Demo 07

k-Nearest Neighbors & Discriminant Analysis

```
from matplotlib import pyplot as plt
import numpy as np
import sklearn

plt.set_cmap('brg')
```

```
<Figure size 640x480 with 0 Axes>
```

```
def plot_decision_boundary(model, X, y, cmap=None, nsamples=128):
    cmap = plt.get_cmap(cmap)
    if len(X.shape) != 2:
        raise ValueError('Can only make 2d plots...')

    plt.legend(*plt.scatter(X[:, 0], X[:, 1], c=y, cmap=cmap, 
edgecolors='w').legend_elements(), title='Classes:')
    xmin, xmax = plt.xlim()
    ymin, ymax = plt.ylim()

    xx1, xx2 = np.meshgrid(np.linspace(xmin, xmax, nsamples), 
np.linspace(ymin, ymax, nsamples))
    XX = np.array([xx1.ravel(), xx2.ravel()]).T
    yy = model.predict_proba(XX).reshape(xx1.shape + (-1, ))
    cmap = cmap.resampled(yy.shape[-1])
    colors = np.array([cmap(idx) for idx in range(yy.shape[-1])])
    img = (yy[..., None] * colors[None, None, ...]).sum(axis=2)
    np.clip(img, 0, 1, out=img)  # Deal with some rounding errors
    plt.imshow(img, extent=(xmin, xmax, ymin, ymax), origin='lower', 
interpolation='bilinear', alpha=0.5)
    plt.contour(xx1, xx2, yy.argmax(axis=2), range(yy.shape[-1]), 
linewidths=0.5, linestyles='dashed', colors='k')

    plt.title('$ŷ(x)$')
    plt.axis('square')
    plt.axis((xmin, xmax, ymin, ymax))
    plt.show()
```

