sheet01-submission

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We are not sure about the status of group registrations and therefore hand in solutions to Exercise sheet 1 individually. The handed-in pdf's for programming and math exercise sheets are identical for all six group members listed above.

1 Programming Sheet 1: Bayes Decision Theory (40 P)

In this exercise sheet, we will apply Bayes decision theory in the context of small two-dimensional problems. For this, we will make use of 3D plotting. We introduce below the basics for constructing these plots in Python/Matplotlib.

1.0.1 The function `numpy.meshgrid`

To plot two-dimensional functions, we first need to discretize the two-dimensional input space. One basic function for this purpose is `numpy.meshgrid`. The following code creates a discrete grid of the rectangular surface $[0, 4] \times [0, 3]$. The function `numpy.meshgrid` takes the discretized intervals as input, and returns two arrays of size corresponding to the discretized surface (i.e. the grid) and containing the X and Y-coordinates respectively.

[1]:
```
import numpy as np
X,Y = np.meshgrid([0,1,2,3,4],[0,1,2,3])
print(X)
print(Y)
```

```
[[0 1 2 3 4]
 [0 1 2 3 4]
 [0 1 2 3 4]
 [0 1 2 3 4]]
[[0 0 0 0 0]
 [1 1 1 1 1]
```

```
 [2 2 2 2 2]
 [3 3 3 3 3]]
```

Note that we can iterate over the elements of the grid by zipping the two arrays `X` and `Y` containing each coordinate. The function `numpy.flatten` converts the 2D arrays to one-dimensional arrays, that can then be iterated element-wise.

[2]:
```
print(list(zip(X.flatten(),Y.flatten())))
```

```
[(0, 0), (1, 0), (2, 0), (3, 0), (4, 0), (0, 1), (1, 1), (2, 1), (3, 1), (4, 1),
(0, 2), (1, 2), (2, 2), (3, 2), (4, 2), (0, 3), (1, 3), (2, 3), (3, 3), (4, 3)]
```

1.0.2 3D-Plotting

To enable 3D-plotting, we first need to load some modules in addition to `matplotlib`:

[3]:
```
import matplotlib
%matplotlib inline
from matplotlib import pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
```

As an example, we would like to plot the L2-norm function $f(x, y) = \sqrt{x^2 + y^2}$ on the subspace $x, y \in [-4, 4]$. First, we create a meshgrid with appropriate size:

[4]:
```
R = np.arange(-4,4+1e-9,0.1)
X,Y = np.meshgrid(R,R)
print(X.shape,Y.shape)
```

```
(81, 81) (81, 81)
```

Here, we have used a discretization with small increments of 0.1 in order to produce a plot with better resolution. The resulting meshgrid has size (81x81), that is, approximately 6400 points. The function f needs to be evaluated at each of these points. This is achieved by applying element-wise operations on the arrays of the meshgrid. The norm at each point of the grid is therefore computed as:

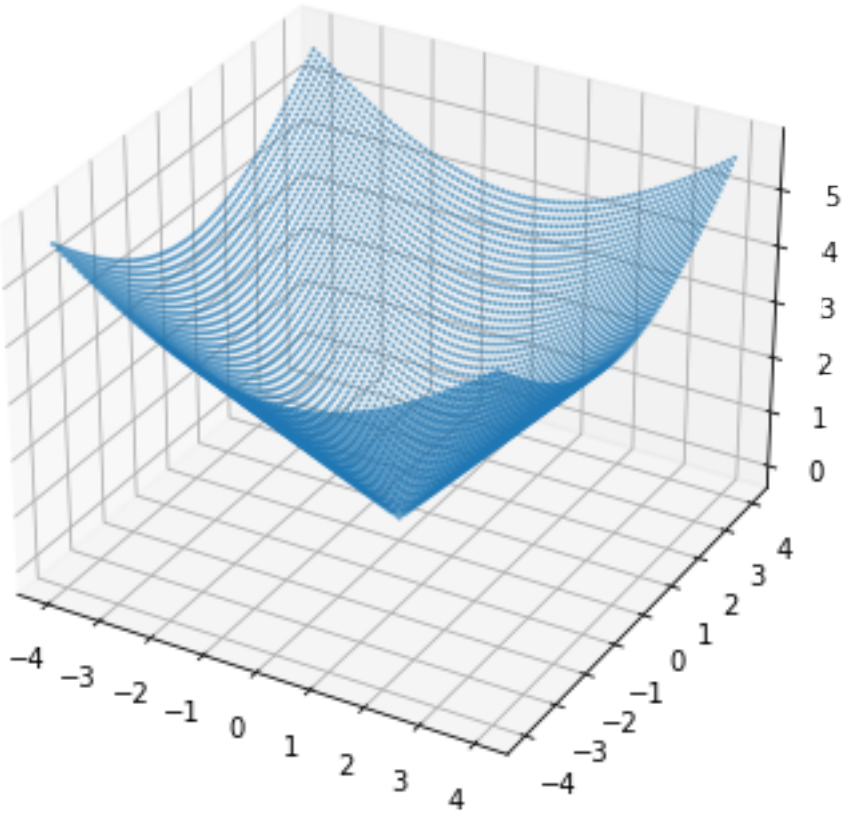
[5]:
```
F = (X**2+Y**2)**.5
print(F.shape)
```

```
(81, 81)
```

