Details about Midterm Exam

Date & Time: Thursday, October 7

Check your email for the time you are scheduled to take the midterm exam. Let me know if there are conflicts well in advance.

- **All exams will be proctored with Honorlock.**

In-class review: Monday, October 4

Post questions in the Midterm Exam Discussion Board until **Sunday, October 3 @ 3 PM**.

- These questions will be addressed in-class on Monday, October 4.

Coverage

Lectures 1-17 (modules 1-4)

Practice Midterm Exam

1. Available in the Assignment-Solutions repo.
2. Practice Canvas Quizzes created to practice Honorlock proctoring and overall exam setup: Pratice Midterm Exam - Honolorck Proctoring
3. Solutions to the practice exam will be posted before the in-class midterm review.
4. One of the questions in the practice exam asks about K-Means clustering, but K-Means clustering will **not** be covered in the Midterm exam.

Allowed Material for the Midterm

- 1-page letter-sized of **formulas** (front and back, handwritten or typed)
- scientific calculator
- Writing and scratch paper to write your answers. I will give an estimate on how many pages to bring in the review lecture.
- Bring a second device (e.g., phone, tablet or other) with the CamScanner or Scannable app installed. This device is only to be used at the end of the exam to take pictures of your handwritten solutions
- **TOTAL TIME:** 2 hours + 15 minutes

Communications between students or anyone else during the exam is considered cheating. Turn off all Slack notifications and other communications channels!

Ten (10) minutes prior to the time you are scheduled to take the exam, you will be able to see the Canvas quiz with your midterm exam.

Lecture 15 - Naive Bayes Classifier; Mixture Models

Naive Bayes Classifier

Therefore, for a given test point $\mathbf{x}^*$, our decision rule is:

$$P(C_1|\mathbf{x}^*) \underset{C_2}{\overset{C_1}{\gtrless}} P(C_2|\mathbf{x}^*)$$

Using the Bayes' rule, we can further rewrite it as:

$$\frac{P(\mathbf{x}^*|C_1)P(C_1)}{P(\mathbf{x}^*)} \underset{C_2}{\overset{C_1}{\gtrless}} \frac{P(\mathbf{x}^*|C_2)P(C_2)}{P(\mathbf{x}^*)}$$

This defines the **Naive Bayes Classifier**.

Training a Generative Classifier

So, **to train the classifier**, what we need to do is to determine the parametric form (and its parameters values) for $p(x|C_1)$, $p(x|C_2)$, $P(C_1)$ and $p(C_2)$.

- For example, we can assume that the data samples coming from either C_1 and C_2 are distributed according to Gaussian distributions. In this case,

$$p(x|C_k) = \frac{1}{(2\pi)^{1/2}|\Sigma_k|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\mu_k)^T\Sigma_k^{-1}(\mathbf{x}-\mu_k)\right\}, \forall k = \{1,2\}$$

For this case, this defines the **Gaussian Naive Bayes Classifier**.

Or, we can consider any other parametric distribution.

- What about the $P(C_1)$ and $P(C_2)$?

We can consider the relative frequency of each class, that is, $P(C_k) = \frac{N_k}{N}$, where N_k is the number of points in class C_k and N is the total number of samples.

MLE Parameter Estimation Steps

For simplification, let's consider the covariance matrix Σ_k for $k = 1, 2$ to be **isotropic** matrices, that is, the covariance matrix is diagonal and the element along the diagonal is the same, or: $\Sigma_k = \sigma_k^2 \mathbf{I}$.

- What are the parameters? The mean and covariance of the Gaussian distribution for both classes.

Given the assumption of the Gaussian form, how would you estimate the parameters for $p(x|C_1)$ and $p(x|C_2)$? We can use **maximum likelihood estimate** for the mean and covariance, because we are looking for the parameters of the distributions that *maximize* the data likelihood!

The MLE estimate for the mean of class C_k is:

$$\mu_{k,\text{MLE}} = \frac{1}{N_k} \sum_{n \in C_k} \mathbf{x}_n$$

where N_k is the number of training data points that belong to class C_k.

Assuming the classes follow a (bivariate or 2-D) Gaussian distribution and, for simplicity, let's assume the covariance matrices are **isotropic**, that is, $\Sigma_k = \sigma_k^2 \mathbf{I}$.

