Density Estimation

September 28, 2018

```
In [5]: import numpy as np
        import math
        %pylab inline
        import matplotlib.pyplot as plt

        class diagonal_gaussian_parametric:
            """
            1. Implement a diagonal Gaussian parametric density estimator. It
            will have to work for data of arbitrary dimension d. As seen in
            the labs, it should have a train() method to learn the parameters
            and a method predict() which calculates the log density.
            """
            def __init__(self):
                pass

            def train(self, train_data):

                # if only one test_data is passed, add dummy dimension
                if len(np.shape(train_data)) == 1:
                    train_data = np.expand_dims(train_data, axis=1)

                self.train_data = train_data

                try:
                    self.n, self.d = np.shape(self.train_data)
                except:
                    self.n = np.shape(self.train_data)
                    self.d = 1

                self.mu = np.sum(self.train_data, axis=0) / self.n
                self.sigma = np.cov(self.train_data.T) * np.eye(self.d)

            def predict(self, test_data, nll=True):

                # if only one test_data is passed, add dummy dimension
                if len(np.shape(test_data)) == 1:
                    test_data = np.expand_dims(test_data, axis=1).T
        self.test_data = test_data
        n_inputs = np.shape(test_data)[0]
        densities = np.zeros(n_inputs)

        sigma_inv = np.linalg.inv(self.sigma)
        sigma_det = np.linalg.det(self.sigma)

        normalizer = 1 / ((2* np.pi)**(self.d / 2) * np.sqrt(sigma_det))

        # we treat each input test_data independently
        for i in range(n_inputs):

            diff = self.test_data[i, :] - self.mu
            exponent = (-0.5) * (diff).T.dot(sigma_inv).dot(diff)

            if nll:
                p = -np.log(normalizer)*exponent
            else:
                p = normalizer*np.exp(exponent)

            # handle edge case where p(x)=0
            if p == 0:
                p = np.finfo(float).eps

            densities[i] = p

        return(densities)

class parzen_density_estimator:
    """
    2. Implement a Parzen density estimator with an isotropic Gaussian
    kernel. It will have to work for data of arbitrary dimension d.
    Likewise it should have a train() method and a predict() method
    that computes the log density.
    """
    def __init__(self):
        pass

    def train(self, train_data, sigma=0):
        self.train_data = np.expand_dims(train_data, axis=1)

        try:
            self.n, self.d = np.shape(self.train_data)
        except:
            self.n = np.shape(self.train_data)
            self.d = 1
        if sigma == 0:
            self.sigma = np.std(self.train_data) # std because isotropic Gaussian
        else:
            self.sigma = sigma

    def predict(self, test_data, nll=True):

        # if only one test_data is passed, add dummy dimension
        if len(np.shape(test_data)) == 1:
            test_data = np.expand_dims(test_data, axis=1).T

        self.test_data = test_data
        n_inputs = np.shape(self.test_data)[0]
        n_train = np.shape(self.train_data)[0]
        densities = np.zeros(n_inputs)
        normalizer = 1/((2*np.pi*self.sigma)**(self.d / 2))

        for i in range(n_inputs):

            # calculate avg dist b/t this training point and all test points
            p = 0
            for j in range(n_train):

                # for gaussian kernel we use euclidean distance
                distance = np.sum((self.test_data[i, :] - self.train_data[j, :])**2)
                exponent = (-0.5) * (distance / self.sigma)

                if nll:
                    p += -np.log(normalizer)*exponent
                else:
                    p += normalizer * np.exp(exponent)

            # handle edge case where p(x)=0
            if p == 0:
                p = np.finfo(float).eps

            # save the average kernel values across all training points
            densities[i] = p/n_train

        return(densities)
```

```
Populating the interactive namespace from numpy and matplotlib


/opt/python/sci_36/lib/python3.6/site-packages/IPython/core/magics/pylab.py:160: UserWarning:
`%matplotlib` prevents importing * from pylab and numpy
  "\n`%matplotlib` prevents importing * from pylab and numpy"
```