The resulting function values are of same size as the meshgrid. Taking `X,Y,F` jointly results in a list of approximately 6400 triplets representing the x-, y-, and z-coordinates in the three-dimensional space where the function should be plotted. The 3d-plot can now be constructed easily by means of the function `scatter` of `matplotlib.pyplot`.

[6]:
```
fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
ax.scatter(X,Y,F,s=1,alpha=0.5)
```

[6]:
```
<mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x116dac8e0>
```



The parameter `s` and `alpha` control the size and the transparency of each data point. Other 3d plotting variants exist (e.g. surface plots), however, the scatter plot is the simplest approach at least conceptually. Having introduced how to easily plot 3D functions in Python, we can now analyze two-dimensional probability distributions with this same tool.

1.1 Exercise 1: Gaussian distributions (5+5+5 P)

Using the technique introduced above, we would like to plot a normal Gaussian probability distribution with mean vector $\mu = (0, 0)$, and covariance matrix $\Sigma = I$ also known as standard normal distribution. We consider the same discretization as above (i.e. a grid from -4 to 4 using step size 0.1). For two-dimensional input spaces, the standard normal distribution is given by:

$$p(x, y) = \frac{1}{2\pi} e^{-0.5(x^2+y^2)}.$$

This distribution sums to 1 when integrated over $\mathbb{R}^2$. However, it does not sum to 1 when summing over the discretized space (i.e. the grid). Instead, we can work with a discretized Gaussian-like distribution:

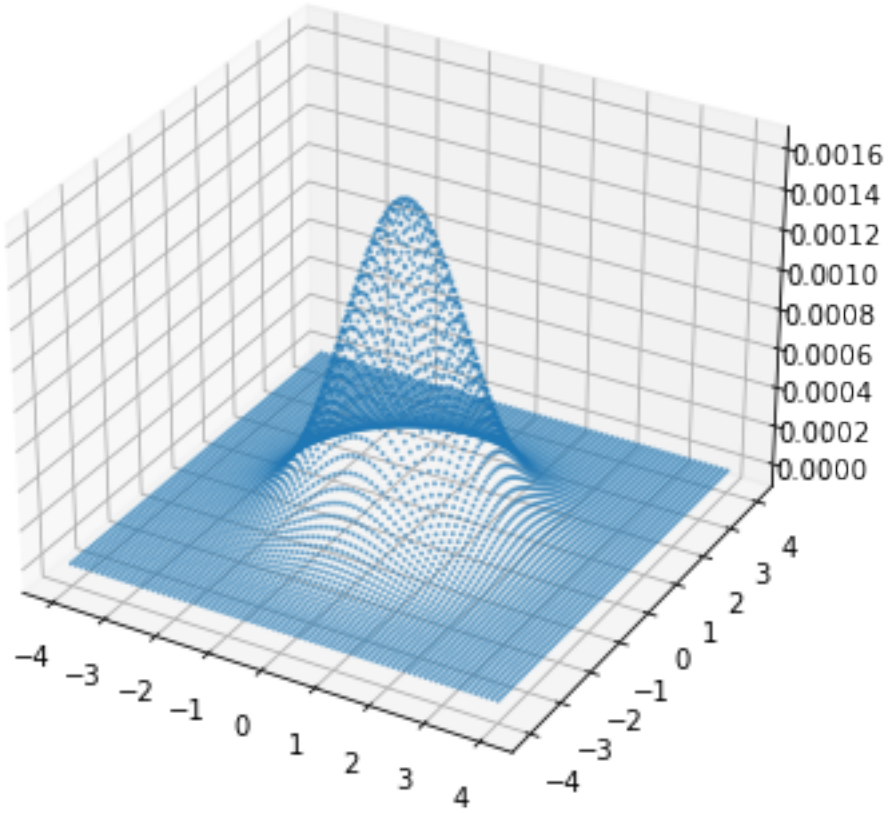
$$P(x, y) = \frac{1}{Z} e^{-0.5(x^2+y^2)} \qquad \text{with} \quad Z = \sum_{x,y} e^{-0.5(x^2+y^2)}$$