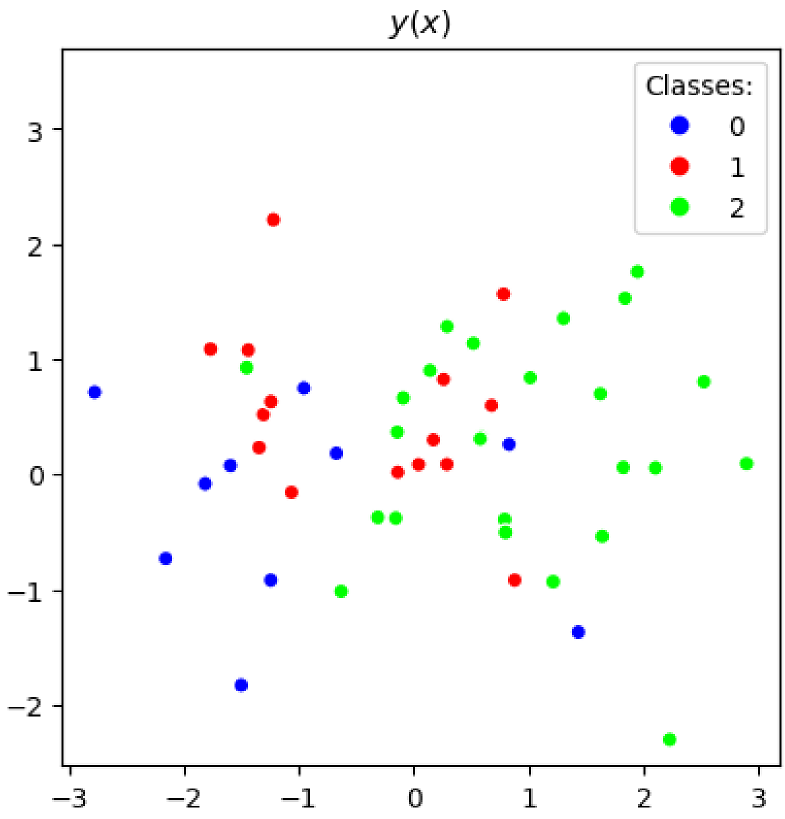
Generate some toy-data

```
from sklearn.datasets import make_blobs
X, y = make_blobs(n_samples=[10, 15, 25], n_features=2, centers=[[-1, 
-1], [0, 1], [1, 0]])
```

```
X, y
```

```
(array([[ 0.79233049, -0.39128381],
        [-1.59164909,  0.07717869],
        [ 1.21331672, -0.93253177],
        [ 1.62411495,  0.7003668 ],
        [ 0.58924034,  0.32656476],
        [ 0.29014318,  0.0883199 ],
        [-1.06147583, -0.15544496],
        [-0.09033047,  0.66432626],
        [-1.30482503,  0.52009523],
        [ 0.51972946,  1.13874622],
        [-1.21890991,  2.21250198],
        [ 0.78271116,  1.56676487],
        [ 0.17160228,  0.29948445],
        [-0.15437322, -0.37976677],
        [-0.14155676,  0.36833106],
        [ 0.79923207, -0.50408184],
        [-1.81221677, -0.08085254],
        [ 0.83132528,  0.26122452],
        [-1.43712877,  1.07987546],
        [ 0.67857281,  0.59876731],
        [-2.15437367, -0.73100775],
        [-0.95385483,  0.7488759 ],
        [ 0.26173165,  0.82631924],
        [ 0.04325531,  0.08647966],
        [-0.31027653, -0.37327116],
        [ 2.10371112,  0.0563056 ],
        [-0.13741687,  0.01830025],
        [ 1.43252778, -1.37046828],
        [ 0.57922099,  0.30792833],
        [ 1.64033236, -0.53944995],
        [ 2.22637668, -2.30389987],
        [-1.76507154,  1.08845403],
        [ 1.83844665,  1.53023005],
        [ 1.30313838,  1.35513838],
        [ 2.89501847,  0.09423781],
        [ 2.52483501,  0.80506931],
        [-1.45098525,  0.92757435],
        [-1.24166816, -0.919044  ],
        [-2.77262465,  0.71440462],
        [ 0.14323189,  0.90242315],
        [-0.67159624,  0.18364606],
        [-1.49795725, -1.83230895],
        [ 0.87896114, -0.91886685],
        [-1.24017565,  0.63228876],
        [ 1.82298363,  0.06068253],
        [ 1.94704992,  1.76035764],
        [-1.34297603,  0.23318425],
        [ 1.01434521,  0.839982  ],
        [ 0.29184587,  1.28524541],
        [-0.62958329, -1.01605826]]),
 array([2, 0, 2, 2, 2, 1, 1, 2, 1, 2, 1, 1, 1, 2, 2, 2, 0, 0, 1, 1, 0,
0,
        1, 1, 2, 2, 1, 0, 2, 2, 2, 1, 2, 2, 2, 2, 2, 0, 0, 2, 0, 0, 1,
1,
        2, 2, 1, 2, 2, 2]))
```

```
plt.legend(*plt.scatter(X[:, 0], X[:, 1], c=y,
edgecolors='w').legend_elements(), title='Classes:')
plt.title('$y(x)$')
plt.axis('square')
plt.show()
```



