Notebook

November 20, 2024

0.1 Run instructions:

Tested in python 3.12.7, within a .conda environment.

(Since the notebook is to be exported as html, requirements.txt is not included, so the dependencies can be installed through: pip install numpy scikit-learn matplotlib pandas)

Figures are configured to be stored in a folder figures within the same directory as the notebook. Make sure there is a folder there if you want to run the notebook.

1 Assignment 1.2 - CAVI

Consider the model defined by Equation (10.21)-(10-23) in Bishop, for which DGM is presented below:

1.0.1 Question 1.2.7:

Implement a function that generates data points for the given model.

```
[21]: # Imports
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from scipy.special import psi, gammaln
```

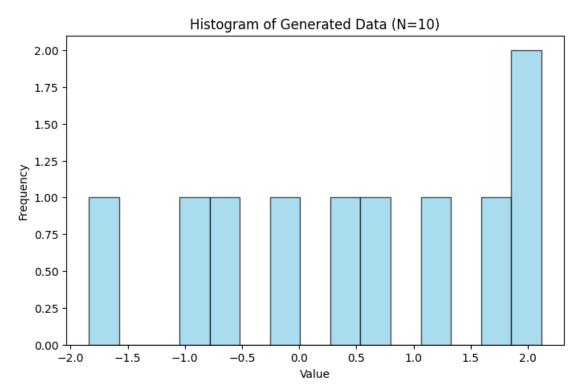
```
[22]: def generate_data(mu, tau, size):
    variance = 1 / tau
    return np.random.normal(mu, np.sqrt(variance), size)
```

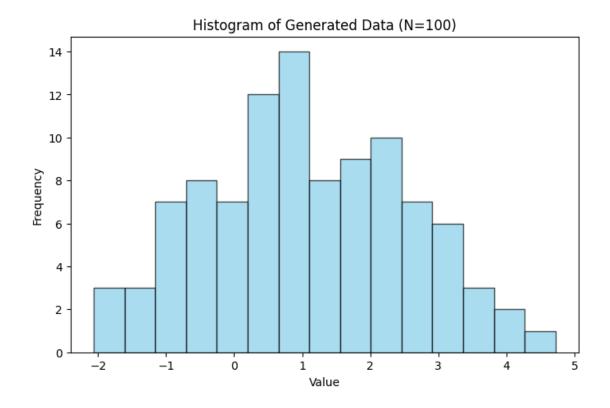
Set = 1, = 0.5 and generate datasets with size N=10,100,1000. Plot the histogram for each of 3 datasets you generated.

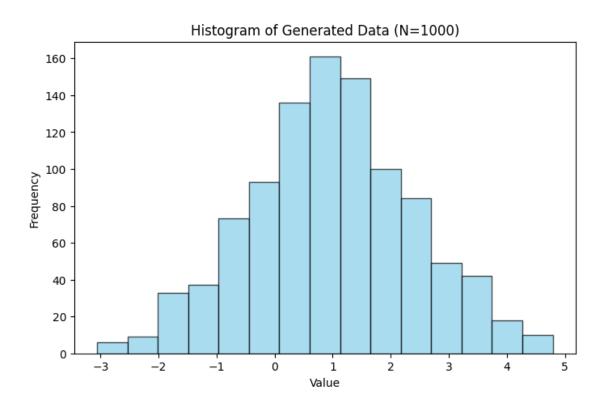
```
[23]: mu = 1
  tau = 0.5
  sizes = [10, 100, 1000]

datasets = {size: generate_data(mu, tau, size) for size in sizes}
```

```
# Visulaize the datasets via histograms
for size, data in datasets.items():
    plt.figure(figsize=(8, 5))
    plt.hist(data, bins=15, color='skyblue', alpha=0.7, edgecolor='black')
    plt.title(f"Histogram of Generated Data (N={size})")
    plt.xlabel("Value")
    plt.ylabel("Frequency")
    plt.savefig(f"figures/{size}_histogram.pdf")
    plt.show()
```