The MLE steps for parameter estimation are:

1. Write down the observed data likelihood, $\mathcal{L}^0$

$$\begin{aligned}
\mathcal{L}^0 &= P(x_1, x_2, \ldots, x_N | C_k) && (1)\\
&= \prod_{n=1}^{N} P(x_n | C_k), \text{ data samples are i.i.d.} && (2)\\
&= \prod_{n=1}^{N} \frac{1}{(2\pi)^{1/2} |\Sigma|^{1/2}} \exp\left\{ -\frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right\} && (3)\\
&= \prod_{n=1}^{N} \frac{1}{(2\pi)^{1/2} |\sigma_k^2 \mathbf{I}|^{1/2}} \exp\left\{ -\frac{1}{2\sigma_k^2} (x_n - \mu_k)^T \mathbf{I} (x_n - \mu_k) \right\} && (4)\\
&= \prod_{n=1}^{N} \frac{1}{(2\pi)^{1/2} (\sigma_k^2)^{1/2}} \exp\left\{ -\frac{1}{2\sigma_k^2} (x_n - \mu_k)^T (x_n - \mu_k) \right\} && (5)
\end{aligned}$$

1. Take the log-likelihood, $\mathbf{L}$. This *trick* helps in taking derivatives.

$$\begin{aligned}
\mathcal{L} &= \ln\left(\mathcal{L}^0\right) && (6)\\
&= \sum_{n=1}^{N} -\frac{1}{2} \ln 2\pi - \frac{1}{2} \ln \sigma_k^2 - \frac{1}{2\sigma_k^2} (x_n - \mu_k)^T (x_n - \mu_k) && (7)
\end{aligned}$$

1. Take the derivative of the log-likelihood function with respect to the parameters of interest. For Gaussian distribution they are the mean and covariance.

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \mu_k} &= 0 && (8)\\
\sum_{n \in C_k} \frac{1}{\sigma_k^2}(x_n - \mu_k) &= 0 && (9)\\
\sum_{n \in C_k} (x_n - \mu_k) &= 0 && (10)\\
\sum_{n \in C_k} x_n - \sum_{n \in C_k} \mu_k &= 0 && (11)\\
\sum_{n \in C_k} x_n - N_k\mu_k &= 0 && (12)\\
\mu_k &= \frac{1}{N_k}\sum_{n \in C_k} x_n && (13)
\end{aligned}
$$

This is the sample mean for each class. And,

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \sigma_k^2} &= 0 && (14)\\
\sum_{n \in C_k} -\frac{1}{2\sigma_k^2} + \frac{2(x_n - \mu_k)^T(x_n - \mu_k)}{(2\sigma_k^2)^2} &= 0 && (15)\\
\sum_{n \in C_k} -1 + \frac{(x_n - \mu_k)^T(x_n - \mu_k)}{\sigma_k^2} &= 0 && (16)\\
\sum_{n \in C_k} \frac{(x_n - \mu_k)^T(x_n - \mu_k)}{\sigma_k^2} &= N_k && (17)\\
\sigma_k^2 &= \sum_{n \in C_k} \frac{(x_n - \mu_k)^T(x_n - \mu_k)}{N_k} && (18)
\end{aligned}
$$

This is the sample variance for each class. Then we can create $\Sigma_k = \sigma_k^2\mathbf{I}$, which is the (biased) sample covariance for each class.

In practice, if we want to estimate an entire covariance matrix, we would have to take the derivative of the log-likelihood function with respect to every entry in the covariance matrix.

We can determine the values for $p(C_1)$ and $p(C_2)$ from the number of data points in each class:

$$p(C_k) = \frac{N_k}{N}$$

where N is the total number of data points.

In [1]:

```
import numpy as np
from scipy.stats import multivariate_normal
import matplotlib.pyplot as plt
plt.style.use('bmh')
```

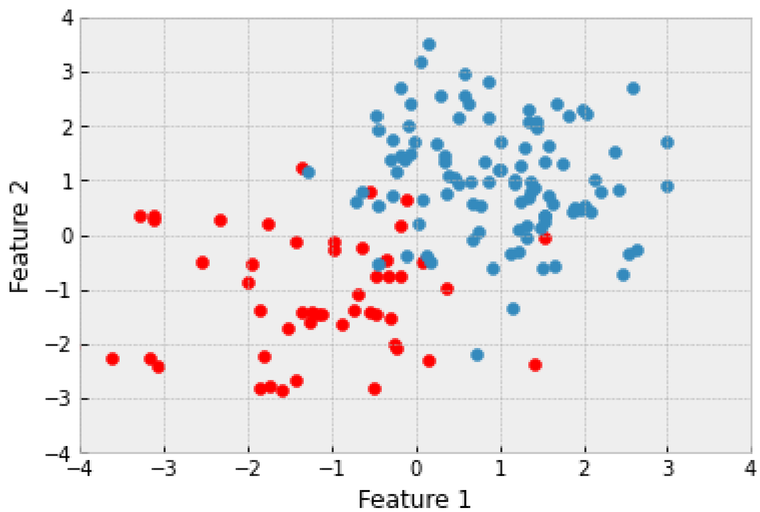
In [2]:

```
def generateData(mean1, mean2, cov1, cov2, N1, N2):
    # We are generating data from two Gaussians to represent two classes
    # In practice, we would not do this - we would just have data from the problem we a
```

```
    data_C1 = np.random.multivariate_normal(mean1, cov1, N1)
    data_C2 = np.random.multivariate_normal(mean2, cov2, N2)

    plt.scatter(data_C1[:,0], data_C1[:,1], c='r')
    plt.scatter(data_C2[:,0], data_C2[:,1])
    plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
    plt.axis([-4,4,-4,4])
    return data_C1, data_C2
```

