decision_boundaries_for_linear_discriminant_analysis

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1 Decision Boundaries For Linear Discriminant Analysis

Assume that a classification is to be made. Given the parameters $\boldsymbol{\theta}$ and the input vector $\mathbf{x}$, the class of the output variable y is to be determined. The probability density function of y being from the class c is modeled using a discrete generative model as follows:

$$p\left(y=c|\mathbf{x},\boldsymbol{\theta}\right)=\frac{p\left(\mathbf{x}|y=c,\boldsymbol{\theta}\right)p\left(y=c|\boldsymbol{\theta}\right)}{p\left(\mathbf{x}|\boldsymbol{\theta}\right)}$$

If a multivariate Gaussian distribution is used to model the class conditional density of the input vector, i.e. $p\left(\mathbf{x}|y=c,\boldsymbol{\theta}\right)$, then this is called the quadratic discriminant analysis:

$$p\left(\mathbf{x}|y=c,\boldsymbol{\theta}\right)=\frac{1}{\left(2\pi\right)^{D/2}\left|\boldsymbol{\Sigma}_c\right|^{1/2}}\exp\left[-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)^T\boldsymbol{\Sigma}_c^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)\right]$$

A special case of the quadratic discriminant analysis is when the covariance matrix of the Gaussian distibution for the class conditional density of the input features is common to all of the classes. That is the mean,

$$\boldsymbol{\Sigma}_c=\boldsymbol{\Sigma}$$

for all of the classes c. Then, $p\left(y=c|\mathbf{x},\boldsymbol{\theta}\right)$ can be calculated as follows:

$$p\left(y=c|\mathbf{x},\boldsymbol{\theta}\right)=\frac{p\left(\mathbf{x}|y=c,\boldsymbol{\theta}\right)p\left(y=c|\boldsymbol{\theta}\right)}{p\left(\mathbf{x}|\boldsymbol{\theta}\right)}=\frac{p\left(\mathbf{x}|y=c,\boldsymbol{\theta}\right)p\left(y=c|\boldsymbol{\theta}\right)}{\sum_{s=1}^{C}p\left(x,y=s|\boldsymbol{\theta}\right)}=\frac{p\left(\mathbf{x}|y=c,\boldsymbol{\theta}\right)p\left(y=c|\boldsymbol{\theta}\right)}{\sum_{s=1}^{C}p\left(\mathbf{x}|y=s,\boldsymbol{\theta}\right)p\left(y=s|\boldsymbol{\theta}\right)}\Rightarrow$$

$$p\left(y=c|\mathbf{x},\boldsymbol{\theta}\right)=\frac{\pi_c p\left(\mathbf{x}|y=c,\boldsymbol{\theta}\right)}{\sum_{s=1}^{C}\pi_s p\left(\mathbf{x}|y=s,\boldsymbol{\theta}\right)}=\frac{\pi_c\frac{1}{\left(2\pi\right)^{D/2}\left|\boldsymbol{\Sigma}\right|^{1/2}}\exp\left[-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)^T\boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)\right]}{\sum_{s=1}^{C}\pi_s\frac{1}{\left(2\pi\right)^{D/2}\left|\boldsymbol{\Sigma}\right|^{1/2}}\exp\left[-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_s\right)^T\boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_s\right)\right]}$$

Let the expression

$$-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)^T\boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)$$

be simplified:

$$-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)^T\boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)=-\frac{1}{2}\left(\mathbf{x}^T-\boldsymbol{\mu}_c^T\right)\left(\boldsymbol{\Sigma}^{-1}\mathbf{x}-\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c\right)=-\frac{1}{2}\left(\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}-\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c-\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\mathbf{x}+\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}$$

$$-\frac{1}{2}\left(\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}-2\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c+\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c\right)=-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}+\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c-\frac{1}{2}\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c$$

The simplified expression is put into the class probability density conditioned on the input and parameters:

$$p\left(y=c|\mathbf{x},\boldsymbol{\theta}\right)=\frac{\pi_c\frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left[-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)^T\boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_c\right)\right]}{\sum_{s=1}^{C}\pi_s\frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left[-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_s\right)^T\boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_s\right)\right]}=\frac{\pi_c\frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left[-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}+\mathbf{x}^T\boldsymbol{\Sigma}}{\sum_{s=1}^{C}\pi_s\frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left[-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}+\mathbf{x}}$$

$$\frac{\frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left(-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}\right)\pi_c\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c-\frac{1}{2}\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c\right]}{\frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left(-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}\right)\sum_{s=1}^{C}\pi_s\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s-\frac{1}{2}\boldsymbol{\mu}_s^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s\right]}=\frac{\pi_c\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c-\frac{1}{2}\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c\right]}{\sum_{s=1}^{C}\pi_s\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s-\frac{1}{2}\boldsymbol{\mu}_s^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s\right]}\Rightarrow$$

$$p\left(y=c|\mathbf{x},\boldsymbol{\theta}\right)=\frac{\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c+\log\pi_c-\frac{1}{2}\boldsymbol{\mu}_c^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_c\right]}{\sum_{s=1}^{C}\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s+\log\pi_s-\frac{1}{2}\boldsymbol{\mu}_s^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s\right]}$$

