Homework 1 - Henrique Gasparini Fiuza do Nascimento

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1 Master M2 MVA 2018/2019 - Graphical models - HWK 1

1.1 Page 1: mathematical formulas and computations

1.1.1 1. Learning in discrete graphical models

Consider the following model : z and x are discrete variables taking respectively M and K different values with $p(z = m) = \pi_m$ and $p(x = k|z = m) = \theta_{mk}$.

Compute the maximum likelihood estimator for π and θ based on an i.i.d. sample of observations. Please provide succinctly your derivations and not just the final answer.

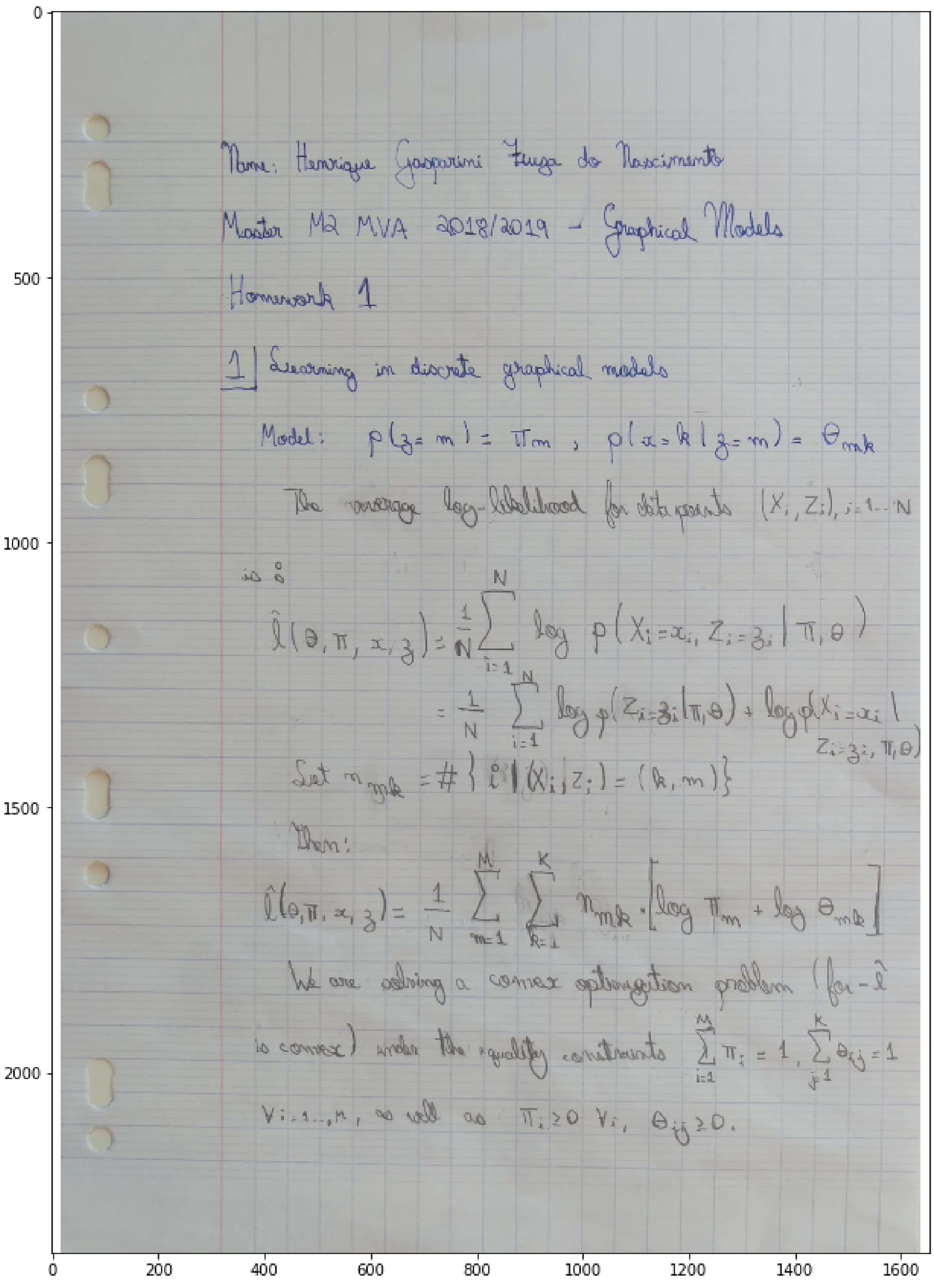
Answer: For variables (X_i, Z_i), $i = 1...N$, let n_{mk} be the number of occurences of $z = m$ and $x = k$. Then:

- $\hat{\pi_m} = \frac{1}{N} \times \sum_{k=1}^{K} n_{mk}$
- $\hat{\theta_{mk}} = \frac{n_{mk}}{\sum_{k=1}^{K} n_{mk}}$

Computations:

In [15]:

Out[15]: <matplotlib.image.AxesImage at 0x7f16f3ff9400>



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Master M2 MVA 2018/2019 – Graphical Models

Homework 1

1| Learning in discrete graphical models

Model: $p(z=m) = \pi_m$, $p(x=k \mid z=m) = \theta_{mk}$

The average log-likelihood for data points $(X_i, Z_i), i=1 \dots N$ is:

$$\hat{l}(\theta, \pi, x, z) = \frac{1}{N} \sum_{i=1}^{N} \log p(X_i = x_i, Z_i = z_i \mid \pi, \theta)$$

$$= \frac{1}{N} \sum_{i=1}^{N} \log p(Z_i = z_i \mid \pi, \theta) + \log p(X_i = x_i \mid Z_i = z_i, \pi, \theta)$$

Set $n_{mk} = \# \{ i \mid (X_i, Z_i) = (k, m) \}$

Then:

$$\hat{l}(\theta, \pi, x, z) = \frac{1}{N} \sum_{m=1}^{M} \sum_{k=1}^{K} n_{mk} \cdot \left[\log \pi_m + \log \theta_{mk} \right]$$

We are solving a convex optimization problem (for $-\hat{l}$ is convex) under the equality constraints $\sum_{i=1}^{M} \pi_i = 1$, $\sum_{j=1}^{K} \theta_{ij} = 1$ $\forall i = 1, \dots, M$, as well as $\pi_i \geq 0$ $\forall i$, $\theta_{ij} \geq 0$.

In [17]:

Out[17]: <matplotlib.image.AxesImage at 0x7f16f3f5e160>

Adding Lagrange constraints:

$$L(\theta, \pi, \lambda) = -\frac{1}{N} \sum_{m=1}^{M} \sum_{k=1}^{K} n_{mk} \left[\log \pi_m + \log \theta_{mk} \right]$$
$$+ \lambda_0 \left(1^T \pi - 1 \right) + \sum_{m=1}^{M} \lambda_m \left(1^T \theta_m - 1 \right)$$

Solving for each π_m individually,

$$\frac{\partial L}{\partial \pi_m} = - \frac{\sum_{k=1}^{K} n_{mk}}{N} \cdot \frac{1}{\hat{\pi}_m} + \lambda_0 = 0$$

$$\Rightarrow \hat{\pi}_m = \frac{1}{N} \sum_{k=1}^{K} n_{mk} \cdot \frac{1}{\lambda_0}$$

Since $\sum_{m=1}^{M} \hat{\pi}_m = 1$, we must have $\lambda_0 = 1$ and

$$\boxed{\hat{\pi}_m = \frac{1}{N} \sum_{k=1}^{K} n_{mk}}$$

Solving for each θ_{mk} individually,

$$\frac{\partial L}{\partial \theta_{mk}} = - \frac{n_{mk}}{N} \cdot \frac{1}{\hat{\theta}_{mk}} + \lambda_m = 0$$

$$\Rightarrow \hat{\theta}_{mk} = \frac{n_{mk}}{N} \cdot \frac{1}{\lambda_m}$$

Since $\sum_{k=1}^{K} \hat{\theta}_{mk} = 1$, we must have:

$$\frac{\sum_{k=1}^{K} n_{mk}}{N} = \lambda_m \Rightarrow \boxed{\hat{\theta}_{mk} = \frac{n_{mk}}{\sum_{k=1}^{K} n_{mk}}}$$

Observation: if for some m, $\sum_{k=1}^{K} n_{mk} = 0$, then $\lambda_m = 0$ and $\frac{\partial L}{\partial \theta_{mk}} = 0$ implies $\hat{\theta}_{mk} = +\infty \; \forall k = 1..K$, which is meaningless (and impossible since θ_{mk} must be smaller or equal to 1). Either way, if $Z = m$ is impossible, by logic $\pi(X = x \mid Z = m)$ is meaningless and does not need to be computed.

1.1.2 2. Linear classification

The files *classificationA.train*, *classificationB.train* and *classificationC.train* contain samples of data (x_n, y_n) where $x_n \in \mathbb{R}^2$ and $y_n \in 0, 1$ (each line of each file contains the 2 components of x_n then y_n.). The goal of this exercise is to implement linear classification methods and to test them on the three data sets. The choice of the programming language is yours (we however recommend Python, Matlab, Scilab, Octave, or R). The source code should be handed in along with results.

Do not forget to use the page formatting imposed in Section 3.

1. Generative model (LDA) Given the class variable, the data are assumed to be Gaussian with different means for different classes but with the same covariance matrix.

$y \sim Bernoulli(\pi), x|y = i \sim Normal(\mu_i, \Sigma)$

(a) Derive the form of the maximum likelihood estimator for this model. Indi- cation : the model was presented in class but not the MLE computations. Compare $p(y = 1|x)$ with the form of logistic regression.

Answer: We compute:

- $\hat{\pi} = \frac{n_1}{n_0 + n_1}$, where n_0 and n_1 are, respectively, the number of 0s and 1s in the training examples
- $\hat{\mu_1} = \frac{\sum\limits_{i=1|y_i=1} x_i}{n_1}$
- $\hat{\mu_0} = \frac{\sum\limits_{i=1|y_i=0} x_i}{n_0}$
- $\hat{\Sigma} = \frac{\sum\limits_{i=1|y_i=1} (x_i - \mu_1)(x_i - \mu_1)^T + \sum\limits_{i=1|y_i=0} (x_i - \mu_0)(x_i - \mu_0)^T}{N}$
- $\mathbb{P}(y = 1|x) = \frac{1}{1 + \frac{\pi}{1-\pi} \exp(-(\mu_1 - \mu_0)^T \Sigma^{-1} (x - \frac{\mu_1 + \mu_0}{2}))}$
- $\log(\frac{\mathbb{P}(y = 1|x)}{\mathbb{P}(y = 0|x)}) = \log(\frac{\pi}{1-\pi}) + (\mu_1 - \mu_0)^T \Sigma^{-1} (x - \frac{\mu_1 + \mu_0}{2})$

We can observe that, as in logistic regression, the log-ratio $\log(\frac{\mathbb{P}(y = 1|x)}{\mathbb{P}(y = 0|x)})$ also is linear on x.