1.0.2 Question 1.2.8:

Find ML estimates of the variables and

```
def ML_est(data):
    mu_ml = np.mean(data)
    tau_ml = 1 / np.var(data)
    return mu_ml, tau_ml

ml_estimates = {size: ML_est(data) for size, data in datasets.items()}

ml_results = pd.DataFrame.from_dict(
    ml_estimates, orient='index', columns=['ML Estimate of ', 'ML Estimate of ', ']
)

print(ml_results)
```

```
ML Estimate of ML Estimate of

10 0.422523 0.617946

100 1.066792 0.449982

1000 0.988250 0.493600
```

1.0.3 Question 1.2.9:

What is the exact posterior? First derive it in closed form, and then implement a function that computes it for the given parameters:

```
{'a_N': 500.0, 'b_N': np.float64(1013.9656178720086), 'mu_N':
np.float64(0.988255621122432), 'lambda_N': 1000.5}
```

1.0.4 Question 1.2.10:

You will implement the VI algorithm for the variational distribution in Equation (10.24) in Bishop. Start with introducing the prior parameters:

```
[26]: # prior parameters
mu_0 = 0
lambda_0 = 1
a_0 = 1
b_0 = 1
```

Continue with a helper function that computes ELBO:

```
[27]: def elbo(x, mu_N, lambda_N, a_N, b_N):
                                                                                       N = len(x)
                                                                                        # Expectations for tau
                                                                                       E_log_tau = psi(a_N) - np.log(b_N)
                                                                                       E_tau = a_N / b_N
                                                                                       # Likelihood term
                                                                                       E_log_p_x_given_mu_tau = (N / 2) * E_log_tau - 0.5 * E_tau * np.sum(x**2 - 0.5 * E_t
                                                                \rightarrow 2 * x * mu_N + mu_N**2 + 1 / lambda_N)
                                                                                        # Prior on mu
                                                                                       E_{log_p_mu_given_tau} = -0.5 * E_{tau} * ((mu_N - mu_0)**2 + 1 / lambda_0)
                                                                                       # Prior on tau
                                                                                       E_{\log_{10} = (a_0 - 1)} * E_{\log_{10} = (a_0 - 
                                                                 \hookrightarrowlog(b_0)
                                                                                        # ELBO
                                                                                       elbo_val = E_log_p_x_given_mu_tau + E_log_p_mu_given_tau + E_log_p_tau
                                                                                       return elbo_val
```

Now, implement the CAVI algorithm:

```
[28]: def CAVI(x, mu_0, lambda_0, a_0, b_0):

# Helpers for calculating updates:
    def update_mu(x, mu_0, lambda_0, E_tau):
        # Update mu, tau from Bishop (10.26, 10.27)
        N = len(x)
        lambda_N = (lambda_0 + N) * E_tau
```

```
mu_N = (N*np.mean(x) + lambda_0 * mu_0) / (lambda_0 + N)
      return mu_N, lambda_N
  def update_tau(x, mu_N, a_0, b_0, lambda_0, lambda_N):
       # Update a_N, b_N from the approximations in Bishop (10.29, 10.30)
      N = len(x)
      a_N = a_0 + (N + 1) / 2
      # b N:s expected mu values
      expected_x_mu_squared = np.sum(x**2 - 2 * x * mu_N + (1 / lambda_N) + 
\rightarrowmu_N**2)
      expected mu mu0_squared = (1 / lambda N) + mu N**2 - 2 * mu_0 * mu_N + L
→mu_0**2
      b_N = b_0 + 0.5 * (expected_x_mu_squared + lambda_0 *_L
→expected_mu_mu0_squared)
      return a_N, b_N
  # Parameter priors
  mu_N = mu_0
  lambda_N = lambda_0
  a_N = a_0
  b_N = b_0
  elbo_history = [elbo(x, mu_N, lambda_N, a_N, b_N)]
  mu_history = [mu_N]
  lambdas_history = [lambda_N]
  estimated_taus_history = [a_N/b_N]
  prev_elbo = -np.inf
  for i in range(100):
      # Update mu and lambda
      E_tau = a_N/b_N
      mu_N, _ = update_mu(x, mu_N, lambda_N, E_tau)
       _, lambda_N = update_mu(x, mu_N, lambda_N, E_tau)
      a_N, _ = update_tau(x, mu_N, a_N, b_N, lambda_0, lambda_N)
       _, b_N = update_tau(x, mu_N, a_N, b_N, lambda_0, lambda_N)
      elbo_value = elbo(x, mu_N, lambda_N, a_N, b_N)
      elbo_history.append(elbo_value)
      mu_history.append(mu_N)
      lambdas_history.append(lambda_N)
```

```
estimated_taus_history.append(a_N/b_N)

print(f"Iteration {i+1}: ELBO = {elbo_value}")

# Early break

if np.abs(elbo_value - prev_elbo) < 1e-6:
        print(f"Converged after {i+1} iterations.")
        return {"a_N": a_N, "b_N": b_N, "mu_N": mu_N, "lambda_N": lambda_N, "elbos": elbo_history, "mus": mu_history, "lambdas": lambdas_history, "taus":
        estimated_taus_history}

prev_elbo = elbo_value

return {"a_N": a_N, "b_N": b_N, "mu_N": mu_N, "lambda_N": lambda_N, "elbos":
        elbo_history, "mus": mu_history, "lambdas": lambdas_history, "taus": usestimated_taus_history}</pre>
```

