SPR Lab 3

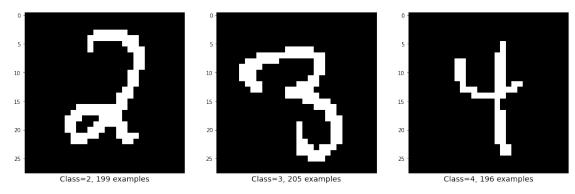
March 3, 2021

1 Multivariate Bernoulli Distribution

Run EM and K-Means algorithm on same dataset and compare the results. ## Reading MNIST dataset

```
[1]: import numpy as np
     import torch
     import pytorch_lightning as pl
     from sklearn.model_selection import train_test_split
     import matplotlib.pyplot as plt
     import scipy
     import seaborn as sns
     np.random.seed(42)
     class Config:
        N = 600
         K = 3
         D = 784
         iterations = 50
     def load_mnist():
         mnist = pd.read_csv('mnist_train.csv').values
         X_train, y_train = mnist[:, 1:], mnist[:, 0]
         # take only digits 2, 3 and 4
         take = (y_train >= 2) & (y_train <= 4)
         X_train, y_train = X_train[take], y_train[take]
         # making arrays have only zeros or ones
         X_{train} = ((X_{train}/255.0) > .5).astype(int)
         # make sure you have a total of 600 examples
         train_size = Config.N / y_train.shape[0]
         X_train, _, y_train, _ = train_test_split(X_train, y_train,_
      →train_size=train_size, stratify=y_train, random_state=42)
         # show one example from each class
         fig, axs = plt.subplots(1, 3, figsize=(18, 6))
```

```
for i, c in enumerate([2, 3, 4]):
    img = X_train[y_train == c][0].reshape((28, 28))
    t = (y_train==c).sum()
    axs[i].imshow(img, cmap='CMRmap')
    axs[i].set(xticks = [])
    axs[i].set_xlabel(f"Class={c}, {t} examples", fontsize=14)
    plt.show()
    return X_train, y_train
X_train, y_train = load_mnist()
```



