Statistical Methods in Image Processing EE-048954

Homework 3: Contrastive Divergence and Noise Contrastive Estimation

Due Date: June 16, 2022

Submission Guidelines

- Submission only in **pairs** on the course website (Moodle).
- Working environment:
  - We encourage you to work in `Jupyter Notebook` online using Google Colab as it does not require any installation.
- You should submit two **separated** files:
  - A `.ipynb` file, with the name: `ee048954_hw3_id1_id2.ipynb` which contains your code implementations.
  - A `.pdf` file, with the name: `ee048954_hw3_id1_id2.pdf` which is your report containing plots, answers, and discussions.
  - **No handwritten submissions** and no other file-types (`.docx`, `.html`, ...) will be accepted.

Mounting your drive for saving/loading stuff

In [ ]:
```
#from google.colab import drive
#drive.mount('/content/drive')
```

Importing relevant libraries

In [1]:
```
## Standard libraries
import os
import math
import time
import numpy as np
import random
import copy

## Scipy optimization routines
from scipy.optimize import minimize

## Progress bar
import tqdm

## Imports for plotting
import matplotlib.pyplot as plt
import matplotlib.animation as animation
%matplotlib inline
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
plt.style.use('ggplot')
```

Part I: Contrastive Divergence (50 points)

Consider the following Gaussian Mixture Model (GMM) distribution

$$p(x;\{\mu_i\}) = \sum_{i=1}^{N} \frac{1}{N}\frac{1}{2\pi}\exp\left\{-\frac{1}{2}||x-\mu_i||^2\right\},$$

where $x, \mu_i \in \mathbb{R}^2$. We will use $N=4$, $\sigma=1$, and $\{\mu_i\} = \{(0,0)^T, (0,3)^T, (3,0)^T, (3,3)^T\}$.

Sampling from GMM

Task 1. Direct sampling: Use your function from HW1 that accepts $\{\mu_i\}$, and returns a sample x from $p(x;\{\mu_i\})$. Draw $J=1000$ samples $\{x\}$ from the distribution $p(x;\{\mu_i\})$ using this function. These will be our **real samples**.

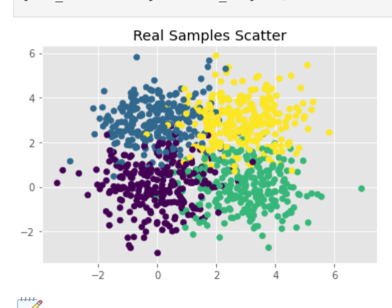
In [2]:
```
def plot_scatter(samples, title, group=None):
    if group is not None:
        plt.scatter(samples[:, 0], samples[:, 1], c=group)
    else:
        plt.scatter(samples[:, 0], samples[:, 1])
    plt.title(title)
    plt.show()
```

In [3]:
```
def sub_plot_scatter(samples_list, titles_list, width, figsize=(15,5)):
    N = len(samples_list)
    fig, axes = plt.subplots(1, 2, figsize=figsize)
    rows = int(N/width)

    for i in range(rows):
        for j in range(width):
            idx = rows * i + j
            if rows > 1:
                axes[i,j] = plt.scatter(samples_list[idx][:, 0], samples_list[idx][:, 1])
                axes[i,j].set_title(titles_list[idx])
            else:
                axes[idx].set_title(titles_list[idx])
                axes[idx].scatter(samples_list[idx][:, 0], samples_list[idx][:, 1])
```

In [4]:
```
def mix_gauss_draw(N=4, sigma=1, mu=[np.array([0,0]),
                                     np.array([0,3]),
                                     np.array([3,0]),
                                     np.array([3,3])], J=1_000):

    Sigma = np.eye(len(mu[0])) * (sigma ** 2)
    X = np.zeros([J, len(mu[0])])
    G = np.zeros([J, 1])

    for i in range(J):
        m = np.random.choice(N,1)
        Mu = mu[int(m)]
        x = np.random.multivariate_normal(mean=Mu, cov=Sigma)
        X[i] = x
        G[i] = m
    return X, G
```

In [5]:
```
real_samples, groups = mix_gauss_draw(sigma=1)
```

In [6]:
```
plot_scatter(samples=real_samples, title='Real Samples Scatter', group=groups)
```



Task 2. Sampling with MCMC: implement the MALA algorithm to draw samples from $p(x;\{\mu_i\})$. The function will get an initial guess $\{\hat{x}_i\}$ and will generate chains of length L. Use $\sqrt{2\varepsilon} = 0.1$ and $N \sim \mathcal{N}(0, I)$.