Run the VI algorithm on the datasets. Compare the inferred variational distribution with the exact posterior and the ML estimate. Visualize the results and discuss your findings.

```
[29]: def plot_results(cavi_results,dataset):
          N = len(dataset)
          elbo history = cavi results["elbos"]
          mu_history = cavi_results["mus"]
          taus_history = cavi_results["taus"]
          # Plot ELBO over iterations
          plt.figure(figsize=(12, 6))
          plt.subplot(1, 2, 1)
          plt.plot(elbo_history, label='ELBO')
          plt.title(f'N = {N}, ELBO Evolution')
          plt.xlabel('Iterations')
          plt.ylabel('ELBO')
          plt.grid(True)
          plt.legend()
          # mu, tau over iterations
          plt.subplot(1, 2, 2)
          plt.plot(mu_history, label='$\mu_N$', color='blue')
          plt.plot(taus_history, label='$a_N/b_N$', color='orange')
          plt.title(f'N = {N}, Variational Parameters Evolution')
          plt.xlabel('Iterations')
          plt.ylabel('Parameter Value')
          plt.grid(True)
          plt.legend()
          plt.tight_layout()
```

```
plt.savefig(f"figures/{N}_ELBOandMuTau.pdf")
  plt.show()
  posterior params = compute_exact_posterior(dataset, a_0, b_0, mu_0,_
→lambda 0)
  ml estimates = ML est(dataset)
  plt.figure(figsize=(8, 5))
  # Exact posterior mean and precision
  plt.axvline(posterior_params["mu_N"], color="g", linestyle="--",__
→label="Exact Posterior (Mean)")
  print(f"Posterior mu: {posterior params["mu N"]}")
  plt.axvline(cavi_results["mu_N"], color="b", linestyle=":", label="CAVI_U"
print(f"CAVI mu: {cavi_results["mu_N"]}")
  # ML estimate
  plt.axvline(ml_estimates[0], color="r", linestyle="-", label="ML Estimate_

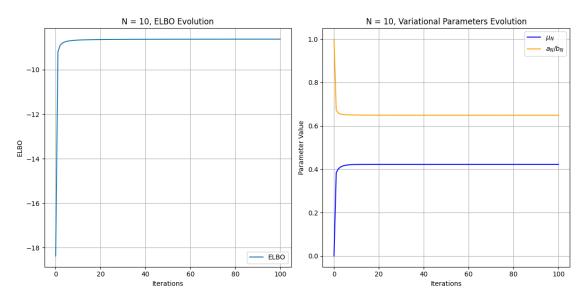
→ (Mean)")
  print(f"ML mu: {ml estimates[0]}")
  plt.title(f"N = {N}, Comparison of Posterior, CAVI, and ML")
  plt.xlabel("Mean ()")
  plt.legend()
  plt.grid()
  #plt.figure(figsize=(8, 5))
  # Exact posterior mean and precision
  plt.axvline(posterior_params["a_N"]/posterior_params["b_N"], color="g", __
→linestyle="--", label="Exact Posterior (tau)")
  print(f"Posterior tau: {posterior_params["a_N"]/posterior_params["b_N"]}")
  # CAVI mean
  plt.axvline(cavi_results["taus"][-1], color="b", linestyle=":", label="CAVI_L
print(f"CAVI tau: {cavi_results["taus"][-1]}")
  # ML estimate
  plt.axvline(ml_estimates[1], color="r", linestyle="-", label="ML Estimate_
print(f"ML tau: {ml_estimates[1]}")
  plt.title(f"N = {N}, Comparison of Posterior, CAVI, and ML")
  plt.xlabel("Value")
  plt.legend()
  plt.grid()
  plt.savefig(f"figures/{N}MLexactCAVIcomp.pdf")
  plt.show()
```

```
<>:19: SyntaxWarning: invalid escape sequence '\m'
<>:19: SyntaxWarning: invalid escape sequence '\m'
```

```
/var/folders/7t/7qxxs14161512g3d5tsqp_xw0000gn/T/ipykernel_56106/247895124.py:19
     : SyntaxWarning: invalid escape sequence '\m'
       plt.plot(mu_history, label='$\mu_N$', color='blue')
[30]: for data in datasets.values():
          cavi_results = CAVI(data, mu_0, lambda_0, a_0, b_0)
          plot_results(cavi_results,data)
     Iteration 1: ELBO = -9.187323262863385
     Iteration 2: ELBO = -8.90285603434964
     Iteration 3: ELBO = -8.801838848750094
     Iteration 4: ELBO = -8.751275155939119
     Iteration 5: ELBO = -8.72158059235591
     Iteration 6: ELBO = -8.702394079451324
     Iteration 7: ELBO = -8.68915702298984