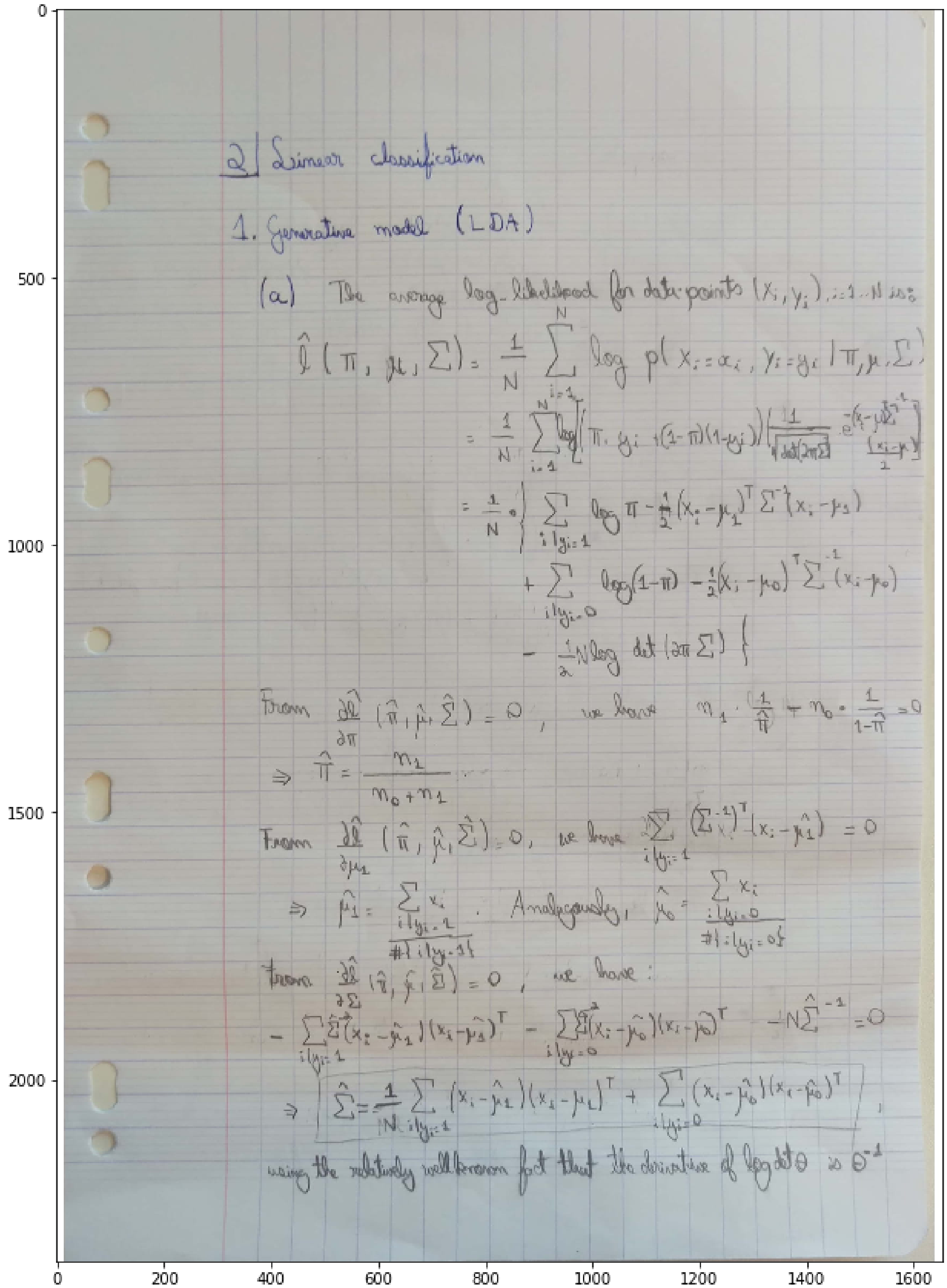
In LDA we allow the intercept (the b term) to be non zero. In logistic regression, to have that, one usually appends an always-1 column to x.

Another remark is that the coefficients for this linear function are obtained from maximizing different log-likelihoods in LDA and logistic regression, and therefore should have different values.

Computations:

In [18]:

Out[18]: <matplotlib.image.AxesImage at 0x7f16f3f38780>



2/ Linear classification

1. Generative model (LDA)

(a) The average log-likelihood for data points $(x_i, y_i)_{i=1..N}$ is:

$$\hat{\ell}(\pi, \mu, \Sigma) = \frac{1}{N} \sum_{i=1}^{N} \log p(X_i = x_i, Y_i = y_i \mid \pi, \mu, \Sigma)$$

$$= \frac{1}{N} \sum_{i=1}^{N} \log\left[(\pi \cdot y_i + (1-\pi)(1-y_i)) \frac{1}{\sqrt{\det(2\pi\Sigma)}} e^{-(x_i-\mu)^T \Sigma^{-1} \frac{(x_i-\mu)}{2}} \right]$$

$$= \frac{1}{N} \cdot \Big\{ \sum_{i|y_i=1} \log \pi - \frac{1}{2}(x_i - \mu_1)^T \Sigma^{-1}(x_i - \mu_1) + \sum_{i|y_i=0} \log(1-\pi) - \frac{1}{2}(x_i - \mu_0)^T \Sigma^{-1}(x_i - \mu_0) - \frac{1}{2} N \log \det(2\pi\Sigma) \Big\}$$

From $\frac{\partial \hat{\ell}}{\partial \pi}(\hat{\pi}, \hat{\mu}, \hat{\Sigma}) = 0$, we have $n_1 \cdot \frac{1}{\hat{\pi}} - n_0 \cdot \frac{1}{1-\hat{\pi}} = 0$

$$\Rightarrow \hat{\pi} = \frac{n_1}{n_0 + n_1}$$

From $\frac{\partial \hat{\ell}}{\partial \mu_1}(\hat{\pi}, \hat{\mu}_1, \hat{\Sigma}) = 0$, we have $\sum_{i|y_i=1} (\hat{\Sigma}^{-1})^T (x_i - \hat{\mu}_1) = 0$

$\Rightarrow \hat{\mu}_1 = \frac{\sum_{i|y_i=1} x_i}{\#\{i|y_i=1\}}$. Analogously, $\hat{\mu}_0 = \frac{\sum_{i|y_i=0} x_i}{\#\{i|y_i=0\}}$

From $\frac{\partial \hat{\ell}}{\partial \Sigma}(\hat{\pi}, \hat{\mu}, \hat{\Sigma}) = 0$, we have:

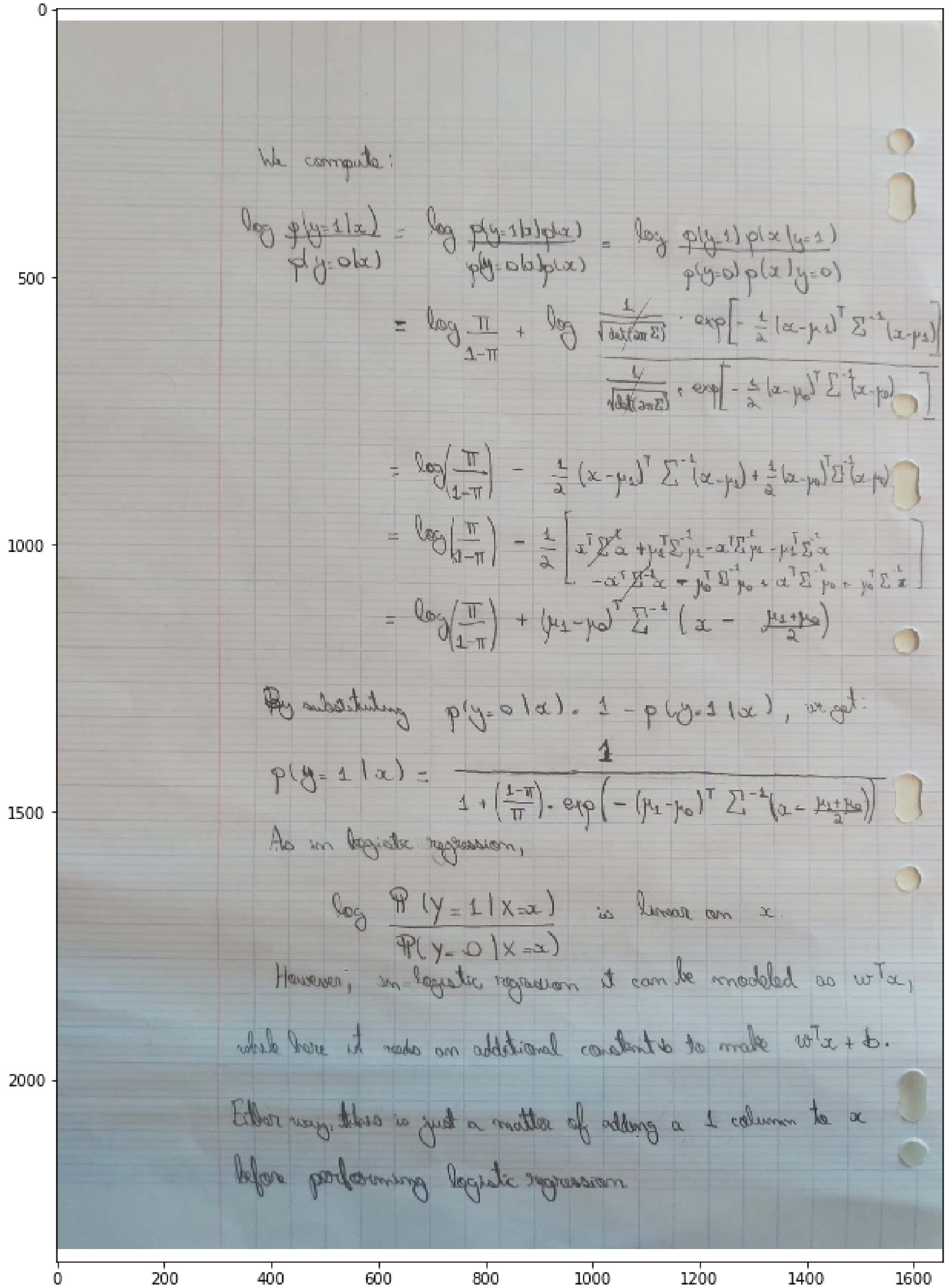
$$- \sum_{i|y_i=1} \hat{\Sigma}^{-2}(x_i - \hat{\mu}_1)(x_i - \hat{\mu}_1)^T - \sum_{i|y_i=0} \hat{\Sigma}^{-2}(x_i - \hat{\mu}_0)(x_i - \hat{\mu}_0)^T - N\hat{\Sigma}^{-1} = 0$$

$$\Rightarrow \boxed{\hat{\Sigma} = \frac{1}{N} \sum_{i|y_i=1} (x_i - \hat{\mu}_1)(x_i - \hat{\mu}_1)^T + \sum_{i|y_i=0} (x_i - \hat{\mu}_0)(x_i - \hat{\mu}_0)^T},$$

using the relatively well-known fact that the derivative of $\log \det \Theta$ is Θ^{-1}

In [19]:

Out[19]: <matplotlib.image.AxesImage at 0x7f16f3e93d68>



We compute:

$$\log \frac{p(y=1|x)}{p(y=0|x)} = \log \frac{p(y=1|x)p(x)}{p(y=0|x)p(x)} = \log \frac{p(y=1)\,p(x|y=1)}{p(y=0)\,p(x|y=0)}$$

$$= \log \frac{\pi}{1-\pi} + \log \frac{\cancel{\frac{1}{\sqrt{\det(2\pi\Sigma)}}} \cdot \exp\left[-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1}(x-\mu_1)\right]}{\cancel{\frac{1}{\sqrt{\det(2\pi\Sigma)}}} \cdot \exp\left[-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1}(x-\mu_0)\right]}$$

$$= \log\left(\frac{\pi}{1-\pi}\right) - \frac{1}{2}(x-\mu_1)^T \Sigma^{-1}(x-\mu_1) + \frac{1}{2}(x-\mu_0)^T \Sigma^{-1}(x-\mu_0)$$

$$= \log\left(\frac{\pi}{1-\pi}\right) - \frac{1}{2}\left[\cancel{x^T \Sigma^{-1} x} + \mu_1^T \Sigma^{-1} \mu_1 - x^T \Sigma^{-1} \mu_1 - \mu_1^T \Sigma^{-1} x - \cancel{x^T \Sigma^{-1} x} - \mu_0^T \Sigma^{-1} \mu_0 + x^T \Sigma^{-1} \mu_0 + \mu_0^T \Sigma^{-1} x\right]$$

$$= \log\left(\frac{\pi}{1-\pi}\right) + (\mu_1-\mu_0)^T \Sigma^{-1}\left(x - \frac{\mu_1+\mu_0}{2}\right)$$

By substituting $p(y=0|x) = 1 - p(y=1|x)$, we get:

$$p(y=1|x) = \frac{1}{1 + \left(\frac{1-\pi}{\pi}\right) \cdot \exp\left(-(\mu_1-\mu_0)^T \Sigma^{-1}\left(x - \frac{\mu_1+\mu_0}{2}\right)\right)}$$

As in logistic regression,

$$\log \frac{\mathbb{P}(Y=1|X=x)}{\mathbb{P}(Y=0|X=x)} \text{ is linear in } x.$$

However, in logistic regression it can be modeled as $w^T x$, while here it needs an additional constant to make $w^T x + b$.