In [7]:
```
def log_gradient_p(x, sigma_2=1,
                   mu=[np.array([0,0]), np.array([0,3]),
                       np.array([3,0]), np.array([3,3])]):
    N = len(mu)
    denominator = 0
    for i in range(N):
        denominator += np.exp((-1/(2*sigma_2)) * np.linalg.norm(x-mu[i], axis=1) ** 2 )
    denominator = np.reshape(denominator, (denominator.shape[0],1))

    nominator = 0
    for i in range(N):
        s = (np.exp((-1/(2*sigma_2)) * np.linalg.norm(x-mu[i], axis=1) ** 2 ))
        d = (mu[i] - x).transpose()
        nominator +=  s * d

    return (1/sigma_2) * nominator.transpose() / denominator
```

In [8]:
```
def p(x, sigma_2=1,mu=[np.array([0,0]), np.array([0,3]),
                      np.array([3,0]), np.array([3,3])]):
    N = len(mu)
    sum_exp = 0
    for n in range(N):
        log_exp = -0.5 * (np.linalg.norm(x-mu[n], axis=1) ** 2)
        sum_exp += np.exp(log_exp)
    return (1/N) * (1 /(2*np.pi)) * sum_exp
```

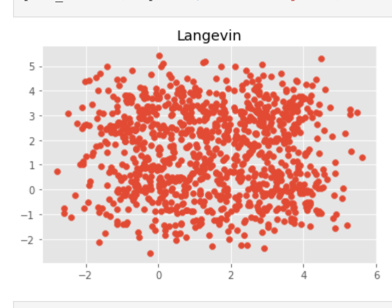
In [9]:
```
def q(x_tag, x, epsilon, mu=[np.array([0,0]), np.array([0,3]),
                             np.array([3,0]), np.array([3,3])]):
    norm = np.linalg.norm(x_tag - x - epsilon * log_gradient_p(x, mu=mu), axis=1) ** 2
    log_q = -norm/(4*epsilon)
    q = np.exp(log_q)
    return q
```

In [10]:
```
def langevin_mala_dynamics(init_guess, steps=5000, samples=1000, sigma_2=1, factored_epsilon=0.1,
                           mu=[np.array([0,0]), np.array([0,3]), np.array([3,0]), np.array([3,3])],
                           MALA=False, verbos=False):
    epsilon = (factored_epsilon ** 2) / 2
    x = init_guess
    mala_reg_update = 0
    mala_alpha_update = 0
    mala_no_update = 0
    for s in tqdm.tqdm(range(steps)):
        noise = np.random.randn(x.shape[0], x.shape[1])
        new_x = x + epsilon * log_gradient_p(x, sigma_2=sigma_2, mu=mu) + factored_epsilon * noise

        if MALA:
            if p(new_x, mu=mu).sum() > p(x, mu=mu).sum():
                x = new_x.copy()
                mala_reg_update += 1
            else:
                p_x = p(x=x, mu=mu).sum()
                p_x_new = p(x=new_x, mu=mu).sum()
                q_x_x_new = q(x_tag=x, x=new_x, epsilon=epsilon, mu=mu).sum()
                q_x_new_x = q(x_tag=new_x, x=x, epsilon=epsilon, mu=mu).sum()
                alpha = (p_x / p_x_new) * (q_x_x_new / q_x_new_x)
                r = np.random.uniform()
                if r < alpha:
                    x = new_x.copy()
                    mala_alpha_update += 1
                else:
                    mala_no_update += 1

        else:
            x = new_x.copy()

    if MALA and verbos:
        print(mala_reg_update / steps)
        print(mala_alpha_update / steps)
        print(mala_no_update / steps)

    return x
```

In [11]:
```
init_guess = np.random.uniform(low=0, high=3, size=(1_000, 2))
x = langevin_mala_dynamics(init_guess=init_guess, steps=10_000, samples=1_000, MALA=False, sigma_2=1)
```

```
100%|██████████| 10000/10000 [00:05<00:00, 180
9.22it/s]
```

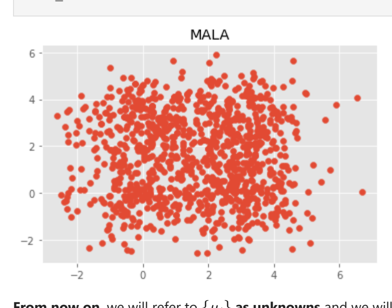
In [12]:
```
plot_scatter(samples=x, title='Langevin')
```



In [13]:
```
init_guess = np.random.uniform(low=0, high=3, size=(1_000, 2))
x = langevin_mala_dynamics(init_guess=init_guess, steps=10_000, samples=1_000, MALA=True, sigma_2=1)
```

```
100%|██████████| 10000/10000 [00:16<00:00, 60
6.90it/s]
```

In [14]:
```
plot_scatter(samples=x, title='MALA')
```



From now on, we will refer to $\{\mu_i\}$ **as unknowns** and we will estimate them using different algorithms.

Estimation of $\{\mu_i\}$

Task 3. Implement Maximum likelihood (ML) estimation of $\{\mu_i\}$ using direct sampling:

- Step 1: Randomly initialize $\{\tilde{\mu}_i\}$ from $U([0,3]^2)$.
- Step 2: Use your function from Task 1 to draw 100 samples $\tilde{x}$ from $p(x;\{\mu_i\})$ using $\{\tilde{\mu}_i\}$.
- Step 3: Update $\{\tilde{\mu}_i\}$ using the ML gradient descent step:

$$\tilde{\mu}_i^{k+1} = \tilde{\mu}_i^k + \eta\left(\langle\nabla_{\mu_i}\log p(x;\{\mu_i\})\rangle_x - \langle\nabla_{\mu_i}\log p(x;\{\mu_i\})\rangle_{\tilde{x}}\right),$$

  where $\langle\cdot\rangle_x$ denotes averaging over the real samples from Task 1 and $\langle\cdot\rangle_{\tilde{x}}$ denotes averaging over the synthetically generated samples from Step 2. Use $\eta = 1$.
- Repeat Step 2 and Step 3 until convergence.