1.1 EM algorithm for Multivariate Bernoulli Mixture

One iteration of EM updates π_k and μ_k as follows

$$P(x|\mu_k) = \prod_{i=1}^{D} \mu_{ki}^{x_i} (1 - \mu_{ki})^{(1-x_i)}$$

$$\gamma_{nk} = \frac{\pi_k P(x_n|\mu_k)}{\sum_{j=1}^{K} \pi_j P(x_n|\mu_j)}$$

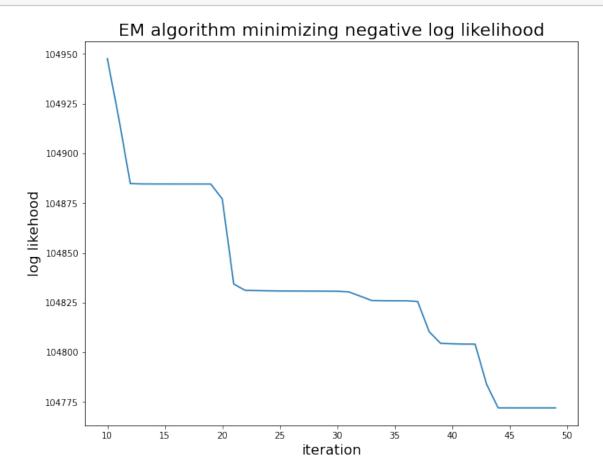
$$N_k = \sum_{n=1}^{N} \gamma_{nk}$$

$$\mu_k = \frac{\sum_{n=1}^{N} \gamma_{nk} x_n}{N_k}$$

```
p_n = np.prod(p_nd, axis=1) # product over dimensions, axis=1
    return p_n
def getGamma(self, X_nd):
    g_kn = np.array([
        self.pi[k, 0] * self.prob(X_nd, k)
        for k in range(Config.K)
    ]) # (k n)
    denom = g_kn.sum(axis=0, keepdims=True)
    denom[denom == 0.0] = 1
    g_kn /= denom # sum over clusters (k) must be one
    return g_kn, denom
def oneIteration(self, X_nd):
    """Performs one iteration of the EM algorithm for bernoulli mix model
    Args
        * X_nd is an np.array with n examples, each of d dimensions
    Function
        * updates Params.mu and Params.pi
    g_kn, denom = self.getGamma(X_nd)
    \# N_k is gamma summed over n
    N_k = g_kn.sum(axis=1, keepdims=True) # shape (k,)
    # new mu is examples averaged over gamma
    mu_kd = np.matmul(g_kn, X_nd)
    self.mu = mu_kd / N_k
    self.pi = N_k / Config.N
    # return log likelihood
    return - np.log(denom).sum()
def fit(self, X_train):
    return [
        self.oneIteration(X_train)
        for i in range(Config.iterations)
    1
```

```
[3]: model = BernoulliMixtureModel()
neg_log_likelihoods = model.fit(X_train)
fig, ax = plt.subplots(figsize=(10, 8))
ax.plot(range(10, Config.iterations), neg_log_likelihoods[10:])
ax.set_ylabel('log likehood', fontsize=16)
ax.set_xlabel('iteration', fontsize=16)
```

ax.set_title('EM algorithm minimizing negative log likelihood', fontsize=20);



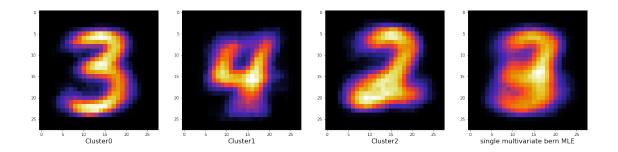
1.2 Most likely estimate for Single Multivariate Bernoulli

$$Z = [z_i] \in \mathbb{R}^d$$

$$Z_{mle} = \frac{\sum_{n=1}^{N} X_i}{N}$$

```
[4]: # display EM algo mus
images = (model.mu * 255).reshape((Config.K, 28, 28)).astype(np.uint8)
fig, axs = plt.subplots(1, 4, figsize=(24, 6))
for k in range(Config.K):
    axs[k].imshow(images[k], cmap='CMRmap')
    axs[k].set_xlabel(f'Cluster{k}', fontsize=16)

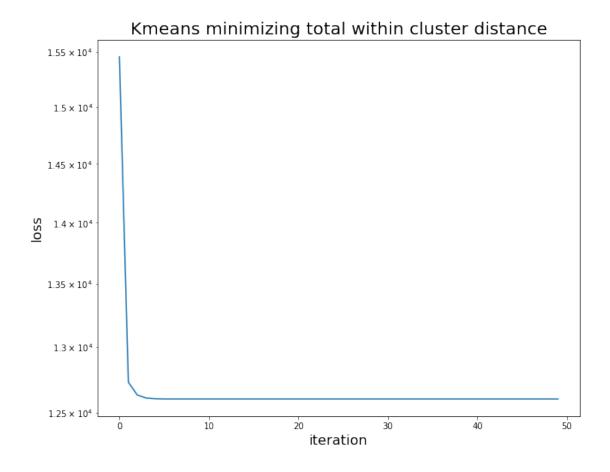
img = (X_train.mean(axis=0) * 255).reshape((28, 28)).astype(np.uint8)
axs[Config.K].imshow(img, cmap='CMRmap')
axs[Config.K].set_xlabel('single multivariate bern MLE', fontsize=16)
plt.show()
```

