

DD2434, Assignment 1A, 2024

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1 Assignment 1A

1.1 Dependencies in a Directed Graphical Model

1.1.1 $w_{n,g} \perp w_{n,g+1} | s_n$?

$w_{n,g} \perp w_{n,g+1} | s_n$ is **false** ($w_{n,g} \leftarrow z_n \rightarrow w_{n,g+1}$, z_n is not observed).

1.1.2 $l_n \perp w_{n,g} | x_{n,g}$?

$l_n \perp w_{n,g} | x_{n,g}$ is **false**. ($x_{n,g}$ is a descendant of $y_{n,g}$ which means that the V-structure does not give independence.)

1.1.3 $z_n \perp x_{n,g} | w_{n,g}, h_{n,g}$?

This is **true**.

(While $w_{n,g}$ and $h_{n,g}$ are observed, for example $w_{n,g+1}$ and $h_{n,g+1}$ are not. These do not have paths to $x_{n,g}$ however. There is a path from $w_{n,g+1}$ to $x_{n,g}$ through l_n , but no descendants of l_n are observed, so there is a independence-giving V-structure there.)

1.1.4 $z_1^n \perp z_M^n | C^n, A_{1:I,1:J}^{1:K}$?

This is **false**. (There is a clear path $z_1^n \rightarrow z_2^n \rightarrow \dots \rightarrow z_{M-1}^n \rightarrow z_M^n$ that does not cross any observed variables.)

1.1.5 $X_1^n \perp X_M^n | X_2^n, C^n$?

This is **true**.

(Because X_2^n is observed, X_1^n can no longer influence X_M^n through $e_{i,r}^k$. Likewise, the paths through z_1^n run into this same issue. It also clearly cannot influence through C^n , due to it being observed.)

1.1.6 $C^n \perp C^{n+1} | z_{1:M}^n, X_{1:M}^n$?

This is **false**. (Both C^n and C^{n+1} depend on π , which is not observed.)

1.2 CAVI

1.2.7 Implement a function that generates data points for the given model. Set $\mu = 1$, $\tau = 0.5$ and generate datasets with size $N = 10, 100, 1000$. Plot the histogram for each of 3 datasets you generated.

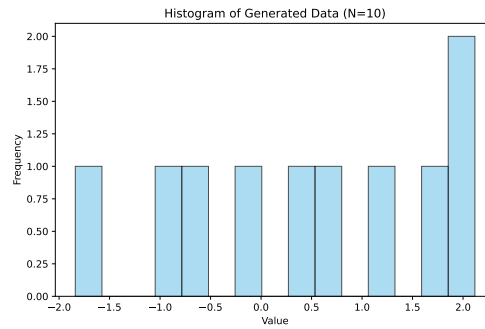


Figure 1: Histogram of data points for $N = 10$

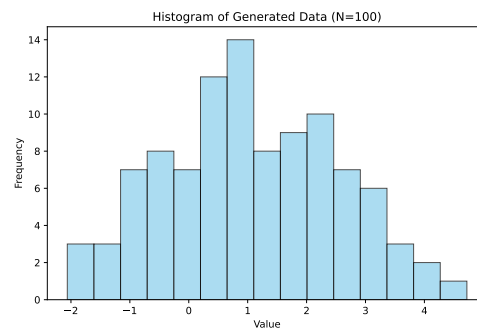


Figure 2: Histogram of data points for $N = 100$

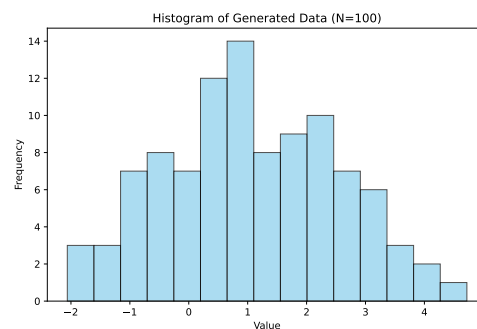


Figure 3: Histogram of data points for $N = 100$

The function is implemented as `generate_data`.

1.2.8 Find ML estimates of the variables μ and τ .

The ML estimates for μ and τ are the mean of the data, and the inverse variance of the data respectively. `ML_est` was implemented to return these values.

1.2.9 What is the exact posterior? (Show your derivations.)

To derive the posterior, we first begin by defining the likelihood and prior:

$$\text{Likelihood: } p(X|\mu, \tau) = \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\left\{-\frac{\tau}{2} \sum_{n=1}^N (x_n - \mu)^2\right\} - \text{As defined in Bishop 10.21} \quad (1)$$

With the given conjugate prior distributions for μ and τ in Bishop 10.22 and 10.23:

$$\begin{aligned} p(\mu|\tau) &= \mathcal{N}(\mu|\mu_0, (\lambda_0\tau)^{-1}) = \frac{\sqrt{\tau\lambda_0}}{\sqrt{2\pi}} \exp\left\{-\frac{\lambda_0\tau(x - \mu)}{2}\right\} \\ p(\tau) &= \text{Gam}(\tau|a_0, b_0) = \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp\{-b_0\tau\} \end{aligned} \quad (2)$$

The posterior is defined through Bayes' theorem, as:

$$p(\mu, \tau|X) \propto p(X|\mu, \tau)p(\mu|\tau)p(\tau), \quad (3)$$

Combining the terms results in the expression:

$$p(\mu, \tau|X) = \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\left\{-\frac{\tau}{2} \sum_{n=1}^N (x_n - \mu)^2\right\} \times \frac{\sqrt{\tau\lambda_0}}{\sqrt{2\pi}} \exp\left\{-\frac{\lambda_0\tau(\mu_0 - \mu)^2}{2}\right\} \times \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp\{-b_0\tau\} \quad (4)$$