The boundary separating two classes c_1 and c_2 is a linear function of $\mathbf{x}$. Hence, this analysis is called the linear discriminant analysis. The equation for this linear boundary can be derived as follows:

$$p\left(y=c_1|\mathbf{x},\boldsymbol{\theta}\right)=p\left(y=c_2|\mathbf{x},\boldsymbol{\theta}\right)\Rightarrow$$

$$\frac{\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}+\log\pi_{c_1}-\frac{1}{2}\boldsymbol{\mu}_{c_1}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}\right]}{\sum_{s=1}^{C}\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s+\log\pi_s-\frac{1}{2}\boldsymbol{\mu}_s^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s\right]}=\frac{\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}+\log\pi_{c_2}-\frac{1}{2}\boldsymbol{\mu}_{c_2}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}\right]}{\sum_{s=1}^{C}\exp\left[\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s+\log\pi_s-\frac{1}{2}\boldsymbol{\mu}_s^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_s\right]}\Rightarrow$$

$$\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}+\log\pi_{c_1}-\frac{1}{2}\boldsymbol{\mu}_{c_1}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}=\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}+\log\pi_{c_2}-\frac{1}{2}\boldsymbol{\mu}_{c_2}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}\Rightarrow$$

$$\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}-\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}=\frac{1}{2}\boldsymbol{\mu}_{c_1}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}-\frac{1}{2}\boldsymbol{\mu}_{c_2}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}+\log\pi_{c_2}-\log\pi_{c_1}\Rightarrow$$

$$\mathbf{x}^T\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}-\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}\right)=\frac{1}{2}\boldsymbol{\mu}_{c_1}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}-\frac{1}{2}\boldsymbol{\mu}_{c_2}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}+\log\pi_{c_2}-\log\pi_{c_1}$$

Assume that there are only two features which means that $\mathbf{x}$ vector is two dimensional. Then, the equation of the boundary is as follows:

$$\beta_1x_1+\beta_2x_2=constant$$

where

$$\mathbf{x}=\begin{bmatrix}x_1\\x_2\end{bmatrix},\boldsymbol{\beta}=\begin{bmatrix}\beta_1\\\beta_2\end{bmatrix}=\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}-\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2},constant=\frac{1}{2}\boldsymbol{\mu}_{c_1}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1}-\frac{1}{2}\boldsymbol{\mu}_{c_2}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}+\log\pi_{c_2}-\log\pi_{c_1}$$

The covariance matrix of the distribution is to be formed. It must be positive definite. Let the distribution's eigenvectors be v_1 and v_2. Let the corresponding eigenvalues be λ_1 and λ_2 respectively. Then:

$$\boldsymbol{\Sigma}_c=\begin{bmatrix}v_1&v_2\end{bmatrix}\begin{bmatrix}\lambda_1&0\\0&\lambda_2\end{bmatrix}\begin{bmatrix}v_1&v_2\end{bmatrix}^{-1}$$

[1]:

```
import numpy as np
v1_t = np.array([1, 3])
v1_t = v1_t / np.linalg.norm(v1_t) # transpose of the first eigenvector
v2_t = np.array([3, -1]) # transpose of the second eigenvector
v2_t = v2_t / np.linalg.norm(v2_t)
eigenvector_matrix = np.array([v1_t, v2_t]).transpose() # eigenvector matrix
```

```
lambda1 = 1 # first eigenvalue
lambda2 = 2 # second eigenvalue
eigenvalue_matrix = np.array([[lambda1, 0],[0, lambda2]])
print("the eigenvector matrix of the distributions:")
print(eigenvector_matrix)
print("the eigenvalue matrix of the distributions")
print(eigenvalue_matrix)
cov = np.matmul(np.matmul(eigenvector_matrix, eigenvalue_matrix), np.linalg.
 ↪inv(eigenvector_matrix))
print("the covariance matrix of the distributions")
print(cov)
```

```
the eigenvector matrix of the distributions:
[[ 0.31622777  0.9486833 ]
 [ 0.9486833  -0.31622777]]
the eigenvalue matrix of the distributions
[[1 0]
 [0 2]]
the covariance matrix of the distributions
[[ 1.9 -0.3]
 [-0.3  1.1]]
```