Either way, this is just a matter of adding a 1 column to x before performing logistic regression.

5. QDA model We finally relax the assumption that the covariance matrices for the two classes are the same. So, given the class label the data are assumed to be Gaussian with means and covariance matrices which are a priori different.

$y \sim Bernoulli(\pi), x \mid y = iNormal(\mu_i, \Sigma_i)$.

Implement the maximum likelihood estimator and apply it to the data.

(a) Derive the form of the maximum likelihood estimator for this model.

Answer: We compute:

- $\hat{\pi} = \dfrac{n_1}{n_0 + n_1}$, where n_0 and n_1 are, respectively, the number of 0s and 1s in the training examples
- $\hat{\mu_1} = \dfrac{\sum\limits_{i=1|y_i=1} x_i}{n_1}$
- $\hat{\mu_0} = \dfrac{\sum\limits_{i=1|y_i=0} x_i}{n_0}$
- $\hat{\Sigma_1} = \dfrac{\sum\limits_{i=1|y_i=1} (x_i - \mu_1)(x_i - \mu_1)^T}{n_1}$
- $\hat{\Sigma_0} = \dfrac{\sum\limits_{i=1|y_i=0} (x_i - \mu_0)(x_i - \mu_0)^T}{n_0}$

Computations:

In [20]:

Out[20]: <matplotlib.image.AxesImage at 0x7f16f3e79400>

5. QDA model

(a) The average log-likelihood for data points (x_i, y_i), $i=1..N$ is:

$$\hat{\ell}(\pi, \mu, \Sigma) = \frac{1}{N} \sum_{i=1}^{N} \log p(X_i = x_i, Y_i = y_i \mid \pi, \mu, \Sigma)$$

$$= \frac{1}{N} \sum_{i=1}^{N} \log p(y_i = y_i \mid \pi) + \log p(X = x_i \mid Y_i = y_i, \mu, \Sigma)$$

$$= \frac{1}{N} \Big\{ \sum_{i \mid y_i = 1} \log \pi - \frac{1}{2}(x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1) - \frac{1}{2} \log \det(2\pi \Sigma_1)$$

$$+ \sum_{i \mid y_i = 0} \log(1-\pi) - \frac{1}{2}(x_i - \mu_0) \Sigma_0^{-1} (x_i - \mu_0) - \frac{1}{2} \log \det(2\pi \Sigma_0) \Big\}$$

From $\frac{\partial \hat{\ell}}{\partial \pi}(\hat{\pi}, \hat{\mu}, \hat{\Sigma}) = 0$, we have $n_1 \frac{1}{\hat{\pi}} - n_0 \frac{1}{1-\hat{\pi}} = 0$

$$\Rightarrow \hat{\pi} = \frac{n_1}{n_0 + n_1}$$

From $\frac{\partial \hat{\ell}}{\partial \mu_1}(\hat{\pi}, \hat{\mu}, \hat{\Sigma}) = 0$, we have $\sum_{i \mid y_i = 1} (\hat{\Sigma}^{-1})^T (x_i - \hat{\mu}_1) = 0$

$\Rightarrow \hat{\mu}_1 = \frac{\sum_{i \mid y_i = 1} x_i}{n_1}$. Analogously $\hat{\mu}_0 = \frac{\sum_{i \mid y_i = 0} x_i}{n_0}$

From $\frac{\partial \hat{\ell}}{\partial \Sigma_1}(\hat{\pi}, \hat{\mu}, \hat{\Sigma}) = 0$, we have:

$$-\sum_{i \mid y_i = 1} (\hat{\Sigma}_1^{-1})^2 (x_i - \hat{\mu}_1)(x_i - \mu_1)^T - n_1 \hat{\Sigma}_1^{-1} = 0$$

$$\Rightarrow \hat{\Sigma}_1 = \frac{1}{n_1} \sum_{i \mid y_i = 1} (x_i - \hat{\mu}_1)(x_i - \hat{\mu}_1)^T$$

Analogously, $\hat{\Sigma}_0 = \frac{1}{n_0} \sum_{i \mid y_i = 0} (x_i - \hat{\mu}_0)(x_i - \hat{\mu}_0)^T$

1.2 Page 2: dataset A

1.2.1 Imports

```
In [332]: import pandas as pd
          import numpy as np
          from scipy.stats import multivariate_normal
          import matplotlib.pyplot as plt
          from sklearn.metrics import accuracy_score
```

1.2.2 Reading the dataset

```
In [321]: dataset_name = 'A'
```

```
In [322]: def read(dataset_name):
              train_path, test_path = ['data/' + filename for filename in ['classification{}.tra
              train_df = pd.read_csv(train_path, delimiter='\t', header=None)
              train_df.columns = ['x1', 'x2', 'y']
              test_df = pd.read_csv(test_path, delimiter='\t', header=None)
              test_df.columns = ['x1', 'x2', 'y']
              return train_df, test_df
```

```
In [323]: train_df, test_df = read(dataset_name)
```

```
In [324]: def points_from_df(df):
              x1s, x2s, ys = df['x1'].values, df['x2'].values, df['y'].values
              return [np.array([x1, x2]) for x1, x2 in zip(x1s, x2s)], ys
```

```
In [325]: X_train, Y_train = points_from_df(train_df)
          X_test, Y_test = points_from_df(test_df)
```

1.2.3 LDA

```
In [227]: class LDAClassifier:
              # Model estimation with MLE
              def fit(self, X, Y):
                  n0, n1 = len([y for y in Y if y == 0.0]), len([y for y in Y if y == 1.0])
                  assert n0 + n1 == Y.shape[0]
                  self.pi = n1 / (n0 + n1)
                  print('Estimated pi = {}'.format(self.pi))

                  self.mu0 = sum([x for x, y in zip(X, Y) if y == 0.0]) / n0
                  print('Estimated mu_0 = {}'.format(self.mu0))
                  self.mu1 = sum([x for x, y in zip(X, Y) if y == 1.0]) / n1
                  print('Estimated mu_1 = {}'.format(self.mu1))

                  self.sigma = np.matrix(1/len(Y) * (sum([(x - self.mu0) * np.atleast_2d(x - sel
                  print('Estimated Sigma = {}'.format(self.sigma))
                  return self
```

```
    def predict_single(self, x):
        log_ratio = np.log(self.pi) - np.log(1 - self.pi) + ((self.mu1 - self.mu0) * n
        return float(int(log_ratio > 0.))

    def predict(self, X):
        return np.array([self.predict_single(x) for x in X])
```

In [228]:
```
clf = LDAClassifier().fit(X_train, Y_train)
```

```
Estimated pi = 0.3333333333333333
Estimated mu_0 = [ 2.89970947 -0.893874  ]
Estimated mu_1 = [-2.69232004  0.866042  ]
Estimated Sigma = [[ 2.44190897 -1.13194024]
 [-1.13194024  0.61375465]]
```

Predict

In [229]:
```
Y_train_pred = clf.predict(X_train)
```

In [230]:
```
Y_pred = clf.predict(X_test)
```

In [231]:
```
print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.9866666666666667
```

In [232]:
```
print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

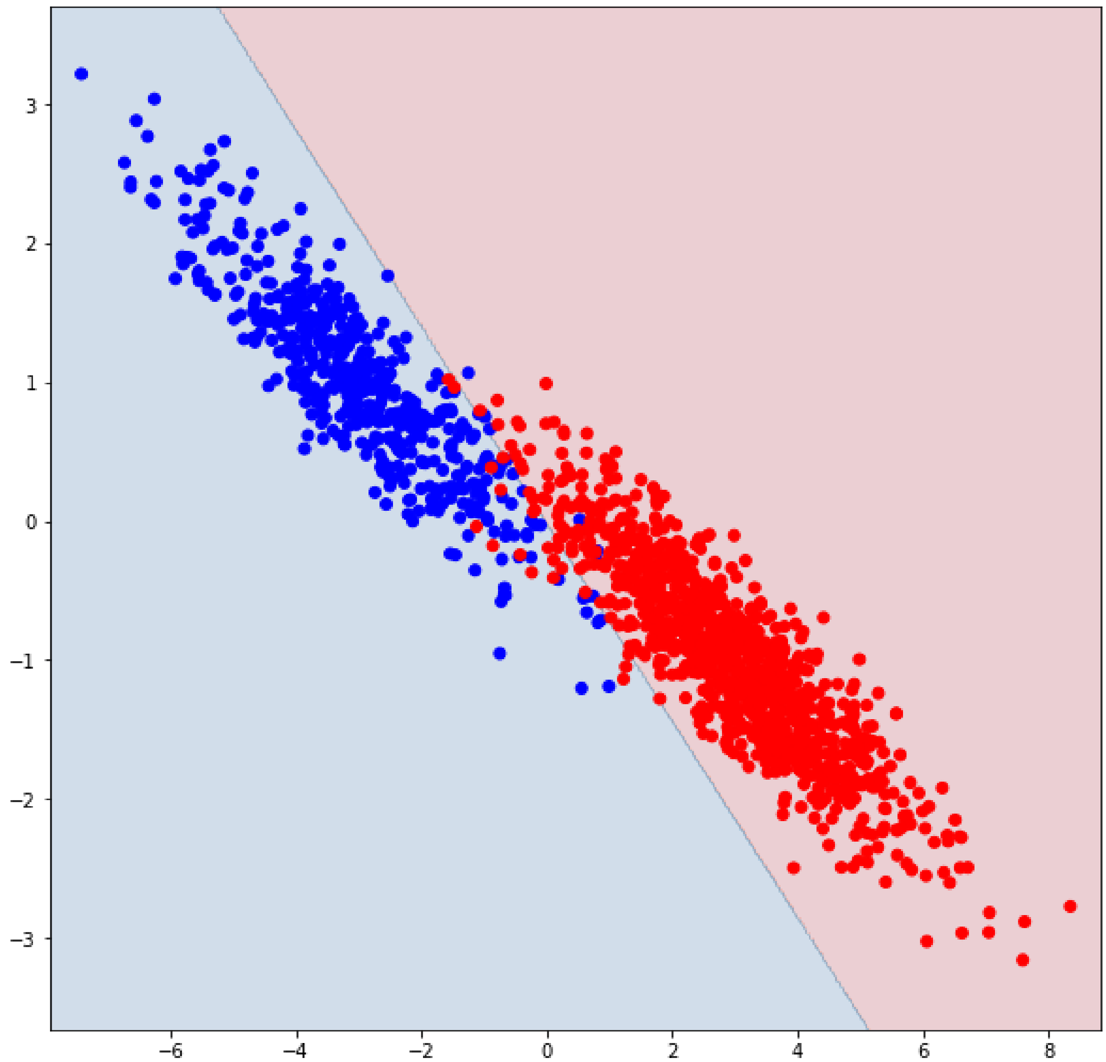
```
Accuracy on test set: 0.98
```

Plot

In [233]:
```
h = .02  # step size in the mesh

x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
```

In [234]:
```
plt.figure(figsize=(10, 10))

cm = plt.cm.RdBu

Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)
```

```
colors = ['b' if y == 1. else 'r' for y in Y_test]
plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

plt.show()
```



1.2.4 Logistic regression

```
In [312]: def sigmoid(z):
              return 1 / (1 + np.exp(-z))


          class LogisticClassifier:
              def compute_hessian(self, w, X, Y):
                  N = sigmoid(w.T * X)
```