Splitting the terms by μ and τ :

$$= \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\{-\tau/2\} \exp\left\{\sum_{n=1}^N (x_n - \mu)^2\right\} \frac{\sqrt{\tau\lambda_0}}{\sqrt{2\pi}} \exp\{\tau\} \exp\left\{-\frac{\lambda_0}{2}(\mu - \mu_0)^2\right\} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp\{-b_0\tau\} \quad (5)$$

The sum and the squared term can be expanded as:

$$\begin{aligned} \sum_{n=1}^N (x_n - \mu)^2 &= \sum_{n=1}^N x_n^2 - 2\mu \sum_{n=1}^N x_n + N\mu^2 \\ \lambda_0(\mu_0 - \mu)^2 &= \lambda_0\mu_0^2 - 2\lambda_0\mu_0\mu + \lambda_0\mu^2 \end{aligned} \quad (6)$$

Together the terms create

$$\begin{aligned} \sum_{n=1}^N (x_n - \mu)^2 + \lambda_0(\mu_0 - \mu)^2 &= (N + \lambda_0)\mu^2 - 2\left(\sum_{n=1}^N x_n + \lambda_0\mu_0\right)\mu + \sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2 \\ &= (N + \lambda_0)\left(\mu^2 - \frac{\sum_{n=1}^N x_n + \lambda_0\mu_0}{N + \lambda_0}\mu + \frac{\sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2}{N + \lambda_0}\right) \end{aligned} \quad (7)$$

We want to be able to express these sums in a more suitable form. This can be done by completing the square $(\mu - \mu^*)$:

$$\begin{aligned} \text{We define } \mu^* \text{ as: } \mu^* &= \frac{\sum_{n=1}^N x_n + \lambda_0\mu_0}{N + \lambda_0} \\ (\text{Eq 7 with } N + \lambda_0 \text{ factored out}) &= \mu^2 - 2\mu^*\mu + \frac{\sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2}{N + \lambda_0} = \\ &= \mu^2 - 2\mu^*\mu + (\mu^*)^2 - (\mu^*)^2 + \frac{\sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2}{N + \lambda_0} = \\ &= (\mu - \mu^*)^2 - (\mu^*)^2 + \frac{\sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2}{N + \lambda_0} = \\ &= (\mu - \mu^*)^2 + \frac{(N + \lambda_0) \left(\sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2 \right) - \left(\sum_{n=1}^N x_n + \lambda_0\mu_0 \right)^2}{(N + \lambda_0)^2} \end{aligned} \quad (8)$$

In equation 5, we now have:

$$\begin{aligned}
 \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\{-\tau/2\} \exp\left\{\sum_{n=1}^N (x_n - \mu)^2\right\} \frac{\sqrt{\tau\lambda_0}}{\sqrt{2\pi}} \exp\{\tau\} \exp\left\{-\frac{\lambda_0}{2}(\mu - \mu_0)^2\right\} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp\{-b_0\tau\} = \\
 \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\{-\tau/2\} \frac{\sqrt{\tau\lambda_0}}{\sqrt{2\pi}} \exp\{\tau\} \exp\{(N + \lambda_0)(\mu - \mu^*)^2\} \\
 \exp\left\{\sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2\right\} \exp\left\{-\frac{\left(\sum_{n=1}^N x_n + \lambda_0\mu_0\right)^2}{N + \lambda_0}\right\} \\
 \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp\{-b_0\tau\}
 \end{aligned} \tag{9}$$

Through combining these terms, we identify:

$$\begin{aligned}
 \mu^* &= \frac{\sum_{n=1}^N x_n + \lambda_0\mu_0}{N + \lambda_0} \\
 \lambda^* &= N + \lambda_0 \\
 a_N &= a_0 + \frac{N}{2} \\
 b_N &= b_0 + \frac{1}{2} \left(\sum_{n=1}^N x_n^2 + \lambda_0\mu_0^2 - \lambda^* \mu^{*2} \right)
 \end{aligned} \tag{10}$$

1.2.10 Implement the VI algorithm for the variational distribution in Equation (10.24) in Bishop. Run the VI algorithm on the datasets. Plot the ELBO results. Compare the inferred variational distribution with the exact posterior and the ML estimate. Visualize the results and discuss your findings.

CAVI is implemented in the notebook, based on the factorized variational approximation from Bishop. This gives the following posterior distributions:

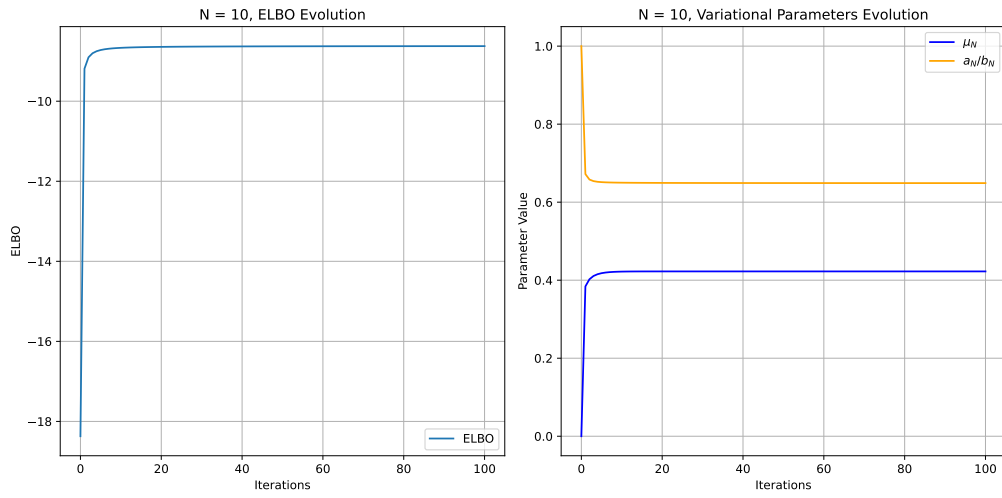
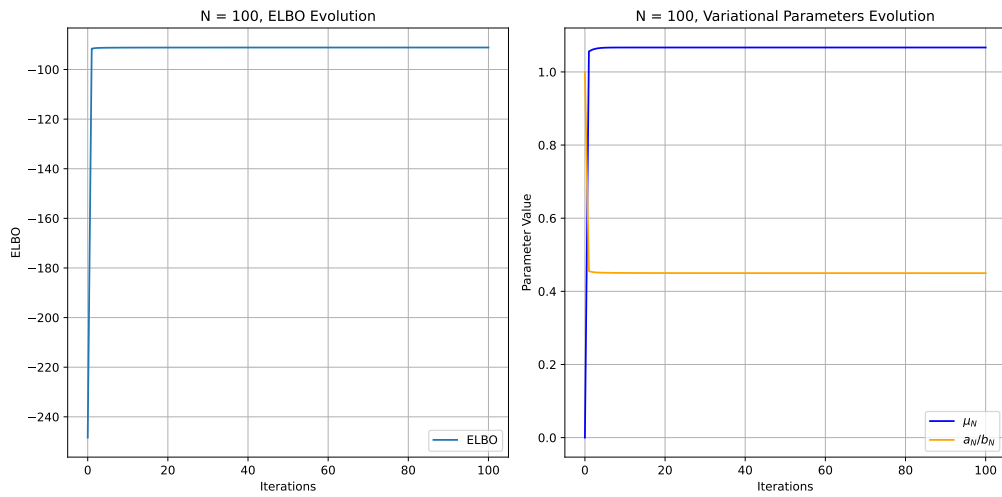
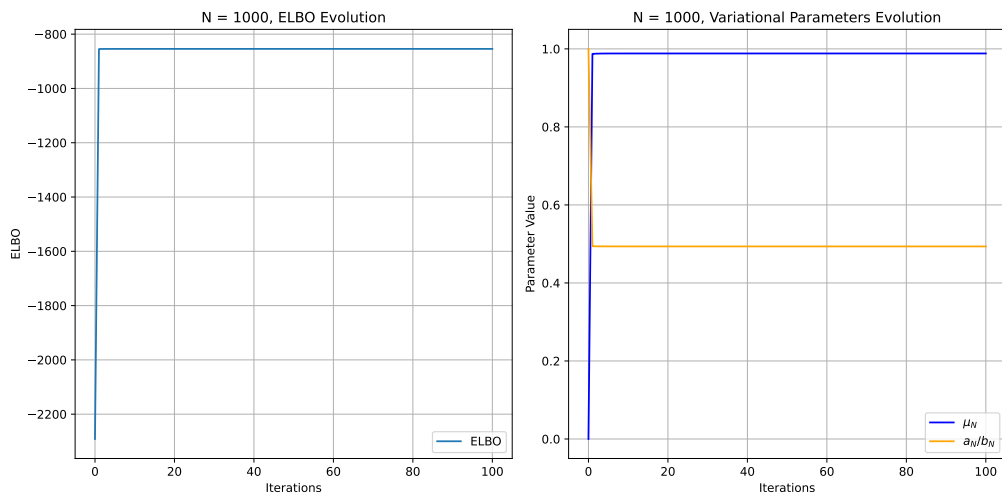
$$\mu_N = \frac{\lambda_0\mu_0 + N\bar{x}}{\lambda_0 + N} \tag{11}$$

$$\lambda_N = (\lambda_0 + N)\mathbb{E}[\tau], \text{ where } \mathbb{E}[\tau] \text{ is estimated as } \frac{a_N}{b_N} \tag{12}$$

$$a_N = a_0 + \frac{N}{2} \tag{13}$$

$$b_N = b_0 + \frac{1}{2} \mathbb{E}_\mu \left[\sum_{n=1}^N (x_n - \mu)^2 + \lambda_0(\mu - \mu_0)^2 \right] \tag{14}$$

Iteration with CAVI and plotting the ELBO:s gave these results over the datasets:

Figure 4: ELBO results and μ_N, τ_N for the dataset of size 10Figure 5: ELBO results and μ_N, τ_N for the dataset of size 100Figure 6: ELBO results and μ_N, τ_N for the dataset of size 1000

Comparing the inferred values μ, τ with the ML estimate and the exact posterior for these datasets:

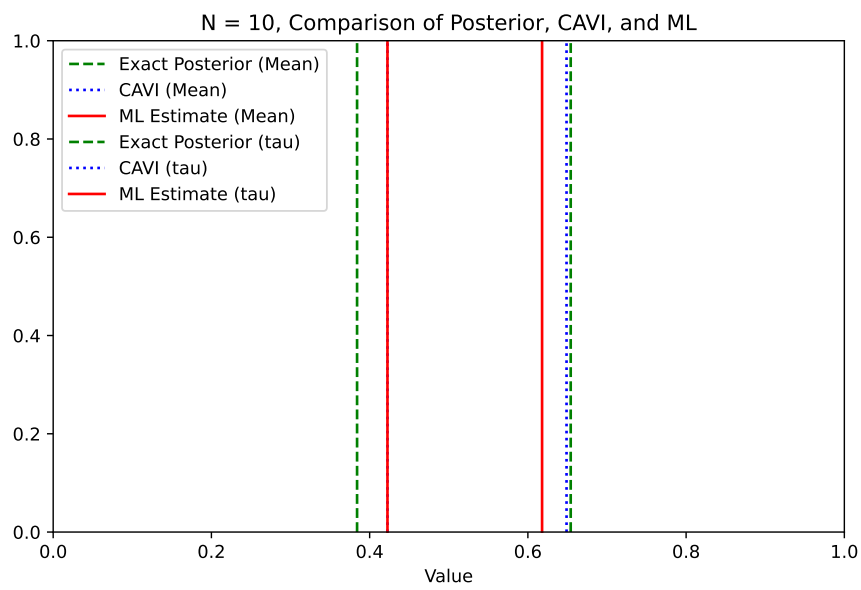


Figure 7: Comparison over the inferred parameters

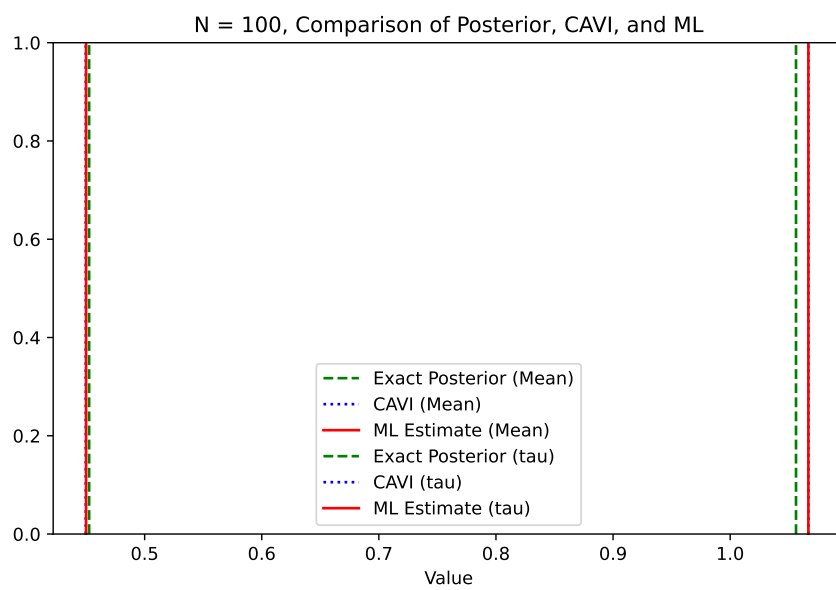


Figure 8: Comparison over the inferred parameters

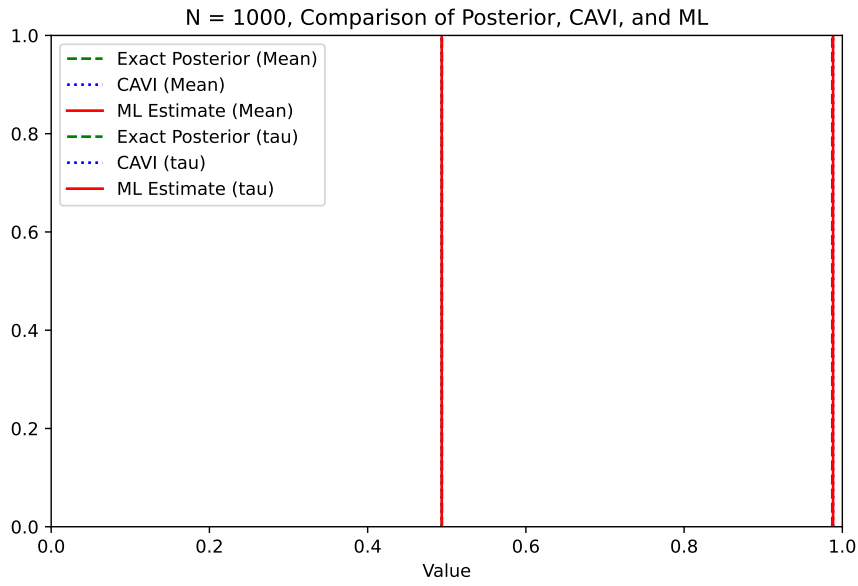


Figure 9: Comparison over the inferred parameters

Analysis

The CAVI algorithm converges very quickly for these datasets, and produces results that are comparable to or closer to the exact posterior compared with the ML estimate, even for the small datasets. Part of this is due to the simple distribution that generated the data, which is just a normal distribution. For the very small datasets, individual points have a large effect, and all methods have a large difference compared with the parameters used to generate the data $\mu = 1, \tau = 0.5$. This difference, as expected, becomes much smaller when the size of the generated data increases, and the parameters converge towards the ones used to generate the datasets.