where the sum runs over the whole discretized space.

- **Compute the distribution $P(x, y)$, and plot it.**
- **Compute the conditional distribution $Q(x, y) = P((x, y)|\sqrt{x^2 + y^2} \geq 1)$, and plot it.**
- **Marginalize the conditioned distribution $Q(x, y)$ over y, and plot the resulting distribution $Q(x)$.**

[7]:
```
R = np.arange(-4,4+1e-9,0.1)
X,Y = np.meshgrid(R,R)

not_normalized_P = np.exp(-0.5*(X**2+Y**2))
P = not_normalized_P/np.sum(not_normalized_P)

fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
ax.scatter(X,Y,P,s=1,alpha=0.5)
```

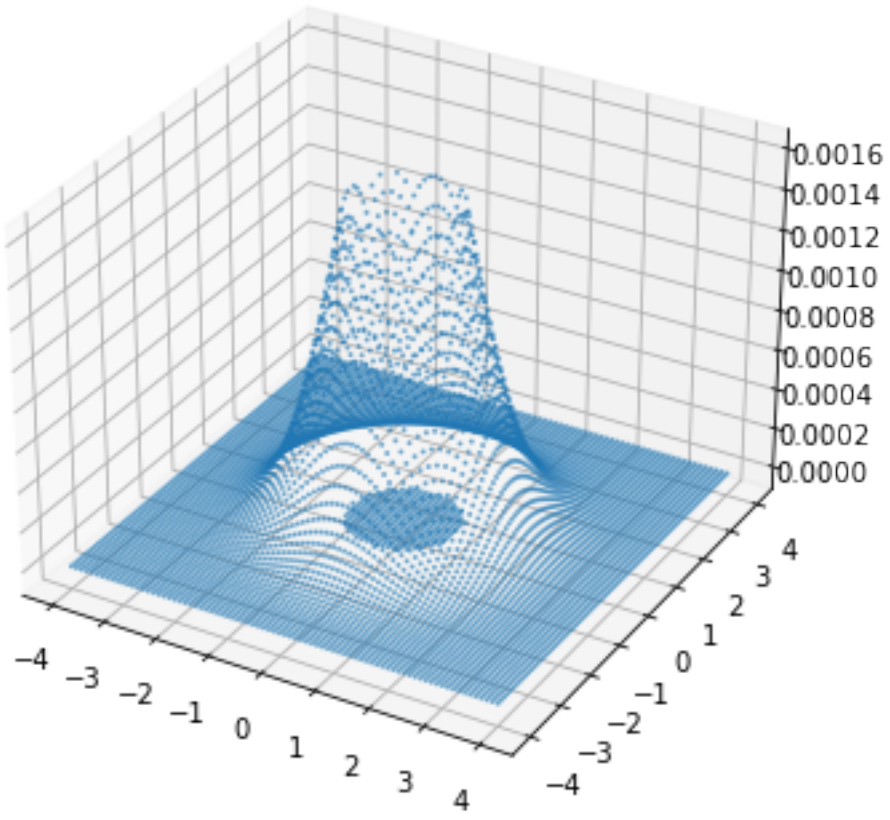
[7]:
```
<mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x116f95cd0>
```