     Iteration 8: ELBO = -8.679563842516467
     Iteration 9: ELBO = -8.672333954458827
     Iteration 10: ELBO = -8.666706758768708
     Iteration 11: ELBO = -8.66220705764017
     Iteration 12: ELBO = -8.658525818553109
     Iteration 13: ELBO = -8.655455269098043
     Iteration 14: ELBO = -8.652851640506002
     Iteration 15: ELBO = -8.650612866644842
     Iteration 16: ELBO = -8.648664775429673
     Iteration 17: ELBO = -8.64695229465658
     Iteration 18: ELBO = -8.645433714355429
     Iteration 19: ELBO = -8.64407686217685
     Iteration 20: ELBO = -8.642856503479164
     Iteration 21: ELBO = -8.641752541195423
     Iteration 22: ELBO = -8.640748747491237
     Iteration 23: ELBO = -8.639831855008577
     Iteration 24: ELBO = -8.63899089516783
     Iteration 25: ELBO = -8.6382167088492
     Iteration 26: ELBO = -8.637501579162814
     Iteration 27: ELBO = -8.636838951959753
     Iteration 28: ELBO = -8.636223220300879
     Iteration 29: ELBO = -8.635649556191492
     Iteration 30: ELBO = -8.635113777710338
     Iteration 31: ELBO = -8.634612242978932
     Iteration 32: ELBO = -8.634141764728263
     Iteration 33: ELBO = -8.633699540850008
     Iteration 34: ELBO = -8.633283097482758
     Iteration 35: ELBO = -8.63289024202373
     Iteration 36: ELBO = -8.632519024070856
     Iteration 37: ELBO = -8.63216770275357
     Iteration 38: ELBO = -8.631834719249909
     Iteration 39: ELBO = -8.63151867354342
     Iteration 40: ELBO = -8.631218304668797
```

```
Iteration 41: ELBO = -8.630932473845293
Iteration 42: ELBO = -8.63066015001403
Iteration 43: ELBO = -8.630400397386522
Iteration 44: ELBO = -8.63015236468411
Iteration 45: ELBO = -8.629915275805518
Iteration 46: ELBO = -8.629688421705449
Iteration 47: ELBO = -8.629471153304461
Iteration 48: ELBO = -8.629262875280254
Iteration 49: ELBO = -8.629063040614936
Iteration 50: ELBO = -8.628871145792958
Iteration 51: ELBO = -8.62868672656077
Iteration 52: ELBO = -8.628509354173078
Iteration 53: ELBO = -8.62833863206166
Iteration 54: ELBO = -8.62817419287229
Iteration 55: ELBO = -8.628015695823196
Iteration 56: ELBO = -8.627862824344982
Iteration 57: ELBO = -8.627715283967772
Iteration 58: ELBO = -8.627572800425714
Iteration 59: ELBO = -8.627435117953338
Iteration 60: ELBO = -8.627301997751452
Iteration 61: ELBO = -8.627173216603097
Iteration 62: ELBO = -8.627048565622943
Iteration 63: ELBO = -8.626927849125147
Iteration 64: ELBO = -8.626810883596848
Iteration 65: ELBO = -8.62669749676609
Iteration 66: ELBO = -8.626587526753944
Iteration 67: ELBO = -8.626480821302396
Iteration 68: ELBO = -8.626377237069942
Iteration 69: ELBO = -8.626276638988237
Iteration 70: ELBO = -8.626178899673626
Iteration 71: ELBO = -8.626083898888252
Iteration 72: ELBO = -8.625991523045814
Iteration 73: ELBO = -8.62590166475786
Iteration 74: ELBO = -8.625814222416665
Iteration 75: ELBO = -8.625729099811384
Iteration 76: ELBO = -8.625646205774363
Iteration 77: ELBO = -8.62556545385494
Iteration 78: ELBO = -8.62548676201823
Iteration 79: ELBO = -8.625410052366663
Iteration 80: ELBO = -8.625335250882422
Iteration 81: ELBO = -8.625262287188786
Iteration 82: ELBO = -8.625191094328935
Iteration 83: ELBO = -8.625121608560702
Iteration 84: ELBO = -8.625053769165874
Iteration 85: ELBO = -8.624987518272963
Iteration 86: ELBO = -8.624922800692259
Iteration 87: ELBO = -8.624859563762266
Iteration 88: ELBO = -8.624797757206538
```