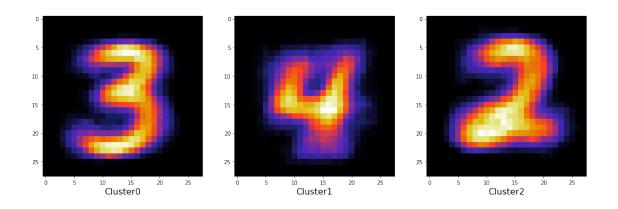


1.3 K-means clustering for MNIST

```
[5]: class Kmeans:
         # standardize data
         def standardize(self, X_train):
             sigma = X_train.std(axis=0, keepdims=True)
             sigma[sigma == 0] = 1
             X_stan = X_train / sigma
             return X_stan, sigma
         def fit(self, X_train):
             # init means as K random points from data
             X_stan, sigma = self.standardize(X_train)
             idx = np.random.choice(np.arange(Config.N), Config.K)
             self.mu = X_stan[idx] * 1.0
             # init assign
             z_n = np.random.choice(np.arange(Config.K), Config.N)
             losses = []
             for i in range(Config.iterations):
                 # calc pairwise dists (ND - K1D -> KN shapes for ref)
                 d_kn = np.linalg.norm(X_stan - self.mu[:,None,:], axis=-1)
                 # assign cluster based on proximity
                 z_n = d_kn.argmin(axis=0) # N
                 losses.append(d_kn.min(axis=0).sum())
                 # update cluster means
                 z_{kn} = np.eye(3)[:, z_n] # 3 N
                 z_kn/= z_kn.sum(axis=1, keepdims=True) # normalize
                 self.mu = z_kn @ X_stan
             self.mu = self.mu * sigma
             return losses
         def predict(self, X):
```

```
d_kn = np.linalg.norm(X - self.mu[:,None,:], axis=-1)
        # assign cluster based on proximity
        z_n = d_kn.argmin(axis=0) # N
       return z_n
   def plot(self, losses, display_means=True):
       fig, ax = plt.subplots(figsize=(10, 8))
       ax.plot(range(Config.iterations), losses)
        ax.set_ylabel('loss', fontsize=16)
        ax.set_xlabel('iteration', fontsize=16)
        ax.set_title('Kmeans minimizing total within cluster distance', __
 →fontsize=20)
       plt.yscale('log')
       plt.show()
        # display the k means
        if display_means:
            images = (model.mu * 255).reshape((Config.K, 28, 28)).astype(np.
→uint8)
           fig, axs = plt.subplots(1, 3, figsize=(18, 6))
            for k in range(Config.K):
                axs[k].imshow(images[k], cmap='CMRmap')
                axs[k].set_xlabel(f'Cluster{k}', fontsize=16)
            plt.show()
model = Kmeans()
losses = model.fit(X_train)
model.plot(losses)
```

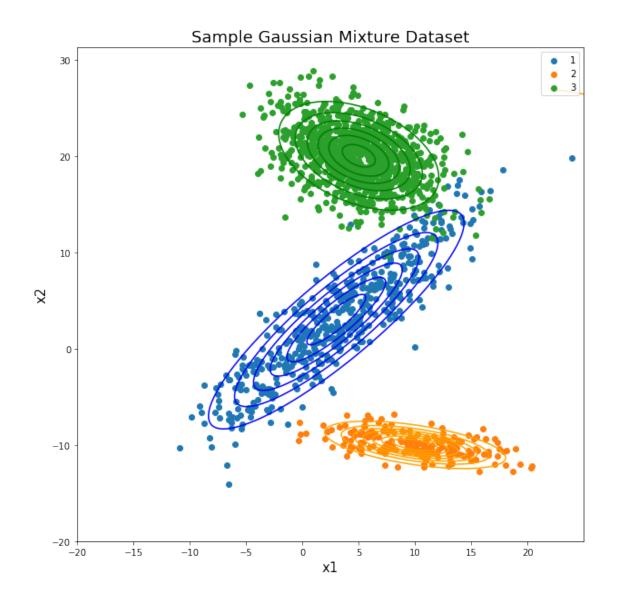




2 GMM on custom data

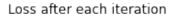
Sample data from univariate and multivariate Gaussian Mixture Models and verify whether EM algorithm is able to retrieve the mixture densities in each of the case.