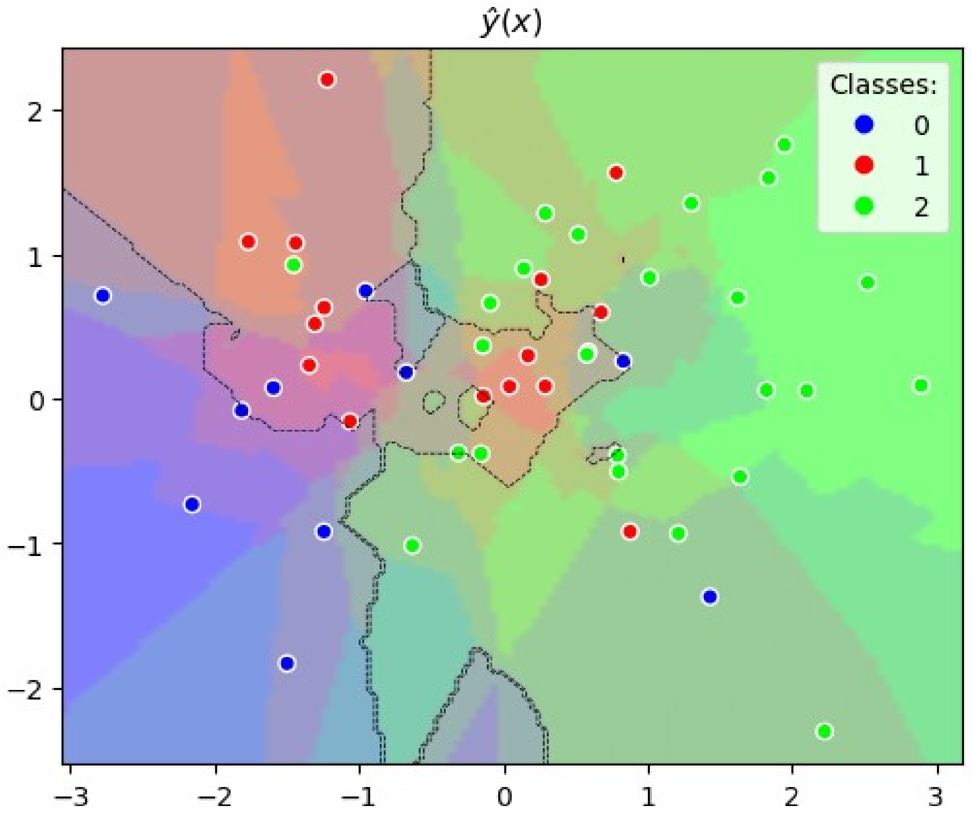
k-Nearest neighbors

```
import sklearn.base
from sklearn.utils.estimator_checks import check_estimator
from sklearn.utils.multiclass import unique_labels
from sklearn.utils.validation import check_is_fitted, validate_data
```

```python
class KNearestNeighbors(sklearn.base.ClassifierMixin,
sklearn.base.BaseEstimator):
    def __init__(self, k=3):
        self.k = k

    def fit(self, X, y):
        X, y = validate_data(self, X, y)
        self.classes_ = unique_labels(y)
        self.fitted_ = True
        # FIT HERE
        self.X_ = X
        self.y_ = (y[:, np.newaxis] == self.classes_)
        return self

    def predict_proba(self, X):
        check_is_fitted(self)
        X = validate_data(self, X, reset=False)
        # PREDICT PROBA HERE
#         print(X.shape, X[:, np.newaxis].shape)
#         print(self.X_.shape, self.X_[np.newaxis, :].shape)
        differences = X[:, np.newaxis] - self.X_[np.newaxis, :]
        sq_distances = np.sqrt(np.sum(differences**2, axis=-1))
        ordered = np.argpartition(sq_distances, self.k, axis=1)
        ordered = ordered[:, :self.k]
#         print(ordered.shape)
#         print(ordered)
        classes = self.y_[ordered]
#         print(classes.shape)
#         print(classes)
        y_proba = np.mean(classes, axis=1)

        return y_proba

    def predict(self, X):
        probas = self.predict_proba(X)
        return self.classes_[np.argmax(probas, axis=1)]
# check_estimator(KNearestNeighbors())

model = KNearestNeighbors(k=5)

model
```

```
KNearestNeighbors(k=5)
```

```python
model.fit(X, y)
y_hat = model.predict(X)

y_hat
plot_decision_boundary(model, X, y)
```