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 $\mu = 1$, $\tau = 0.5$ 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]

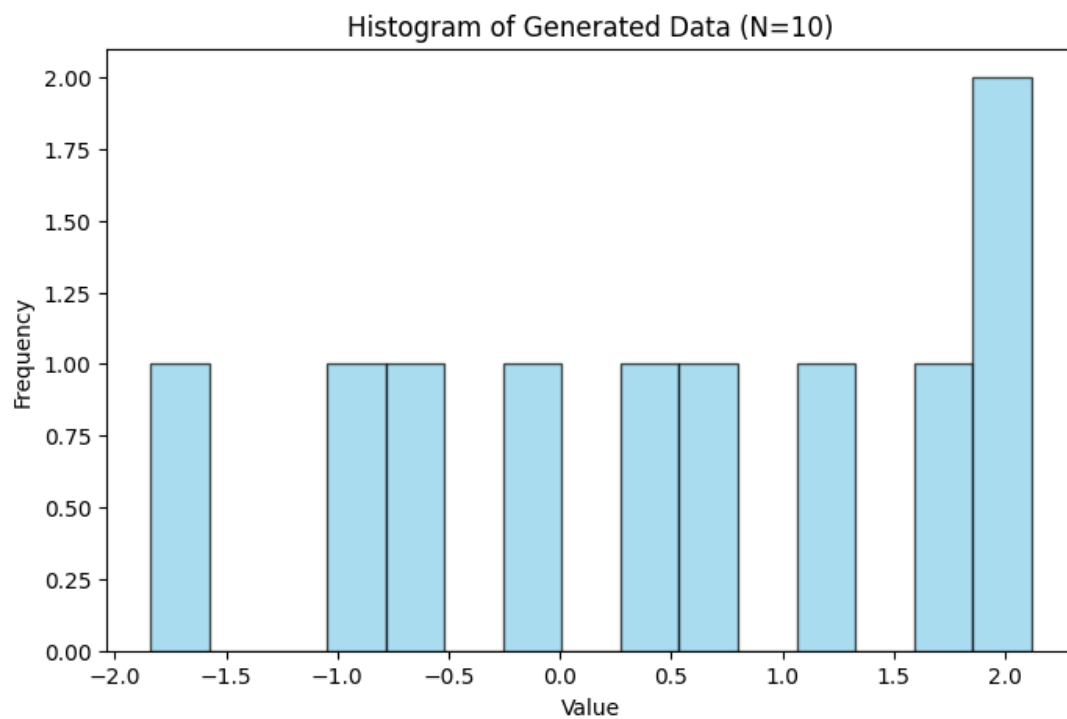
datasets = {size: generate_data(mu, tau, size) for size in sizes}
```

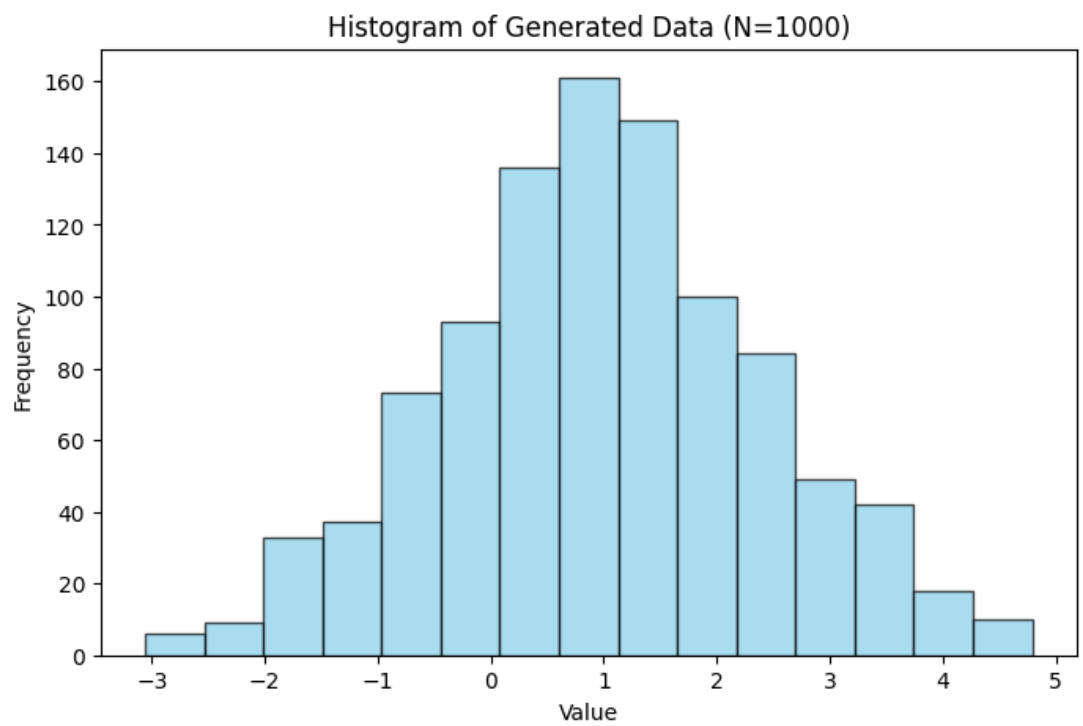
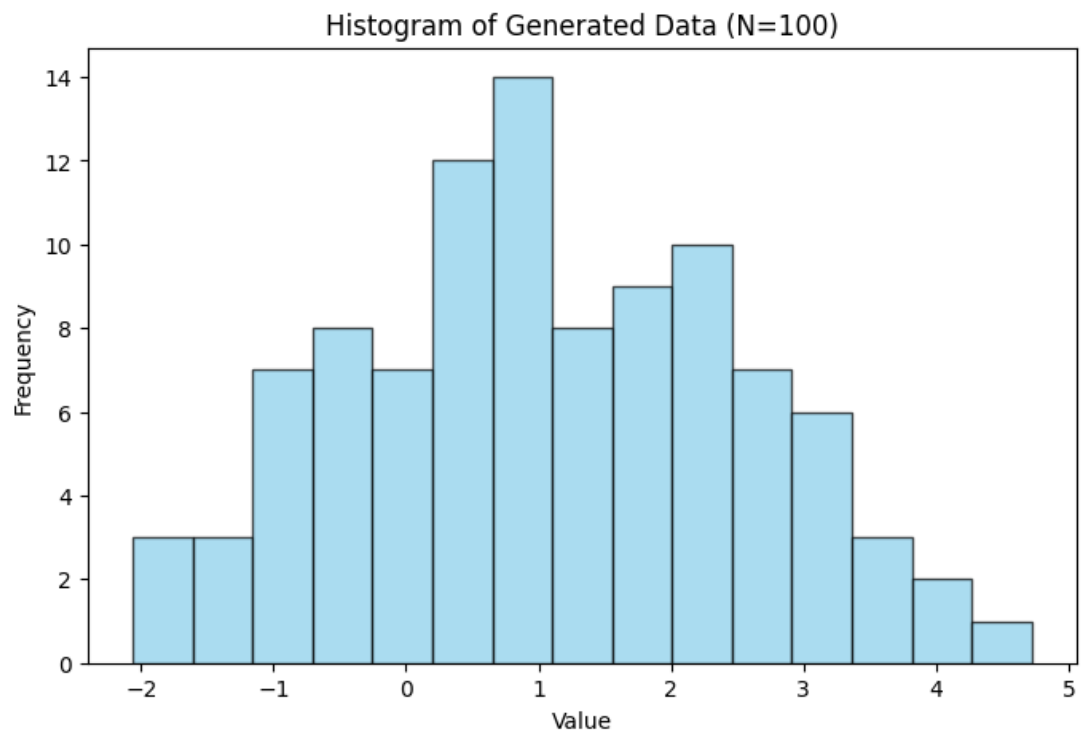


