```
from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split

X, y = make_classification(
    n_samples=100_000, n_features=20, n_informative=2, n_redundant=10, random_stat
)

X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.99, random_state=42
)

# %%
# Calibration curves
# ------------------
#
# Gaussian Naive Bayes
# ^^^^^^^^^^^^^^^^^^^^
#
# First, we will compare:
#
# * :class:`~sklearn.linear_model.LogisticRegression` (used as baseline
#   since very often, properly regularized logistic regression is well
#   calibrated by default thanks to the use of the log-loss)
# * Uncalibrated :class:`~sklearn.naive_bayes.GaussianNB`
# * :class:`~sklearn.naive_bayes.GaussianNB` with isotonic and sigmoid
#   calibration (see :ref:`User Guide <calibration>`)
#
# Calibration curves for all 4 conditions are plotted below, with the average
# predicted probability for each bin on the x-axis and the fraction of positive
# classes in each bin on the y-axis.

import matplotlib.pyplot as plt
from matplotlib.gridspec import GridSpec

from sklearn.calibration import CalibratedClassifierCV, CalibrationDisplay
from sklearn.linear_model import LogisticRegression
from sklearn.naive_bayes import GaussianNB

lr = LogisticRegression(C=1.0)
gnb = GaussianNB()
gnb_isotonic = CalibratedClassifierCV(gnb, cv=2, method="isotonic")
gnb_sigmoid = CalibratedClassifierCV(gnb, cv=2, method="sigmoid")

clf_list = [
    (lr, "Logistic"),
    (gnb, "Naive Bayes"),
    (gnb_isotonic, "Naive Bayes + Isotonic"),
    (gnb_sigmoid, "Naive Bayes + Sigmoid"),
]

# %%
fig = plt.figure(figsize=(10, 10))
gs = GridSpec(4, 2)
```

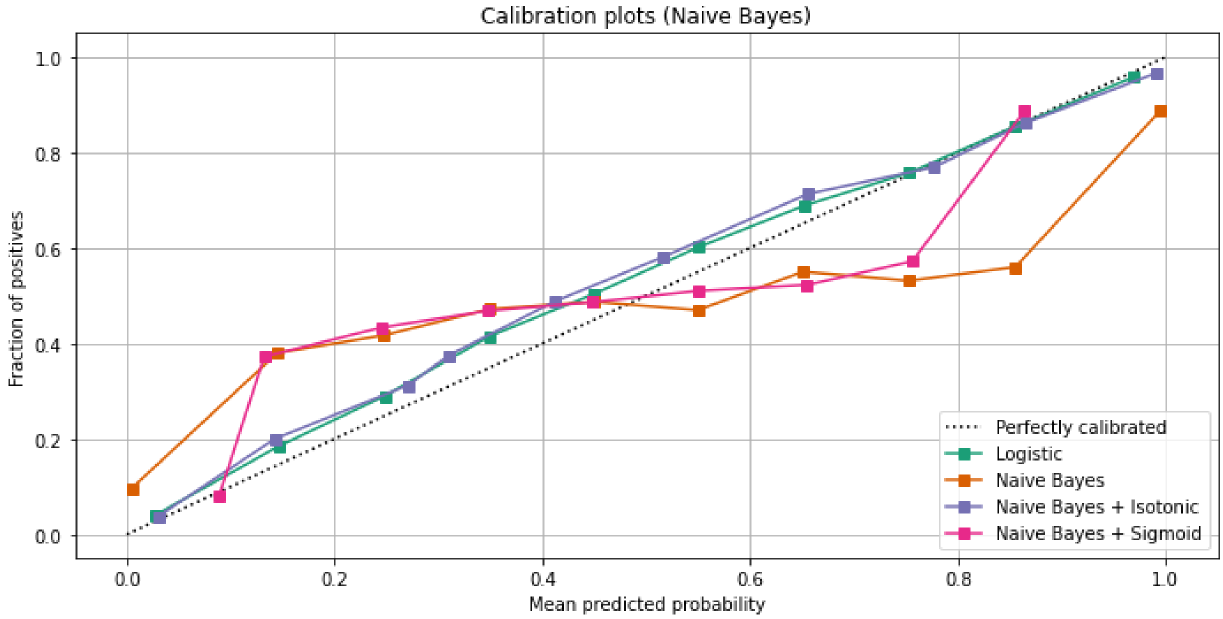
```
colors = plt.cm.get_cmap("Dark2")

ax_calibration_curve = fig.add_subplot(gs[:2, :2])
calibration_displays = {}
for i, (clf, name) in enumerate(clf_list):
    clf.fit(X_train, y_train)
    display = CalibrationDisplay.from_estimator(
        clf,
        X_test,
        y_test,
        n_bins=10,
        name=name,
        ax=ax_calibration_curve,
        color=colors(i),
    )
    calibration_displays[name] = display

ax_calibration_curve.grid()
ax_calibration_curve.set_title("Calibration plots (Naive Bayes)")

# Add histogram
grid_positions = [(2, 0), (2, 1), (3, 0), (3, 1)]
for i, (_, name) in enumerate(clf_list):
    row, col = grid_positions[i]
    ax = fig.add_subplot(gs[row, col])

    ax.hist(
        calibration_displays[name].y_prob,
        range=(0, 1),
        bins=10,
        label=name,
        color=colors(i),
    )
    ax.set(title=name, xlabel="Mean predicted probability", ylabel="Count")

plt.tight_layout()
plt.show()

# %%
# Uncalibrated :class:`~sklearn.naive_bayes.GaussianNB` is poorly calibrated
# because of
# the redundant features which violate the assumption of feature-independence
# and result in an overly confident classifier, which is indicated by the
# typical transposed-sigmoid curve. Calibration of the probabilities of
# :class:`~sklearn.naive_bayes.GaussianNB` with :ref:`isotonic` can fix
# this issue as can be seen from the nearly diagonal calibration curve.
# :ref:sigmoid regression `<sigmoid_regressor>` also improves calibration
# slightly,
# albeit not as strongly as the non-parametric isotonic regression. This can be
# attributed to the fact that we have plenty of calibration data such that the
# greater flexibility of the non-parametric model can be exploited.
#
# Below we will make a quantitative analysis considering several classification
# metrics: :ref:`brier_score_loss`, :ref:`log_loss`,
```