Linear Discriminant Analysis

Bayes formula

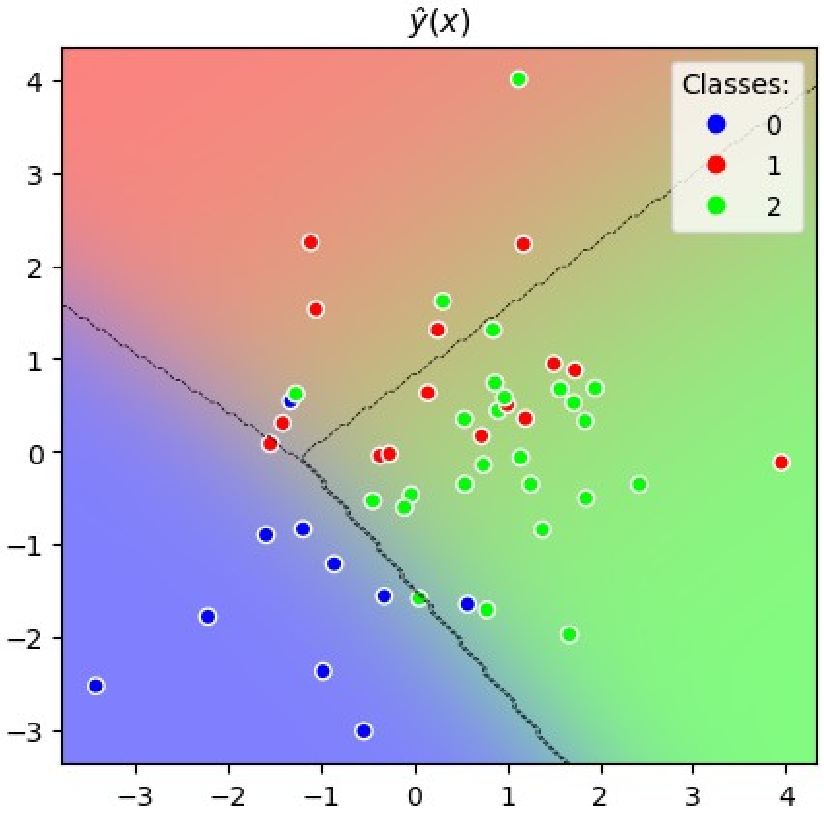
$$P(y \vee x) \propto P(x \vee y) \cdot P(y)$$

Multivariate Gaussian distribution

$$P(x \vee y) = \sqrt{\left|1/2\pi\Sigma^{-1}\right|}\, e^{-1/2(x-\mu_y)^{\mathrm{T}}\Sigma^{-1}(x-\mu_y)}$$

```
class LinearDA(sklearn.base.ClassifierMixin,
sklearn.base.BaseEstimator):
    def fit(self, X, y):
        X, y = validate_data(self, X, y)
        self.classes_ = unique_labels(y)
        self.counts_ = np.count_nonzero(y[:, np.newaxis] ==
self.classes_, axis=0)
        self.means_ = {c: np.mean(X[y == c, :], axis=0) for c in
self.classes_}
        cov = np.cov([x_i - self.means_[y_i] for x_i, y_i in zip(X,
y)], ddof=0, rowvar=False)
```

```
        self.inv_cov_ = np.linalg.inv(cov)
        return self

    def predict_proba(self, X):
        X = validate_data(self, X, reset=False)
        check_is_fitted(self)
        y_proba = self.counts_ * np.exp([[-0.5 * (x_i - self.means_[y_i]) @ self.inv_cov_ @ (x_i - self.means_[y_i]) for y_i in self.classes_] for x_i in X])
        y_proba = y_proba / np.sum(y_proba, axis=1, keepdims=True)
        return y_proba

    def predict(self, X):
        probas = self.predict_proba(X)
        return self.classes_[np.argmax(probas, axis=1)]
# check_estimator(LinearDA())

model = LinearDA()

model

LinearDA()

model.fit(X, y)
y_hat = model.predict(X)

y_hat
plot_decision_boundary(model, X, y)
```



