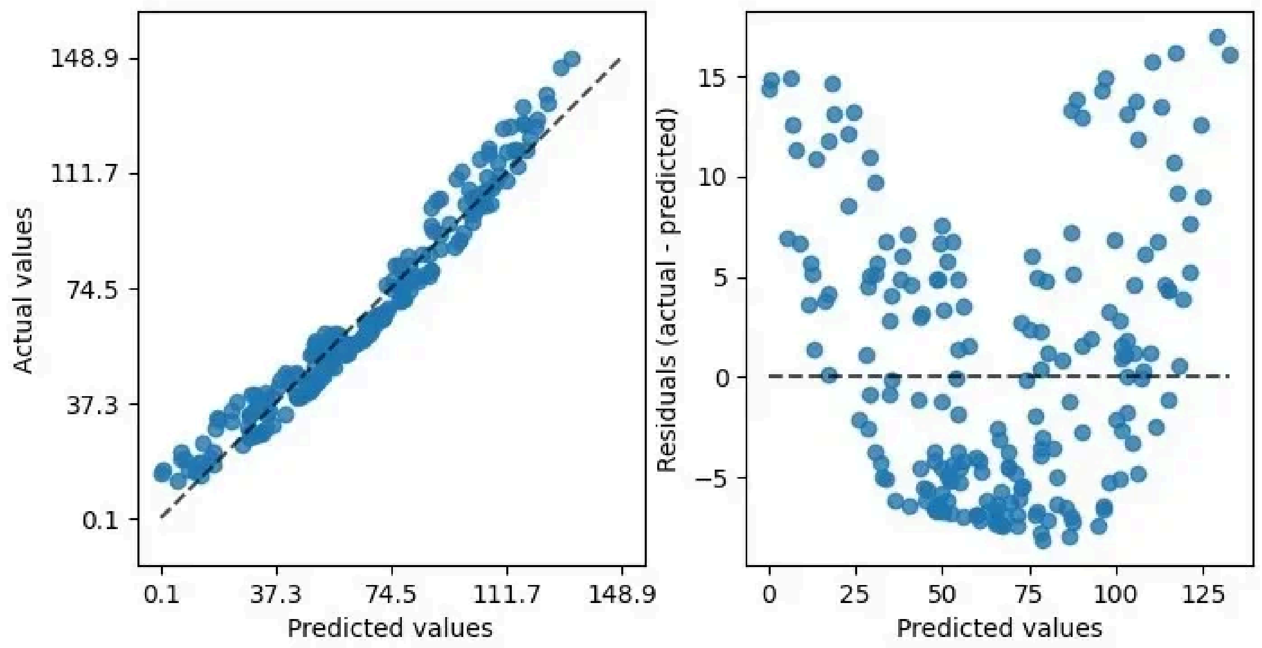
Scikit-learn's metrics.PredictionErrorDisplay helps assess regression models.

```
from sklearn.svm import SVR
from sklearn.metrics import PredictionErrorDisplay

rng = np.random.default_rng(42)
X = rng.random(size=(200, 2)) * 10
y = X[:, 0]**2 + 5 * X[:, 1] + 10 + rng.normal(loc=0.0, scale=0.1, size=(200,))

reg = make_pipeline(StandardScaler(), SVR(kernel='linear', C=10))
reg.fit(X, y)

fig, axes = plt.subplots(1, 2, figsize=(8, 4))
PredictionErrorDisplay.from_estimator(reg, X, y, ax=axes[0], kind="actual_vs_predicted"
```



Two charts were drawn by PredictionErrorDisplay.

As shown, it can draw two kinds of graphs. The left shows predicted vs. actual values – good for linear regression.