In [15]:
```
def grad_mu_log_p(x, mu):
    N = len(mu)
    denominator = 0
    for n in range(N):
        log_exp = -0.5 * (np.linalg.norm(x-mu[n]) ** 2)
        denominator += np.exp(log_exp)

    nominator = np.zeros([N,2])

    for n in range(N):
        log_exp = -0.5 * (np.linalg.norm(x-mu[n]) ** 2)
        exp = np.exp(log_exp)
        nominator[n] = exp * (x-mu[n])

    return (1/denominator) * nominator
```

In [16]:
```
def avg_grad_mu_log_p(x, mu):
    grad = np.zeros(shape=mu.shape)
    for x_i in x:
        grad += grad_mu_log_p(x=x_i, mu=mu)
    return grad / x.shape[0]
```

In [17]:
```
def ML_DS(N, real_samples, etta=1, draw_mcmc=False, init_task_1=False):
    mu_hat = np.random.uniform(size=[N,2]) * 3
    step_idx = 0
    while True:
        if draw_mcmc:
            if init_task_1:
                init_guess, _ = mix_gauss_draw(N=N, sigma=1, J=100) # using original mu's
                x_hat = langevin_mala_dynamics(init_guess=init_guess, steps=10, samples=100, MALA=True, sigma_2
            else:
                init_guess = np.random.randn(100, 2) * np.sqrt(2) + 1.5
                x_hat = langevin_mala_dynamics(init_guess=init_guess, steps=1_000, samples=100, MALA=True, sigm
        else:
            x_hat, _ = mix_gauss_draw(N=N, sigma=1, mu=mu_hat, J=100)
        avg_mu_grad_estim = avg_grad_mu_log_p(x_hat, mu_hat)
        avg_mu_grad_real = avg_grad_mu_log_p(real_samples, mu_hat)

        old_mu = mu_hat.copy()
        mu_hat = mu_hat + etta * (avg_mu_grad_real - avg_mu_grad_estim)

        step_norm = np.linalg.norm(mu_hat - old_mu)

        if step_norm < 1e-1:
            print(step_norm)
            break

        if step_idx % 10 == 0:
            print(step_norm)
        step_idx += 1

    return mu_hat
```

In [18]:
```
real_samples, groups = mix_gauss_draw(sigma=1)
estim_mu = ML_DS(N=4, real_samples=real_samples, etta=1)
print("Estimated MU:\n", estim_mu)
```

```
0.2558766679562691
0.21107447927951567
0.1263122438198493
0.08803442535979092
Estimated MU:
 [[ 3.01091859  0.03061885]
 [-0.01691787  3.00878443]
 [ 2.9861965   2.99639136]
 [-0.07696866 -0.04974094]]
```

Task 4. Implement Maximum likelihood (ML) estimation of $\{\mu_i\}$ using MCMC:

- Step 1: Randomly initialize $\{\tilde{\mu}_i\}$ from $U([0,3]^2)$.
- Step 2: Use your function from Task 2 to draw 100 samples $\tilde{x}$ from $p(x;\{\mu_i\})$ using $\{\tilde{\mu}_i\}$. Initialize the chains with $\hat{x}_i \sim \mathcal{N}(1.5, 2)$ and use chains length of $L = 1000$.
- Step 3: Update $\{\tilde{\mu}_i\}$ using the ML gradient descent step:

$$\tilde{\mu}_i^{k+1} = \tilde{\mu}_i^k + \eta\left(\langle\nabla_{\mu_i}\log p(x;\{\mu_i\})\rangle_x - \langle\nabla_{\mu_i}\log p(x;\{\mu_i\})\rangle_{\tilde{x}}\right),$$

  where $\langle\cdot\rangle_x$ denotes averaging over the real samples from Task 1 and $\langle\cdot\rangle_{\tilde{x}}$ denotes averaging over the synthetically generated samples from Step 2. Use $\eta = 1$.
- Repeat Step 2 and Step 3 until convergence.