[2]:

```
mean_1_t = np.array([1.0, 1.0]) # the mean vector of the first distribution
print("transpose of the mean vector of the first distribution")
print(mean_1_t)
```

```
transpose of the mean vector of the first distribution
[1. 1.]
```

[3]:

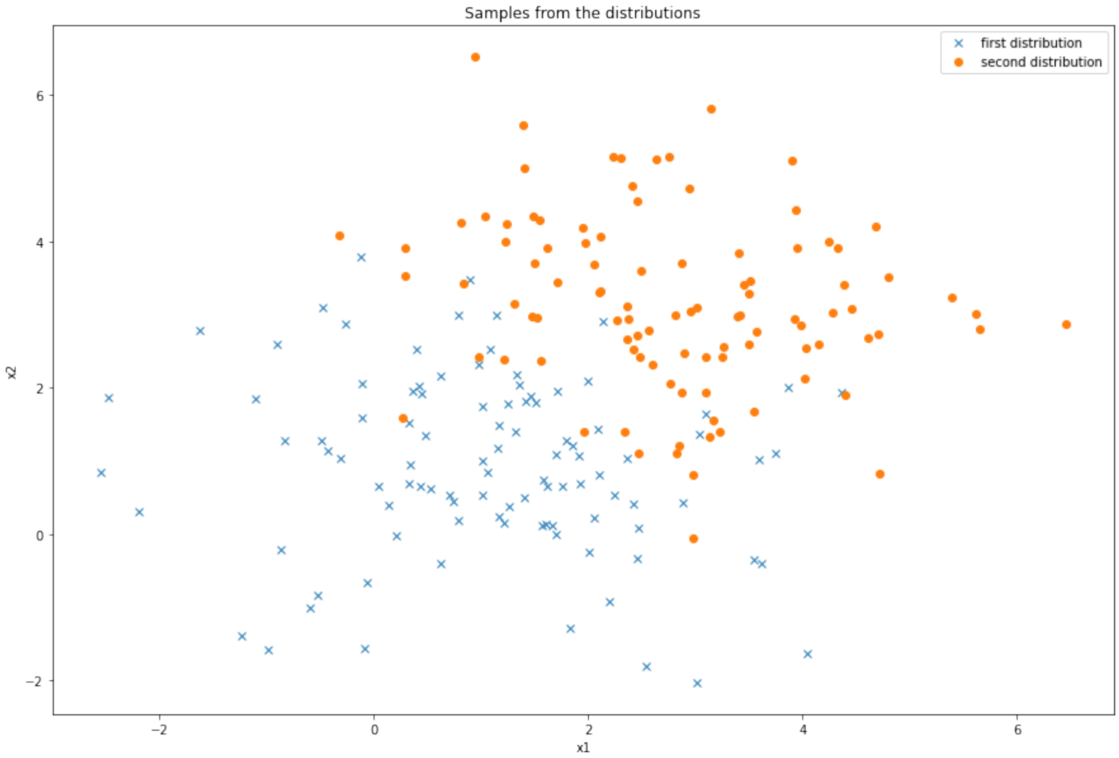
```
mean_2_t = np.array([3.0, 3.0]) # the mean vector of the second distribution
print("transpose of the mean vector of the second distribution")
print(mean_2_t)
```

```
transpose of the mean vector of the second distribution
[3. 3.]
```

[4]:

```
import matplotlib.pyplot as plt

# samples from the first distribution
x1_s, y1_s = np.random.default_rng().multivariate_normal(mean_1_t, cov, 100).T

# samples from the second distribution
x2_s, y2_s = np.random.default_rng().multivariate_normal(mean_2_t, cov, 100).T

fig, ax = plt.subplots(figsize=(15, 10))
_ = ax.plot(x1_s, y1_s, 'x', label='first distribution')
_ = ax.plot(x2_s, y2_s, 'o', label='second distribution')
```