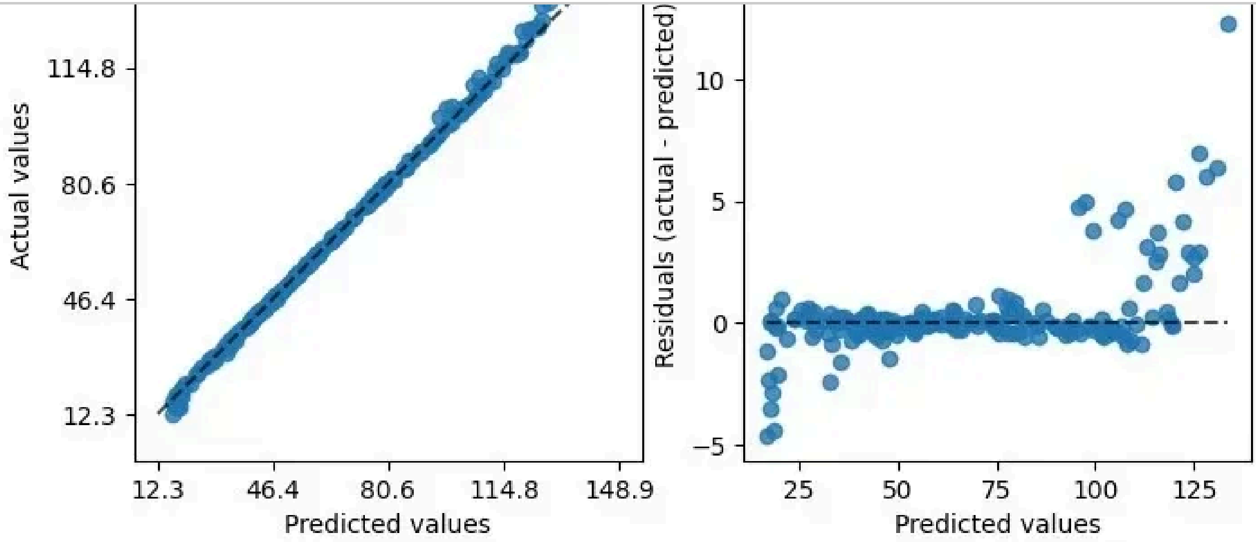
However, not all data is perfectly linear. For that, use the right graph.

It compares real vs. predicted differences, a residuals plot.

This plot's banana shape suggests our data might not fit linear regression.

Switching from a linear to an rbf kernel can help.

```
reg = make_pipeline(StandardScaler(), SVR(kernel='rbf', C=10))
```



A visual demonstration of the improved model performance.

See, with rbf, the residual plot looks better.

Using model_selection.LearningCurveDisplay for learning curves

After assessing performance, let's look at optimization with LearningCurveDisplay.

First up, learning curves – how well the model generalizes with different training and testing data, and if it suffers from variance or bias.

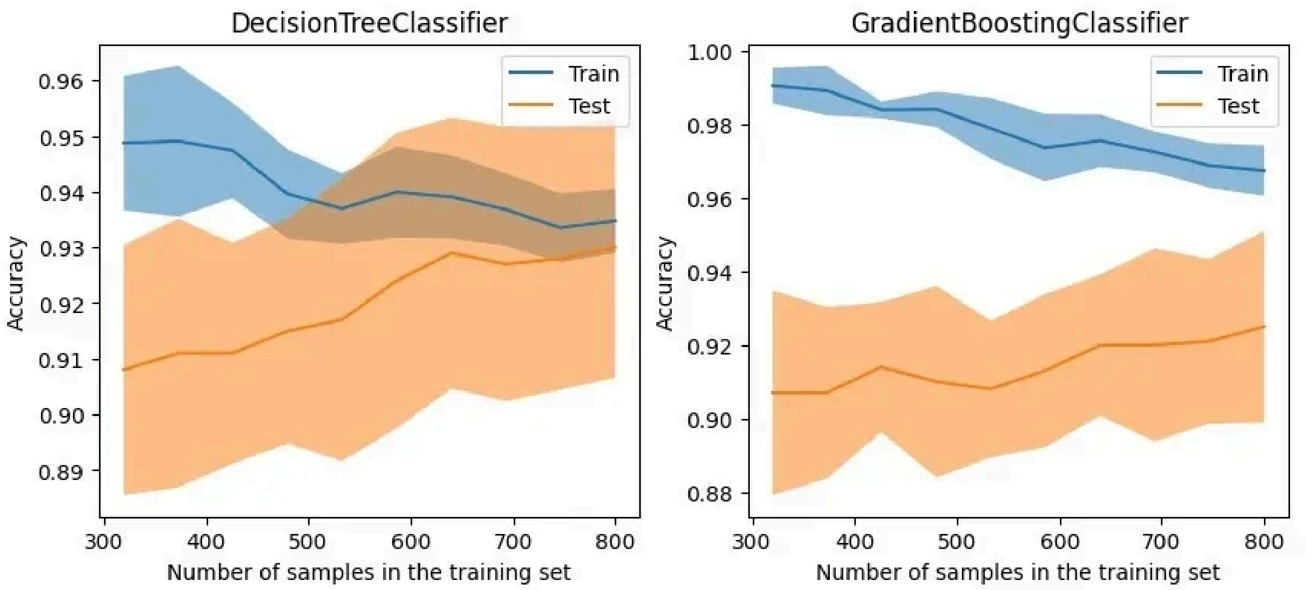
As shown below, we compare a DecisionTreeClassifier and a GradientBoostingClassifier to see how they do as training data changes.