Quadratic Discriminant Analysis

Bayes formula

$$P(y \vee x) \propto P(x \vee y) \cdot P(y)$$

Multivariate Gaussian distribution

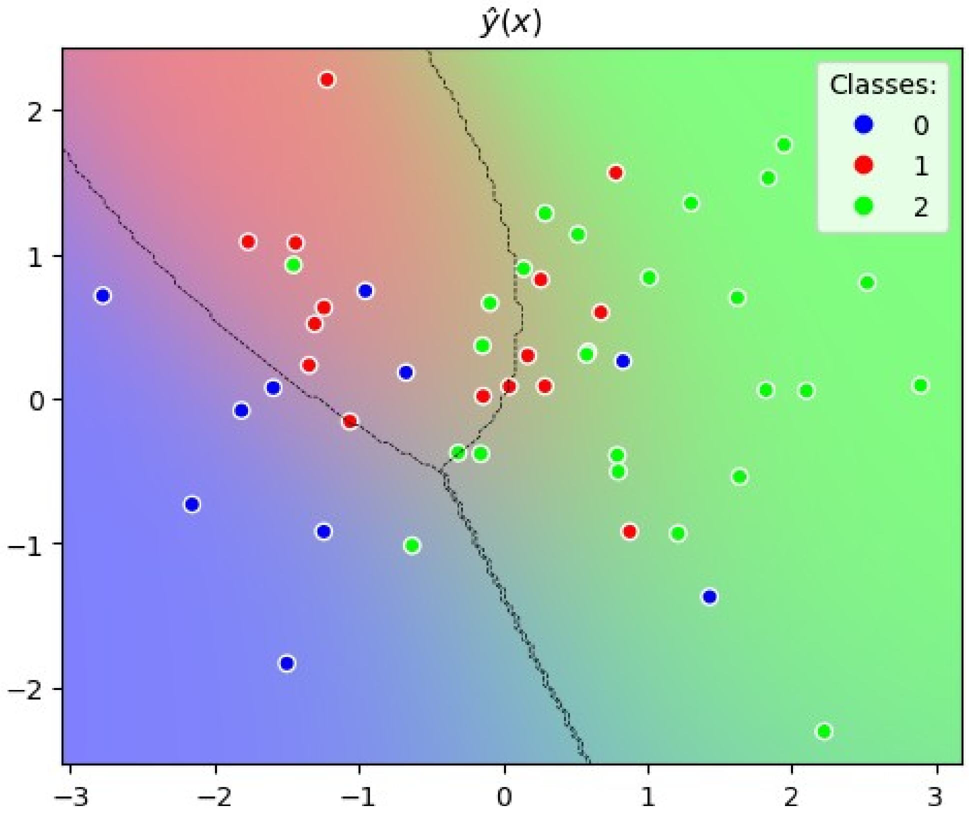
$$P(x \vee y) = \sqrt{\left|1/2\pi\Sigma_y^{-1}\right|}\, e^{-1/2(x-\mu_y)^{\mathrm{T}}\Sigma_y^{-1}(x-\mu_y)}$$

```
class QuadraticDA(sklearn.base.ClassifierMixin,
sklearn.base.BaseEstimator):
    def fit(self, X, y):
        X, y = validate_data(self, X, y)
        self.classes_ = unique_labels(y)
        self.counts_ = np.count_nonzero(y[:, np.newaxis] ==
self.classes_, axis=0)
        self.means_ = {c: np.mean(X[y == c, :], axis=0) for c in
self.classes_}
        self.inv_covs_ = {c: np.linalg.inv(np.cov([x_i -
self.means_[y_i] for x_i, y_i in zip(X, y) if y_i == c], ddof=1,
rowvar=False)) for c in self.classes_}
```

```
        return self

    def predict_proba(self, X):
        X = validate_data(self, X, reset=False)
        check_is_fitted(self)
        y_proba = self.counts_ *
np.sqrt([np.linalg.det(self.inv_covs_[c]) for c in self.classes_]) *
np.exp([[-0.5 * (x_i - self.means_[y_i]) @ self.inv_covs_[y_i] @ (x_i
- self.means_[y_i]) for y_i in self.classes_] for x_i in X])
        y_proba = y_proba / np.sum(y_proba, axis=1, keepdims=True)
        return y_proba

    def predict(self, X):
        probas = self.predict_proba(X)
        return self.classes_[np.argmax(probas, axis=1)]

model = QuadraticDA()

model
```