In [13]:

```
mean1 = [-1, -1]
mean2 = [1, 1]
cov1 = [[1,0],[0,1]]
cov2 = [[1,0],[0,1]]
N1 = 50
N2 = 100

data_C1, data_C2 = generateData(mean1, mean2, cov1, cov2, N1, N2)
```



In [14]:

```
data_C1.shape
```

Out[14]:

```
(50, 2)
```

In [15]:

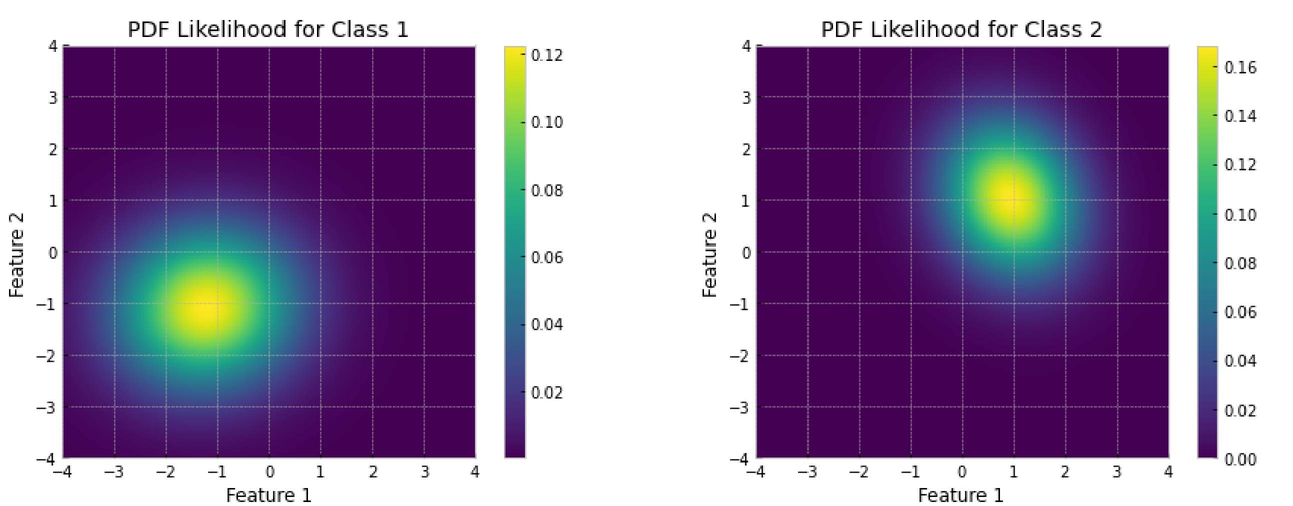
```
# Estimate the mean and covariance for each class from the training data

mu1 = np.mean(data_C1, axis=0)
print('Mean of Class 1: ', mu1)


cov1 = np.cov(data_C1.T) # because np.cov assumes data comes in as DxN
print('Covariance of Class 1: ',cov1)


mu2 = np.mean(data_C2, axis=0)
print('Mean of Class 2: ',mu2)


cov2 = np.cov(data_C2.T)
print('Covariance of Class 2: ',cov2)
```

```python
# Estimate the prior for each class

pC1 = data_C1.shape[0]/(data_C1.shape[0]+data_C2.shape[0])
print('Probability of  Class 1: ',pC1)

pC2 = data_C2.shape[0]/(data_C1.shape[0]+data_C2.shape[0])
print('Probability of Class 2: ',pC2)
```

```
Mean of Class 1:  [-1.21519443 -1.10616409]
Covariance of Class 1:  [[1.44725922 0.06498299]
 [0.06498299 1.16522598]]
Mean of Class 2:  [0.95239041 1.03401998]
Covariance of Class 2:  [[ 0.83583401 -0.13410859]
 [-0.13410859  1.08745696]]
Probability of  Class 1:  0.3333333333333333
Probability of Class 2:  0.6666666666666666
```