```

# 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 μ and λ

```
[24]: 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  $\mu$ ', 'ML Estimate of  $\lambda$ ']
)

print(ml_results)
```

	ML Estimate of μ	ML Estimate of λ
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:

```
[25]: def compute_exact_posterior(D, a_0, b_0, mu_0, lambda_0):
    N = len(D)
    x_mean = np.mean(D)
    lambda_N = lambda_0 + N
    a_N = a_0 + N / 2
    mu_N = (lambda_0 * mu_0 + np.sum(D)) / (lambda_0 + N)
    # Same expressions from derivation and from wikipedia - exact same value
    # returned
    b_N = b_0 + 1/2 * (np.sum(np.power(D,2)) + lambda_0*mu_0**2 -
    lambda_N*mu_N**2)
    # b_N = b_0 + 1/2 * np.sum(np.power(D-x_mean,2)) + N*lambda_0/(N+lambda_0) *
    ((x_mean - mu_0)**2)/2

    return {"a_N": a_N, "b_N": b_N, "mu_N": mu_N, "lambda_N": lambda_N}

print(compute_exact_posterior(datasets[1000],0,1,1,0.5))
```

```
{'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 -
↪ 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_p_tau = (a_0 - 1) * E_log_tau - b_0 * E_tau - gammaln(a_0) + a_0 * np.
↪ log(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) +
↪mu_N**2)
    expected_mu_mu0_squared = (1 / lambda_N) + mu_N**2 - 2 * mu_0 * mu_N +
↪mu_0**2

    b_N = b_0 + 0.5 * (expected_x_mu_squared + lambda_0 *
↪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":
    ↪ estimated_taus_history}

```

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"]}")
# CAVI mean
plt.axvline(cavi_results["mu_N"], color="b", linestyle=":", label="CAVI
↳(Mean)")
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
↳(tau)")
print(f"CAVI tau: {cavi_results["taus"][-1]}")
# ML estimate
plt.axvline(ml_estimates[1], color="r", linestyle="-", label="ML Estimate
↳(tau)")
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'

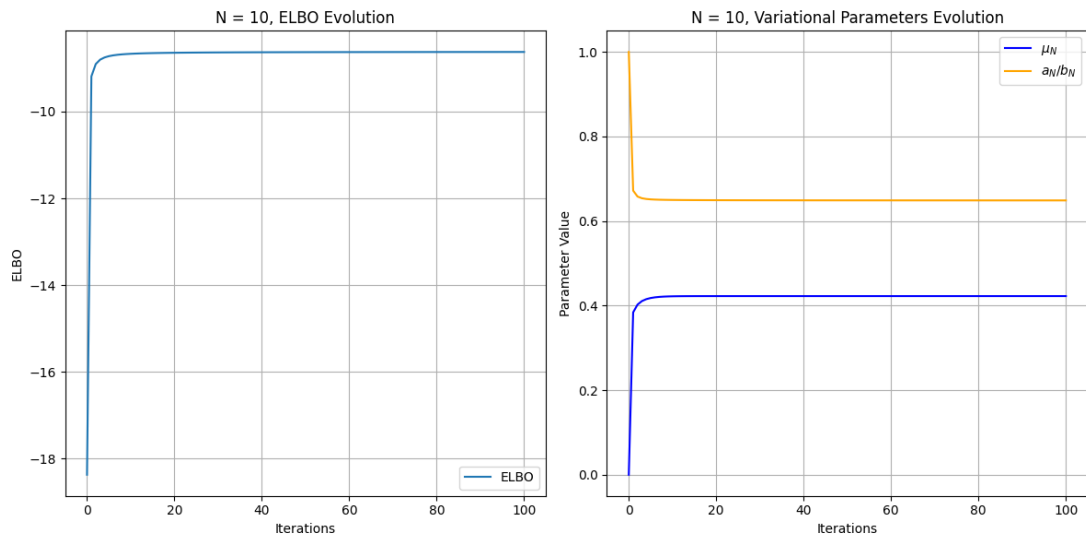
```
/var/folders/7t/7qxxs14161512g3d5tsqp_xw0000gn/T/ipykernel_56106/247895124.py:19
: SyntaxWarning: invalid escape sequence '\m'
plt.plot(mu_history, label='$\mu_N$', color='blue')
```

```
[30]: for data in datasets.values():
      cavi_results = CAVI(data, mu_0, lambda_0, a_0, b_0)
      plot_results(cavi_results, data)
```