[8]:
```
R = np.arange(-4,4+1e-9,0.1)
X,Y = np.meshgrid(R,R)
```

```
not_normalized_P = np.exp(-0.5*(X**2+Y**2))

check_condition = lambda x,y,p: ((x**2+y**2)**.5 >= 1) * p  # first part␣
↪produces boolean: false if x,y are not in unit circle. multiplying with p:␣
↪false blanks out probabilities that would be in unit circle
not_normalized_Q = check_condition(X,Y,not_normalized_P)

Q = not_normalized_Q/np.sum(not_normalized_Q)

fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
ax.scatter(X,Y,Q,s=1,alpha=0.5)
```

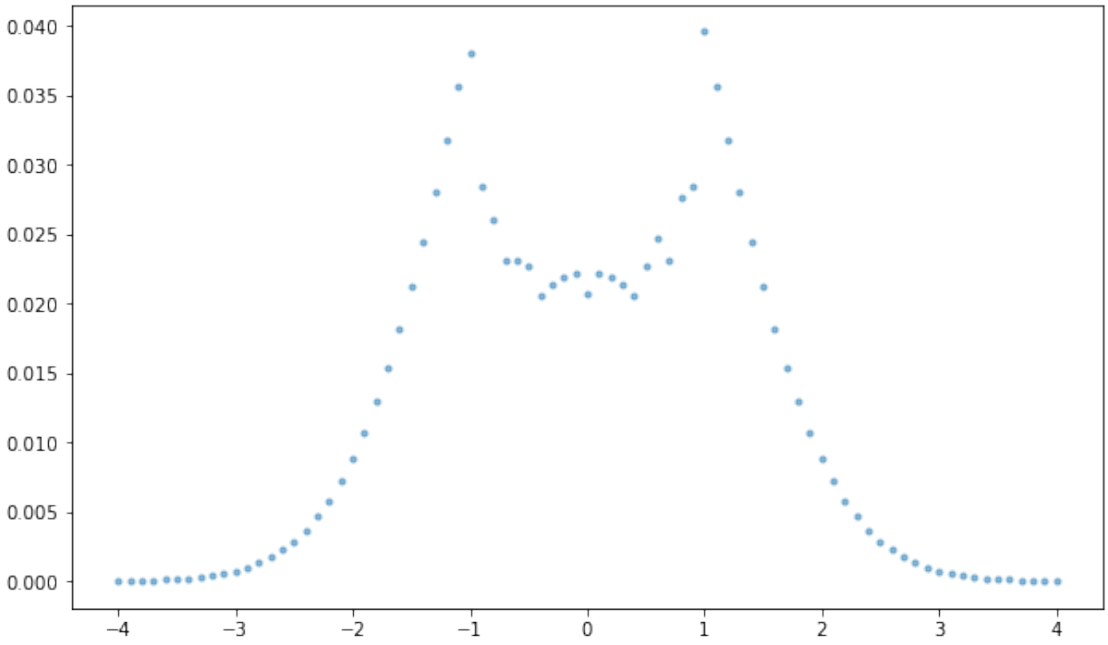
[8]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x1172b8a00>



[9]:
```
# ... extending upon last cell, run in order

Q_x = np.sum(Q, axis=0)
```

```
X_x = X[0]

fig = plt.figure(figsize=(10,6))
ax = plt.axes()
ax.scatter(X_x,Q_x,s=10,alpha=0.5)
```

[9]: <matplotlib.collections.PathCollection at 0x117505f10>



1.2 Exercise 2: Bayesian Classification (5+5+5 P)

Let the two coordinates x and y be now representated as a two-dimensional vector $\boldsymbol{x}$. We consider two classes ω_1 and ω_2 with data-generating Gaussian distributions $p(\boldsymbol{x}|\omega_1)$ and $p(\boldsymbol{x}|\omega_2)$ of mean vectors

$$\boldsymbol{\mu}_1 = (-0.5, -0.5) \quad \text{and} \quad \boldsymbol{\mu}_2 = (0.5, 0.5)$$

respectively, and same covariance matrix

$$\Sigma = \begin{pmatrix} 1.0 & 0 \\ 0 & 0.5 \end{pmatrix}.$$

Classes occur with probability $P(\omega_1) = 0.9$ and $P(\omega_2) = 0.1$. Analysis tells us that in such scenario, the optimal decision boundary between the two classes should be linear. We would like to verify this computationally by applying Bayes decision theory on grid-like discretized distributions.