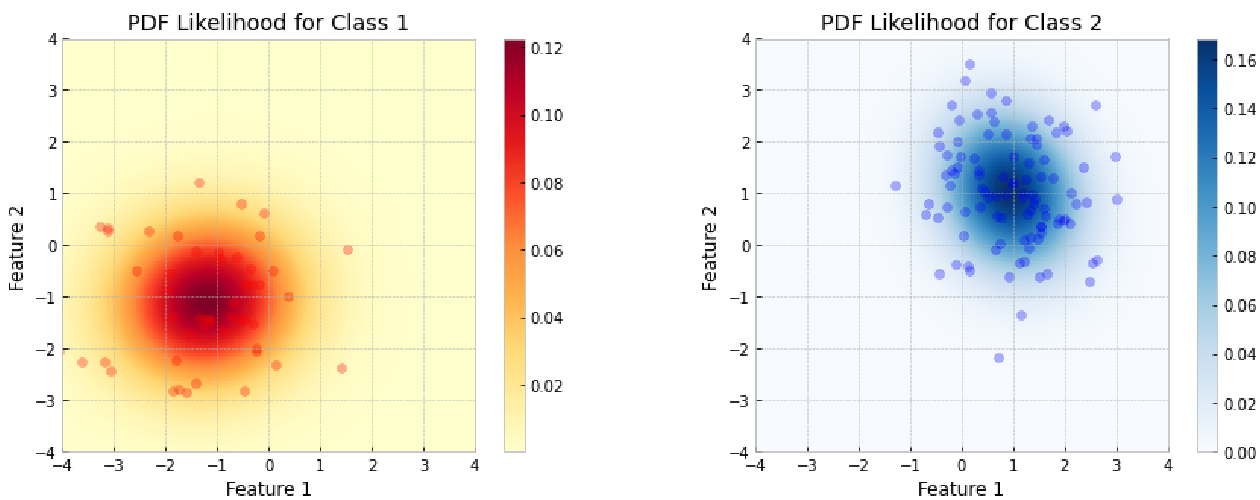
In [16]:

```python
# Compute a grid of values for x and y
x = np.linspace(-4, 4, 100)
y = np.linspace(-4, 4, 100)
xm, ym = np.meshgrid(x, y)
X = np.flip(np.dstack([xm,ym]),axis=0)

# Let's plot the probabaility density function (pdf) for each class
y1 = multivariate_normal.pdf(X, mean=mu1, cov=cov1) # P(x|C1)
y2 = multivariate_normal.pdf(X, mean=mu2, cov=cov2) # P(x|C2)


fig =plt.figure(figsize=(15,5))
fig.add_subplot(1,2,1)
plt.imshow(y1, extent=[-4,4,-4,4])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('PDF Likelihood for Class 1')

fig.add_subplot(1,2,2)
plt.imshow(y2, extent=[-4,4,-4,4])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('PDF Likelihood for Class 2');
```



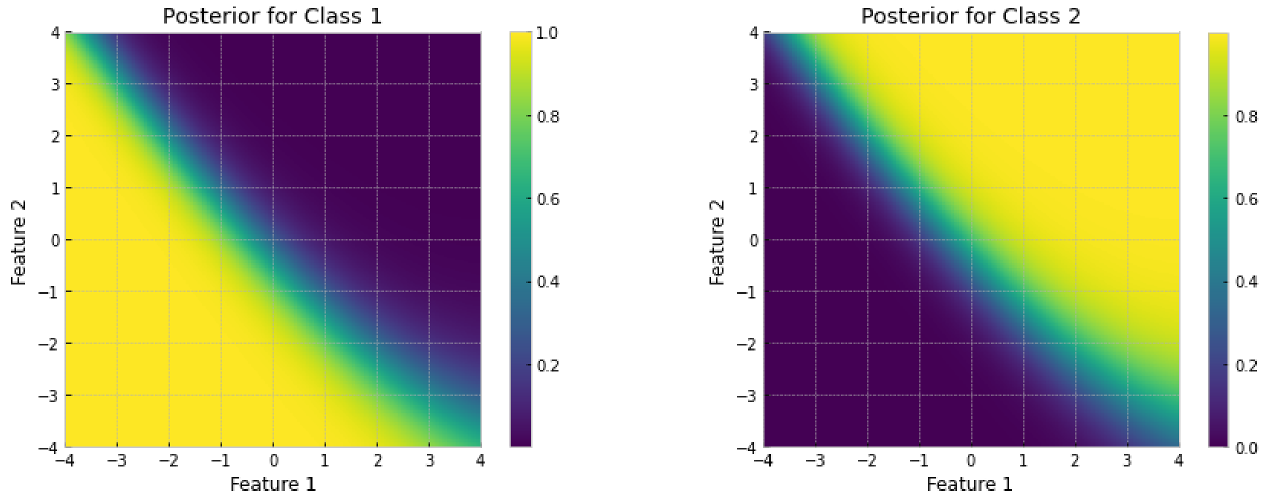
In [17]:

```
fig =plt.figure(figsize=(15,5))
fig.add_subplot(1,2,1)
plt.scatter(data_C1[:,0], data_C1[:,1], c='r',alpha=0.3)
plt.imshow(y1, extent=[-4,4,-4,4],cmap='YlOrRd')
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('PDF Likelihood for Class 1')

fig.add_subplot(1,2,2)
plt.scatter(data_C2[:,0], data_C2[:,1], c='b',alpha=0.3)
plt.imshow(y2, extent=[-4,4,-4,4], cmap='Blues')
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('PDF Likelihood for Class 2');
```