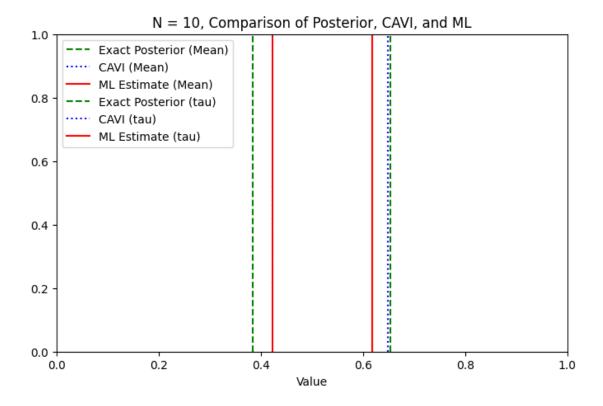
Iteration 89: ELBO = -8.624737333000121
Iteration 90: ELBO = -8.624678245244917
Iteration 91: ELBO = -8.624620450053225
Iteration 92: ELBO = -8.62456390543879
Iteration 93: ELBO = -8.624508571214973
Iteration 94: ELBO = -8.6245440408899311
Iteration 95: ELBO = -8.624401381624098
Iteration 96: ELBO = -8.624349454052576
Iteration 97: ELBO = -8.624298592300265
Iteration 98: ELBO = -8.62424876386109
Iteration 99: ELBO = -8.624199937538
Iteration 100: ELBO = -8.624152083377703