In [19]:
```
estim_mu_mala = ML_DS(N=4, real_samples=real_samples, etta=1, draw_mcmc=True)
print("Estimated MU:\n", estim_mu_mala)
```

```
100%|██████████| 1000/1000 [00:00<00:00, 115
3.55it/s]
0.45575212224887335
100%|██████████| 1000/1000 [00:00<00:00, 119
4.50it/s]
100%|██████████| 1000/1000 [00:00<00:00, 124
3.23it/s]
100%|██████████| 1000/1000 [00:00<00:00, 122
6.41it/s]
100%|██████████| 1000/1000 [00:00<00:00, 124
4.78it/s]
100%|██████████| 1000/1000 [00:00<00:00, 126
9.71it/s]
100%|██████████| 1000/1000 [00:00<00:00, 127
1.85it/s]
100%|██████████| 1000/1000 [00:00<00:00, 123
9.83it/s]
100%|██████████| 1000/1000 [00:00<00:00, 123
3.35it/s]
100%|██████████| 1000/1000 [00:00<00:00, 126
6.69it/s]
100%|██████████| 1000/1000 [00:00<00:00, 116
3.90it/s]
0.12004580897410269
100%|██████████| 1000/1000 [00:00<00:00, 109
7.99it/s]
0.09669773564672267
Estimated MU:
 [[ 2.73926735  3.1403476 ]
 [ 3.07690851  0.132218  ]
 [-0.06140892  0.06579094]
 [-0.10931543  3.10781589]]
```

Task 5. Implement Contrastive Divergence (CD) estimation of $\{\mu_i\}$ using MCMC sampling:

- Step 1: Randomly initialize $\{\tilde{\mu}_i\}$ from $U([0,3]^2)$.
- Step 2: Use your function from Task 2 to draw 100 samples $\tilde{x}$ from $p(x;\{\mu_i\})$ using $\{\tilde{\mu}_i\}$. Initialize the chains with **100 samples randomly chosen from the real set of examples from Task 1**, and use only $L = 10$ update steps.
- Step 3: Update $\{\tilde{\mu}_i\}$ using the CD gradient descent step:

$$\tilde{\mu}_i^{k+1} = \tilde{\mu}_i^k + \eta\left(\langle\nabla_{\mu_i}\log p(x;\{\mu_i\})\rangle_x - \langle\nabla_{\mu_i}\log p(x;\{\mu_i\})\rangle_{\tilde{x}}\right),$$

  where $\langle\cdot\rangle_x$ denotes averaging over the 100 real samples used for initialization of the chains in Step 2 and $\langle\cdot\rangle_{\tilde{x}}$ denotes averaging over the MCMC generated samples from Step 3. Use $\eta = 1$.
- Repeat Step 2 and Step 3 until convergence.

In [22]:
```
estim_mu_mala_init_task_1 = ML_DS(N=4, real_samples=real_samples, etta=1, draw_mcmc=True, init_task_1=True)
print("Estimated MU:\n", estim_mu_mala_init_task_1)
```

```
100%|██████████| 10/10 [00:00<00:00, 248
6.84it/s]
0.2707670236008407
100%|██████████| 10/10 [00:00<00:00, 248
5.66it/s]
100%|██████████| 10/10 [00:00<00:00, 252
7.30it/s]
100%|██████████| 10/10 [00:00<00:00, 248
4.92it/s]
100%|██████████| 10/10 [00:00<00:00, 200
5.02it/s]
100%|██████████| 10/10 [00:00<00:00, 125
3.04it/s]
100%|██████████| 10/10 [00:00<00:00, 166
8.58it/s]
100%|██████████| 10/10 [00:00<00:00, 245
8.70it/s]
100%|██████████| 10/10 [00:00<00:00, 247
4.22it/s]
100%|██████████| 10/10 [00:00<00:00, 250
6.61it/s]
100%|██████████| 10/10 [00:00<00:00, 167
1.37it/s]
0.1205612773427741
100%|██████████| 10/10 [00:00<00:00, 143
2.33it/s]
100%|██████████| 10/10 [00:00<00:00, 200
9.83it/s]
0.09028178109519877
Estimated MU:
 [[ 3.29127853  0.60871475]
 [ 1.08688689 -0.55987471]
 [ 2.44252935  3.45389101]
 [ 0.05760177  2.03691587]]
```

Task 6. Present the estimated $\{\mu_i\}$ and the final random samples $\{\tilde{x}_i\}$ generated with each of the three algorithms in Tasks 3-5. Discuss the differences in convergence.

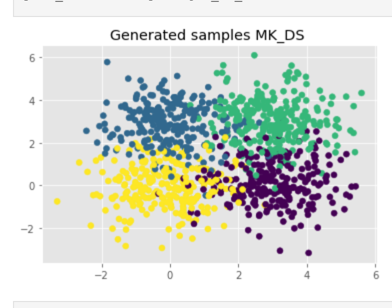
In [23]:
```
import itertools
def calc_diff_mu(mu_hat, mu=[np.array([0,0]), np.array([0,3]), np.array([3,0]), np.array([3,3])]):
    mu = np.array(mu)
    permutations = np.array(list(itertools.permutations(mu_hat)))
    min_tot_err = 1e6

    for perm in permutations:
        tot_err = np.linalg.norm(mu-perm) ** 2

        if tot_err <  min_tot_err:
            min_tot_err = tot_err

    return min_tot_err
```

In [24]:
```
print("Task 3:\n", estim_mu)
print("Squared Error: ", calc_diff_mu(mu_hat=estim_mu))
print("\nTask 4:\n", estim_mu_mala)
print("Squared Error: ", calc_diff_mu(mu_hat=estim_mu_mala))
print("\nTask 5:\n", estim_mu_mala_init_task_1)
print("Squared Error: ", calc_diff_mu(mu_hat=estim_mu_mala_init_task_1))
```