- ** Using the same grid as in Exercise 1, discretize the two data-generating distributions $p(\boldsymbol{x}|\omega_1)$ and $p(\boldsymbol{x}|\omega_2)$ (i.e. create discrete distributions $P(\boldsymbol{x}|\omega_1)$ and $P(\boldsymbol{x}|\omega_2)$ on the grid), and plot them with different colors.**

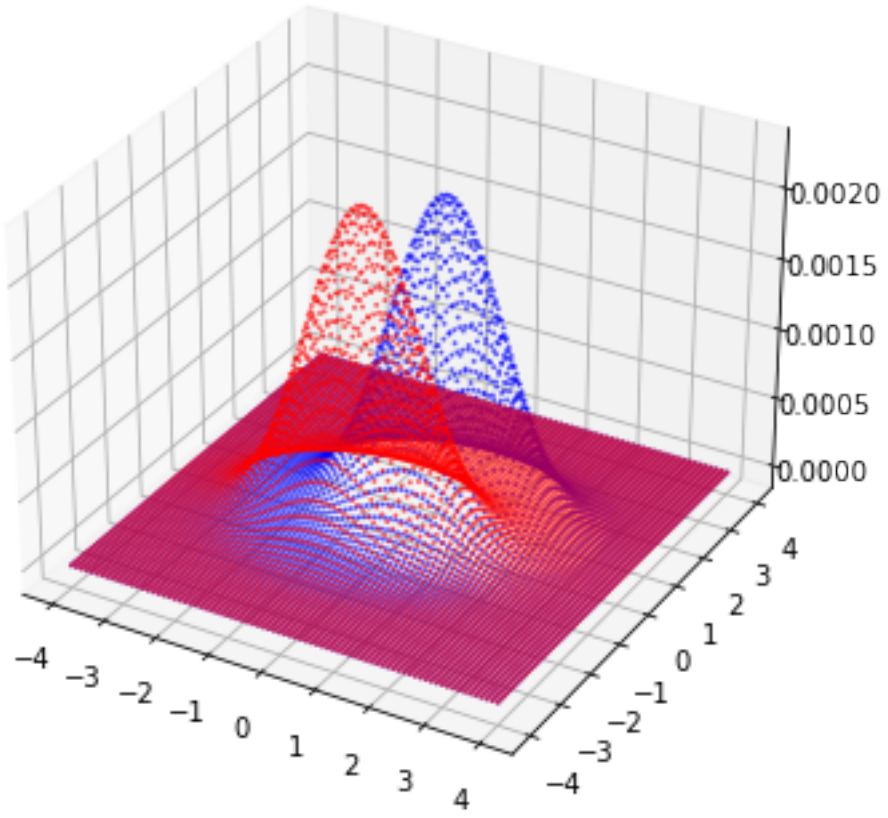
- **From these distributions, compute the total probability distribution $P(\boldsymbol{x}) = \sum_{c\in\{1,2\}} P(\boldsymbol{x}|\omega_c) \cdot P(\omega_c)$, and plot it.**
- **Compute and plot the class posterior probabilities $P(\omega_1|\boldsymbol{x})$ and $P(\omega_2|\boldsymbol{x})$, and print the Bayes error rate for the discretized case.**

[10]:
```
from scipy.stats import multivariate_normal

mu_1 = [-.5,-.5]
sig_1 = [[1.,0.],[0., .5]]
P_1 = .9

mu_2 = [.5,.5]
sig_2 = sig_1
P_2 = .1
```

Plotting $p(\boldsymbol{x}|\omega_1)$ (red) and $p(\boldsymbol{x}|\omega_2)$ (blue):