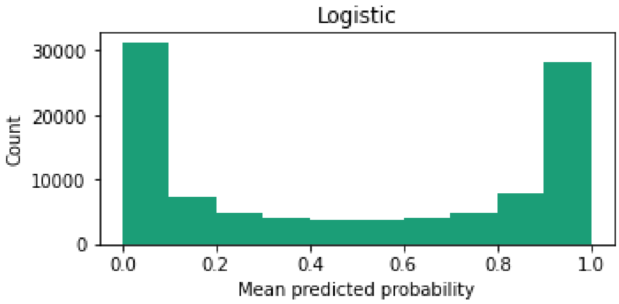
```
# :ref:`precision, recall, F1 score <precision_recall_f_measure_metrics>` and
# :ref:`ROC AUC <roc_metrics>`.

from collections import defaultdict

import pandas as pd

from sklearn.metrics import (
    precision_score,
    recall_score,
    f1_score,
    brier_score_loss,
    log_loss,
    roc_auc_score,
)

scores = defaultdict(list)
for i, (clf, name) in enumerate(clf_list):
    clf.fit(X_train, y_train)
    y_prob = clf.predict_proba(X_test)
    y_pred = clf.predict(X_test)
    scores["Classifier"].append(name)

    for metric in [brier_score_loss, log_loss]:
        score_name = metric.__name__.replace("_", " ").replace("score", "").capita
        scores[score_name].append(metric(y_test, y_prob[:, 1]))

    for metric in [precision_score, recall_score, f1_score, roc_auc_score]:
        score_name = metric.__name__.replace("_", " ").replace("score", "").capita
        scores[score_name].append(metric(y_test, y_pred))

    score_df = pd.DataFrame(scores).set_index("Classifier")
    score_df.round(decimals=3)

score_df

# %%
# Notice that although calibration improves the :ref:`brier_score_loss` (a
# metric composed
# of calibration term and refinement term) and :ref:`log_loss`, it does not
# significantly alter the prediction accuracy measures (precision, recall and
# F1 score).
# This is because calibration should not significantly change prediction
# probabilities at the location of the decision threshold (at x = 0.5 on the
# graph). Calibration should however, make the predicted probabilities more
# accurate and thus more useful for making allocation decisions under
# uncertainty.
# Further, ROC AUC, should not change at all because calibration is a
# monotonic transformation. Indeed, no rank metrics are affected by
# calibration.
#
# Linear support vector classifier
# ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
# Next, we will compare:
```

