Pattern Recognition
and Applications Lab

The Gaussian Classifier
Machine Learning – Laboratory

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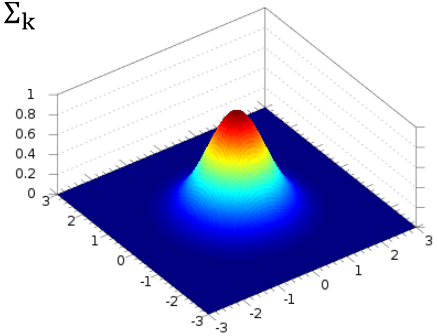
Gaussian Classifier - Prediction

- Bayesian classifier that uses MAP for predictions: $y_k^\star = \arg\max_{y_k} p(y_k|x) = \dfrac{p(x|y_k)p_k}{p(x)}$

- The likelihood is computed using a multivariate Gaussian distribution
  - This means that each class is modeled as Gaussian, with parameters μ_k, Σ_k

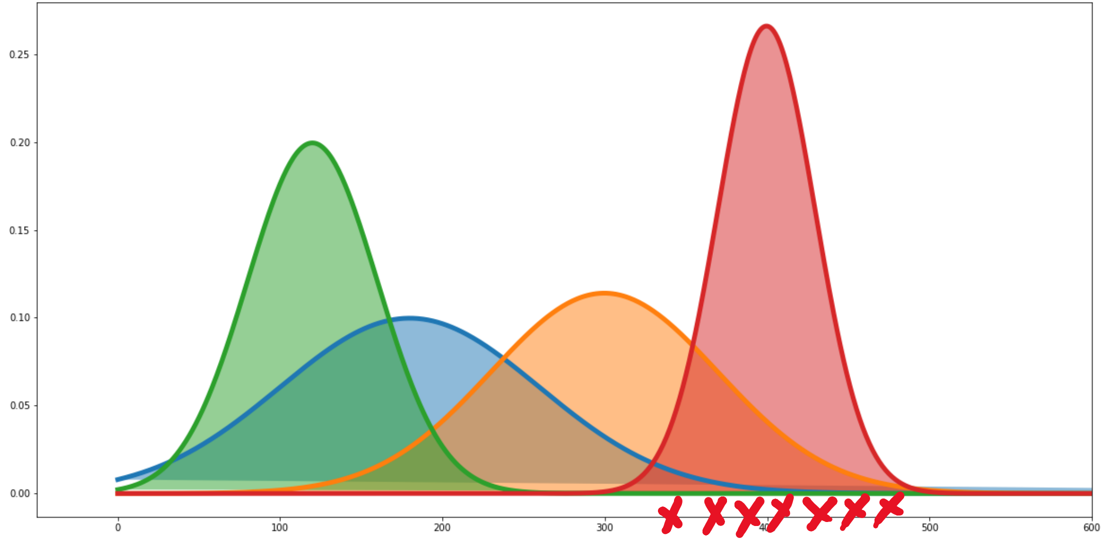
$$p(x|y_k) = \mathrm{g}(x; \mu_k, \Sigma_k) = \frac{1}{\sqrt{(2\pi)^d \det \Sigma_k}} \exp\left(-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1}(x-\mu_k)\right)$$



- Recall also that:
  - p_k is the prior probability of class y_k;
  - the evidence is obtained, as usual, by marginalization over the classes, i.e., $p(x) = \sum_k p(x|y_k)p_k$

Gaussian Classifier - Training

- During training, we aim to fit one Gaussian distribution per class.
  - But how do we find the best parameters μ_k, Σ_k for each Gaussian?
  - What is the meaning of *best parameters* here?



Which of these Gaussian distributions is a better fit to the 'x' data points? Why?

Gaussian Classifier - Training

- **Maximum Likelihood Estimation (MLE).** MLE defines the best parameters of our model $\theta^\star$ as those maximizing the likelihood L that the data $x_1, \ldots, x_n$ is generated by the model:

$$\theta^\star = \underset{\theta}{\operatorname{argmax}}\, L(x_1, \ldots, x_n\, |\theta)$$

- In our case, we aim to fit one Gaussian distribution per class. Thus, for each class,
  - we first extract the samples $x_1, \ldots, x_n$ for that class, and then
  - estimate the parameters $\theta = (\mu_k, \Sigma_\mathrm{k})$ for that class via MLE.

- **Good news:** MLE for Gaussian fitting can be solved in closed form!
  - The optimal $\mu_k^\star, \Sigma_\mathrm{k}^\star$ values are obtained as the **sample mean** and the **sample covariance**

$$\mu_k^\star = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\Sigma_k^\star = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \mu_k^\star)(x_i - \mu_k^\star)^\mathrm{T}$$

  - ... and these equations are already implemented in many statistical tools and libraries!