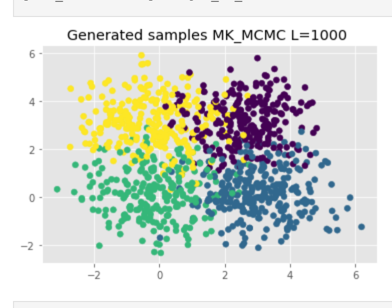
```
Task 3:
 [[ 3.01091859  0.03061885]
 [-0.01691787  3.00878443]
 [ 2.9861965   2.99639136]
 [-0.07696866 -0.04974094]]
Squared Error:  0.010022005521795623

Task 4:
 [[ 2.73926735  3.1403476 ]
 [ 3.07690851  0.132218  ]
 [-0.06140892  0.06579094]
 [-0.10931543  3.10781589]]
Squared Error:  0.1427491165494605

Task 5:
 [[ 3.29127853  0.60871475]
 [ 1.08688689 -0.55987471]
 [ 2.44252935  3.45389101]
 [ 0.05760177  2.03691587]]
Squared Error:  3.3977992119222185
```

In [25]:
```
gen_mu_3, g_3=mix_gauss_draw(mu=estim_mu)
gen_mu_4, g_4=mix_gauss_draw(mu=estim_mu_mala)
gen_mu_5, g_5=mix_gauss_draw(mu=estim_mu_mala_init_task_1)
```

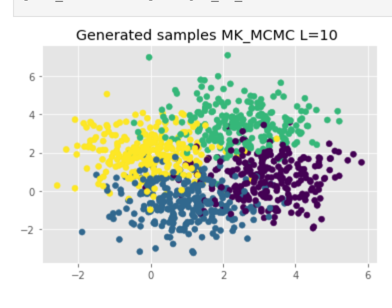
In [26]:
```
plot_scatter(samples=gen_mu_3, title='Generated samples MK_DS ', group=g_3)
```



In [27]:
```
plot_scatter(samples=gen_mu_4, title='Generated samples MK_MCMC L=1000 ', group=g_4)
```



In [28]:
```
plot_scatter(samples=gen_mu_5, title='Generated samples MK_MCMC L=10 ', group=g_5)
```



Discussion:

From the plots it's very hard to see any pattern even on the real data. So, to distinguish between the generated samples is even harder.

In order to estimate the diffrences beween the $\hat{\mu}$ we calculated the squared error beween each one and the real μ. Results shows as excpected that the ML estimation based on the real results are the best and the generated samples based on L=10 are worse that generated MCMC samples based on L=1000 as excpected since the L=10 will not converge as good to the real data distribution as L=1000.

Part II: Noise Contrastive Estimation (50 points)

Consider the distribution

$$p_m(x;\{\mu_i\}) = \frac{1}{Z}\sum_{i=1}^{N}\exp\left\{-\frac{1}{2\sigma^2}||x-\mu_i||^2\right\},$$

where $Z \in \mathbb{R}$ is a normalization constant, and $x, \mu_i \in \mathbb{R}^2$.

Sampling from GMM

Task 7. What is the value of Z?

Easy to see that: $\Sigma = I\sigma^2$

$$\Rightarrow \frac{1}{Z} = \frac{1}{N}\cdot\det(2\pi\Sigma)^{-1/2} = \frac{1}{2\pi N\sigma^2}$$

$$\Rightarrow Z = 2\pi N\sigma^2$$

Task 8. Use $N=4$, $\sigma=1$, and $\{\mu_i\} = \{(0,0)^T, (0,3)^T, (3,0)^T, (3,3)^T\}$. Draw $J=1000$ samples $\{x_j\}$ from the distribution $p_m(x;\{\mu_i\})$ using the function from Task 1.

In [29]:
```
real_samples, groups = mix_gauss_draw(N=4, sigma=1, mu=[np.array([0,0]),
                                                        np.array([0,3]),
                                                        np.array([3,0]),
                                                        np.array([3,3])], J=1_000)
```

From now on, we will refer to $\{\mu_i\}$ **as unknowns** and we will estimate them using the Noise Contrastive Estimation method.

Estimation of $\{\mu_i\}$

Task 9. Implement Noise Contrastive Estimation of $\{\mu_i\}$:

- Step 1: Generating the artificial data-set of noise: Draw $J=1000$ samples $\{y_j\}$ from

$$p_n(y;\mu_n) = \frac{1}{2\pi\sigma_n^2}\exp\left\{-\frac{1}{2\sigma_n^2}||y-\mu_n||^2\right\}$$

  using $\mu_n = (1,1)^T$ and $\sigma_n = 2$.
- Step 2: Randomly select an initial guess for the model means $\{\tilde{\mu}_i\}$ from $U([0,3]^2)$.
- Step 3: Update $\{\tilde{\mu}_i\}$ by **maximizing**:

$$\{\tilde{\mu}_i\} = \underset{\{\mu_i\}}{\arg\max}\sum_{j=1}^{J}\left[\ln(h(x_j;\{\mu_i\})) + \ln(1-h(y_j;\{\mu_i\}))\right],$$

  where

$$h(u;\{\mu_i\}) = \frac{p_m(u;\{\mu_i\})}{p_m(u;\{\mu_i\}) + p_n(u;\mu_n)}.$$

  Implementation Tip: This step can be executed using the function `scipy.optimize.minimize` which finds the **minimum** of an (unconstrained) optimization problem (e.g. using the `'BFGS'` method), given a function that calculates the objective and an initial guess (see scipy documentation for more details). In our case, for **maximization**, implement a function that calculates the **minus** of the objective above.