```
            D = np.diag(np.multiply(N, 1. - N).tolist()[0])
            return - X * D * X.T

        def update(self, w, X, Y):
            N = sigmoid(w.T * X)
            D = np.diag(np.multiply(N, 1. - N).tolist()[0])
            hessian = - X * D * X.T
            return w + np.linalg.inv(hessian) * X * (Y - N.T)

        # Model estimation with IRSL in the update method
        def fit(self, X, Y):
            augmented_X = [np.concatenate([x, [1.]]) for x in X_train]
            w = np.matrix(np.zeros((3, 1)))
            input_X, input_Y = np.matrix(augmented_X).T, np.matrix(Y).T
            hessian = self.compute_hessian(w, input_X, input_Y)
            cnt = 0
            while np.abs(np.linalg.det(hessian)) > 10**-7 and cnt < 100:
                w = self.update(w, input_X, input_Y)
                hessian = self.compute_hessian(w, input_X, input_Y)
                cnt += 1
            self.w = w
            return self

        def predict_single(self, x):
            return float(int(np.dot(self.w.T, np.concatenate([x, [1.]])) < 0))

        def predict(self, X):
            return np.array([self.predict_single(x) for x in X])
```

```
In [313]: clf = LogisticClassifier().fit(X_train, Y_train)
```

```
/home/hfiuza/Programs/virtualenv/ds/lib/python3.6/site-packages/ipykernel_launcher.py:2: Runtime
```

Predict

```
In [314]: Y_train_pred = clf.predict(X_train)
```

```
In [315]: Y_pred = clf.predict(X_test)
```

```
In [316]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.9933333333333333
```

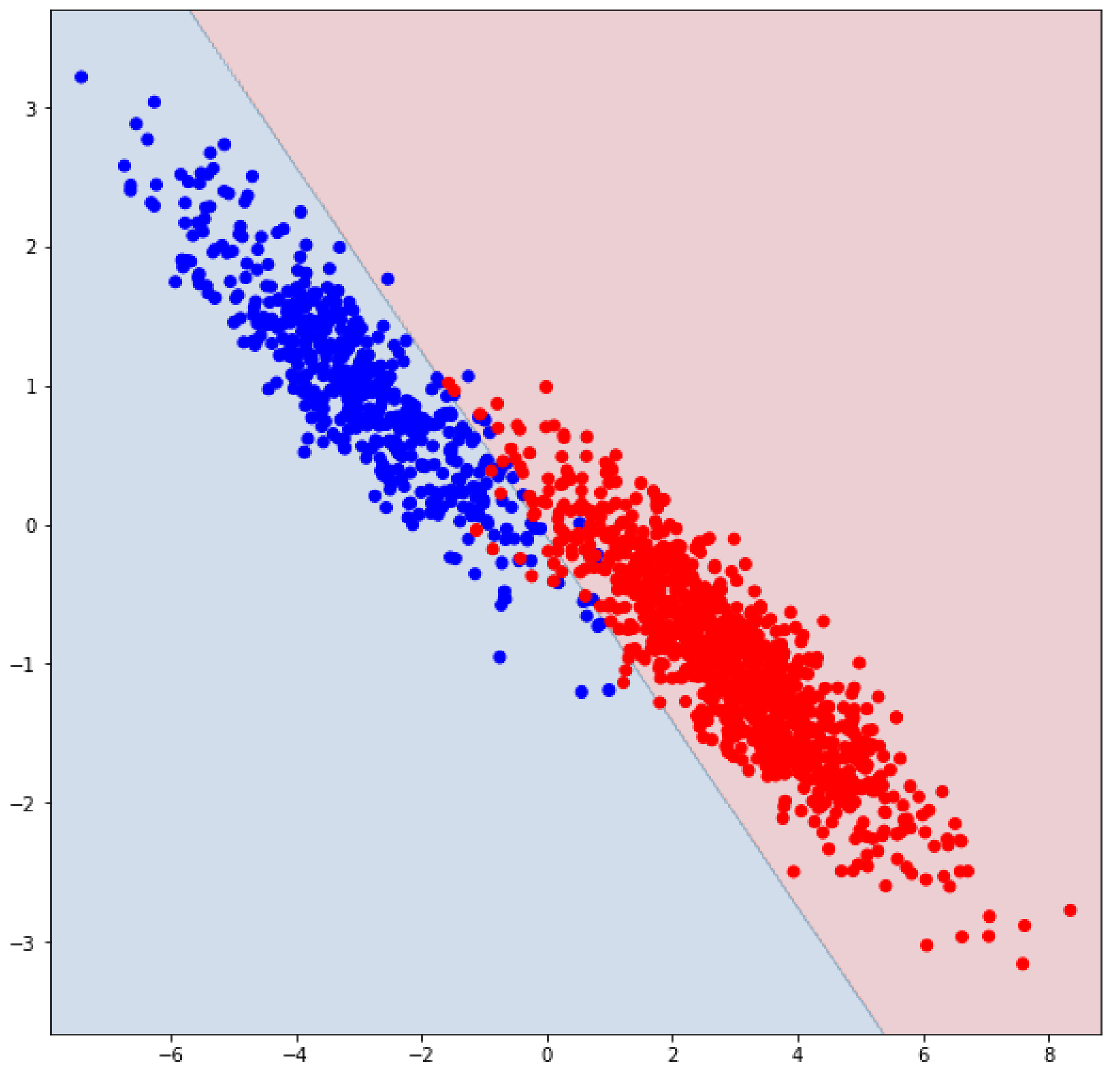
```
In [317]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9806666666666667
```

Plot

```
In [318]: h = .02  # step size in the mesh

          x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
          y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
          xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                               np.arange(y_min, y_max, h))
```

```
In [319]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

          colors = ['b' if y == 1. else 'r' for y in Y_test]
          plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

          plt.show()
```



1.2.5 Linear regression

```
In [326]: class LinearClassifier:

              def mle_w(self, X, Y):
                  return np.linalg.inv(X.T * X) * X.T * Y

              def fit(self, X, Y):
                  augmented_X = [np.concatenate([x, [1.]]) for x in X_train]
                  input_X, input_Y = np.matrix(augmented_X), np.matrix(Y).T

                  self.w = self.mle_w(input_X, input_Y)
                  return self
```

```
    def predict_single(self, x):
        return float(int(np.dot(self.w.T, np.concatenate([x, [1.]])) > 0.5))

    def predict(self, X):
        return np.array([self.predict_single(x) for x in X])
```

```
In [327]: clf = LinearClassifier().fit(X_train, Y_train)
```

Predict

```
In [328]: Y_train_pred = clf.predict(X_train)
```

```
In [329]: Y_pred = clf.predict(X_test)
```

```
In [330]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.9866666666666667
```

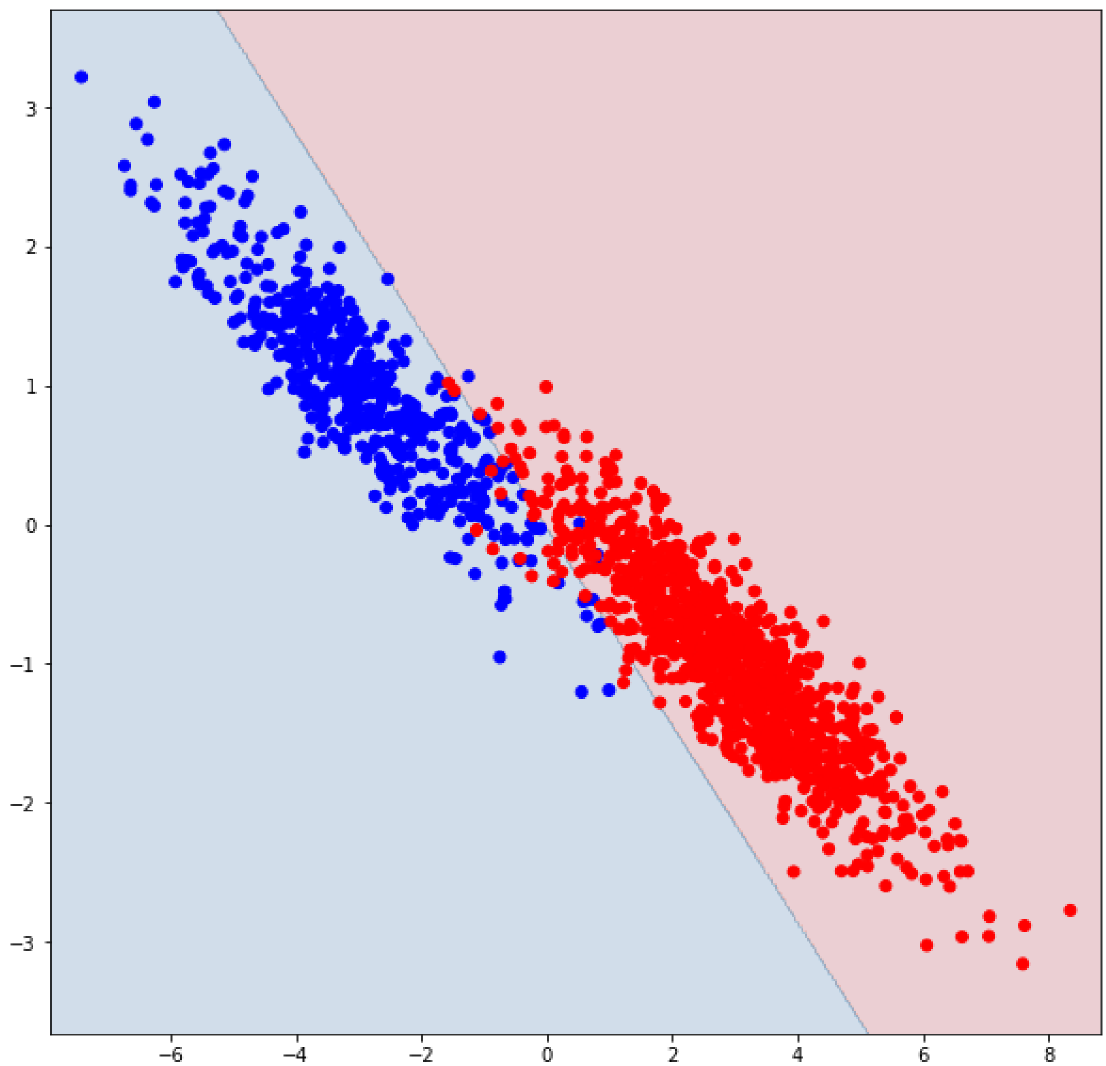
```
In [331]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9793333333333333
```

Plot

```
In [249]: h = .02  # step size in the mesh

          x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
          y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
          xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                               np.arange(y_min, y_max, h))
```

```
In [250]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

          colors = ['b' if y == 1. else 'r' for y in Y_test]
          plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

          plt.show()
```



1.2.6 Results summary up to now

```
In [251]: lda_train_accuracy, lda_test_accuracy = 0.9866666666666667, 0.98
          logistic_train_accuracy, logistic_test_accuracy = 0.9933333333333333, 0.9806666666666
          linear_train_accuracy, linear_test_accuracy = 0.9866666666666667, 0.9793333333333333
```

Comment: the Logistic model gives a slightly better accuracy score in the the test set, but it should not be relevant. The three models give very good results, close to 98% accuracy.

1.2.7 QDA

```
In [333]: class QDAClassifier:
              # Model estimation with MLE
              def fit(self, X, Y):
```