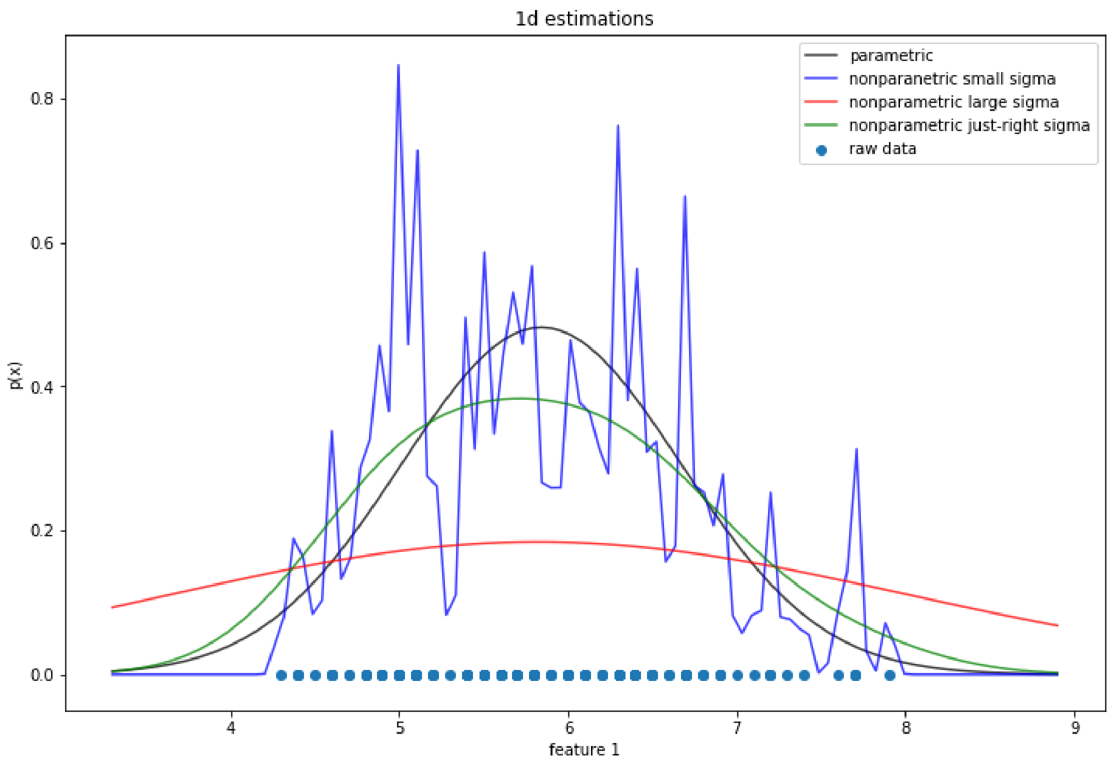
0.1 1D Densities

From the Iris dataset examples, choose a subset corresponding to one of the classes (of your choice), and one of the characteristic features, so that we will be in dimension d = 1 and produce a single graph (using the plot function) including:

- the data points of the subset (displayed on the x axis).
- a plot of the density estimated by your parametric Gaussian estimator.
- a plot of the density estimated by the Parzen estimator with a hyper-parameter (standard deviation) too small.
- a plot of the density estimated by the Parzen estimator with the hyper-parameter being a little too big.
- a plot of the density estimated by the Parzen estimator with the hyper-parameter that you consider more appropriate. Use a different color for each plot, and provide your graph with a clear legend.
- Explain how you chose your hyper-parameter .

```
In [6]: # load data
        iris = np.loadtxt("iris.txt")
        iris_subset = iris[:,0]
        n = len(iris_subset)

        # general plotting variables
        n_bins = 100
        axes_min = np.min(iris_subset)-1
        axes_max = np.max(iris_subset)+1
        alpha=0.75

        small_sig = 0.001
        large_sig = 4
        moyen_sig = 0.25

        x = np.atleast_2d(np.linspace(axes_min, axes_max, n_bins)).T

        # (a) -- raw data
        plt.figure(figsize=(12, 8))
        plt.scatter(iris_subset, np.zeros(len(iris_subset)))

        # (b) -- parametric model
        flower = diagonal_gaussian_parametric()
        flower.train(iris_subset)
        density = flower.predict(x, nll=False)
        plt.plot(x, density, color='black', alpha=alpha)

        # (c) -- nonparametric small sigma
        flower = parzen_density_estimator()
        flower.train(iris_subset, sigma=small_sig)
        density2 = flower.predict(x, nll=False)
        plt.plot(x, density2, color='blue', alpha=alpha)
```

```
# (d) -- nonparametric large sigma
flower = parzen_density_estimator()
flower.train(iris_subset, sigma=large_sig)
density = flower.predict(x, nll=False)
plt.plot(x, density, color='red', alpha=alpha)

# (e) -- nonparametric just-right sigma
flower = parzen_density_estimator()
flower.train(iris_subset, sigma=moyen_sig)
density = flower.predict(x, nll=False)
plt.plot(x, density, color='green', alpha=alpha)

# legend
plt.legend(['parametric',
            'nonparanetric small sigma',
            'nonparametric large sigma',
            'nonparametric just-right sigma',
            'raw data'])

plt.title('1d estimations')
plt.xlabel('feature 1')
plt.ylabel('p(x)')
plt.show()
```