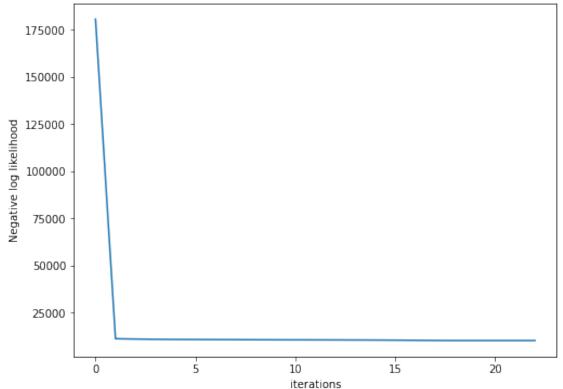
```
[6]: # Config has hardcoded values and are not meant to be changed at all for this.
      \rightarrownotebook
     class Config:
         N = 1700
         K = 3 \# theser
         D = 2 # dont change this we need 2d for interpretting plots
         iterations = 75
         eps = 1e-3
     class Actual:
         mu = np.array([[3,3], [10, -10], [5, 20]])
         cov_norot = [
             [[4, 0], [0, 64]],
             [[16, 0], [0, 1]],
             [[16, 0], [0, 6]]
         ]
         cov = []
         rots = [45, 10, 30]
         sizes = [500, 200, 1000]
     def rotate2D(theta):
         c, s = np.cos(theta), np.sin(theta)
         return np.array([[c, -s],[s, c]])
     def sampleMultiGaussian(mu, cov, theta, size):
         R = rotate2D(theta)
         Actual.cov.append(R.T @ cov @ R)
         return np.random.multivariate normal(mu, Actual.cov[-1], size=size)
     def sampleDistriubtion():
         fig, ax = plt.subplots(figsize=(10, 10))
         X train = []
         y_train = []
         x_grid = np.arange(-20, 25, .02)
         y_grid = np.arange(-20, 27, .02)
         x_grid, y_grid = np.meshgrid(x_grid, y_grid)
         coordinates = np.array([x_grid.ravel(), y_grid.ravel()]).T
         colors = ['blue', 'orange', 'green']
         for i in range(Config.K):
             samples = sampleMultiGaussian(Actual.mu[i], Actual.cov_norot[i],
                         theta=np.radians(Actual.rots[i]), size=Actual.sizes[i])
             labels = np.ones(Actual.sizes[i]) * i
             X_train.append(samples)
             y_train.append(labels)
             ax.scatter(samples[:,0], samples[:, 1], label=str(i+1))
```



```
if len(nll) > 1 and np.abs(loss - nll[-2]) < Config.eps:
               break
       return nll
   # helpers
   def prob(self, X_nd, k): # (examples, k) -> [P(example1 | k),__
\rightarrow P(example2|k), ...]
       mu 1d = self.mu[k:k+1]
       cov_dd = self.cov[k]
       z_nd = X_nd - mu_1d
       A_nd = (z_nd @ np.linalg.inv(cov_dd))
       z_n = (A_nd * z_nd).sum(axis=1)
       p_n = (2*np.pi) ** (- Config.D / 2) * np.linalg.det(cov_dd) ** -.5 *_
\rightarrownp.exp(-.5 * z_n)
       return p_n
   def getGamma(self, X_nd):
       g_kn = np.array([
           self.pi[k, 0] * self.prob(X_nd, k)
           for k in range(Config.K)
       ]) # (k n)
       denom = g_kn.sum(axis=0, keepdims=True)
       denom[denom == 0.0] = 1
       g_kn /= denom # sum over clusters (k) must be one
       return g_kn, denom
   def em_one_iteration(self, X_nd):
       """Performs one iteration of the EM algorithm for gaussian mixture model
           * X_nd is an np.array with n examples, each of d dimensions
       Function
           * updates Params.mu, Params.cov and Params.pi
       g_kn, denom = self.getGamma(X_nd)
       \# N_k is gamma summed over n
       N_k1 = g_{n.sum}(axis=1, keepdims=True) # shape (k,1)
       # new mu is examples averaged over gamma
       self.mu = np.matmul(g_kn, X_nd) / N_k1
       self.pi = N_k1 / Config.N
       # new mean is used to calculate new cov
       # calculate cov as E[x-mu] but over dist of reponse coeff
       for k in range(Config.K):
           g_n1 = g_kn[k:k+1].T
```

```
z_nd = X_nd - self.mu[k:k+1]
            self.cov[k] = ((g_n1 * z_nd).T @ z_nd) / N_k1[k]
        # return log likelihood
        neg_log_likelihood = - np.log(denom).sum()
        return neg_log_likelihood
model = GaussianMixtureModel()
nll = model.fit(X_train)
fig, ax = plt.subplots(figsize=(8, 6))
plt.plot(nll)
plt.xlabel('iterations')
plt.ylabel('Negative log likelihood')
plt.title('Loss after each iteration')
plt.show()
print("Model means:")
print(model.mu)
print()
print("Actual means:")
print(Actual.mu)
```