```
            n0, n1 = len([y for y in Y if y == 0.0]), len([y for y in Y if y == 1.0])
            assert n0 + n1 == Y.shape[0]
            self.pi = n1 / (n0 + n1)
            print('Estimated pi = {}'.format(self.pi))

            self.mu0 = sum([x for x, y in zip(X, Y) if y == 0.0]) / n0
            print('Estimated mu_0 = {}'.format(self.mu0))
            self.mu1 = sum([x for x, y in zip(X, Y) if y == 1.0]) / n1
            print('Estimated mu_1 = {}'.format(self.mu1))

            self.sigma0 = np.matrix(1/n0 * sum([(x - self.mu0) * np.atleast_2d(x - self.mu
            print('Estimated Sigma_0 = {}'.format(self.sigma0))
            self.sigma1 = np.matrix(1/n1 * sum([(x - self.mu1) * np.atleast_2d(x - self.mu
            print('Estimated Sigma_1 = {}'.format(self.sigma1))

            self.var0 = multivariate_normal(mean=self.mu0, cov=self.sigma0)
            self.var1 = multivariate_normal(mean=self.mu1, cov=self.sigma1)
            return self

        def predict_single(self, x):
            return float(int(self.var1.pdf(x) > self.var0.pdf(x)))

        def predict(self, X):
            return np.array([self.predict_single(x) for x in X])
```

```
In [335]: clf = QDAClassifier().fit(X_train, Y_train)
```

```
Estimated pi = 0.3333333333333333
Estimated mu_0 = [ 2.89970947 -0.893874  ]
Estimated mu_1 = [-2.69232004  0.866042  ]
Estimated Sigma_0 = [[ 2.31065259 -1.04748461]
 [-1.04748461  0.57578403]]
Estimated Sigma_1 = [[ 2.70442172 -1.3008515 ]
 [-1.3008515   0.68969588]]
```

Predict

```
In [336]: Y_train_pred = clf.predict(X_train)
```

```
In [337]: Y_pred = clf.predict(X_test)
```

```
In [338]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.9866666666666667
```

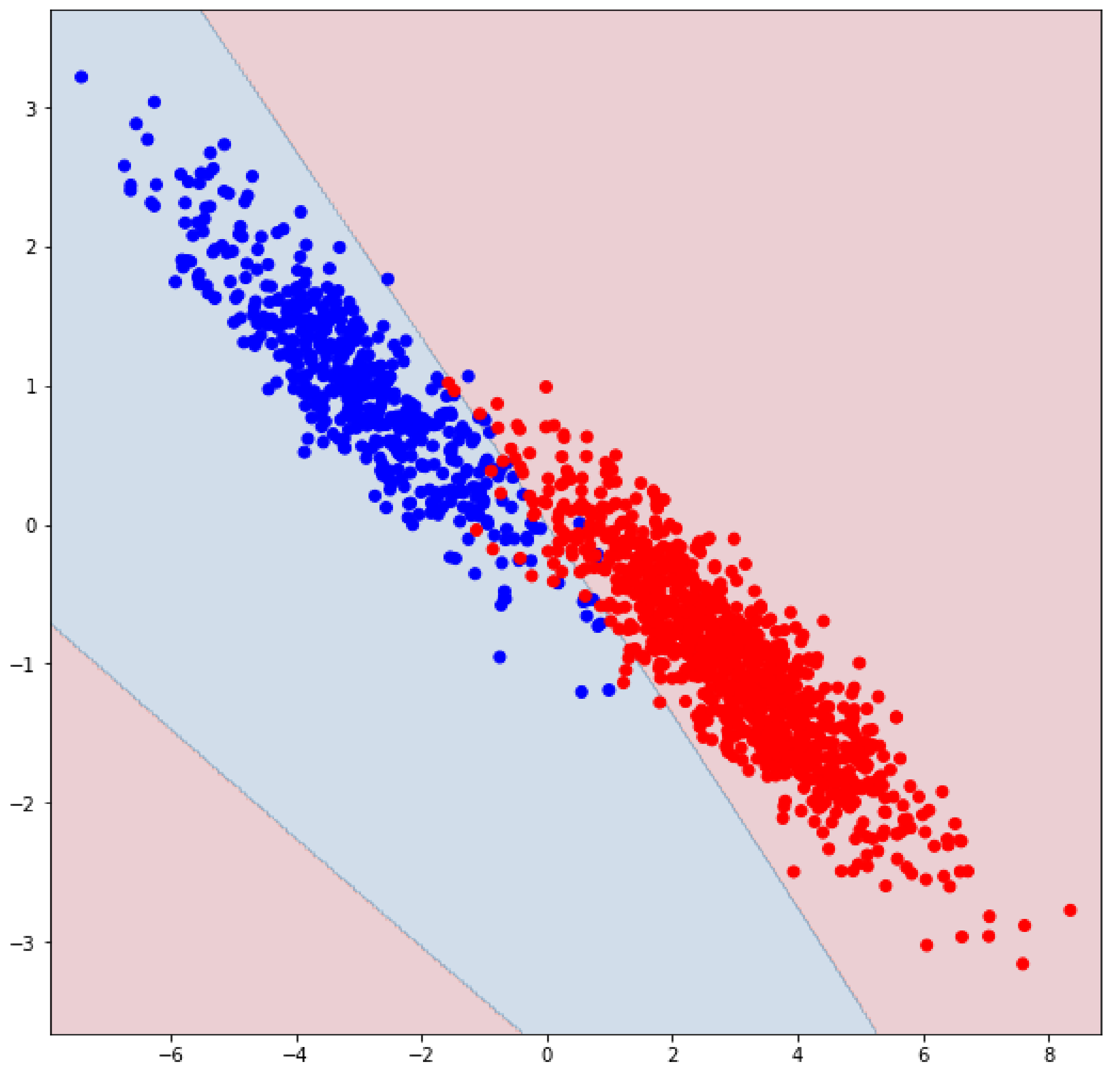
```
In [339]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.976
```

Plot

In [340]:
```
h = .02  # step size in the mesh

x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
```

In [341]:
```
plt.figure(figsize=(10, 10))

cm = plt.cm.RdBu

Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

colors = ['b' if y == 1. else 'r' for y in Y_test]
plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

plt.show()
```



Comments This dataset is almost linearly separable, so the QDA model should not bring any advantages. In fact, we observe that it overfits to the training data more than the LDA did, producing worse results than the other 3 models in the test set.

It is also interesting to observe that the estimates for the covariance matrices in QDA are quite close to each other, confirming (well, not so rigorously) that the assumption of LDA was reasonable.

1.3 Page 3: dataset B

1.3.1 Reading the dataset

```
In [343]: dataset_name = 'B'
```

```
In [344]: def read(dataset_name):
              train_path, test_path = ['data/' + filename for filename in ['classification{}.tra
```

```
        train_df = pd.read_csv(train_path, delimiter='\t', header=None)
        train_df.columns = ['x1', 'x2', 'y']
        test_df = pd.read_csv(test_path, delimiter='\t', header=None)
        test_df.columns = ['x1', 'x2', 'y']
        return train_df, test_df
```

In [345]:
```
train_df, test_df = read(dataset_name)
```

In [346]:
```
def points_from_df(df):
    x1s, x2s, ys = df['x1'].values, df['x2'].values, df['y'].values
    return [np.array([x1, x2]) for x1, x2 in zip(x1s, x2s)], ys
```

In [347]:
```
X_train, Y_train = points_from_df(train_df)
X_test, Y_test = points_from_df(test_df)
```

1.3.2 LDA

In [348]:
```
clf = LDAClassifier().fit(X_train, Y_train)
```

```
Estimated pi = 0.5
Estimated mu_0 = [ 3.34068896 -0.83546333]
Estimated mu_1 = [-3.21670734  1.08306733]
Estimated Sigma = [[ 3.34623467 -0.13516489]
 [-0.13516489  1.73807475]]
```

Predict

In [349]:
```
Y_train_pred = clf.predict(X_train)
```

In [350]:
```
Y_pred = clf.predict(X_test)
```

In [351]:
```
print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.97
```

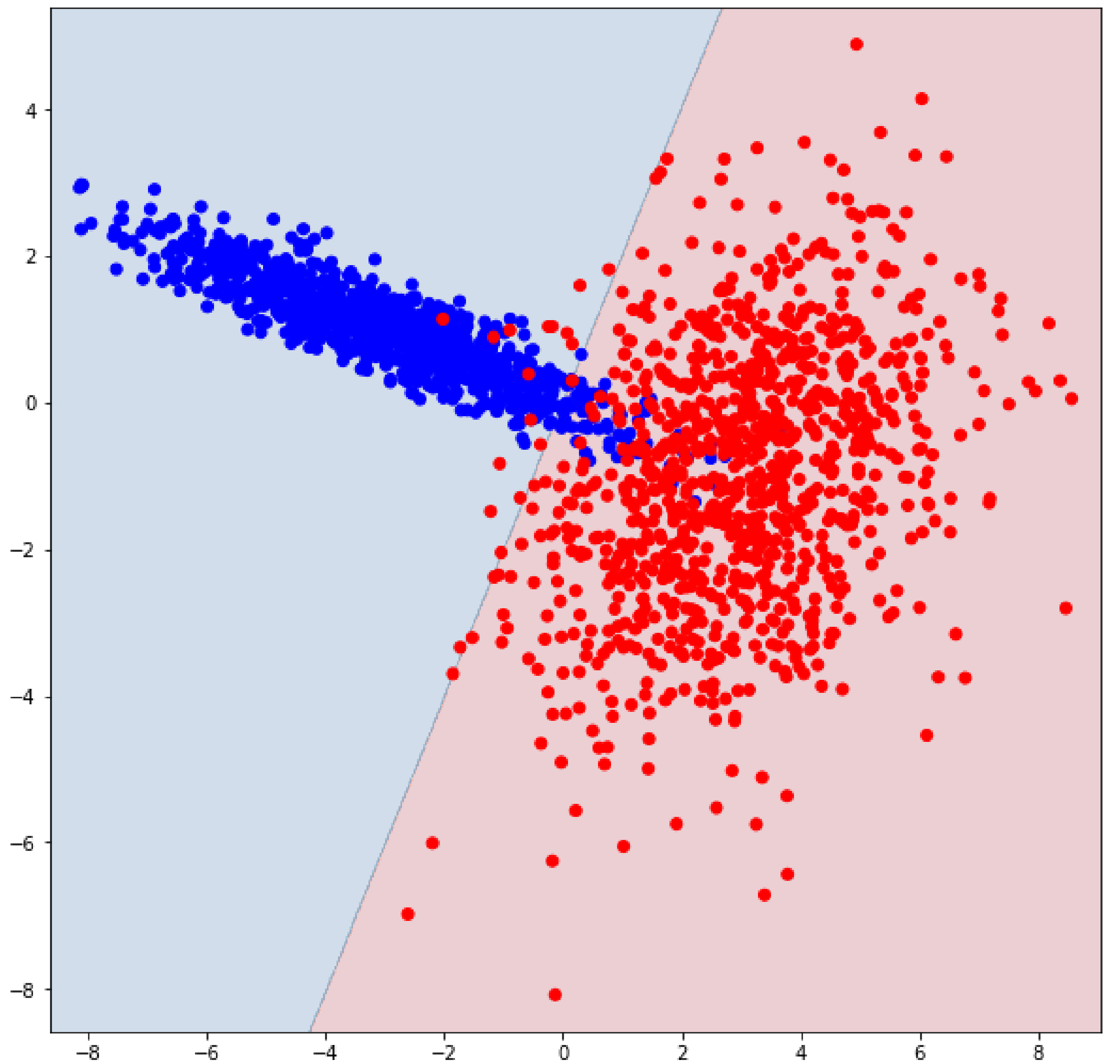
In [352]:
```
print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9585
```

Plot

In [262]:
```
h = .02  # step size in the mesh

x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
```

```
In [263]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

          colors = ['b' if y == 1. else 'r' for y in Y_test]
          plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

          plt.show()
```



1.3.3 Logistic regression

```
In [264]: clf = LogisticClassifier().fit(X_train, Y_train)
```

```
/home/hfiuza/Programs/virtualenv/ds/lib/python3.6/site-packages/ipykernel_launcher.py:2: Runtime
```

Predict