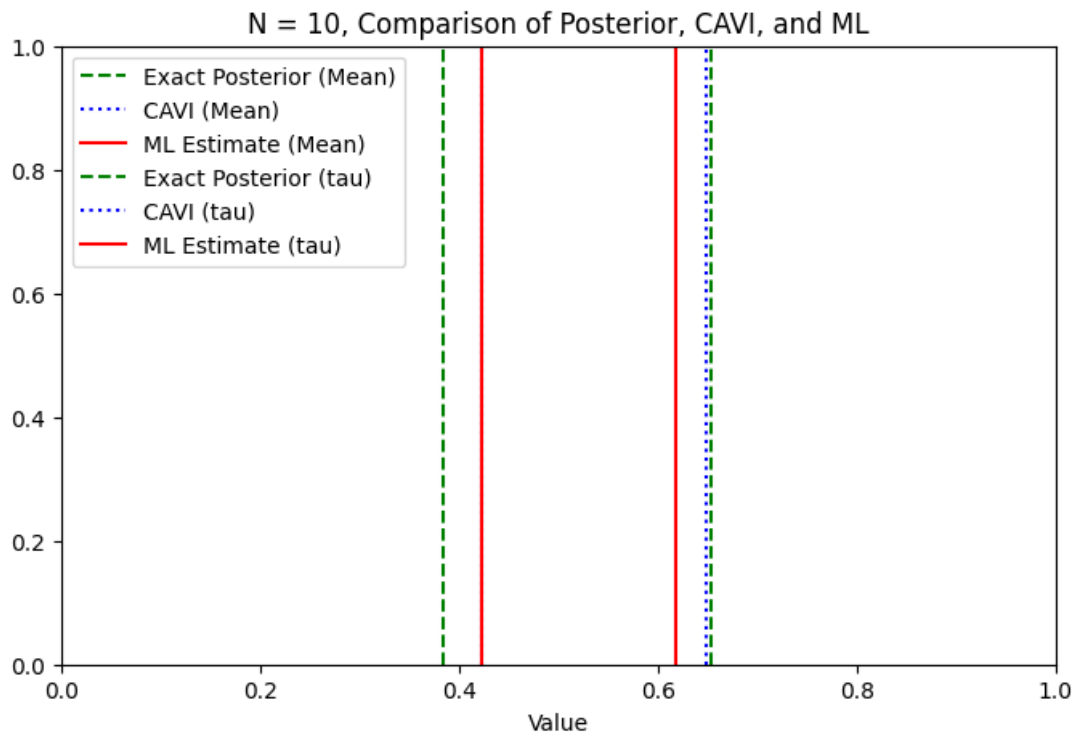
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Iteration 40: ELBO = -8.631218304668797
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Posterior mu: 0.3841121169952442
 CAVI mu: 0.42252332869476866
 ML mu: 0.4225233286947686
 Posterior tau: 0.6541310166157251
 CAVI tau: 0.6488655557317343
 ML tau: 0.6179456690768029