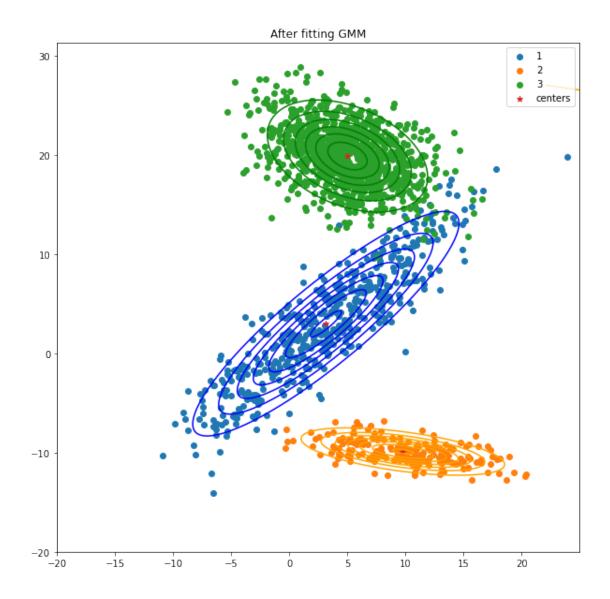


```
Model means:
[[ 5.00015899 19.8556918 ]
  [ 9.76671785 -9.90188685]
  [ 3.14197768 2.97072897]]

Actual means:
[[ 3 3]
  [ 10 -10]
  [ 5 20]]
```

2.1 Plotting learned distributions

```
[8]: fig, ax = plt.subplots(figsize=(10, 10))
     parts = np.cumsum([0] + Actual.sizes)
     x_grid = np.arange(-20, 25, .02)
     y_grid = np.arange(-20, 27, .02)
     x_grid, y_grid = np.meshgrid(x_grid, y_grid)
     coordinates = np.array([x_grid.ravel(), y_grid.ravel()]).T
     colors = ['green', 'orange', 'blue']
     for k in range(Config.K):
         x = X_train[parts[k]:parts[k+1]]
         ax.scatter(x[:,0], x[:,1], label=str(k+1))
         z grid = scipy.stats.multivariate_normal(model.mu[k], model.cov[k]).
      \rightarrowpdf(coordinates).reshape(x_grid.shape)
         ax.contour(x_grid, y_grid, z_grid, colors=colors[k])
     ax.scatter(model.mu[:,0], model.mu[:,1], marker='*', label='centers')
     ax.set_title('After fitting GMM')
     plt.legend();
```



3 Parzen Window and K-means on the same custom data

Run K-Means and Parzen Window/Kernel density estimation on dataset generated in question 2 and compare the results with EM algorithm. Try different window sizes and different kernels for Kernel density estimation. Compare it with histogram based density estimation.

```
[9]: model = Kmeans()
losses = model.fit(X_train)
model.plot(losses, display_means=False)
labels = model.predict(X_train)

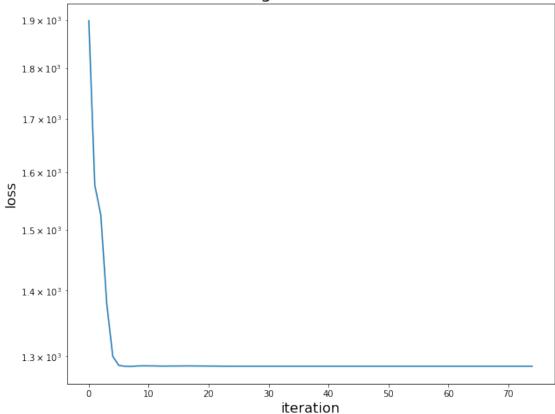
# plotting clusters got by model
fig, ax = plt.subplots(figsize=(10, 10))
```