```
In [265]: Y_train_pred = clf.predict(X_train)
```

```
In [266]: Y_pred = clf.predict(X_test)
```

```
In [267]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.9733333333333334
```

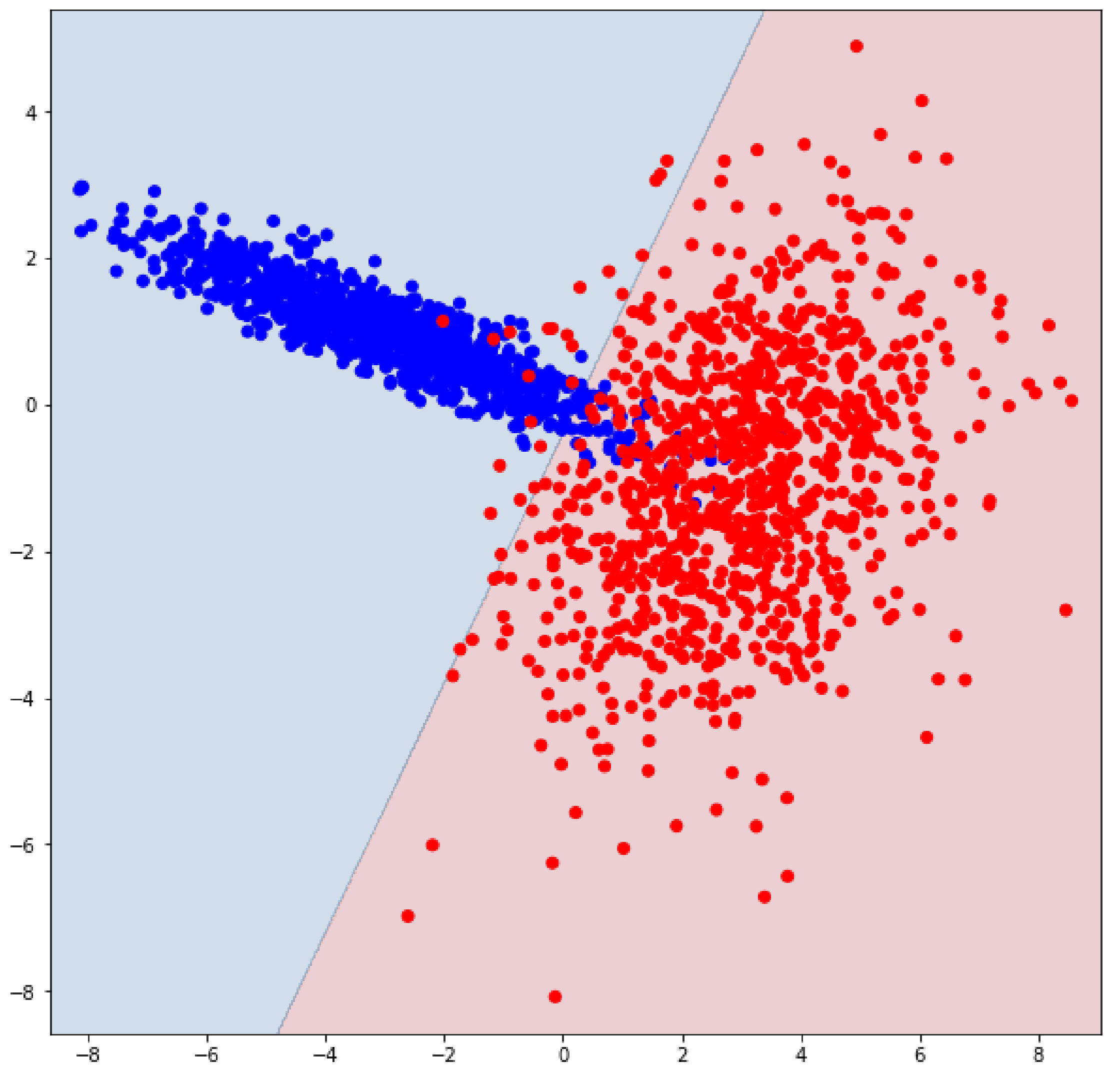
```
In [268]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.962
```

Plot

```
In [269]: h = .02  # step size in the mesh

          x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
          y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
          xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                               np.arange(y_min, y_max, h))
```

```
In [270]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

          colors = ['b' if y == 1. else 'r' for y in Y_test]
          plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

          plt.show()
```



1.3.4 Linear regression

```
In [271]: clf = LinearClassifier().fit(X_train, Y_train)
```

Predict

```
In [272]: Y_train_pred = clf.predict(X_train)
```

```
In [273]: Y_pred = clf.predict(X_test)
```

```
In [274]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.97
```

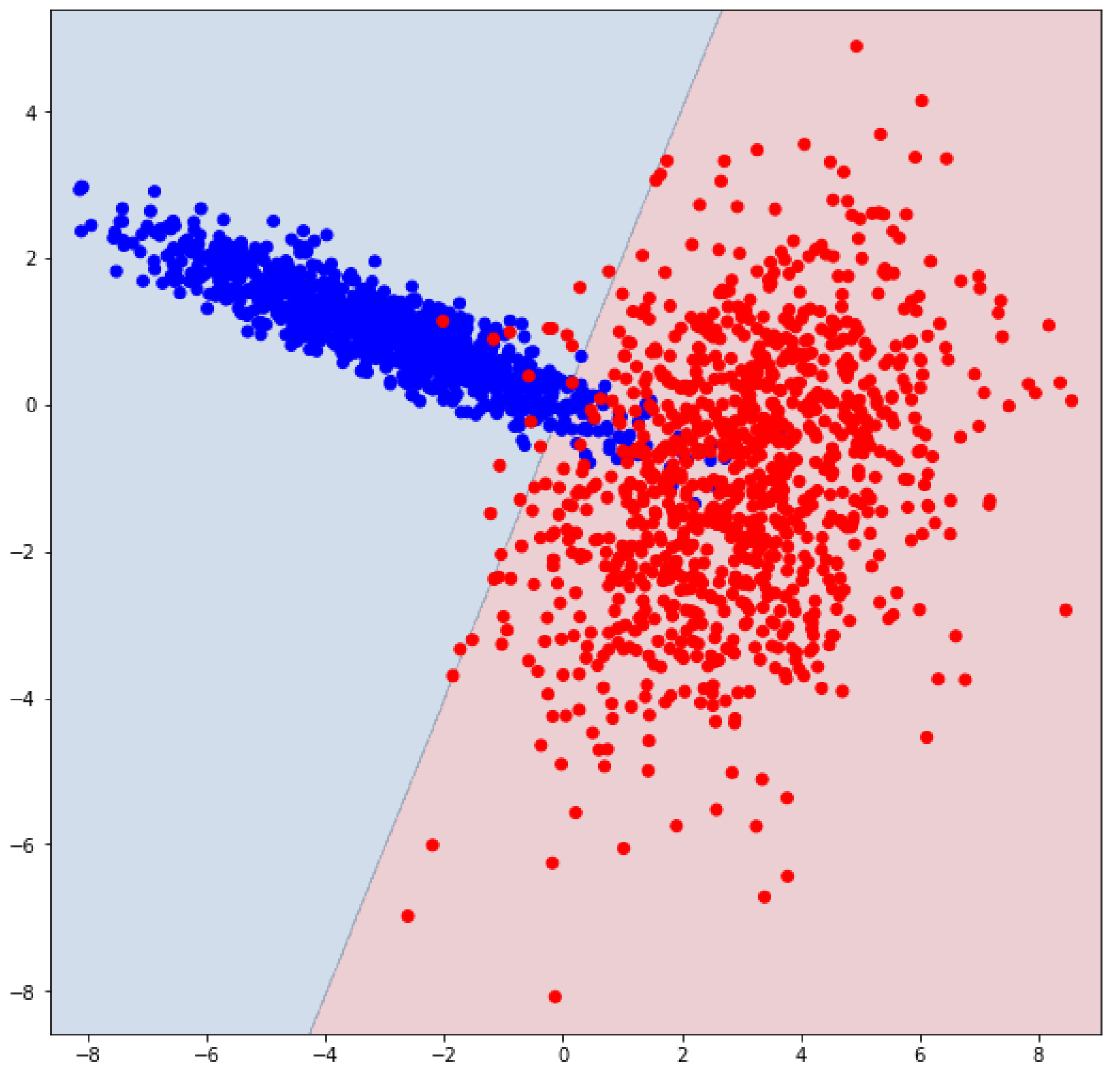
```
In [275]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9585
```

Plot

```
In [276]: h = .02  # step size in the mesh

          x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
          y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
          xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                               np.arange(y_min, y_max, h))
```

```
In [277]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

          colors = ['b' if y == 1. else 'r' for y in Y_test]
          plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

          plt.show()
```



1.3.5 Results summary up to now

```
In [353]: lda_train_accuracy, lda_test_accuracy = 0.97, 0.959
          logistic_train_accuracy, logistic_test_accuracy = 0.9733333333333334, 0.962
          linear_train_accuracy, linear_test_accuracy = 0.97, 0.9585
```

Comment: the Logistic model again gives a slightly better accuracy score in the the test set, and this time one could say it's considerably higher (96.2% > 95.9%).

1.3.6 QDA

```
In [354]: clf = QDAClassifier().fit(X_train, Y_train)
```

```
Estimated pi = 0.5
Estimated mu_0 = [ 3.34068896 -0.83546333]
```

```
Estimated mu_1 = [-3.21670734  1.08306733]
Estimated Sigma_0 = [[2.53885859 1.0642112 ]
 [1.0642112  2.96007891]]
Estimated Sigma_1 = [[ 4.15361075 -1.33454097]
 [-1.33454097  0.51607059]]
```

Predict