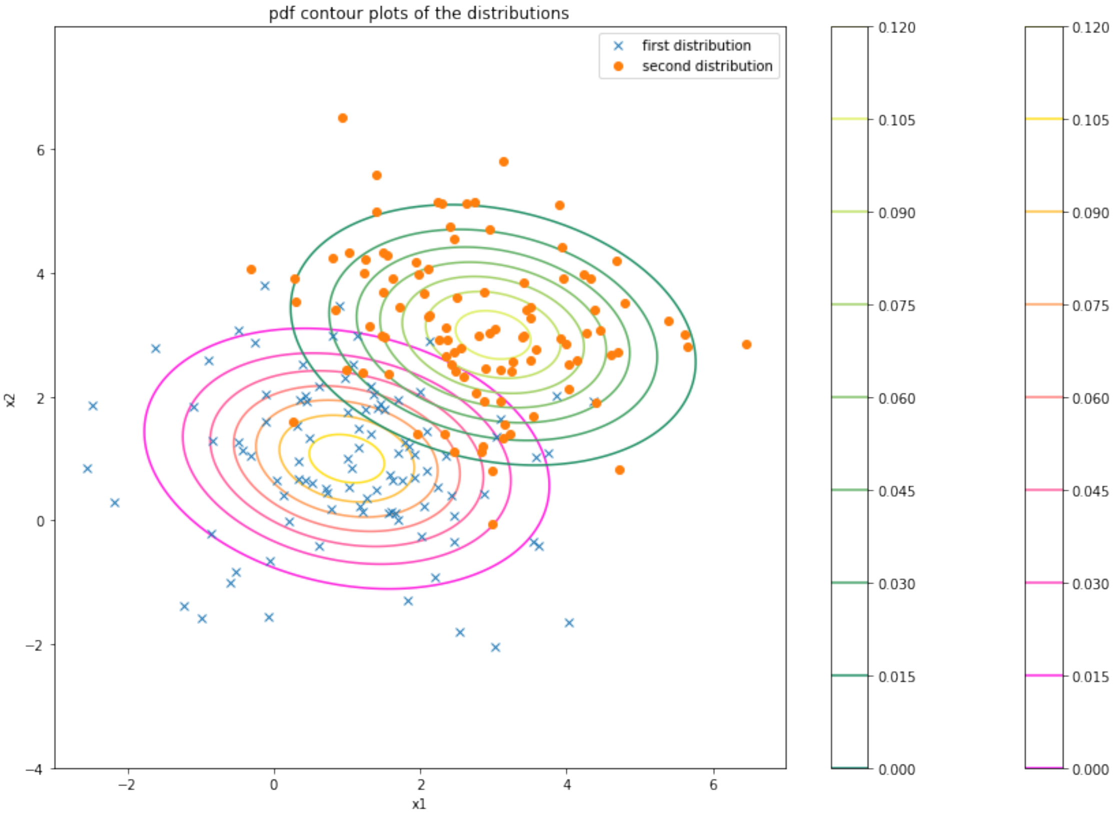
```
handles, labels = ax.get_legend_handles_labels()
_ = ax.legend(handles, labels)
_ = ax.set_title('Samples from the distributions')
_ = plt.xlabel('x1')
_ = plt.ylabel('x2')
```



[5]:

```
from scipy.stats import multivariate_normal

x_min = -3.0
x_max = 7.0
y_min = -4.0
y_max = 8.0
x, y = np.mgrid[x_min:x_max:.01, y_min:y_max:.01]
pos = np.empty(x.shape + (2,))
pos[:, :, 0] = x; pos[:, :, 1] = y

rv1 = multivariate_normal(mean_1_t, cov)
rv2 = multivariate_normal(mean_2_t, cov)

cmap1 = plt.cm.get_cmap("spring")
cmap2 = plt.cm.get_cmap("summer")

fig, ax = plt.subplots(figsize=(15, 10))
```

```
contour_plot_1 = ax.contour(x, y, rv1.pdf(pos), cmap=cmap1)
contour_plot_2 = ax.contour(x, y, rv2.pdf(pos), cmap=cmap2)
_ = fig.colorbar(contour_plot_1, ax=ax)
_ = fig.colorbar(contour_plot_2, ax=ax)

_ = ax.plot(x1_s, y1_s, 'x', label='first distribution')
_ = ax.plot(x2_s, y2_s, 'o', label='second distribution')
handles, labels = ax.get_legend_handles_labels()
_ = ax.legend(handles, labels)

_ = ax.set_title('pdf contour plots of the distributions')
_ = plt.xlabel('x1')
_ = plt.ylabel('x2')
```