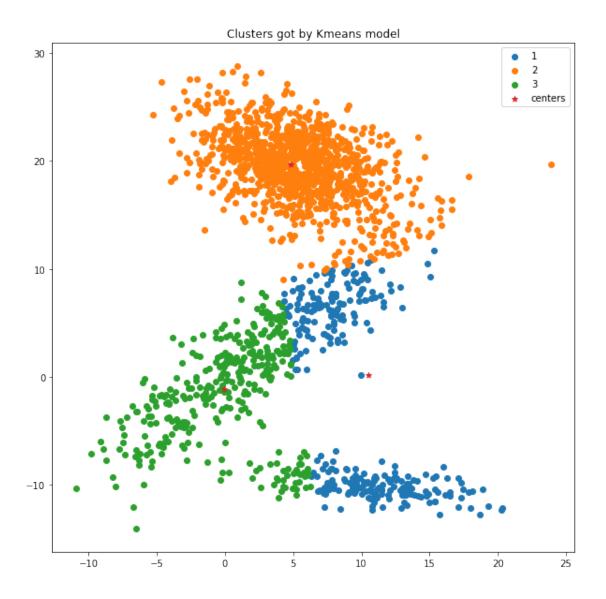
```
colors = ['blue', 'green', 'orange']

for k in range(Config.K):
    x = X_train[labels == k]
    ax.scatter(x[:,0], x[:,1], label=str(k+1))

ax.scatter(model.mu[:,0], model.mu[:,1], marker='*', label='centers')
ax.set_title('Clusters got by Kmeans model')
plt.legend();
```





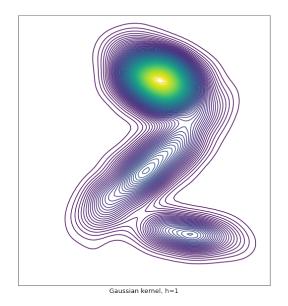


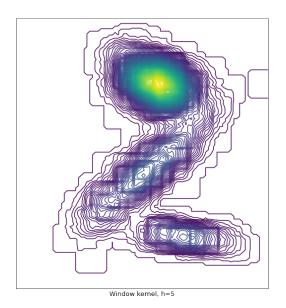
```
def __init__(self, X_train, h, kernel='gaussian'):
    self.X = X_train
    self.h = h
    if kernel.lower() == 'gaussian':
        self.kernel = gaussianKernel
    else:
        self.kernel = windowKernel

def predict(self, X_t):
    z_mtd = (X_t - self.X[:,None,:]) / self.h
    phi_t = self.kernel(z_mtd, self.h)
    return phi_t
```

```
[11]: x_{grid} = np.arange(-20, 25, .5)
      y_grid = np.arange(-20, 33, .5)
      x_grid, y_grid = np.meshgrid(x_grid, y_grid)
      coordinates = np.array([x_grid.ravel(), y_grid.ravel()]).T
      model_gk = ParzenWindow(X_train, 2, 'gaussian')
      density_g = model_gk.predict(coordinates).reshape(x_grid.shape)
      model_wk = ParzenWindow(X_train, 5, 'window')
      density_w = model_wk.predict(coordinates).reshape(x_grid.shape)
      fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(20, 10))
      fig.suptitle('Parzen window density estimation', fontsize=18)
      ax1.contour(x_grid, y_grid, density_g, levels=np.linspace(density_g.min(),_
      →density_g.max(), num=100))
      ax1.set_xlabel('Gaussian kernel, h=1', fontsize=13)
      ax1.set(xticks=[], yticks=[])
      ax2.contour(x_grid, y_grid, density_w, levels=np.linspace(density_w.min(),_

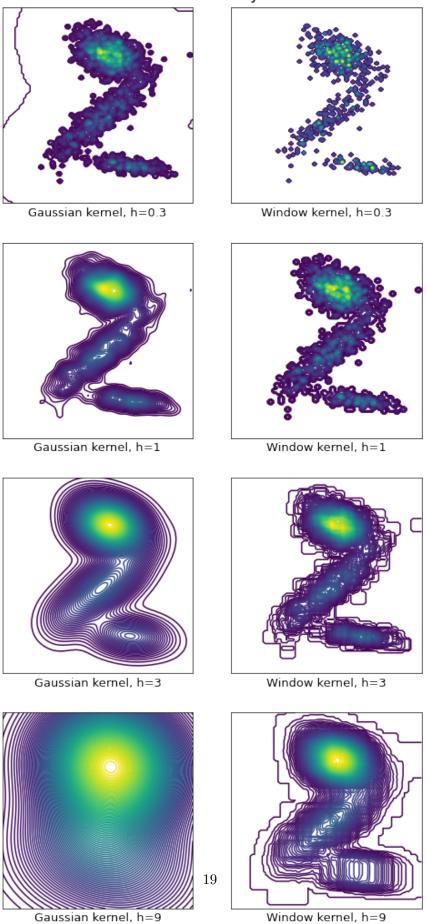
density_w.max(), num=100))
      ax2.set_xlabel('Window kernel, h=5', fontsize=13)
      ax2.set(xticks=[], yticks=[]);
```