```
In [355]: Y_train_pred = clf.predict(X_train)
```

```
In [356]: Y_pred = clf.predict(X_test)
```

```
In [357]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.9866666666666667
```

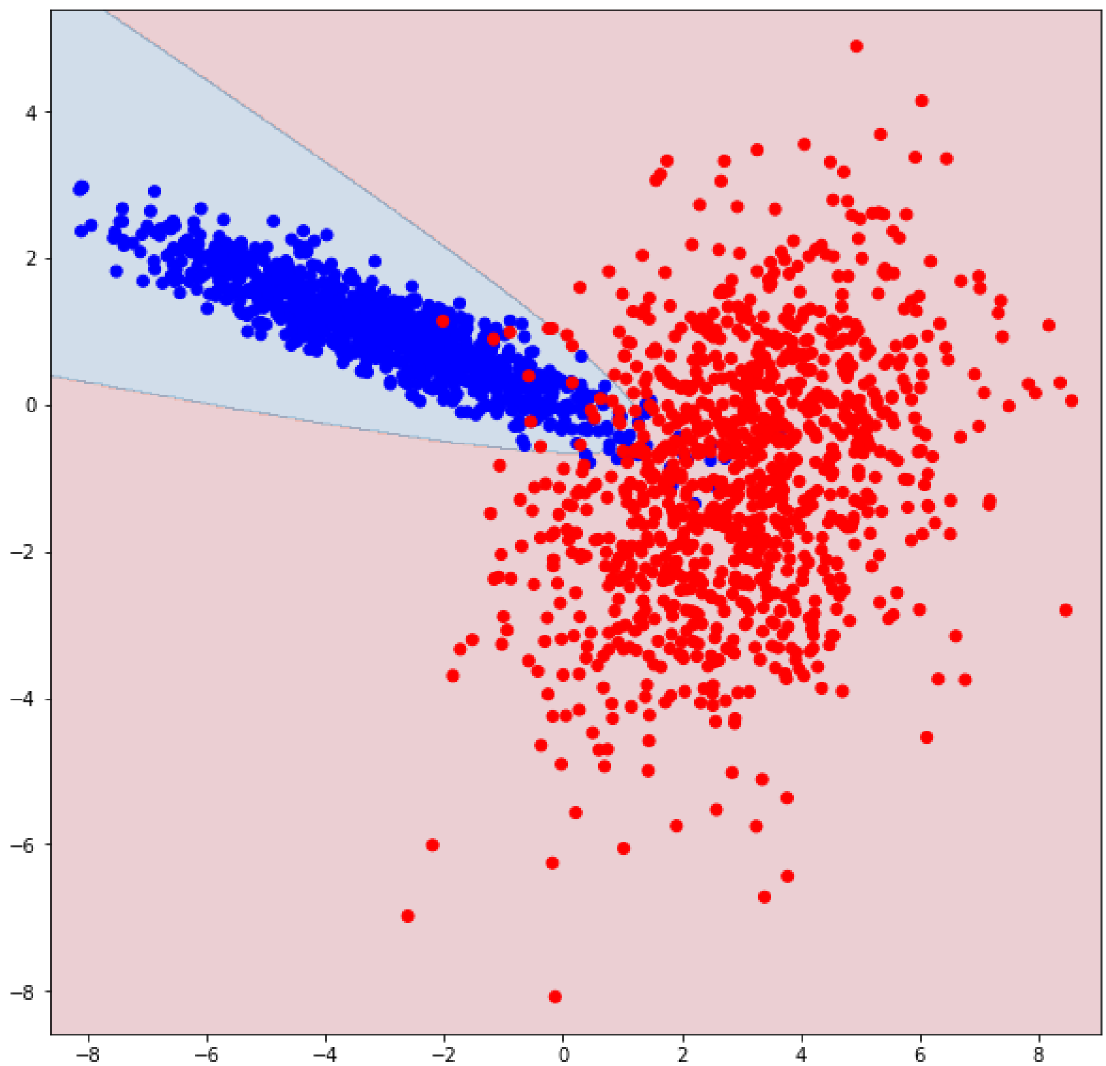
```
In [358]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.98
```

Plot

```
In [359]: h = .02  # step size in the mesh

          x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
          y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
          xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                               np.arange(y_min, y_max, h))
```

```
In [360]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

          colors = ['b' if y == 1. else 'r' for y in Y_test]
          plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

          plt.show()
```



Comments This dataset is not linearly separable, so the LDA model was not able to discriminate correctly for some points. On the other hand, the QDA model could find good natural region delimiters and reduce in 50% the error rate.

In addition, one could argue from the visualization that these classes definitely do not share the same covariance matrices. In fact, the estimates from QDA of Σ_0 and Σ_1 are quite different from each other.

1.4 Page 3: dataset C

1.4.1 Reading the dataset

```
In [361]: dataset_name = 'C'
```

```
In [362]: def read(dataset_name):
              train_path, test_path = ['data/' + filename for filename in ['classification{}.tra
```

```
        train_df = pd.read_csv(train_path, delimiter='\t', header=None)
        train_df.columns = ['x1', 'x2', 'y']
        test_df = pd.read_csv(test_path, delimiter='\t', header=None)
        test_df.columns = ['x1', 'x2', 'y']
        return train_df, test_df
```

In [363]:
```
train_df, test_df = read(dataset_name)
```

In [364]:
```
def points_from_df(df):
    x1s, x2s, ys = df['x1'].values, df['x2'].values, df['y'].values
    return [np.array([x1, x2]) for x1, x2 in zip(x1s, x2s)], ys
```

In [365]:
```
X_train, Y_train = points_from_df(train_df)
X_test, Y_test = points_from_df(test_df)
```

1.4.2 LDA

In [284]:
```
clf = LDAClassifier().fit(X_train, Y_train)
```

```
Estimated pi = 0.625
Estimated mu_0 = [ 2.79304824 -0.83838667]
Estimated mu_1 = [-2.94232885 -0.9578284 ]
Estimated Sigma = [[ 2.88039225 -0.63405081]
 [-0.63405081  5.19952435]]
```

Predict

In [285]:
```
Y_train_pred = clf.predict(X_train)
```

In [286]:
```
Y_pred = clf.predict(X_test)
```

In [287]:
```
print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.945
```

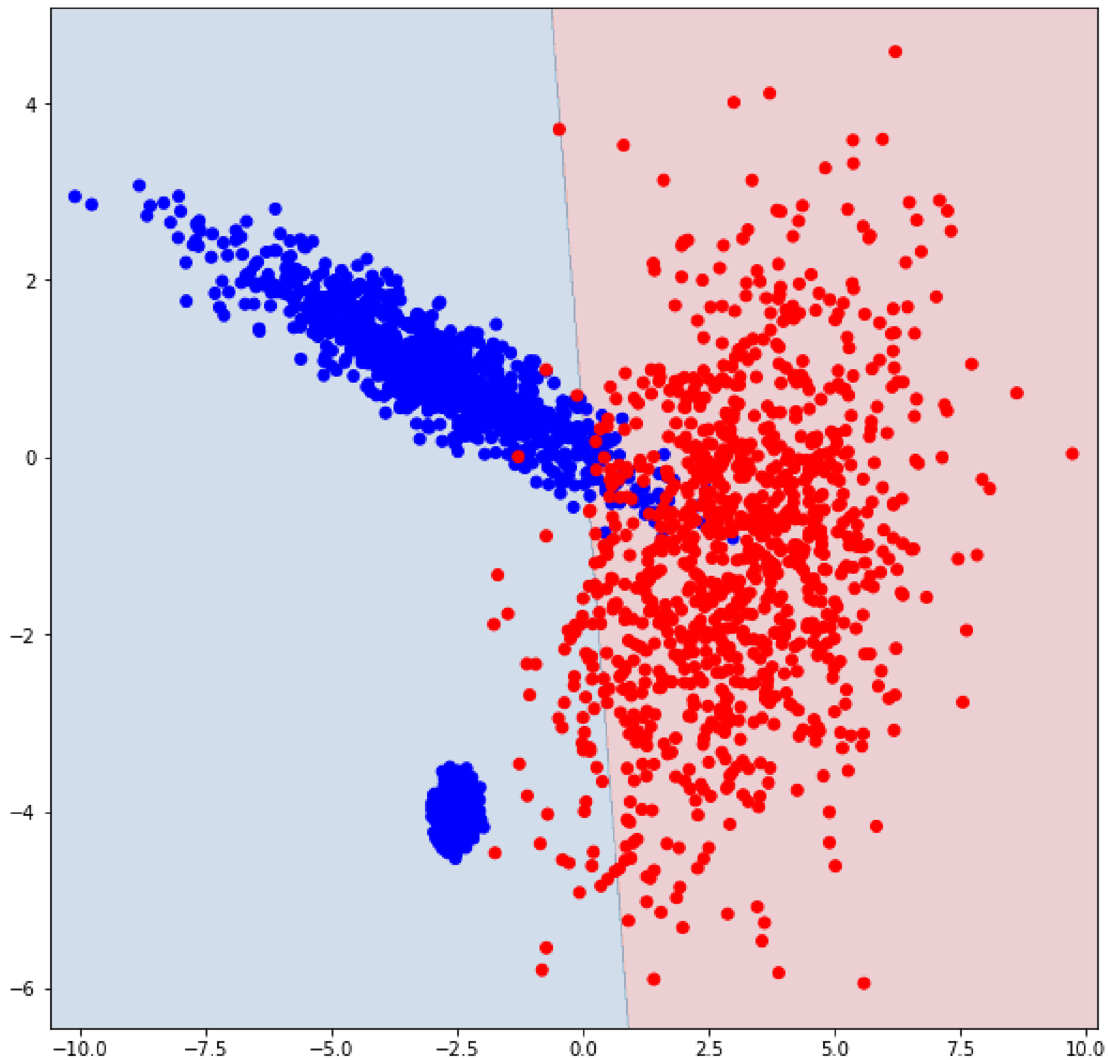
In [288]:
```
print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9576666666666667
```

Plot

In [289]:
```
h = .02  # step size in the mesh

x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
```

In [290]:
```
plt.figure(figsize=(10, 10))

cm = plt.cm.RdBu

Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

colors = ['b' if y == 1. else 'r' for y in Y_test]
plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

plt.show()
```



1.4.3 Logistic regression

```
In [291]: clf = LogisticClassifier().fit(X_train, Y_train)
```

```
/home/hfiuza/Programs/virtualenv/ds/lib/python3.6/site-packages/ipykernel_launcher.py:2: Runtime
```

Predict

```
In [292]: Y_train_pred = clf.predict(X_train)
```

```
In [293]: Y_pred = clf.predict(X_test)
```

```
In [294]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.945
```

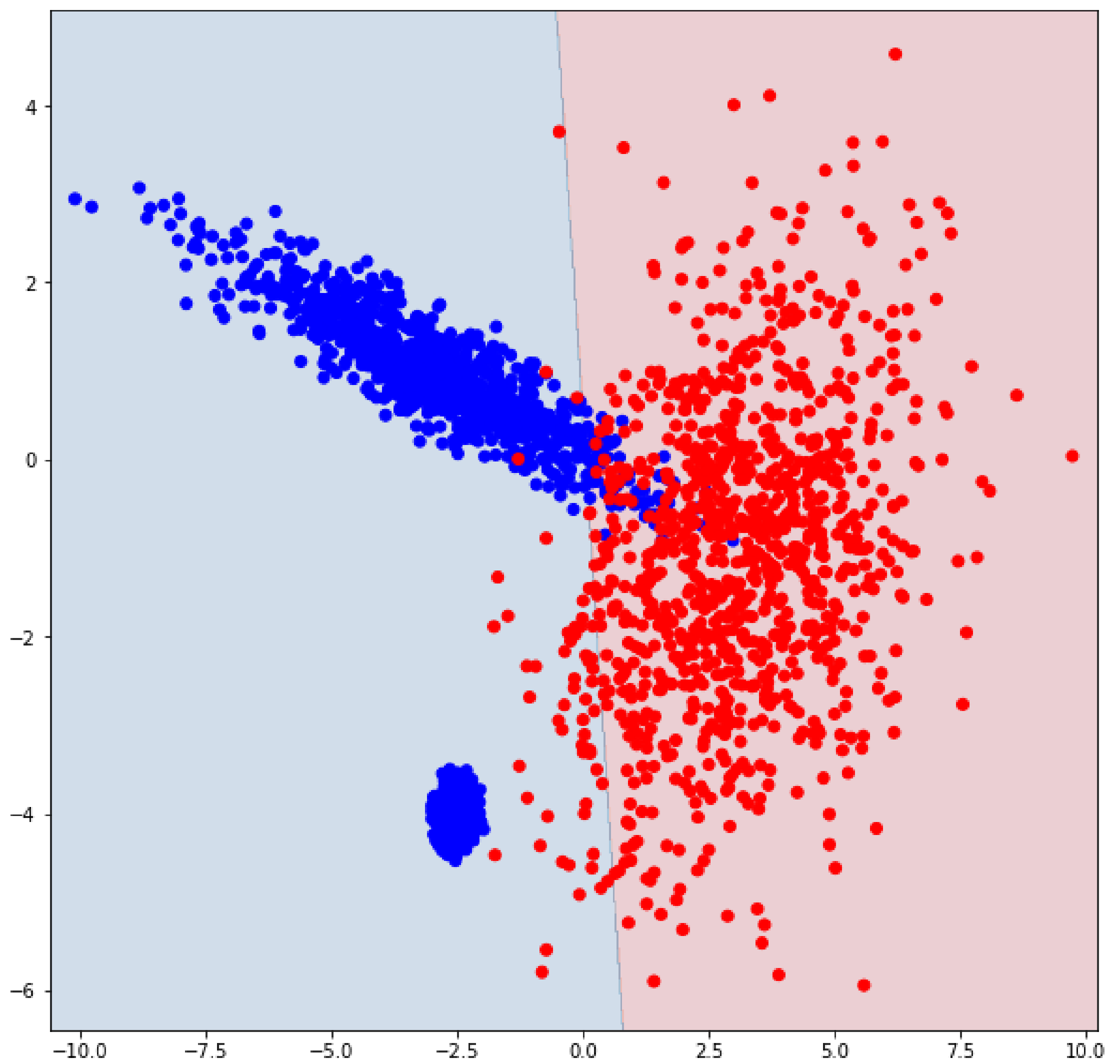
```
In [295]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9586666666666667
```

Plot