We chose sigma based on how it looked on the plot. The very large sigma (4) was chosen to encompase lots of empty feature space and the very small sigma (0.001) was chosen to be very sensitive to each data point. For the 'just right' sigma (0.25), we chose a value that mostly covered the data distribution without it encompasing too much empty feature space.

0.2 2D Densities

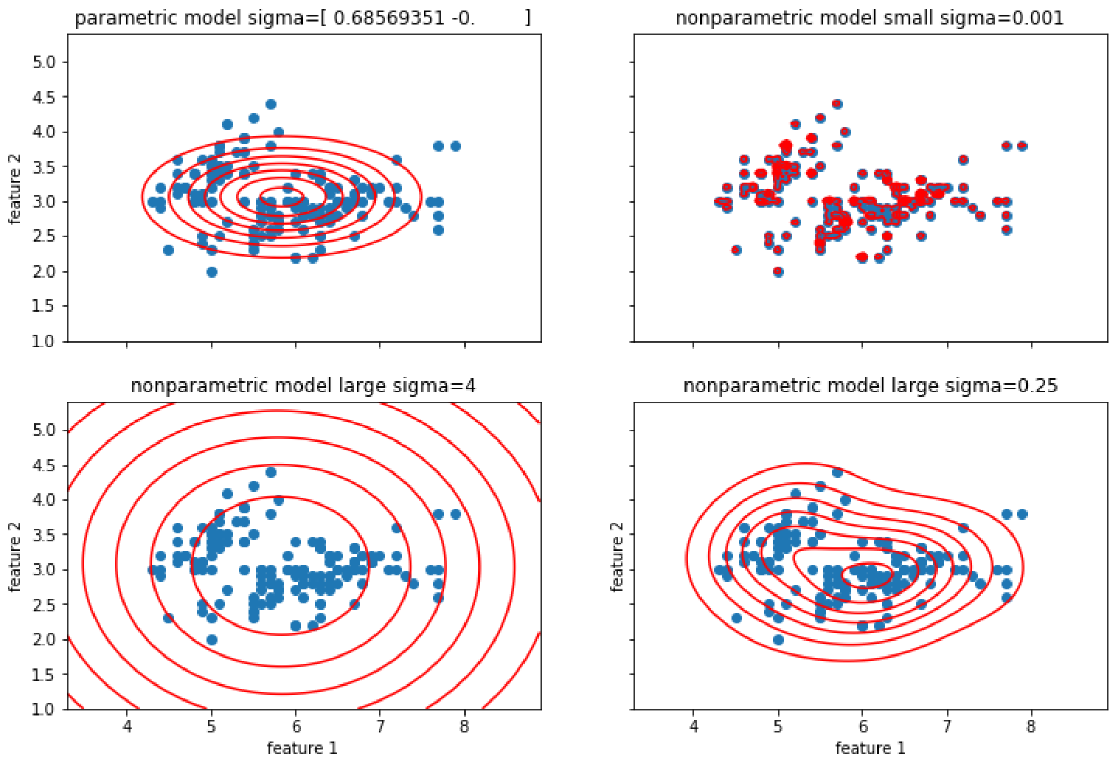
Now add a second characteristic feature of Iris, in order to have entries in d = 2 and produce 4 plots, each displaying the points of the subset of the data (with the plot function), and the contour lines of the density estimated (using the contour function):