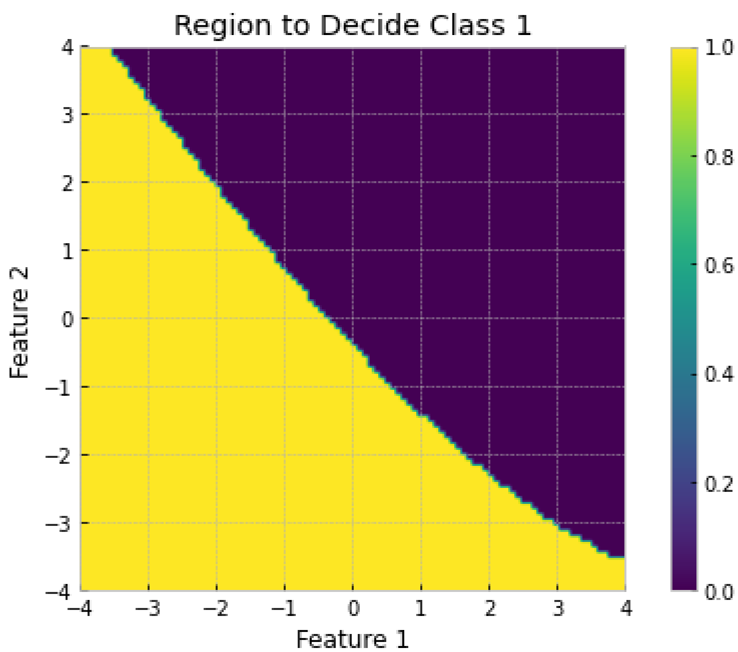


In [18]:

```
# Let's take a look at the posterior distributions: they represent our classification d
pos1 = (y1*pC1)/(y1*pC1 + y2*pC2) # P(C1|x)
pos2 = (y2*pC2)/(y1*pC1 + y2*pC2) # P(C2|x)

fig =plt.figure(figsize=(15,5))
fig.add_subplot(1,2,1)
plt.imshow(pos1, extent=[-4,4,-4,4])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('Posterior for Class 1')

fig.add_subplot(1,2,2)
plt.imshow(pos2, extent=[-4,4,-4,4])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('Posterior for Class 2');
```



In [19]:
```
# Look at the decision boundary:
plt.figure(figsize=(8,5))
plt.imshow(pos1 > pos2, extent=[-4,4,-4,4])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('Region to Decide Class 1');
```



- Let's use this classifier to predict the class label for point $[1, 1]$:

In [21]:
```
x = [1,1]

# Data Likelihoods
y1_newPoint = multivariate_normal.pdf(x, mean=mu1, cov=cov1) # p(x|C1)
y2_newPoint = multivariate_normal.pdf(x, mean=mu2, cov=cov2) # p(x|C2)

print('Data likelihoods:')
print('P(x|C1) = ', y1_newPoint)
print('P(x|C2) = ', y2_newPoint,'\n')

# Posterior Probabilities
```

```
y1_pos = y1_newPoint*pC1/(y1_newPoint*pC1 + y2_newPoint*pC2)
y2_pos = y2_newPoint*pC2/(y1_newPoint*pC1 + y2_newPoint*pC2)

print('Posterior probabilities:')
print('P(C1|x) = ', y1_pos)
print('P(C2|x) = ', y2_pos,'\n')

if y1_pos > y2_pos:
    print('x = ',x,' belongs to class 1')
else:
    print('x = ',x,' belongs to class 2')
```

```
Data likelihoods:
P(x|C1) =  0.003983945876533317
P(x|C2) =  0.16833065178108447

Posterior probabilities:
P(C1|x) =  0.011695292633899514
P(C2|x) =  0.9883047073661004

x =  [1, 1]  belongs to class 2
```

- What about $x = [2, 4]$?