```
In [296]: h = .02  # step size in the mesh

          x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
          y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
          xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                               np.arange(y_min, y_max, h))
```

```
In [297]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

          colors = ['b' if y == 1. else 'r' for y in Y_test]
          plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

          plt.show()
```



1.4.4 Linear regression

```
In [298]: clf = LinearClassifier().fit(X_train, Y_train)
```

Predict

```
In [299]: Y_train_pred = clf.predict(X_train)
```

```
In [300]: Y_pred = clf.predict(X_test)
```

```
In [301]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.945
```

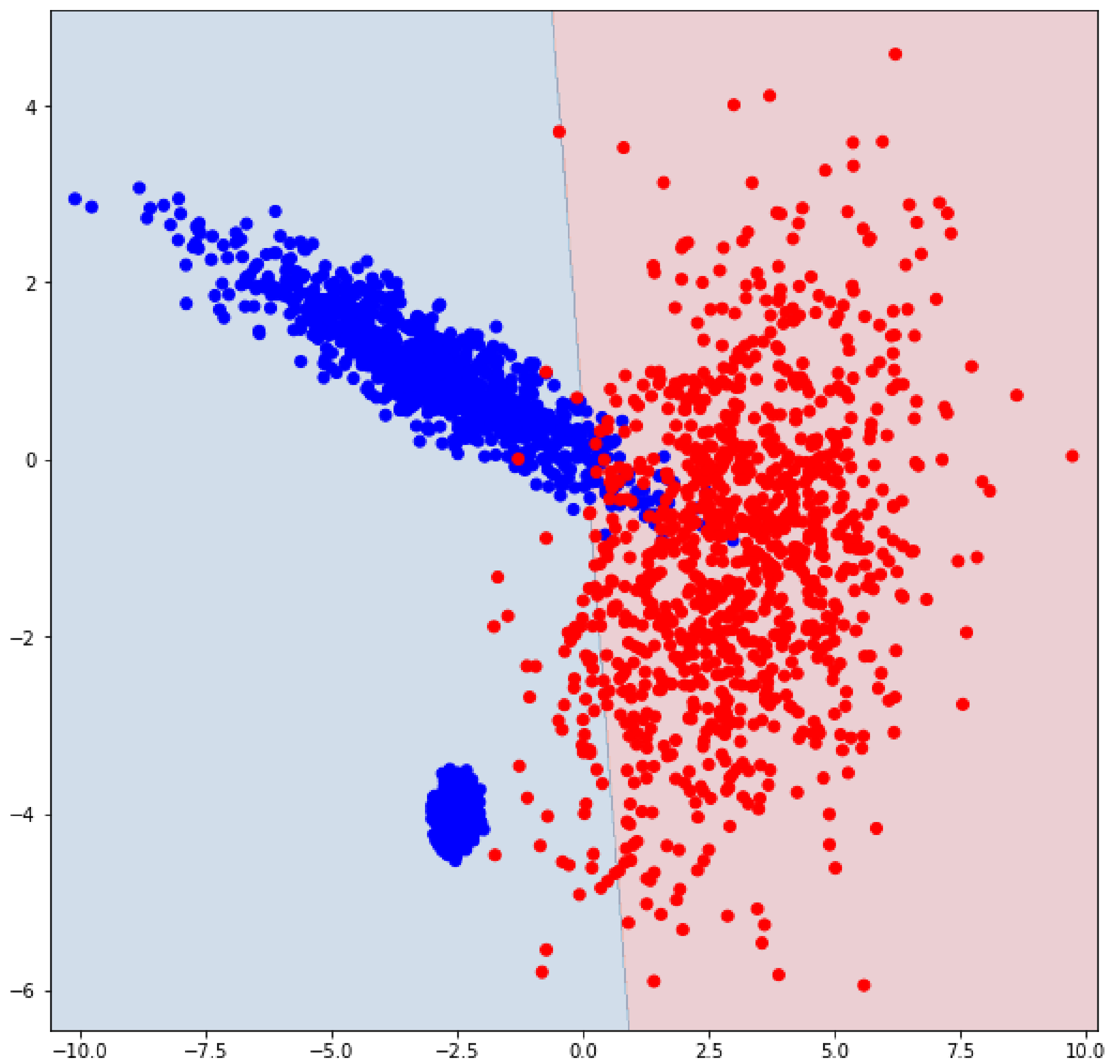
In [302]:
```
print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9576666666666667
```

Plot

In [303]:
```
h = .02  # step size in the mesh

x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
```

In [304]:
```
plt.figure(figsize=(10, 10))

cm = plt.cm.RdBu

Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)

colors = ['b' if y == 1. else 'r' for y in Y_test]
plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

plt.show()
```



1.4.5 Results summary

```
In [305]: lda_train_accuracy, lda_test_accuracy = 0.9475, 0.9606666666666667
          logistic_train_accuracy, logistic_test_accuracy = 0.945, 0.9586666666666667
          linear_train_accuracy, linear_test_accuracy = 0.945, 0.9576666666666667
```

Comment: the LDA classifier gives the best accuracies for both the training and test set, although it's weird that the later is better than the former. One should pick it but do not expect that the 96.06% accuracy rate will be attained in real data.

From the visualization, we can see that:

- the data is not linearly separable;
- the classes could have been generated by 3 Gaussian distributions with different covariance matrices.

These observations, specially the second one, contradict basic assumptions of LDA. We should be very happy to still have 96.06% accuracy on the test set.

1.4.6 QDA

```
In [366]: clf = QDAClassifier().fit(X_train, Y_train)
```

```
Estimated pi = 0.625
Estimated mu_0 = [ 2.79304824 -0.83838667]
Estimated mu_1 = [-2.94232885 -0.9578284 ]
Estimated Sigma_0 = [[2.89913927 1.24581553]
 [1.24581553 2.92475448]]
Estimated Sigma_1 = [[ 2.86914403 -1.76197061]
 [-1.76197061  6.56438626]]
```

Predict

```
In [367]: Y_train_pred = clf.predict(X_train)

In [368]: Y_pred = clf.predict(X_test)

In [369]: print('Accuracy on training set: {}'.format(accuracy_score(Y_train_pred, Y_train)))
```

```
Accuracy on training set: 0.955
```

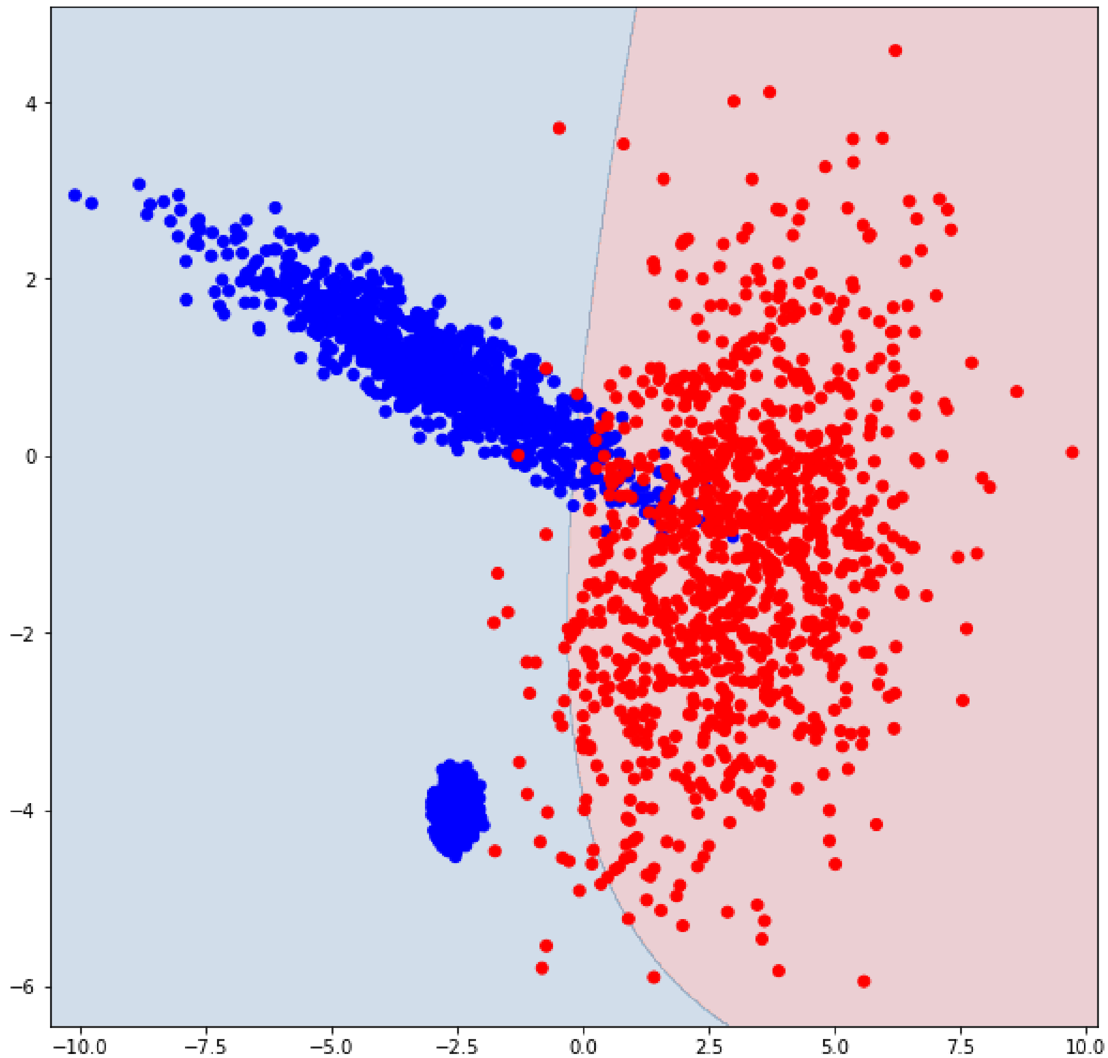
```
In [370]: print('Accuracy on test set: {}'.format(accuracy_score(Y_pred, Y_test)))
```

```
Accuracy on test set: 0.9643333333333334
```

Plot

```
In [371]: h = .02  # step size in the mesh

          x_min, x_max = min([x[0] for x in X_test]) - .5, max([x[0] for x in X_test]) + .5
          y_min, y_max = min([x[1] for x in X_test]) - .5, max([x[1] for x in X_test]) + .5
          xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                               np.arange(y_min, y_max, h))

In [374]: plt.figure(figsize=(10, 10))

          cm = plt.cm.RdBu

          Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          plt.contourf(xx, yy, Z, cmap=cm, alpha=.2)
```

```
colors = ['b' if y == 1. else 'r' for y in Y_test]
plt.scatter([x[0] for x in X_test], [x[1] for x in X_test], c=colors)

plt.show()
```



Comments This dataset is not linearly separable, so the LDA model was not able to discriminate correctly for some points.

On the other hand, the QDA model also failed to find the correct natural regions because it assumes that each class is generated by a single Gaussian distribution. However, for this dataset, the class 1 is generated from two Gaussian distributions.

In spite of this, QDA still gave better accuracies than the other models for both training and test sets.