[11]:
```
X,Y = np.mgrid[-4:4+1e-9:.1, -4:4+1e-9:.1]
pos = np.dstack((X,Y))

var_1 = multivariate_normal(mean=mu_1, cov=sig_1)
P_x_w1 = var_1.pdf(pos) / 100

var_2 = multivariate_normal(mean=mu_2, cov=sig_2)
P_x_w2 = var_2.pdf(pos) / 100


fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
ax.scatter(X,Y,P_x_w1,s=1,alpha=0.5,c='r')
ax.scatter(X,Y,P_x_w2,s=1,alpha=0.5,c='b')
```

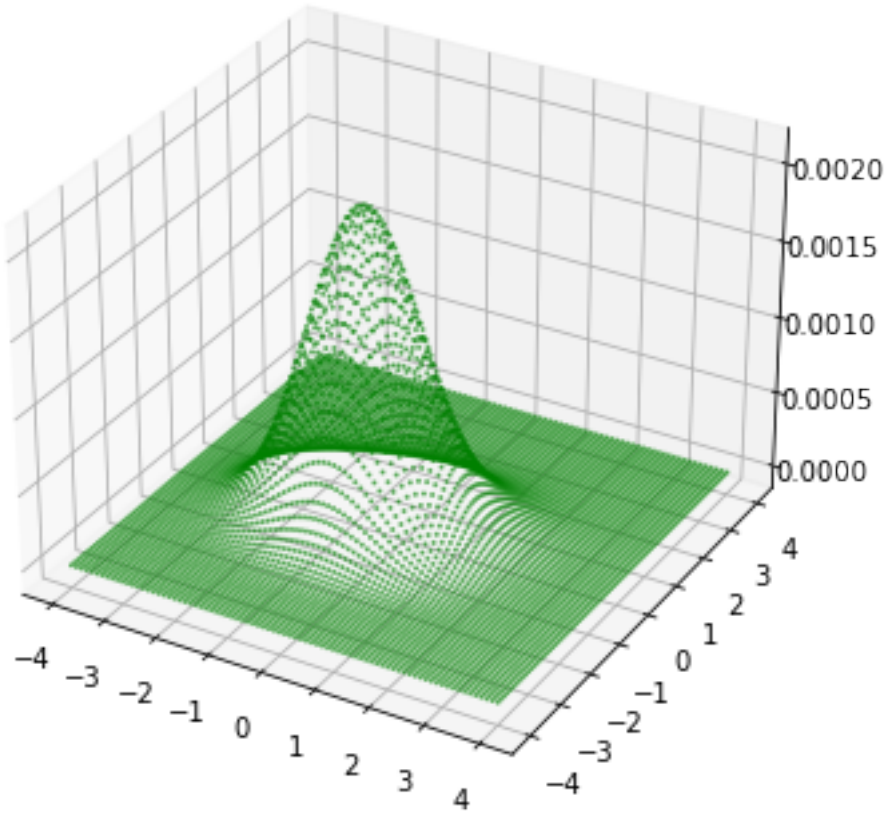
[11]:
```
<mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x119ae2580>
```



Plotting $P(\boldsymbol{x}) = \sum_{c \in \{1,2\}} P(\boldsymbol{x}|\omega_c) \cdot P(\omega_c)$:

[12]:
```
P_x = P_x_w1 * P_1 + P_x_w2 * P_2

fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
ax.scatter(X,Y,P_x,s=1,alpha=0.5,c='g')
```