In [23]:

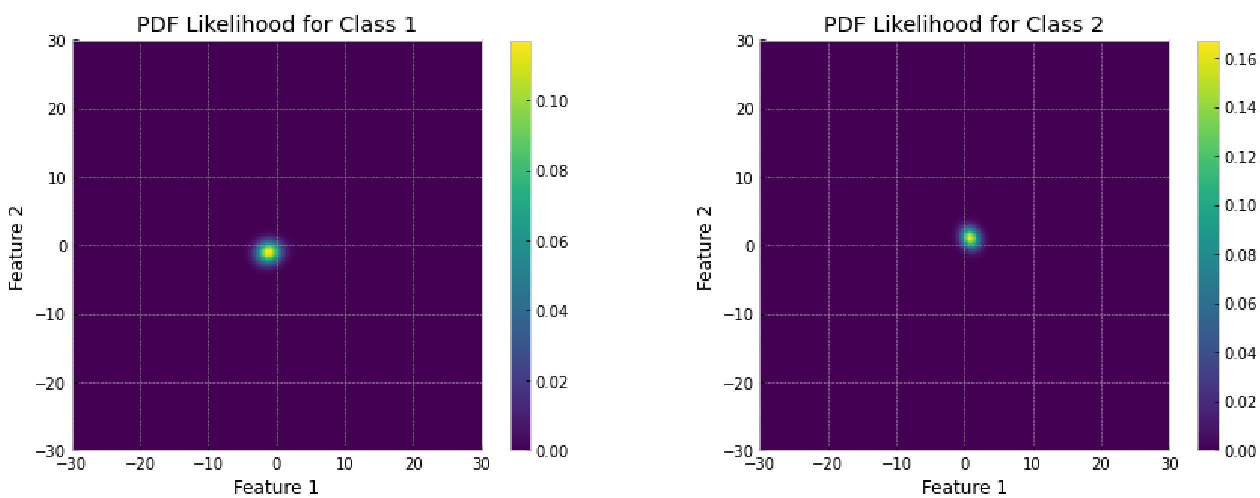
```
x = [2,4]

# Data Likelihoods
y1_newPoint = multivariate_normal.pdf(x, mean=mu1, cov=cov1) # p(x|C1)
y2_newPoint = multivariate_normal.pdf(x, mean=mu2, cov=cov2) # p(x|C2)

print('Data likelihoods:')
print('P(x|C1) = ', y1_newPoint)
print('P(x|C2) = ', y2_newPoint,'\n')

# Posterior Probabilities
y1_pos = y1_newPoint*pC1/(y1_newPoint*pC1 + y2_newPoint*pC2)
y2_pos = y2_newPoint*pC2/(y1_newPoint*pC1 + y2_newPoint*pC2)

print('Posterior probabilities:')
print('P(C1|x) = ', y1_pos)
print('P(C2|x) = ', y2_pos,'\n')

if y1_pos > y2_pos:
    print('x = ',x,' belongs to class 1')
else:
    print('x = ',x,' belongs to class 2')
```

```
Data likelihoods:
P(x|C1) =  8.676399018565161e-08
P(x|C2) =  0.000872588499860459

Posterior probabilities:
P(C1|x) =  4.971396988221305e-05
P(C2|x) =  0.9999502860301178

x =  [2, 4]  belongs to class 2
```

Let's expand the decision surface view:

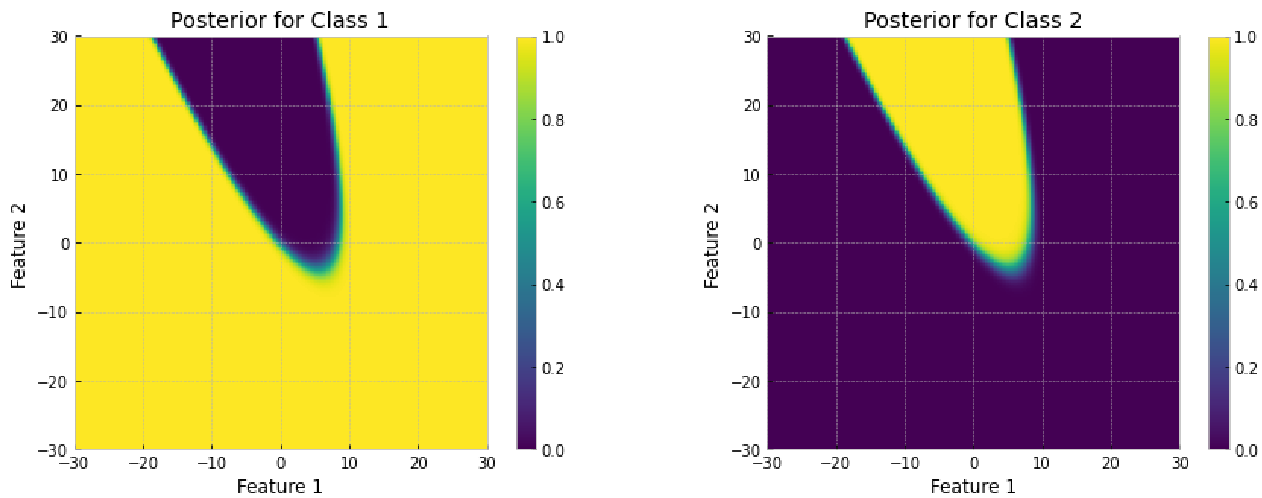
In [41]:

```python
nd=30

# Compute a grid of values for x and y
x = np.linspace(-nd, nd, 100)
y = np.linspace(-nd, nd, 100)
xm, ym = np.meshgrid(x, y)
X = np.flip(np.dstack([xm,ym]),axis=0)

# Let's plot the probabaility density function (pdf) for each class
y1 = multivariate_normal.pdf(X, mean=mu1, cov=cov1) # P(x|C1)
y2 = multivariate_normal.pdf(X, mean=mu2, cov=cov2) # P(x|C2)


fig =plt.figure(figsize=(15,5))
fig.add_subplot(1,2,1)
plt.imshow(y1, extent=[-nd,nd,-nd,nd])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('PDF Likelihood for Class 1')

fig.add_subplot(1,2,2)
plt.imshow(y2, extent=[-nd,nd,-nd,nd])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('PDF Likelihood for Class 2');
```



In [42]:

```python
# Let's take a look at the posterior distributions: they represent our classification d
pos1 = (y1*pC1)/(y1*pC1 + y2*pC2) # P(C1|x)
pos2 = (y2*pC2)/(y1*pC1 + y2*pC2) # P(C2|x)

fig =plt.figure(figsize=(15,5))
fig.add_subplot(1,2,1)
plt.imshow(pos1, extent=[-nd,nd,-nd,nd])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('Posterior for Class 1')

fig.add_subplot(1,2,2)
plt.imshow(pos2, extent=[-nd,nd,-nd,nd])
plt.colorbar()
plt.xlabel('Feature 1'); plt.ylabel('Feature 2')
plt.title('Posterior for Class 2');
```



- What about $x = [10, 10]$?

In [43]:

```
x = [10,10]

# Data Likelihoods
y1_newPoint = multivariate_normal.pdf(x, mean=mu1, cov=cov1) # p(x|C1)
y2_newPoint = multivariate_normal.pdf(x, mean=mu2, cov=cov2) # p(x|C2)

print('Data likelihoods:')
print('P(x|C1) = ', y1_newPoint)
print('P(x|C2) = ', y2_newPoint,'\n')

# Posterior Probabilities
y1_pos = y1_newPoint*pC1/(y1_newPoint*pC1 + y2_newPoint*pC2)
y2_pos = y2_newPoint*pC2/(y1_newPoint*pC1 + y2_newPoint*pC2)

print('Posterior probabilities:')
print('P(C1|x) = ', y1_pos)
print('P(C2|x) = ', y2_pos,'\n')

if y1_pos > y2_pos:
    print('x = ',x,' belongs to class 1')
else:
    print('x = ',x,' belongs to class 2')
```

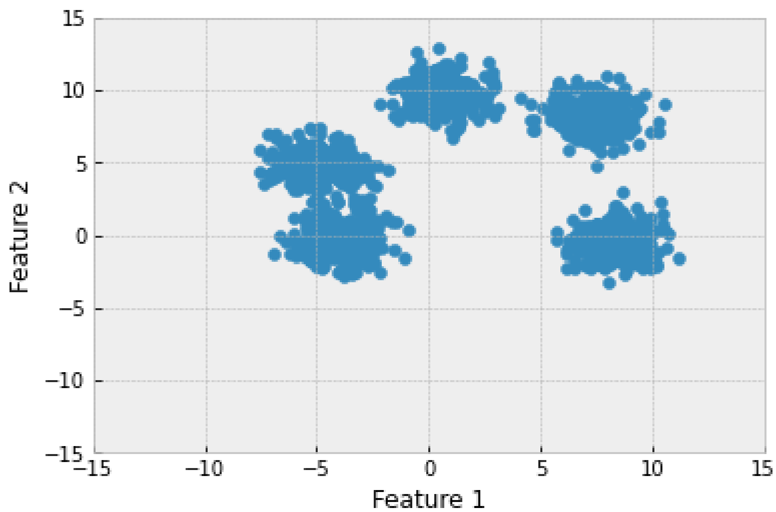
```
Data likelihoods:
P(x|C1) =  1.640177424643123e-41
P(x|C2) =  7.103322349039243e-45

Posterior probabilities:
P(C1|x) =  0.9991345844764138
P(C2|x) =  0.0008654155235862463

x =  [10, 10]  belongs to class 1
```