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.model_selection import LearningCurveDisplay

X, y = make_classification(n_samples=1000, n_classes=2, n_features=10,
                           n_informative=2, n_redundant=0, n_repeated=0)

tree_clf = DecisionTreeClassifier(max_depth=3, random_state=42)
gb_clf = GradientBoostingClassifier(n_estimators=50, max_depth=3, tol=1e-3)

train_sizes = np.linspace(0.4, 1.0, 10)
fig, axes = plt.subplots(1, 2, figsize=(10, 4))
LearningCurveDisplay.from_estimator(tree_clf, X, y,
                                    train_sizes=train_sizes,
                                    ax=axes[0],
                                    scoring='accuracy')
axes[0].set_title('DecisionTreeClassifier')
LearningCurveDisplay.from_estimator(gb_clf, X, y,
                                    train_sizes=train_sizes,
                                    ax=axes[1],
                                    scoring='accuracy')
```



Comparison of the learning curve of two different models.

The graph shows that although the tree-based GradientBoostingClassifier maintains good accuracy on the training data, its generalization capability on test data does not have a significant advantage over the DecisionTreeClassifier.

Using model_selection.ValidationCurveDisplay for visualizing parameter tuning

So, for models that don't generalize well, you might try adjusting the model's regularization parameters to tweak its performance.

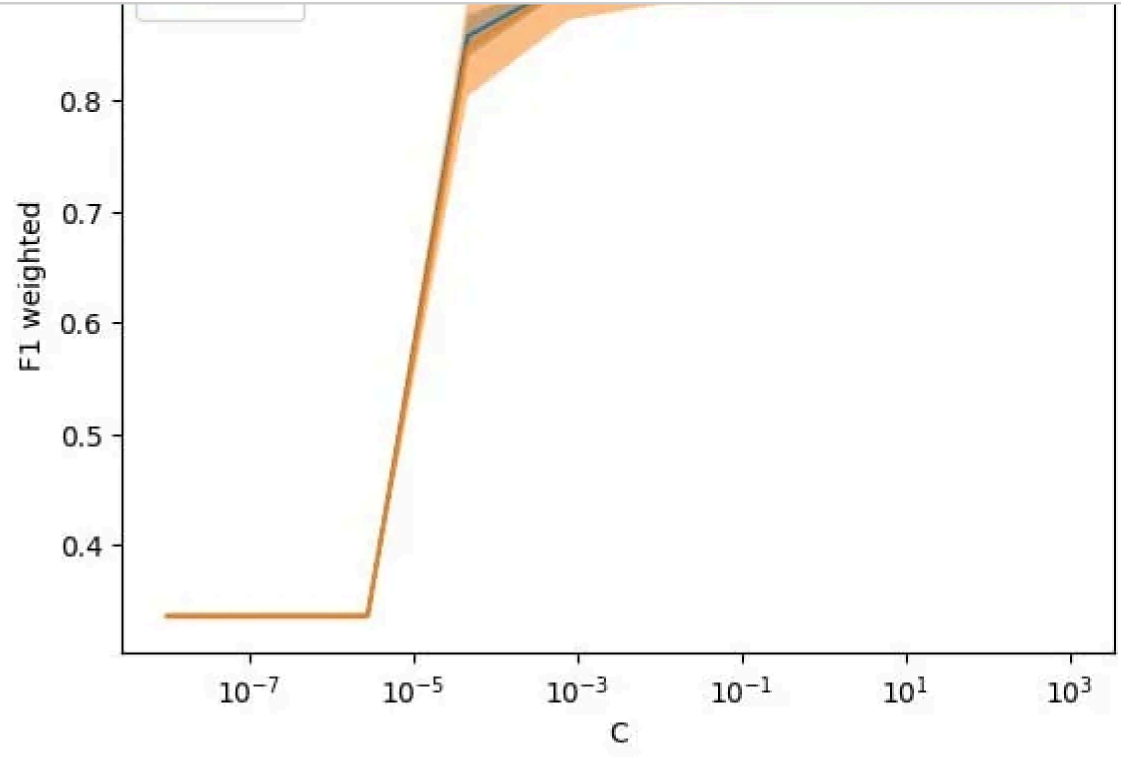
The traditional approach is to use tools like GridSearchCV or Optuna to tune the model, but these methods only give you the overall best-performing model and the tuning process is not very intuitive.

For scenarios where you want to adjust a specific parameter to test its effect on the model, I recommend using model_selection.ValidationCurveDisplay to visualize how the model performs as the parameter changes.