[12]:
```
<mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x119d78f10>
```

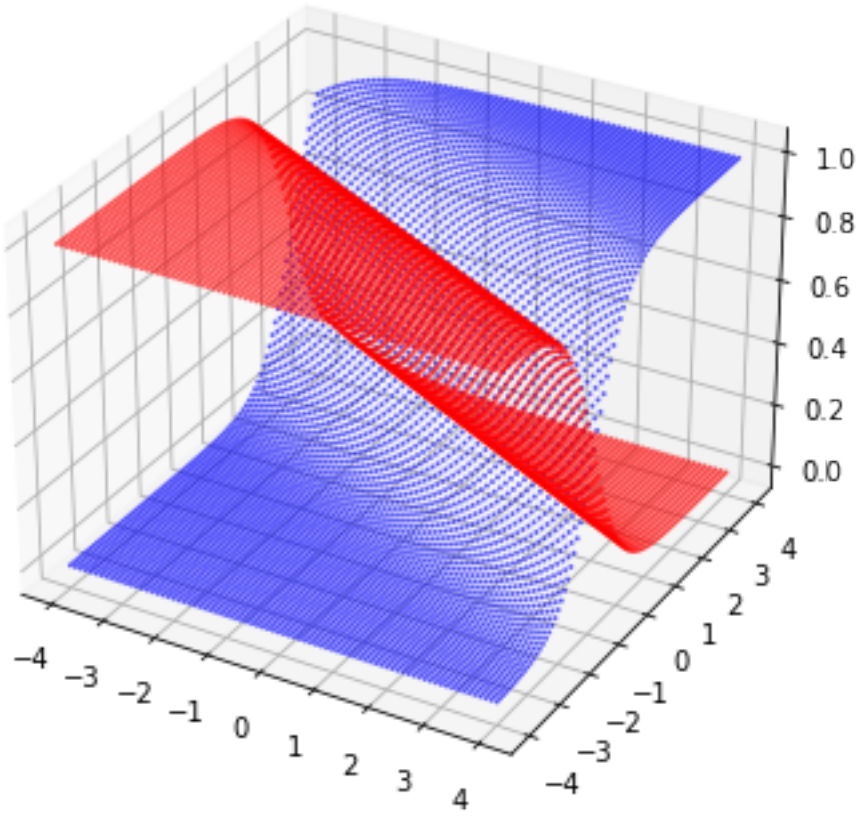


Plotting the class posterior probabilities $P(\omega_1|\boldsymbol{x})$ (red) and $P(\omega_2|\boldsymbol{x})$ (blue):

[13]:
```
P_w1_x = P_x_w1 * P_1 / P_x
P_w2_x = P_x_w2 * P_2 / P_x

bayes_error = np.sum(np.minimum(P_w1_x, P_w2_x) * P_x)
print('Bayes error rate:', bayes_error)

fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
ax.scatter(X,Y,P_w1_x,s=1,alpha=0.5,c='r')
ax.scatter(X,Y,P_w2_x,s=1,alpha=0.5,c='b')
```

```
Bayes error rate: 0.08040553760622296
```

[13]:
```
<mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x11a00e700>
```



Clearly displaying decision boundary:

[14]:
```
# class2ismorelikely = P_w1_x < P_w2_x

# fig = plt.figure(figsize=(10,6))
# ax = plt.axes(projection='3d')
# ax.scatter(X,Y,class2ismorelikely,s=1,alpha=0.5,c='g')
```