Mixture Models

In this example, we look at a relatively simple model where we model each class with a single Gaussian probability density function (pdf).

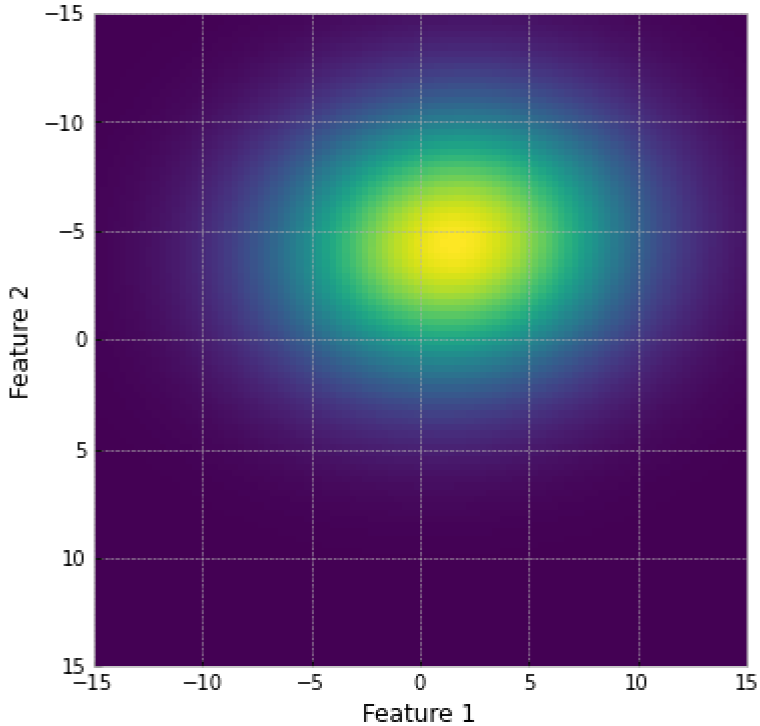
- What if the data for a single class looked like the plot below?

In [26]:
```
from sklearn.datasets import make_blobs

data, _ = make_blobs(n_samples = 1500, centers = 5)

plt.scatter(data[:,0],data[:,1]); plt.axis([-15,15,-15,15])
plt.xlabel('Feature 1'); plt.ylabel('Feature 2');
```



If we assume a single Gaussian distribution, we would obtain a very poor estimate of the true underlying data likelihood:

In [27]:
```
# Compute a grid of values for x and y
x = np.linspace(-15, 15, 100)
y = np.linspace(-15,15, 100)
xm, ym = np.meshgrid(x, y)
X = np.flip(np.dstack([xm,ym]),axis=0)

y1 = multivariate_normal.pdf(X, mean=np.mean(data, axis=0), cov=np.cov(data.T))

plt.figure(figsize=(6,6))
plt.imshow(y1, extent=[-15,15,15,-15])
plt.xlabel('Feature 1'); plt.ylabel('Feature 2');
```



Mixture Models

We can better represent this data with a **mixture model**:

$$p(x|\Theta) = \sum_{k=1}^{K} \pi_k P(x|\Theta_k)$$

where $\Theta = \{\Theta_k\}_{k=1}^{K}$ are set of parameters that define the distributional form in the probabilistic model $P(\bullet|\Theta_k)$ and

$$0 \leq \pi_k \leq 1 \tag{19}$$
$$\sum_k \pi_k = 1 \tag{20}$$

If the probabilistic model $P(\bullet|\Theta_k)$ is assumed to be a Gaussian distribution, then the above mixture model is a **Gaussian Mixture Model (GMM)**

$$P(x|\Theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$

where $\Theta_k = \{\mu_k, \Sigma_k, \pi_k\}, \forall k$ are the mean, covariance and weight of each Gaussian distribution, and, again, $0 \leq \pi_k \leq 1$ with $\sum_k \pi_k = 1$.