- by the diagonal Gaussian parametric estimator.
- by the Parzen estimator with the hyper-parameter (standard deviation) being too small.
- by the Parzen estimator with the hyper-parameter being a little too big.
- by the Parzen estimator with the hyper-parameter that you consider more appropriate.
- Explain how you chose your hyper-parameter

```
In [7]: def make_dimensions(x_min, x_max, y_min, y_max, n_bins):
            X = np.atleast_2d(np.linspace(x_min, x_max, n_bins)).T
            Y = np.atleast_2d(np.linspace(y_min, y_max, n_bins)).T
            l = len(X) * len(Y)
            Z = np.zeros([l, 2])
            i = 0
            for x in X:
                for y in Y:
                    Z[i, 0] = x
                    Z[i, 1] = y
                    i += 1

            return X, Y, Z
```

```
In [9]: # new data subset
        iris_subset = iris[:,0:2]

        # general plotting variables
        n_bins = 100
        x_min = np.min(iris_subset[:,0])-1
        x_max = np.max(iris_subset[:,0])+1
        y_min = np.min(iris_subset[:,1])-1
        y_max = np.max(iris_subset[:,1])+1
        alpha=0.75

        # plot time
        f, ((ax1, ax2), (ax3, ax4)) = plt.subplots(2, 2, figsize=(12, 8), sharex=True,
                                                                           sharey=True)

        # add raw data
```

```python
ax1.scatter(iris_subset[:, 0], iris_subset[:, 1])
ax2.scatter(iris_subset[:, 0], iris_subset[:, 1])
ax3.scatter(iris_subset[:, 0], iris_subset[:, 1])
ax4.scatter(iris_subset[:, 0], iris_subset[:, 1])

# (b) -- parametric model
flower = diagonal_gaussian_parametric()
flower.train(iris_subset)
X, Y, Z = make_dimensions(x_min, x_max, y_min, y_max, n_bins)
X, Y = np.meshgrid(X, Y)
density = flower.predict(Z, nll=False).reshape(n_bins, n_bins)
ax1.contour(X, Y, density.T, colors='red')
ax1.set_title('parametric model sigma={}'.format(flower.sigma[0]))
ax1.set_ylabel('feature 2')

# (c) -- nonparametric model, small sigma
flower = parzen_density_estimator()
flower.train(iris_subset, sigma=small_sig)
X, Y, Z = make_dimensions(x_min, x_max, y_min, y_max, n_bins)
X, Y = np.meshgrid(X, Y)
density = flower.predict(Z, nll=False).reshape(n_bins, n_bins)
ax2.contour(X, Y, density.T, colors='red')
ax2.set_title('nonparametric model small sigma={}'.format(small_sig))

# (d) -- nonparametric model, large sigma
flower = parzen_density_estimator()
flower.train(iris_subset, sigma=large_sig)
X, Y, Z = make_dimensions(x_min, x_max, y_min, y_max, n_bins)
X, Y = np.meshgrid(X, Y)
density = flower.predict(Z, nll=False).reshape(n_bins, n_bins)
ax3.contour(X, Y, density.T, colors='red')
ax3.set_title('nonparametric model large sigma={}'.format(large_sig))
ax3.set_xlabel('feature 1')
ax3.set_ylabel('feature 2')

# (e) -- nonparametric model, just right sigma
flower = parzen_density_estimator()
flower.train(iris_subset, sigma=moyen_sig)
X, Y, Z = make_dimensions(x_min, x_max, y_min, y_max, n_bins)
X, Y = np.meshgrid(X, Y)
density = flower.predict(Z, nll=False).reshape(n_bins, n_bins)
ax4.contour(X, Y, density.T, colors='red')
ax4.set_title('nonparametric model large sigma={}'.format(moyen_sig))
ax4.set_xlabel('feature 1')
ax4.set_ylabel('feature 2')

plt.show()
```



We chose sigma based on how it looked on the plot. The very large sigma (4) was chosen to encompase lots of empty feature space and the very small sigma (0.001) was chosen to tightly wrap each data point. For the 'just right' sigma (0.25), we chose a value that mostly covered the data distribution without it encompasing too much empty feature space.