Posterior mu: 0.3841121169952442 CAVI mu: 0.42252332869476866 ML mu: 0.4225233286947686

Posterior tau: 0.6541310166157251 CAVI tau: 0.6488655557317343

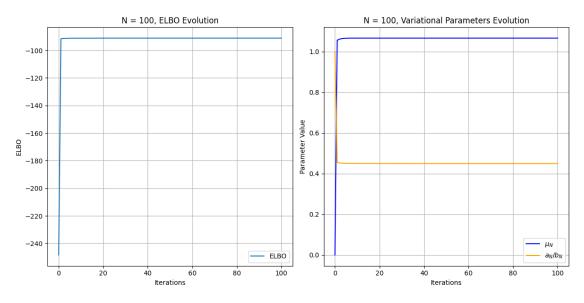
ML tau: 0.6179456690768029



```
Iteration 1: ELBO = -91.58168991703877
Iteration 2: ELBO = -91.35537097890905
Iteration 3: ELBO = -91.28579282079392
Iteration 4: ELBO = -91.25134286406013
Iteration 5: ELBO = -91.22991085598186
Iteration 6: ELBO = -91.21495968713218
Iteration 7: ELBO = -91.2038697834088
Iteration 8: ELBO = -91.19532610918294
Iteration 9: ELBO = -91.18856242121484
Iteration 10: ELBO = -91.18309055218947
Iteration 11: ELBO = -91.17858236783403
Iteration 12: ELBO = -91.1748093922292
Iteration 13: ELBO = -91.17160830822048
Iteration 14: ELBO = -91.16885981111402
Iteration 15: ELBO = -91.16647506219832
Iteration 16: ELBO = -91.16438674773254
Iteration 17: ELBO = -91.16254304273174
Iteration 18: ELBO = -91.16090345755161
Iteration 19: ELBO = -91.15943593042796
Iteration 20: ELBO = -91.1581147591426
Iteration 21: ELBO = -91.15691910694878
Iteration 22: ELBO = -91.15583190750611
Iteration 23: ELBO = -91.15483905114054
```

```
Iteration 24: ELBO = -91.15392877226483
Iteration 25: ELBO = -91.15309118259775
Iteration 26: ELBO = -91.15231791142237
Iteration 27: ELBO = -91.15160182539616
Iteration 28: ELBO = -91.15093680816443
Iteration 29: ELBO = -91.15031758542334
Iteration 30: ELBO = -91.14973958487208
Iteration 31: ELBO = -91.1491988232054
Iteration 32: ELBO = -91.14869181424824
Iteration 33: ELBO = -91.14821549376036
Iteration 34: ELBO = -91.14776715748563
Iteration 35: ELBO = -91.14734440980354
Iteration 36: ELBO = -91.14694512092483
Iteration 37: ELBO = -91.1465673910179
Iteration 38: ELBO = -91.14620951999079
Iteration 39: ELBO = -91.14586998191622
Iteration 40: ELBO = -91.14554740328713
Iteration 41: ELBO = -91.14524054445104
Iteration 42: ELBO = -91.14494828369244
Iteration 43: ELBO = -91.14466960353461
Iteration 44: ELBO = -91.14440357890678
Iteration 45: ELBO = -91.14414936688715
Iteration 46: ELBO = -91.14390619778253
Iteration 47: ELBO = -91.14367336734573
Iteration 48: ELBO = -91.14345022996437
Iteration 49: ELBO = -91.14323619268362
Iteration 50: ELBO = -91.14303070994475
Iteration 51: ELBO = -91.14283327894252
Iteration 52: ELBO = -91.14264343551768
Iteration 53: ELBO = -91.14246075051457
Iteration 54: ELBO = -91.14228482654202
Iteration 55: ELBO = -91.14211529508825
Iteration 56: ELBO = -91.14195181394435
Iteration 57: ELBO = -91.14179406489878
Iteration 58: ELBO = -91.14164175166975
Iteration 59: ELBO = -91.14149459804861
Iteration 60: ELBO = -91.14135234622808
Iteration 61: ELBO = -91.14121475529495
Iteration 62: ELBO = -91.14108159986824
Iteration 63: ELBO = -91.14095266886827
Iteration 64: ELBO = -91.14082776439895
Iteration 65: ELBO = -91.14070670073497
Iteration 66: ELBO = -91.14058930340026
Iteration 67: ELBO = -91.14047540832877
Iteration 68: ELBO = -91.14036486109993
Iteration 69: ELBO = -91.14025751623988
Iteration 70: ELBO = -91.14015323658221
Iteration 71: ELBO = -91.14005189268474
```