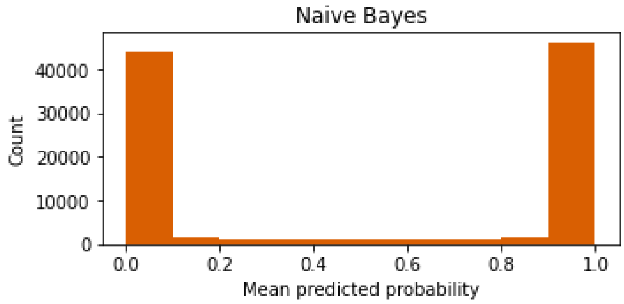
```
#
# * :class:`~sklearn.linear_model.LogisticRegression` (baseline)
# * Uncalibrated :class:`~sklearn.svm.LinearSVC`. Since SVC does not output
#   probabilities by default, we naively scale the output of the
#   :term:`decision_function` into [0, 1] by applying min-max scaling.
# * :class:`~sklearn.svm.LinearSVC` with isotonic and sigmoid
#   calibration (see :ref:`User Guide <calibration>`)

import numpy as np

from sklearn.svm import LinearSVC


class NaivelyCalibratedLinearSVC(LinearSVC):
    """LinearSVC with `predict_proba` method that naively scales
    `decision_function` output for binary classification."""

    def fit(self, X, y):
        super().fit(X, y)
        df = self.decision_function(X)
        self.df_min_ = df.min()
        self.df_max_ = df.max()

    def predict_proba(self, X):
        """Min-max scale output of `decision_function` to [0, 1]."""
        df = self.decision_function(X)
        calibrated_df = (df - self.df_min_) / (self.df_max_ - self.df_min_)
        proba_pos_class = np.clip(calibrated_df, 0, 1)
        proba_neg_class = 1 - proba_pos_class
        proba = np.c_[proba_neg_class, proba_pos_class]
        return proba


# %%

lr = LogisticRegression(C=1.0)
svc = NaivelyCalibratedLinearSVC(max_iter=10_000)
svc_isotonic = CalibratedClassifierCV(svc, cv=2, method="isotonic")
svc_sigmoid = CalibratedClassifierCV(svc, cv=2, method="sigmoid")

clf_list = [
    (lr, "Logistic"),
    (svc, "SVC"),
    (svc_isotonic, "SVC + Isotonic"),
    (svc_sigmoid, "SVC + Sigmoid"),
]

# %%
fig = plt.figure(figsize=(10, 10))
gs = GridSpec(4, 2)

ax_calibration_curve = fig.add_subplot(gs[:2, :2])
calibration_displays = {}
for i, (clf, name) in enumerate(clf_list):
    clf.fit(X_train, y_train)
```

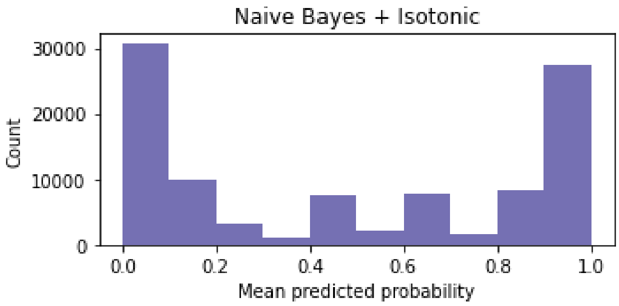
```python
    clf.fit(X_train, y_train)
    display = CalibrationDisplay.from_estimator(
        clf,
        X_test,
        y_test,
        n_bins=10,
        name=name,
        ax=ax_calibration_curve,
        color=colors(i),
    )
    calibration_displays[name] = display

ax_calibration_curve.grid()
ax_calibration_curve.set_title("Calibration plots (SVC)")

# Add histogram
grid_positions = [(2, 0), (2, 1), (3, 0), (3, 1)]
for i, (_, name) in enumerate(clf_list):
    row, col = grid_positions[i]
    ax = fig.add_subplot(gs[row, col])

    ax.hist(
        calibration_displays[name].y_prob,
        range=(0, 1),
        bins=10,
        label=name,
        color=colors(i),
    )
    ax.set(title=name, xlabel="Mean predicted probability", ylabel="Count")

plt.tight_layout()
plt.show()

# %%
# :class:`~sklearn.svm.LinearSVC` shows the opposite
# behavior to :class:`~sklearn.naive_bayes.GaussianNB`; the calibration
# curve has a sigmoid shape, which is typical for an under-confident
# classifier. In the case of :class:`~sklearn.svm.LinearSVC`, this is caused
# by the margin property of the hinge loss, which focuses on samples that are
# close to the decision boundary (support vectors). Samples that are far
# away from the decision boundary do not impact the hinge loss. It thus makes
# sense that :class:`~sklearn.svm.LinearSVC` does not try to separate samples
# in the high confidence region regions. This leads to flatter calibration
# curves near 0 and 1 and is empirically shown with a variety of datasets
# in Niculescu-Mizil & Caruana [1]_.
#
# Both kinds of calibration (sigmoid and isotonic) can fix this issue and
# yield similar results.
#
# As before, we show the :ref:`brier_score_loss`, :ref:`log_loss`,
# :ref:`precision, recall, F1 score <precision_recall_f_measure_metrics>` and
# :ref:`ROC AUC <roc_metrics>`.

scores = defaultdict(list)
for i, (clf, name) in enumerate(clf_list):
```