Exercise 1

- Implement a Gaussian classifier that
  1. fits a Gaussian distribution to each training class
  2. predicts test samples by assigning them to the class with the max. a-posteriori probability (MAP)

- Test it on some Gaussian dataset
  - Measure test error
  - Visualize the decision regions

Solution (small excerpt from the notebook code)

```
class CClassifierGaussian:
    """
    Class implementing a Gaussian classifier
    """

    def fit(self, x, y):
        """Estimate priors, centroids and covariances with
        maximum likelihood estimates from the training data x,y.
        """
        n_classes = np.unique(y).size
        n_features = x.shape[1]

        self._priors = np.zeros(shape=(n_classes,))
        self._centroids = np.zeros(shape=(n_classes, n_features))
        self._covariances = np.zeros(shape=(n_classes, n_features, n_features))

        for k in range(n_classes):
            self._centroids[k, :] = x[y == k, :].mean(axis=0)
            self._priors[k] = (y == k).mean()
            self._covariances[k, :, :] = np.cov(x[y == k, :].T)

        self._priors /= self._priors.sum()  # ensure priors sum up to 1
        return self
```

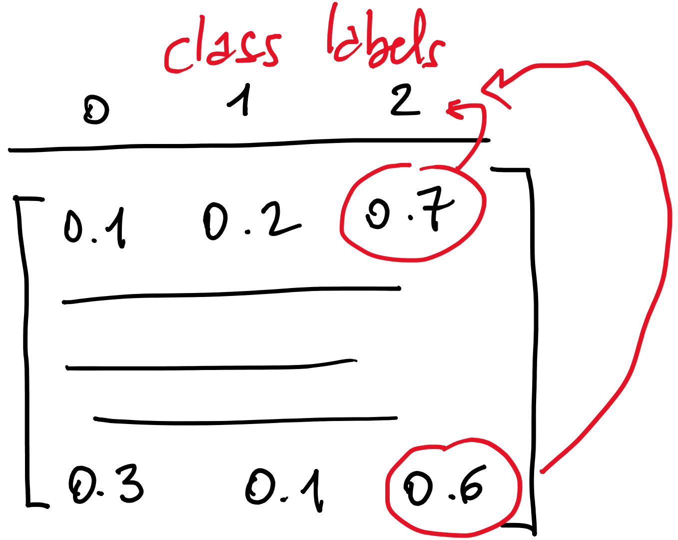
These are the maximum-likelihood estimates for the parameters of each class

Solution (small excerpt from the notebook code)

```
def decision_function(self, x):
    """Return posterior estimates for each class""»

    n_samples = x.shape[0]
    n_classes = self._centroids.shape[0]
    scores = np.zeros(shape=(n_samples, n_classes))
```

The matrix *scores* will contain, for each row (sample), the posterior probability predicted for each class.

Each sample will then be assigned to the class exhibiting the maximum a-posteriori probability estimate



Solution (small excerpt from the notebook code)

```
def decision_function(self, x):
    """Return posterior or joint probability estimates for each class,
    depending on whether posterior=True or False."""
    n_samples = x.shape[0]
    n_classes = self._centroids.shape[0]
    scores = np.zeros(shape=(n_samples, n_classes))
    for k in range(n_classes):
        likelihood_k = mvn.pdf(
            x, mean=self._centroids[k, :], cov=self._covariances[k, :, :])
        scores[:, k] = self._priors[k] * likelihood_k  # joint probability

    if self.posterior:
        # if posterior probs are required, divide joint probs by evidence
        evidence = scores.sum(axis=1)
        for k in range(n_classes):
            # normalize per row to estimate posterior
            scores[:, k] /= evidence
    return scores


def predict(self, x):
    """Return predicted labels."""
    scores = self.decision_function(x)
    y_pred = np.argmax(scores, axis=1)
    return y_pred
```

Compute Gaussian PDF at x.
This is our likelihood:

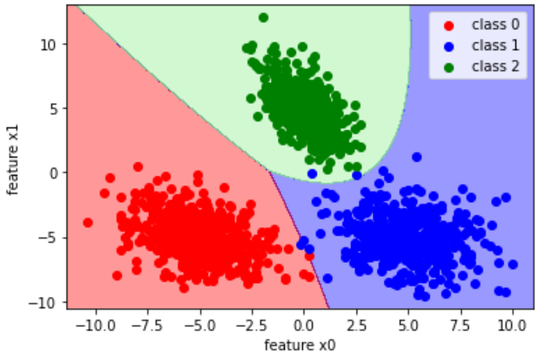
$$\frac{1}{\sqrt{(2\pi)^d \det \Sigma_k}} \exp\left(-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1}(x-\mu_k)\right)$$