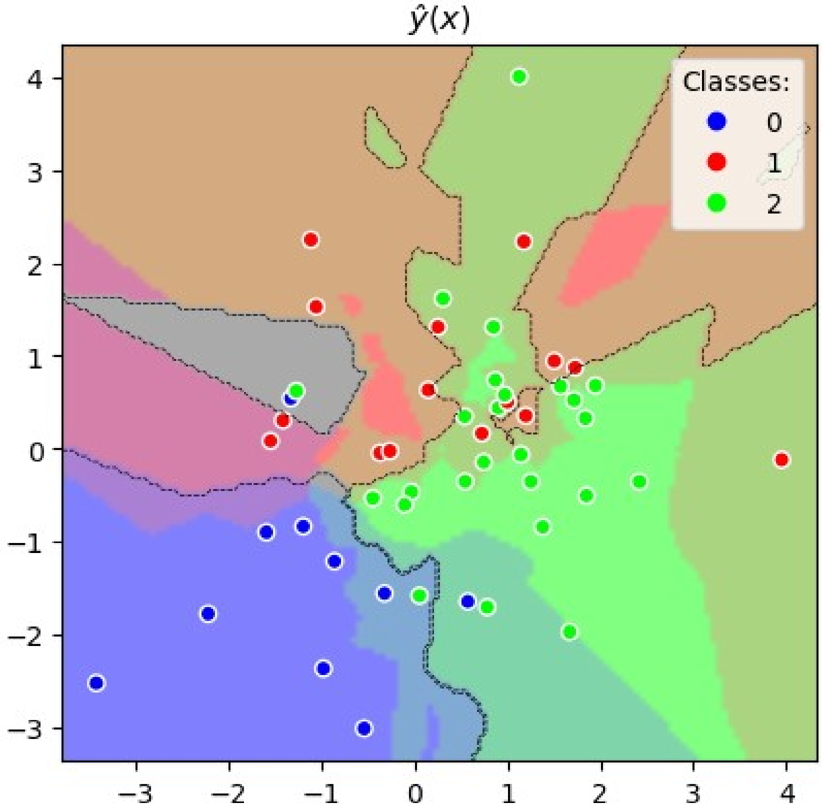
```
QuadraticDA()
```

```
model.fit(X, y)
y_hat = model.predict(X)

y_hat
plot_decision_boundary(model, X, y)
```