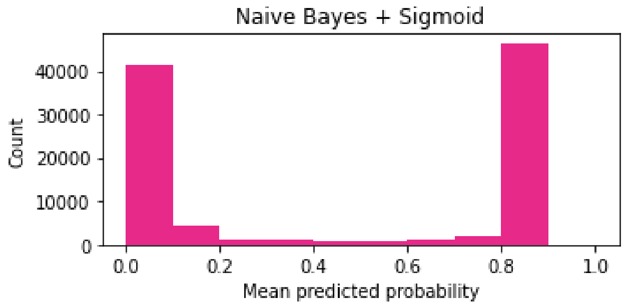
```
for i, (clf, name) in enumerate(clf_list):
    clf.fit(X_train, y_train)
    y_prob = clf.predict_proba(X_test)
    y_pred = clf.predict(X_test)
    scores["Classifier"].append(name)

    for metric in [brier_score_loss, log_loss]:
        score_name = metric.__name__.replace("_", " ").replace("score", "").capita
        scores[score_name].append(metric(y_test, y_prob[:, 1]))

    for metric in [precision_score, recall_score, f1_score, roc_auc_score]:
        score_name = metric.__name__.replace("_", " ").replace("score", "").capita
        scores[score_name].append(metric(y_test, y_pred))

    score_df = pd.DataFrame(scores).set_index("Classifier")
    score_df.round(decimals=3)

score_df
```