Then multiply it by the prior to obtain the joint probability, and divide by the evidence p(x) to obtain the posterior

Take the index of the maximum posterior to predict the class label

Solution

```
n_samples = [500, 500, 500]
centroids = [[-5, -5],
             [+5, -5],
             [0, +5]]
cov=[[[3, -1],
      [-1, 3]],
     [[3, -0.5],
      [-0.5, 3]],
     [[1, -1],
      [-1, 3]]]

# generate data
x_tr, y_tr = make_gaussian_dataset(n_samples, centroids, cov=cov)
x_ts, y_ts = make_gaussian_dataset(n_samples, centroids, cov=cov)

clf = CClassifierGaussian()
clf.fit(x_tr, y_tr)
plot_decision_regions(x_tr, y_tr, classifier=clf)
plot_dataset(x_tr, y_tr)
plt.show()

scores = clf.decision_function(x_ts)
y_pred = clf.predict(x_ts)

print('Estimated priors: ', clf.priors)
print('Estimated centroids (with MLE): ', clf.centroids)
print('Estimated covariances (with MLE): ', clf.covariances)

print('Test error (%): ', (y_pred != y_ts).mean()*100)
```




```
Estimated priors:
[0.33333333 0.33333333 0.33333333]

Estimated centroids (with MLE):
[[-5.02818576 -5.07365035]
 [ 4.95564731 -5.04938789]
 [-0.03591899 4.87763586]]

Estimated covariances (with MLE):
[[[ 2.89255506 -1.05314784]
  [-1.05314784 2.77306075]]

 [[ 2.88868113 -0.46682182]
  [-0.46682182 3.04256309]]

 [[ 1.04041627 -1.09369177]
  [-1.09369177 3.26337424]]]

Test error (%): 0.26666666666666666
```

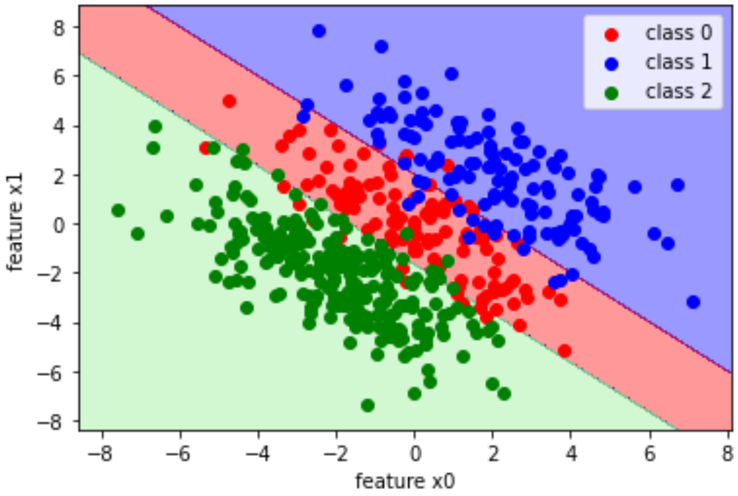
Exercise 2

- Visualize the optimal decision regions for a 3-class Gaussian Classifier with parameters:
  - $p_0 = p_1 = \frac{1}{4}, \; p_2 = \frac{1}{2}$
  - $\mu_0 = [0, 0]^T, \; \mu_1 = [2, 2]^T, \; \mu_2 = [-2, -2]^T$
  - $\Sigma_0 = \Sigma_1 = \Sigma_2 = \begin{bmatrix} 4 & -3 \\ -3 & 4 \end{bmatrix}$