In [30]:
```
def p(x, sigma_squared, means_vec, Z=None):
    N = len(means_vec)
    if Z is None:
        Z = N*2*np.pi*sigma_squared

    sum_exp = 0
    for n in range(N):
        log_exp = -(0.5/sigma_squared) * (np.linalg.norm(x-means_vec[n], axis=1) ** 2)
        sum_exp += np.exp(log_exp)
    return 1/Z * sum_exp


def h(x, mu, Z = None):
    pm = p(x=x, sigma_squared=1,means_vec=mu, Z=Z)
    pn = p(x=x, sigma_squared=4,means_vec=np.array([1,1]))
    return pm/(pm+pn)

def objective(params, *args):

    sum = 0
    real_samples, noise_samples = args[0], args[1]

    mu = params.reshape(-1,2)
    sum = np.sum(np.log(h(x=real_samples, mu=mu)) + np.log(1-h(x=noise_samples, mu=mu)))
    return -sum
```

In [31]:
```
J = 1000
sigma_n=2
mu_n=[np.array([1,1])]
noise_samples_9 = np.random.randn(J, 2) * np.sqrt(sigma_n) + 1
mu_hat_9 = np.random.uniform(size=[4,2]) * 3
```

In [32]:
```
results = minimize(method='BFGS', fun=objective, x0=mu_hat_9, args=(real_samples, noise_samples_9)) #, options=
mu_task_9 = results.x.reshape(-1,2)
print(mu_task_9)
```

```
[[-0.37680239 -0.2867889 ]
 [-0.36224257  3.48330967]
 [ 3.22317244  3.04671973]
 [ 3.26963204 -0.16830731]]
```

We will now regard both $\{\mu_i\}$ **and the normalization constant** Z as unknowns, and will estimate them using Noise Contrastive Estimation.

Task 10. Implement Noise Contrastive Estimation with an **un-normalized** probability model:

- Step 1: Generating the artificial data-set of noise: Draw $J=1000$ samples $\{y_j\}$ from

$$p_n(y;\mu_n) = \frac{1}{2\pi\sigma_n^2}\exp\left\{-\frac{1}{2\sigma_n^2}||y-\mu_n||^2\right\}$$

  using $\mu_n = (1,1)^T$ and $\sigma_n = 2$.
- Step 2: Randomly select an initial guess for the model means $\{\tilde{\mu}_i\}$ from $U([0,3]^2)$, and for the normalization constant Z from $U([0.1,1])$
- Step 3: Update $\{\tilde{\mu}_i\}$ and Z by **maximizing**:

$$\{\tilde{\mu}_i\}, Z = \underset{\{\mu_i\},Z}{\arg\max}\sum_{j=1}^{J}\left[\ln(h(x_j;\{\mu_i\},Z)) + \ln(1-h(y_j;\{\mu_i\},Z))\right],$$

  where

$$h(u;\{\mu_i\},Z) = \frac{p_m(u;\{\mu_i\},Z)}{p_m(u;\{\mu_i\},Z) + p_n(u;\mu_n)}.$$

In [33]:
```
def Objective_Z(params, *args):
    obj_sum = 0
    real_samples, noise_samples = args[0], args[1]
    mu_hat = params[:-1].reshape(-1,2)
    Z = params[-1]
    obj_sum = np.sum(np.log(h(x=real_samples, mu=mu_hat, Z=Z)) + np.log(1-h(x=noise_samples, mu=mu_hat, Z=Z)))

    return -obj_sum
```

In [46]:
```
J = 1000
sigma=2
mu=[np.array([1,1])]
noise_samples_10 = np.random.randn(J, 2) * np.sqrt(2) + 1
mu_hat_10 = np.random.uniform(size=[4,2]) * 3
Z_10 = np.random.uniform() * 0.9 + 0.1
mu_hat_Z = np.append(mu_hat_10, Z_10)
```

In [47]:
```
results_Z = minimize(method='BFGS', fun=Objective_Z, x0=mu_hat_Z, args=(real_samples, noise_samples_10))
mu_task_10 = results_Z.x[:8].reshape(-1,2)
Z_task_10 = results_Z.x[8]
print(Z_task_10)
print(mu_task_10)
```