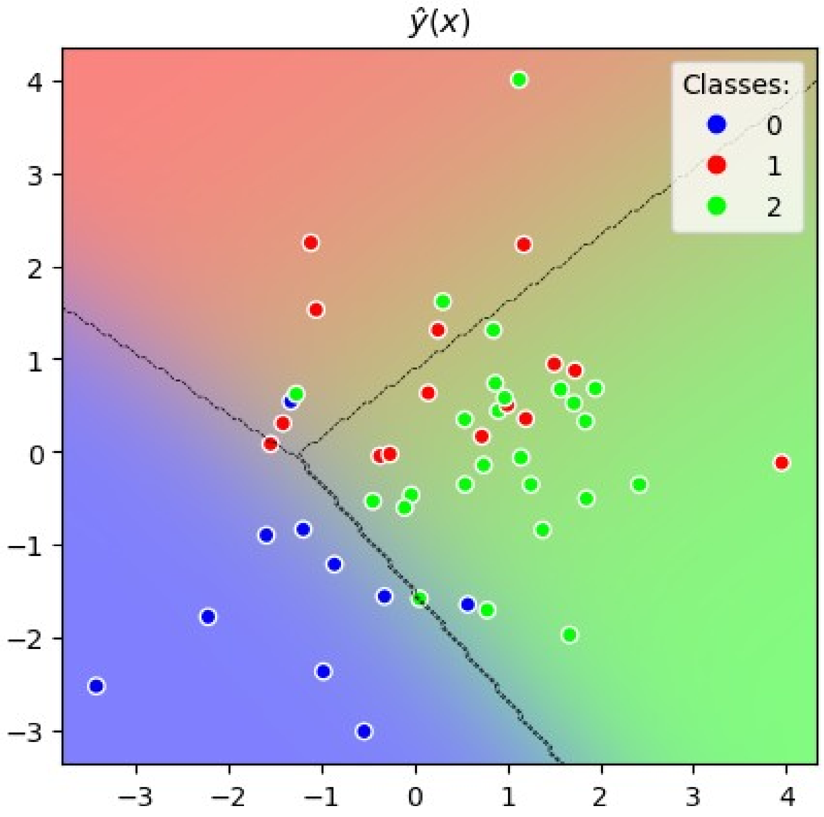


Scikit-learn

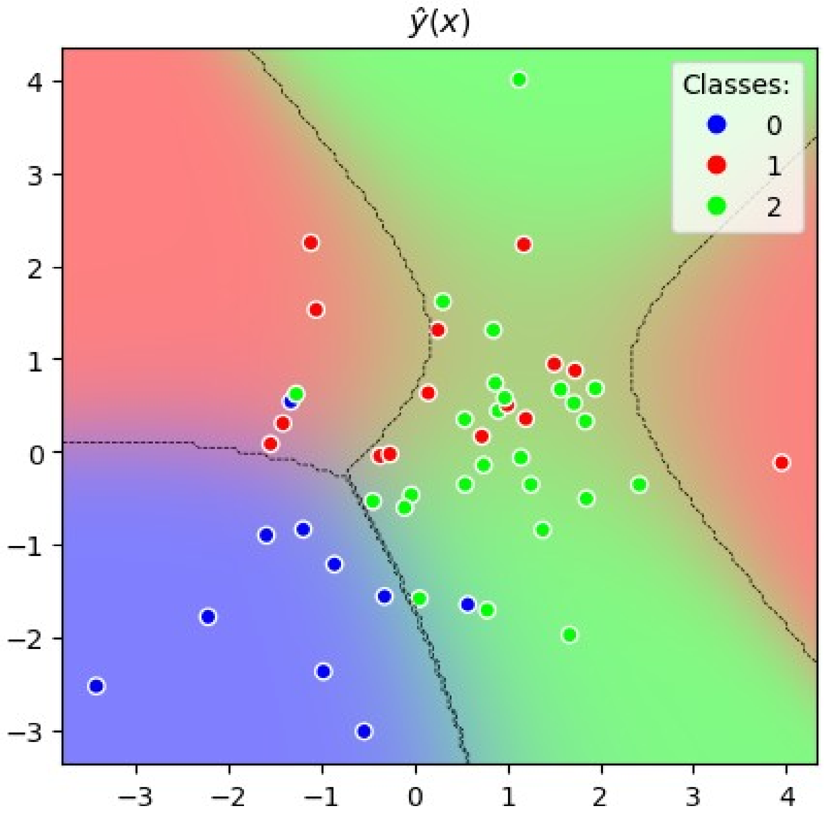
```
from sklearn.neighbors import KNeighborsClassifier
model = KNeighborsClassifier(n_neighbors=3)
model.fit(X, y)

model

KNeighborsClassifier(n_neighbors=3)

y_hat = model.predict(X)

y_hat
plot_decision_boundary(model, X, y)
```



```
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
model = LinearDiscriminantAnalysis()
model.fit(X, y)

model

LinearDiscriminantAnalysis()

y_hat = model.predict(X)

y_hat
plot_decision_boundary(model, X, y)
```



```
from sklearn.discriminant_analysis import
QuadraticDiscriminantAnalysis
model = QuadraticDiscriminantAnalysis()
model.fit(X, y)

model

QuadraticDiscriminantAnalysis()

y_hat = model.predict(X)

y_hat
plot_decision_boundary(model, X, y)
```