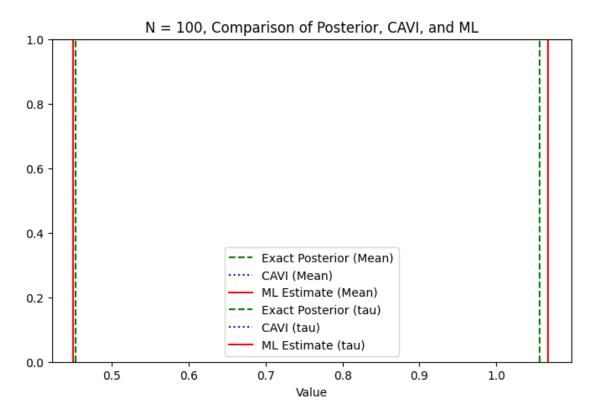
Iteration 72: ELBO = -91.13995336229168Iteration 73: ELBO = -91.13985752984318Iteration 74: ELBO = -91.13976428602189Iteration 75: ELBO = -91.13967352733792Iteration 76: ELBO = -91.13958515574554Iteration 77: ELBO = -91.13949907828916Iteration 78: ELBO = -91.13941520677808Iteration 79: ELBO = -91.13933345748467Iteration 80: ELBO = -91.13925375086552Iteration 81: ELBO = -91.13917601130349Iteration 82: ELBO = -91.139100166868 Iteration 83: ELBO = -91.13902614909352Iteration 84: ELBO = -91.13895389277323Iteration 85: ELBO = -91.1388833357677Iteration 86: ELBO = -91.13881441882585 Iteration 87: ELBO = -91.13874708541972Iteration 88: ELBO = -91.13868128159005Iteration 89: ELBO = -91.13861695580108Iteration 90: ELBO = -91.1385540588069Iteration 91: ELBO = -91.13849254352493Iteration 92: ELBO = -91.13843236491937 Iteration 93: ELBO = -91.13837347989Iteration 94: ELBO = -91.13831584717009Iteration 95: ELBO = -91.13825942723008 Iteration 96: ELBO = -91.13820418218624Iteration 97: ELBO = -91.13815007571665Iteration 98: ELBO = -91.13809707298147Iteration 99: ELBO = -91.13804514054773Iteration 100: ELBO = -91.13799424631947



Posterior mu: 1.0562298179442813 CAVI mu: 1.0667921161237242 ML mu: 1.0667921161237242

Posterior tau: 0.45261338017085945

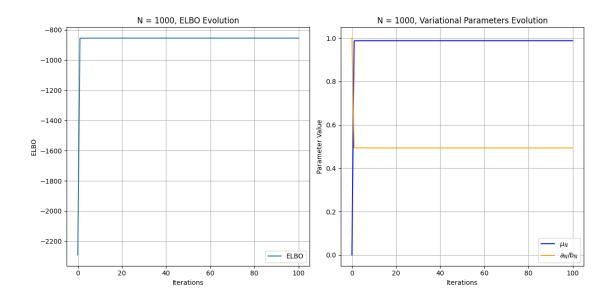
CAVI tau: 0.4497396428472921 ML tau: 0.4499819818276406



Iteration 1: ELBO = -854.7426719244954Iteration 2: ELBO = -854.4958466164718Iteration 3: ELBO = -854.4142098448644Iteration 4: ELBO = -854.3734310868642Iteration 5: ELBO = -854.348888327698Iteration 6: ELBO = -854.3324555490261Iteration 7: ELBO = -854.3206702591896Iteration 8: ELBO = -854.3118028228499Iteration 9: ELBO = -854.3048897783746Iteration 10: ELBO = -854.2993504256987Iteration 11: ELBO = -854.2948133669037 Iteration 12: ELBO = -854.2910298427438Iteration 13: ELBO = -854.2878269563269Iteration 14: ELBO = -854.2850808267947Iteration 15: ELBO = -854.2827003966447Iteration 16: ELBO = -854.2806172574069

```
Iteration 17: ELBO = -854.2787790342159
Iteration 18: ELBO = -854.2771449572036
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Posterior mu: 0.9872624864465467

CAVI mu: 0.9882497489329933 ML mu: 0.9882497489329932

Posterior tau: 0.4938620077824699 CAVI tau: 0.49361078527716995 ML tau: 0.49360018564056446