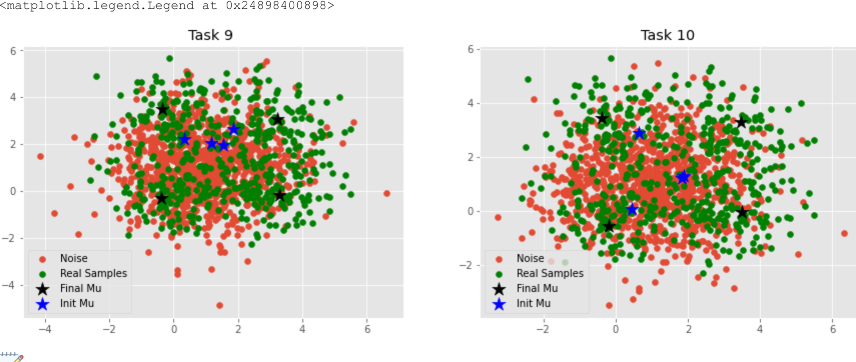
```
19.623383237463372
[[-0.19051958 -0.55742932]
 [-0.38375688  3.44490873]
 [ 3.46101388  3.29148425]
 [ 3.50002984 -0.0390691 ]]
```

Evaluating the Results

Task 11. Visually: plot the estimates of $\{\mu_i\}$ of Tasks 9 and 10 (two separate figures). Include the model samples, the noise samples, the initial guess for the model means, and the final estimates of $\{\tilde{\mu}_i\}$.

In [48]:
```
fig, axes = plt.subplots(1,2, figsize=(15,5))

axes[0].scatter(noise_samples_9[:,0], noise_samples_9[:,1], label='Noise')
axes[0].scatter(real_samples[0:500][:,0], real_samples[0:500][:,1], c='green', label='Real Samples')
axes[0].scatter(mu_task_9[:,0], mu_task_9[:,1], marker="*", s=200, c='black', label='Final Mu')
axes[0].scatter(mu_hat_9[:,0], mu_hat_9[:,1], marker="*", s=200, c='blue', label='Init Mu')
axes[0].set_title('Task 9 ')
axes[0].legend()

axes[1].scatter(noise_samples_10[:,0], noise_samples_10[:,1], label='Noise')
axes[1].scatter(real_samples[0:500][:,0], real_samples[0:500][:,1], c='green', label='Real Samples')
axes[1].scatter(mu_task_10[:,0], mu_task_10[:,1], marker="*", s=200, c='black', label='Final Mu')
axes[1].scatter(mu_hat_10[:,0], mu_hat_10[:,1], marker="*", s=200, c='blue', label='Init Mu')
axes[1].set_title('Task 10 ')
axes[1].legend()
```

Out[48]: `<matplotlib.legend.Legend at 0x24898400898>`



Task 12. Quantitatively: repeat Tasks 9 and 10, this time with $J = 100\times[1,5,10,20,30,50]$. For each value of J repeat the estimation process for 50 times, each time with different realizations for $\{x_j\}$ and $\{y_j\}$ and initial guesses for the estimands ($\{\mu_i\}$ in Task 9 and $\{\mu_i\}, Z$ in Task 10.

For each value of J, calculate the MSE between the true parameter values and their estimates (the mean will be taken over the different realizations). Note that for the model means, the MSE should be calculated to the closest true μ_i for each estimation. If at the same run two estimated μ_is pick the same true μ_i, then this run should be declared as a failure and should be disregarded. Report the number of failure runs.

In [97]:
```
def calc_dist(mu_hat, mu=np.array([[0,0],[0,3],[3,0],[3,3]])):
    map_order = {}
    err = 0
    for idx, m in enumerate(mu_hat):
        err += np.min(np.linalg.norm(mu-m, axis=1) ** 2)
        map_order[idx] = np.argmin(np.linalg.norm(mu-m, axis=1) ** 2)

    if not len(set(map_order.values())) == len(map_order):
        return False, err

    return True, err
```