Solution

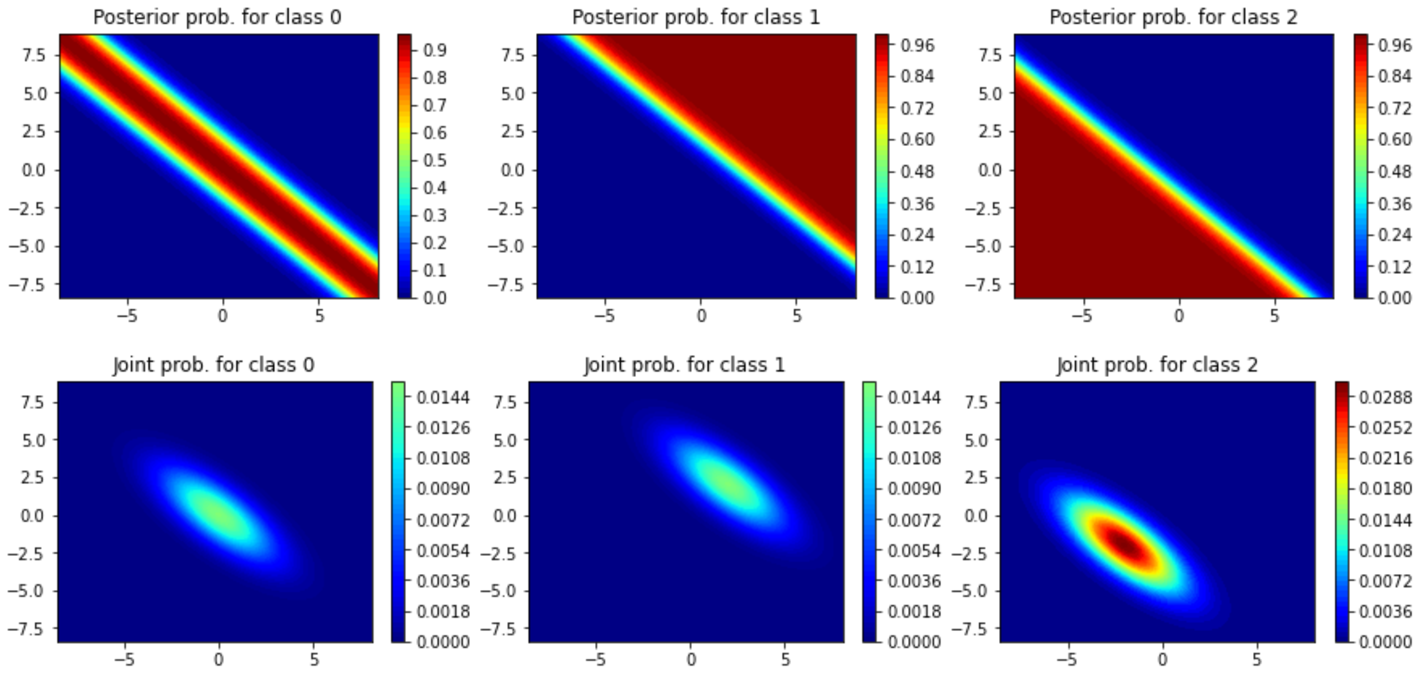
- In this case, we set the parameters directly to the Gaussian Classifier (instead of estimating them via *fit*), and then visualize the decision regions and boundaries

```
priors = np.array([1/4, 1/4, 1/2])
centroids = [[0, 0],
             [2, 2],
             [-2, -2]]
cov=[[[4, -3], [-3, 4]],
     [[4, -3], [-3, 4]],
     [[4, -3], [-3, 4]]]

clf = CClassifierGaussian()
# we do not estimate the parameters here,
# but use the true ones
# clf.fit(x_tr, y_tr)
clf._priors = np.array(priors)
clf._centroids = np.array(centroids)
clf._covariances = np.array(cov)
plot_decision_regions(x_tr, y_tr, classifier=clf)
plot_dataset(x_tr, y_tr)
plt.show()
```



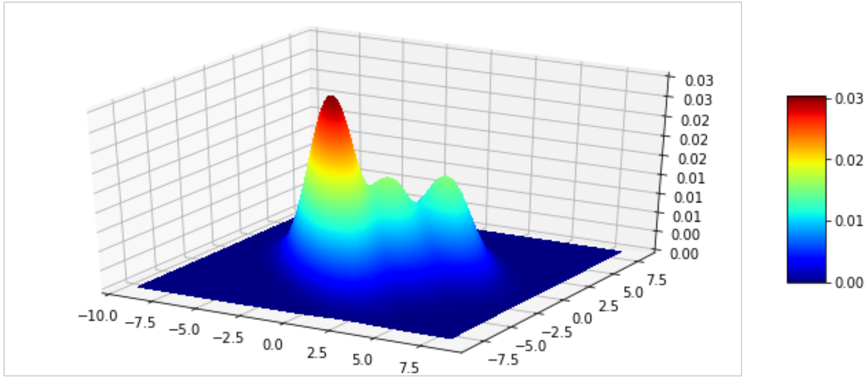
Solution

- We can also visualize the posterior and joint probabilities for each class



Solution

- Finally, we also plot the evidence *p(x)* along the z-axis in a 3D plot



- Note here the overlap among the three Gaussian distributions, one per class, and that the Gaussian associated to the highest prior (1/2) has a higher peak