[12]: h_list = [0.3, 1, 3, 9] fig, axs = plt.subplots(len(h_list), 2, figsize=(8, 16),__ ⇒gridspec_kw=dict(left=0.1, right=0.9, bottom=0.1, top=0.96)) plt.subplots_adjust(top=0.8) fig.suptitle('Parzen window density estimation', fontsize=18) for i, h in enumerate(h_list): model_gk = ParzenWindow(X_train, h, 'gaussian') density_g = model_gk.predict(coordinates).reshape(x_grid.shape) model_wk = ParzenWindow(X_train, h, 'window') density_w = model_wk.predict(coordinates).reshape(x_grid.shape) ax1, ax2 = axs[i,0], axs[i,1]ax1.contour(x_grid, y_grid, density_g, levels=np.linspace(density_g.min(),_ density_g.max(), num=100)) ax1.set_xlabel(f'Gaussian kernel, h={h}', fontsize=13) ax1.set(xticks=[], yticks=[]) ax2.contour(x_grid, y_grid, density_w, levels=np.linspace(density_w.min(),_ density_w.max(), num=100)) ax2.set_xlabel(f'Window kernel, h={h}', fontsize=13) ax2.set(xticks=[], yticks=[]); plt.show()

Parzen window density estimation



- As the window size increases, the density function becomes smoother and smoother.
- Small window sizes => density function changes over small changes in position
- Large window sizes => even if we add points in a small region, a larger surrounding will have its density function value changed because of the large window size. The contour plot is a graphical representation of the same.

3.1 GD GMM

- $\pi_k \in [0,1]$ and $\sum \pi_k = 1$ then we declare a unconstrained variable ξ_k such that $\pi = softmax(\xi)$
- The covariance matrices must be positive semidefinite. so we declare unconstrained matrices M_k such that $\sum_{k=1}^{\infty} M_k M_k^T$