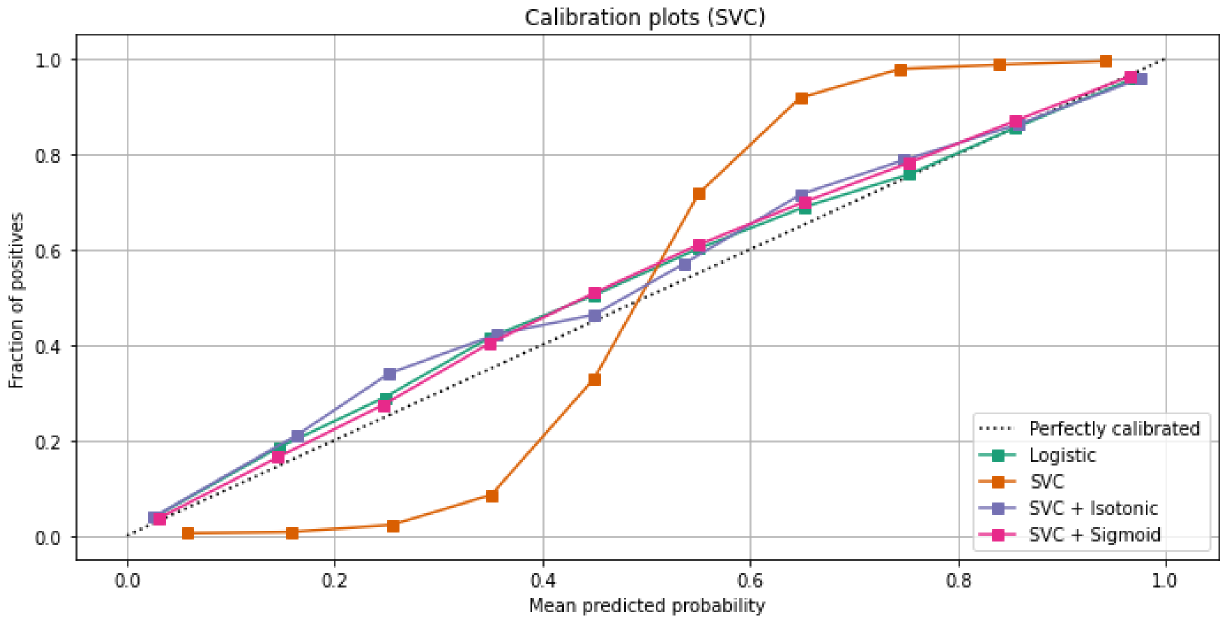

Calibration plots (Naive Bayes)
Fraction of positives
Mean predicted probability
Perfectly calibrated
Logistic
Naive Bayes
Naive Bayes + Isotonic
Naive Bayes + Sigmoid

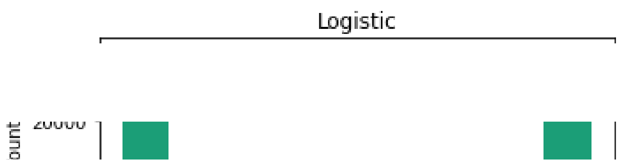

Logistic
Count
Mean predicted probability

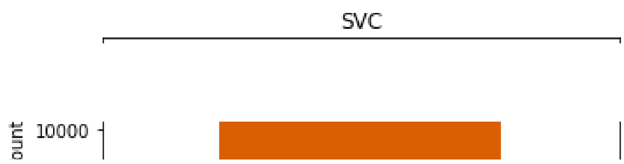

Naive Bayes
Count
Mean predicted probability

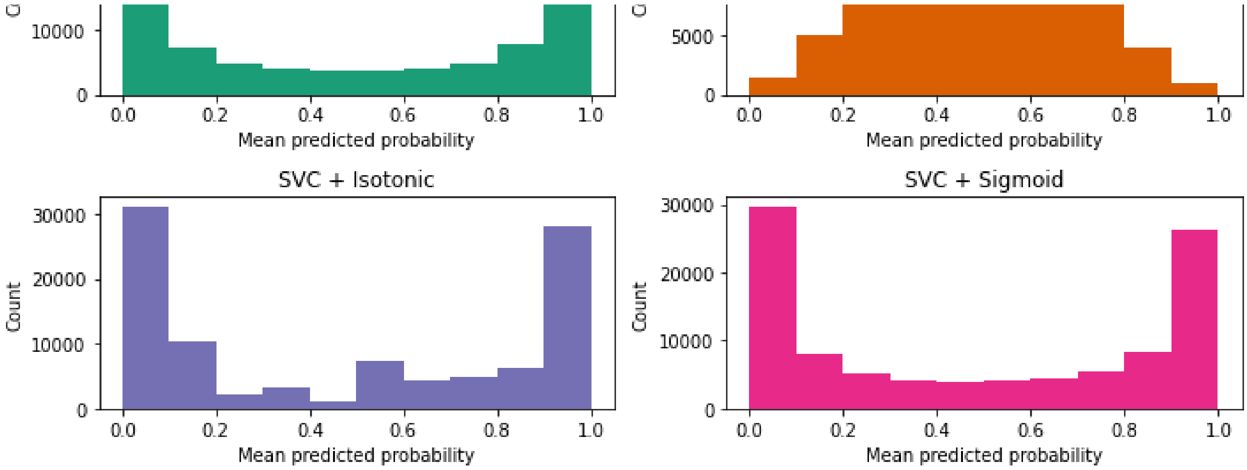

Naive Bayes + Isotonic
Count
Mean predicted probability


Naive Bayes + Sigmoid
Count
Mean predicted probability


Calibration plots (SVC)
Fraction of positives
Mean predicted probability
Perfectly calibrated
Logistic
SVC
SVC + Isotonic
SVC + Sigmoid


Logistic


SVC



Classifier	Brier loss	Log loss	Precision	Recall	F1	Roc auc
Logistic	0.098921	0.323178	0.872009	0.851408	0.861586	0.863157
SVC	0.144944	0.465647	0.872201	0.851772	0.861865	0.863420
SVC + Isotonic	0.099827	0.374535	0.853032	0.878041	0.865356	0.863306