In [101…
```
dic_res = {}
for J in [100, 150, 1_000, 2_000, 3_000, 5_000]:

    num_fail_9 = 0
    num_fail_10 = 0

    tot_err_9 = 0
    tot_err_10 = 0

    for i in tqdm.tqdm(range(50)):
        real_samples, groups = mix_gauss_draw(N=4, sigma=1, mu=[np.array([0,0]),
                                                                np.array([0,3]),
                                                                np.array([3,0]),
                                                                np.array([3,3])], J=J)

        noise_samples_9 = np.random.randn(J, 2) * np.sqrt(2) + 1
        mu_hat_9 = np.random.uniform(size=[4,2]) * 3

        results = minimize(method='BFGS', fun=objective, x0=mu_hat_9, args=(real_samples, noise_samples_9))
        mu_task_9 = results.x.reshape(-1,2)

        suc, err = calc_dist(mu_task_9)
        num_fail_9 += int(not(suc))
        tot_err_9 += err

        noise_samples_10 = np.random.randn(J, 2) * np.sqrt(2) + 1
        mu_hat_10 = np.random.uniform(size=[4,2]) * 3
        Z_10 = np.random.uniform() * 0.9 + 0.1
        mu_hat_Z = np.append(mu_hat_10, Z_10)

        results_Z = minimize(method='BFGS', fun=Objective_Z, x0=mu_hat_Z, args=(real_samples, noise_samples_10)
        mu_task_10 = results_Z.x[:8].reshape(-1,2)
        Z_task_10 = results_Z.x[8]

        suc, err = calc_dist(mu_task_10)
        num_fail_10 += int(not(suc))
        tot_err_10 += err


    dic_res[(9, J)] = (num_fail_9, tot_err_9)
    dic_res[(10, J)] = (num_fail_10, tot_err_10)
```

```
 10%|█████                                              | 5/50 [00:01<00:08,
5.01it/s]C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\scipy\optimize\optimize.py:663: RuntimeWarning: invalid value encountered in double_scalars
  grad[k] = (f(*((xk + d,) + args)) - f0) / d[k]
C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: invalid value encountered in log

 56%|████████████████████████████                       | 28/50 [00:05<00:05,
4.15it/s]C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: invalid value encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\scipy\optimize\optimize.py:663: RuntimeWarning: invalid value encountered in double_scalars
  grad[k] = (f(*((xk + d,) + args)) - f0) / d[k]
C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: invalid value encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

100%|██████████████████████████████████████████████████| 50/50 [00:10<00:00,
4.66it/s]
 44%|██████████████████████                             | 22/50 [00:04<00:06,
4.43it/s]C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: invalid value encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\scipy\optimize\optimize.py:663: RuntimeWarning: invalid value encountered in double_scalars
  grad[k] = (f(*((xk + d,) + args)) - f0) / d[k]
C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: invalid value encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

100%|██████████████████████████████████████████████████| 50/50 [00:11<00:00,
4.31it/s]
 22%|███████████                                        | 11/50 [00:07<00:25,
1.55it/s]C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\scipy\optimize\optimize.py:663: RuntimeWarning: invalid value encountered in double_scalars
  grad[k] = (f(*((xk + d,) + args)) - f0) / d[k]
C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: divide by zero encountered in log

C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\ipykernel_launcher.py:6: RuntimeWarning: invalid value encountered in log

100%|██████████████████████████████████████████████████| 50/50 [00:34<00:00,
1.47it/s]
100%|██████████████████████████████████████████████████| 50/50 [01:01<00:00,
1.23s/it]
100%|██████████████████████████████████████████████████| 50/50 [01:26<00:00,
1.74s/it]
 74%|█████████████████████████████████████              | 37/50 [01:40<00:38,
2.96s/it]C:\Users\neria\anaconda3\envs\deep_learn\lib\site-packages\scipy\optimize\optimize.py:1013: RuntimeWarning: divide by zero encountered in double_scalars
  rhok = 1.0 / (numpy.dot(yk, sk))
100%|██████████████████████████████████████████████████| 50/50 [02:16<00:00,
2.74s/it]
```

In [106…

```python
nine_task_j_acc = {}
ten_task_j_acc = {}
for key, val in dic_res.items():
    print("Task:", key[0], "J=", key[1])
    print("Failuers:", val[0], "Avg Err:", val[1]/(50-val[0]))

    if key[0] == 9:
        nine_task_j_acc[key[1]] = val[1]/(50-val[0])
    if key[0] == 10:
        ten_task_j_acc[key[1]] = val[1]/(50-val[0])

    print("="*10)
```

```
Task: 9 J= 100
Failuers: 2 Avg Err: 2.5393292646359957
==========
Task: 10 J= 100
Failuers: 20 Avg Err: 566.2526486742096
==========
Task: 9 J= 150
Failuers: 0 Avg Err: 1.6880837649611724
==========
Task: 10 J= 150
Failuers: 26 Avg Err: 2646.624648537139
==========
Task: 9 J= 1000
Failuers: 0 Avg Err: 0.7642552780696296
==========
Task: 10 J= 1000
Failuers: 24 Avg Err: 14442.679453818524
==========
Task: 9 J= 2000
Failuers: 0 Avg Err: 0.696888466449651
==========
Task: 10 J= 2000
Failuers: 29 Avg Err: 50842.81310065304
==========
Task: 9 J= 3000
Failuers: 0 Avg Err: 0.678179897579023
==========
Task: 10 J= 3000
Failuers: 27 Avg Err: 39854.68709802683
==========
Task: 9 J= 5000
Failuers: 0 Avg Err: 0.6487374382663149
==========
Task: 10 J= 5000
Failuers: 34 Avg Err: 135038.9161081356
==========
```

Task 13. Discussion: How does the number of samples J affect the accuracy of the estimation? How does the addition of Z as an unknown affect the accuracy?

In [126…

```python
fig, axes = plt.subplots(1,2, figsize=(15,5))
axes[1].plot(list(ten_task_j_acc.keys()), list(ten_task_j_acc.values()), label="Error")
axes[1].legend()
axes[1].set_title("Task 10")
axes[1].set_xlabel("J")
axes[1].set_ylabel("Avg Err")

axes[0].plot(list(nine_task_j_acc.keys()), list(nine_task_j_acc.values()), label="Error")
axes[0].legend()
axes[0].set_title("Task 9")
axes[0].set_xlabel("J")
axes[0].set_ylabel("Avg Err")
```

Out[126…

```
Text(0, 0.5, 'Avg Err')
```


Discussion:

In case we know Z the error decrease with J.

In the other case where Z need to be estimated we both have higher number of errors and worst error duo to stabillity issues.