The equation to be solved for determining the decision boundary and the related variables are repeated:

$$\beta_1 x_1 + \beta_2 x_2 = constant$$

where

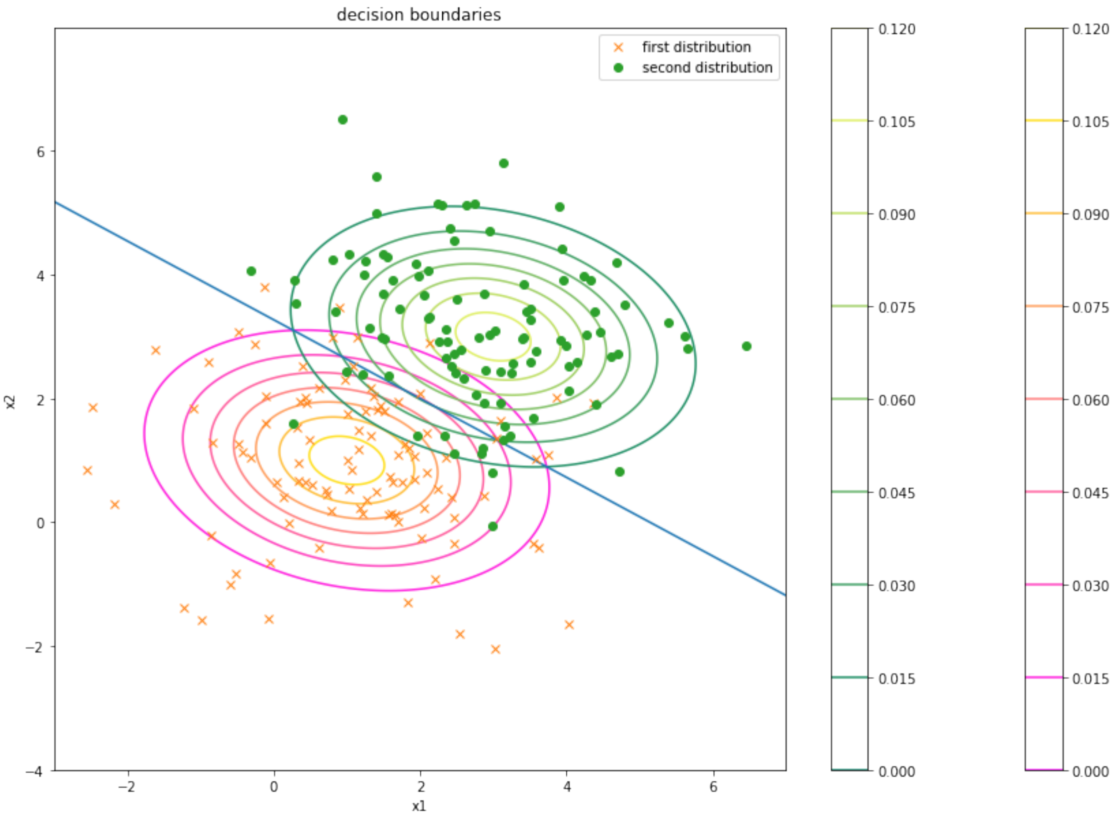
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1} - \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2}, constant = \frac{1}{2}\boldsymbol{\mu}_{c_1}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_1} - \frac{1}{2}\boldsymbol{\mu}_{c_2}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{c_2} + \log\pi_{c_2} - \log\pi_{c_1}$$

[6]:

```
beta = np.matmul(np.linalg.inv(cov), (mean_1_t-mean_2_t))
beta1 = beta[0]
beta2 = beta[1]
pi_c1 = 0.5
pi_c2 = 0.5
constant = 0.5*((mean_1_t*np.matmul(np.linalg.inv(cov), mean_1_t)).sum()-
                (mean_2_t*np.matmul(np.linalg.inv(cov), mean_2_t)).sum())+np.
 ↪log(pi_c2)-np.log(pi_c1)

x1 = np.arange(x_min, x_max, step=0.01)
x2 = (-beta1*x1 + constant)/beta2
```

[7]:

```
fig, ax = plt.subplots(figsize=(15.0, 10.0))
_ = ax.plot(x1, x2)
contour_plot_1 = ax.contour(x, y, rv1.pdf(pos), cmap=cmap1)
contour_plot_2 = ax.contour(x, y, rv2.pdf(pos), cmap=cmap2)
_ = fig.colorbar(contour_plot_1, ax=ax)
_ = fig.colorbar(contour_plot_2, ax=ax)

_ = ax.plot(x1_s, y1_s, 'x', label='first distribution')
_ = ax.plot(x2_s, y2_s, 'o', label='second distribution')
handles, labels = ax.get_legend_handles_labels()
_ = ax.legend(handles, labels)

_ = ax.set_title('decision boundaries')
_ = plt.xlabel('x1')
_ = plt.ylabel('x2')
```



2 References

Machine Learning A Probabilistic Perspective, Kevin P. Murphy