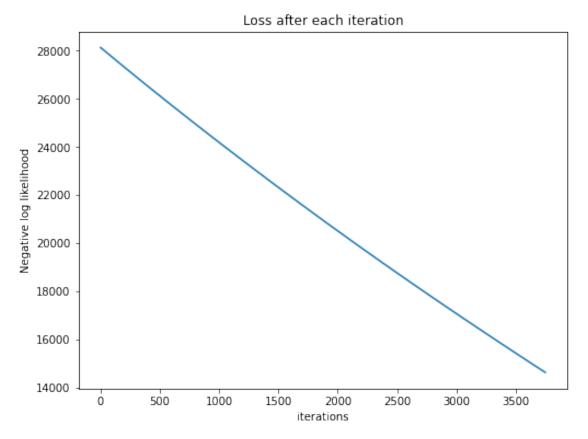
```
[13]: np.random.seed(42)
      class GaussianMixtureModelGrad:
          def fit(self, X_train):
              self.si = np.zeros((Config.K,1))
                                                                                 \# pi_k
              # pi is softmax(si)
              idx = np.random.choice(np.arange(Config.N), Config.K)
              self.mu = X_train[idx] * 1.0 # choose K samples randomly from dist
              # correct mu
      #
                self.mu = np.array([[3,3], [10, -10], [5, 20]]).astype(np.float32)
              self.precision = np.array([np.random.randn(Config.D, Config.D) for i in_
       →range(Config.K)]) # init K covs to identity
              self.eta = 2e-3/Config.N
              nll = []
              for i in range(Config.iterations*50):
                  loss = self.gd_one_iteration(X_train)
                  nll.append(loss)
              return nll
          # helpers
          def prob(self, X_nd, k): # (examples, k) -> [P(example1 | k),
       \rightarrow P(example2/k), ...]
              mu_1d = self.mu[k:k+1]
                inv\_cov\_dd = self.precision[k] @ self.precision[k].T
              inv_cov_dd = np.linalg.inv(Actual.cov[k])
              z_nd = X_nd - mu_1d
              A_nd = z_nd @ inv_cov_dd
              z_n = (A_nd * z_nd).sum(axis=1)
              p_n = (2*np.pi) ** (- Config.D / 2) * np.linalg.det(inv_cov_dd) ** .5_U
       \rightarrow* np.exp(-.5 * z_n)
              return p_n
```

```
def getGamma(self, X_nd):
       g_kn = np.array([
            np.exp(self.si[k, 0]) * self.prob(X_nd, k)
           for k in range(Config.K)
       ]) # (k n)
       denom = g_kn.sum(axis=0, keepdims=True)
       denom[denom == 0.0] = 1
       g kn /= denom # sum over clusters (k) must be one
       return g_kn, denom
   def gd_one_iteration(self, X_nd):
        """Performs one iteration of the gradient descent for gaussian mixture_\sqcup
\hookrightarrow model
       Args
            * X_nd is an np.array with n examples, each of d dimensions
       Function
            * updates Params.mu, Params.cov and Params.pi
       g_kn, denom = self.getGamma(X_nd)
       \# N_k is gamma summed over n
       N_k1 = g_{kn.sum}(axis=1, keepdims=True) # shape (k,1)
       # new mu is examples averaged over gamma
       for k in range(Config.K):
            z_nd = X_nd - self.mu[k:k+1]
           g_n1 = g_kn[k:k+1].T
              inv_cov = self.precision[k] @ self.precision[k].T
            inv_cov = np.linalg.inv(Actual.cov[k])
            delta_mu = g_n1.T @ (inv_cov @ z_nd.T).T
            # delta\_cov = .5 * (inv\_cov @ ((q\_n1 * z\_nd).T @ z\_nd) @ inv\_cov -__
\hookrightarrow N_k1[k] * inv_cov)
              delta_precision = np.linalq.inv(self.precision[k].T) * N_k1[k] - 1
\rightarrow self.precision[k] @ ((g_n1 * z_nd).T @ z_nd)
              self.precision[k] += self.eta * delta_precision
            self.mu[k:k+1] += self.eta * delta_mu
       delta_si = N_k1
       self.si += self.eta * delta_si
       # return log likelihood
       neg_log_likelihood = - np.log(denom).sum()
       return neg_log_likelihood
```

```
model = GaussianMixtureModelGrad()
nll = model.fit(X_train)
fig, ax = plt.subplots(figsize=(8, 6))
plt.plot(nll)
plt.xlabel('iterations')
plt.ylabel('Negative log likelihood')
plt.title('Loss after each iteration')
plt.show()

print("Model means:")
print(model.mu)
print()
print("Actual means:")
print(Actual.mu)

print(model.si)
```



```
Model means:
[[ 9.56550783 17.95945598]
[ 4.56785114 15.78477678]
```

```
[ 6.97719713 18.4234213 ]]
     Actual means:
     [[ 3
             3]
      [ 10 -10]
      [ 5 20]]
     [[2.89094286]
      [0.40089697]
      [4.20816017]]
[14]: fig, ax = plt.subplots(figsize=(10, 10))
      parts = np.cumsum([0] + Actual.sizes)
      x_grid = np.arange(-20, 25, .02)
      y_grid = np.arange(-20, 27, .02)
      x_grid, y_grid = np.meshgrid(x_grid, y_grid)
      coordinates = np.array([x_grid.ravel(), y_grid.ravel()]).T
      colors = ['green', 'orange', 'blue']
      for k in range(Config.K):
          x = X_train[parts[k]:parts[k+1]]
          ax.scatter(x[:,0], x[:,1], label=str(k+1))
          cov = np.linalg.inv(model.precision[k] @ model.precision[k].T)
          z_grid = scipy.stats.multivariate_normal(model.mu[k], cov).pdf(coordinates).
       →reshape(x_grid.shape)
          ax.contour(x_grid, y_grid, z_grid, colors=colors[k])
      ax.scatter(model.mu[:,0], model.mu[:,1], marker='*', label='centers')
      ax.set_title('After fitting GMM')
      plt.legend();
```