1.3 Exercise 3: Reducing the Variance (5+5 P)

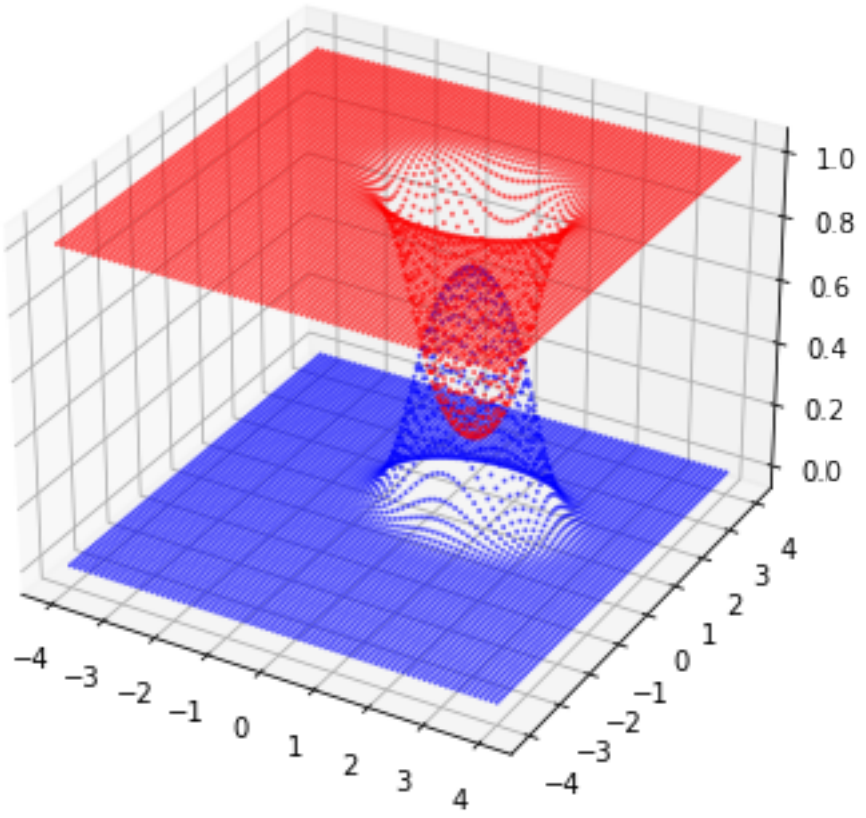
Suppose that the data generating distribution for the second class changes to produce samples much closer to the mean. This variance reduction for the second class is implemented by keeping the first covariance the same (i.e. $\Sigma_1 = \Sigma$) and dividing the second covariance matrix by 4 (i.e. $\Sigma_2 = \Sigma/4$). For this new set of parameters, we can perform the same analysis as in Exercise 2.

- **Plot the new class posterior probabilities $P(\omega_1|\boldsymbol{x})$ and $P(\omega_2|\boldsymbol{x})$ associated to the new covariance matrices, and print the new Bayes error rate.**

[15]:
```
mu_1 = [-.5,-.5]
sig_1 = np.array([[1.,0.],[0., .5]])
P_1 = .9

mu_2 = [.5,.5]
sig_2 = sig_1 / 4
P_2 = .1

X,Y = np.mgrid[-4:4+1e-9:.1, -4:4+1e-9:.1]
pos = np.dstack((X,Y))

var_1 = multivariate_normal(mean=mu_1, cov=sig_1)
P_x_w1 = var_1.pdf(pos) / 100

var_2 = multivariate_normal(mean=mu_2, cov=sig_2)
P_x_w2 = var_2.pdf(pos) / 100

P_x = P_x_w1 * P_1 + P_x_w2 * P_2

P_w1_x = P_x_w1 * P_1 / P_x
P_w2_x = P_x_w2 * P_2 / P_x

bayes_error = np.sum(np.minimum(P_w1_x, P_w2_x) * P_x)
print('Bayes error rate:', bayes_error)

fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
ax.scatter(X,Y,P_w1_x,s=1,alpha=0.5,c='r')
ax.scatter(X,Y,P_w2_x,s=1,alpha=0.5,c='b')
```

```
Bayes error rate: 0.07290160794820309
```

[15]:
```
<mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x11a408190>
```



Clearly displaying decision boundary:

[16]:
```
# class2ismorelikely = P_w1_x < P_w2_x

# fig = plt.figure(figsize=(10,6))
# ax = plt.axes(projection='3d')
# ax.scatter(X,Y,class2ismorelikely,s=1,alpha=0.5,c='g')
```

Intuition tells us that by variance reduction and resulting concentration of generated data for class 2 in a smaller region of the input space, it should be easier to predict class 2 with certainty at this location. Paradoxally, in this new "dense" setting, we observe that class 2 does not reach full certainty anywhere in the input space, whereas it did in the previous exercise.

- **Explain this paradox.**

The lower variance of our second distribution results in it being denser, but since this narrow center of density overlaps with the first distribution, the probability of a given point in that region being part of the first class is still considerably higher than in our previous example where our linear boundary (and wider variance) allowed for a higher probability when points were closer to either of the two means. In the previous example, the further we are from the mean of the first distribution,

the more likely we are dealing with our second class (and vice versa), in this case, with such a strong overlap of distributions, it makes sense that we do not have as much certainty anywhere as we did before. Another way of looking at this is that the first example has a linear relationship between certainty and distance from the mean, whereas our second example has a more complex (quadratic) relationship between class membership probability and distance from the means of our distributions.