```
from sklearn.model_selection import ValidationCurveDisplay
from sklearn.linear_model import LogisticRegression

param_name, param_range = "C", np.logspace(-8, 3, 10)
lr_clf = LogisticRegression()

ValidationCurveDisplay.from_estimator(lr_clf, X, y,
                                      param_name=param_name,
                                      param_range=param_range,
                                      scoring='f1_weighted',
                                      cv=5, n_jobs=-1)
plt.show()
```



Fine-tuning of model parameters plotted with ValidationCurveDisplay.

Some regrets

After trying out all these Displays, I must admit some regrets:

- The biggest one is that most of these APIs lack detailed tutorials, which is probably why they're not well-known compared to Scikit-learn's thorough documentation.
- These APIs are scattered across various packages, making it hard to reference them from a single place.
- The code is still pretty basic. You often need to pair it with Matplotlib's APIs to get the job done. A typical example is DecisionBoundaryDisplay
, where after plotting the decision boundary, you still need Matplotlib to plot the data distribution.
- They're hard to extend. Besides a few methods validating parameters, it's tough to simplify my model visualization process with tools or methods; I end up rewriting a lot.

I hope these APIs get more attention, and as versions upgrade, visualization APIs become even easier to use.

Conclusion

In the journey of machine learning, explaining models with visualization is as important as training them.

This article introduced various plotting APIs in the current version of scikit-learn.

With these APIs, you can simplify some Matplotlib code, ease your learning curve, and streamline your model evaluation process.

Now it's your turn. What are your expectations for visualizing machine learning methods? Feel free to leave a comment and discuss.

This article was originally published on my personal blog Data Leads Future.

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czubilicious • 1d ago

Very nicely done. Thanks. Do you use seaborn? I really like it, as it also can plot interactive diagrams.

13 Reply Share ...

qtalen OP • 1d ago

Explaining models often requires customized visualization methods. Seaborn, which is a high-level encapsulation of matplotlib, is not very satisfactory in terms of customization. If you're interested in Seaborn objects interface, you can read my other article:

https://www.dataleadsfuture.com/seaborn-0-12-an-insightful-guide-to-the-objects-interface-and-declarative-graphics/

7 Reply Share ...

databot_ • 14h ago

you can also use sklearn-evaluation, it has a bunch of extra things: https://sklearn-evaluation.ploomber.io/en/latest/intro.html

4 Reply Share ...

qtalen OP • 12h ago

Thank you for sharing, it's a really nice resource.

1 Reply Share ...

Corpulos • 14h ago

ubiond • 13h ago

thanks!

2 Reply Share ...

Training_Butterfly70 • 9h ago

Helpful for quick plots for sure! I personally love using plotly with dash for dashboards

2 Reply Share ...

pach812 • 8h ago

Awesome post! You should also explore scikit-plot! Have really good graphs and they are easy to use.

2 Reply Share ...

qtalen OP • 7h ago

Thank you for your suggestion. Scikit-plot is indeed very user-friendly. Therefore, when I wrote this article, I added a constraint: considering that some production systems may not be able to install third-party libraries. Finally, I regret to say that, compared to other APIs, sklearn's Display API is indeed still quite rudimentary.

1 Reply Share ...

Ill_Race_2060 • 16h ago

i have been working as a data scientist for last 3 years,

i struggle a lot in managing datas from diffrent sources, and Data Cleaning,

whats yours

2 Reply Share ...

qtalen OP • 12h ago

No offense taken, but I don't think working for three years qualifies someone to be called a "scientist". I've been working in the big data field for nearly 20 years, and my biggest confusion is that technology is developing so fast that I'm starting to fall behind. So I learn and share at the same time. I hope this method helps me remember new knowledge better.

3 Reply Share ...

jotunman • 11h ago

What is your background? All this is pretty basic for modern statisticians, because they have to know how to communicate the statistics, models used and what the data says. If they can't, they're not very good statisticians.

Also, this is much easier in R, at least in my opinion. If communication through visualizations is the goal, you can make some sexy shit with R!

2 Reply Share ...

plotting APIs. For simple model evaluation, you only need to use these APIs instead of mastering third-party libraries. That's why the article seems very straightforward.

2 Reply Share ...