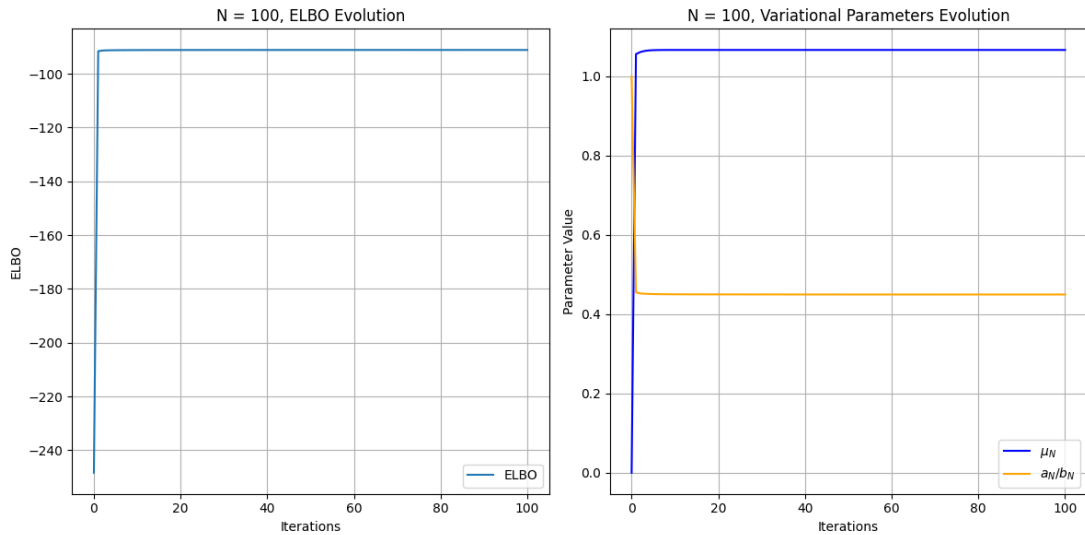
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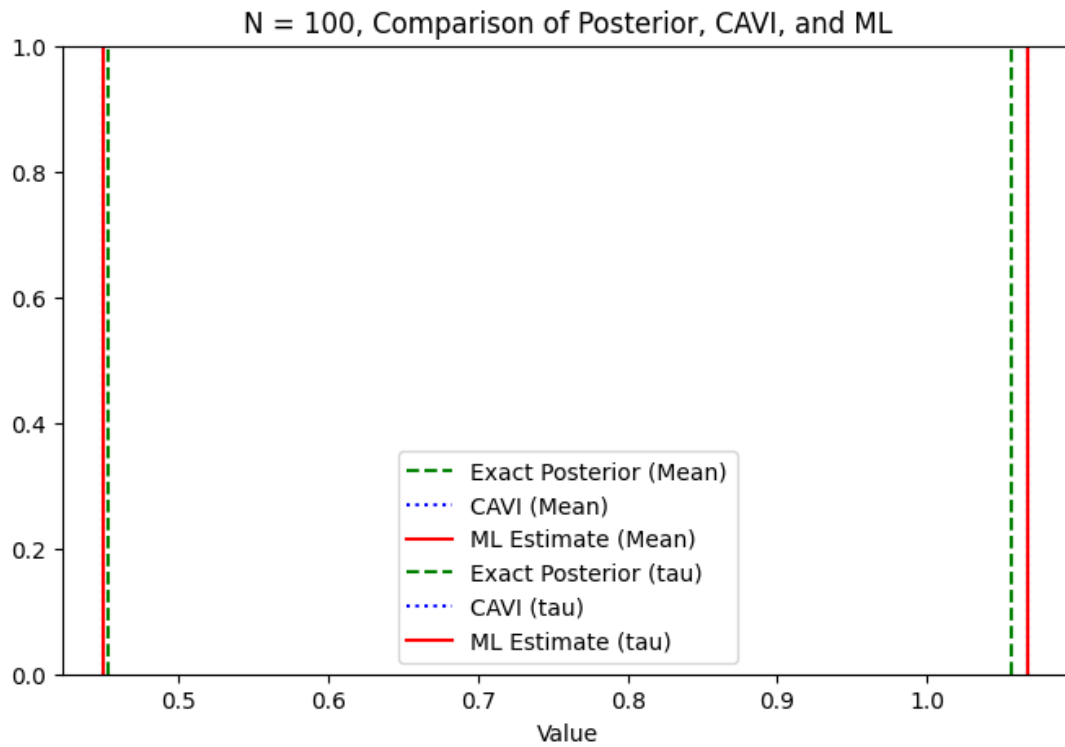
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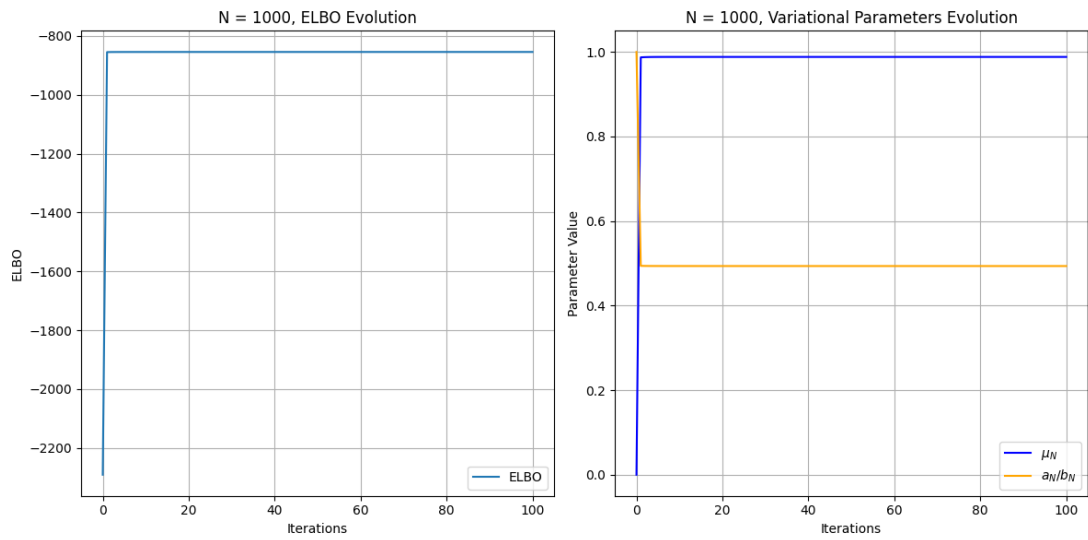
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CAVI mu: 1.0667921161237242
ML mu: 1.0667921161237242
Posterior tau: 0.45261338017085945
CAVI tau: 0.4497396428472921
ML tau: 0.4499819818276406



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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