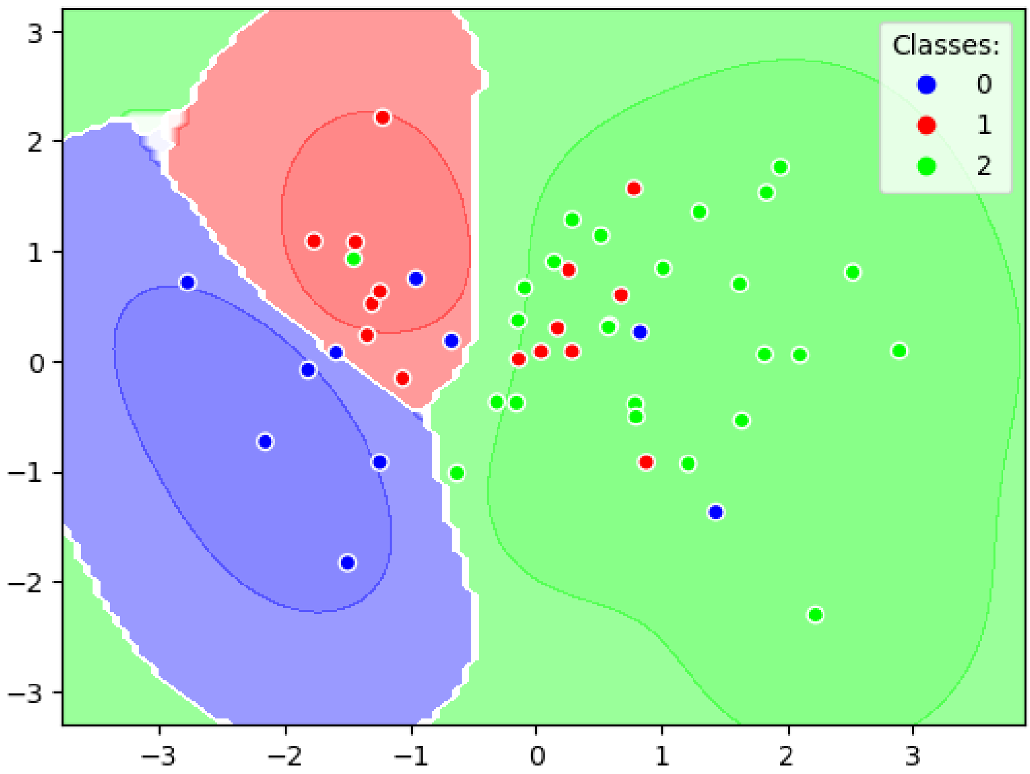


```
from sklearn.svm import SVC
model = SVC(kernel='rbf')
model.fit(X, y)
model
```

```
SVC()
```

```
sklearn.inspection.DecisionBoundaryDisplay.from_estimator(model, X,
multiclass_colors=plt.get_cmap().name, alpha=0.5)
plt.legend(*plt.scatter(X[:, 0], X[:, 1], c=y,
edgecolors='w').legend_elements(), title='Classes:')
```

```
<matplotlib.legend.Legend at 0x7f9706ee6d10>
```


Classes:
0
1
2
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3