Assignment 3 Report
CS-726: Advanced Machine Learning

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1 Task 0

The output provided on running the program is:

```
Using device: cuda

--- Model Architecture ---
EnergyRegressor(
    (net): Sequential(
        (0): Linear(in_features=784, out_features=4096, bias=True)
        (1): ReLU(inplace=True)
        (2): Linear(in_features=4096, out_features=2048, bias=True)
        (3): ReLU(inplace=True)
        (4): Linear(in_features=2048, out_features=1024, bias=True)
        (5): ReLU(inplace=True)
        (6): Linear(in_features=1024, out_features=512, bias=True)
        (7): ReLU(inplace=True)
        (8): Linear(in_features=512, out_features=256, bias=True)
        (9): ReLU(inplace=True)
        (10): Linear(in_features=256, out_features=128, bias=True)
        (11): ReLU(inplace=True)
        (12): Linear(in_features=128, out_features=64, bias=True)
        (13): ReLU(inplace=True)
        (14): Linear(in_features=64, out_features=32, bias=True)
        (15): ReLU(inplace=True)
        (16): Linear(in_features=32, out_features=16, bias=True)
        (17): ReLU(inplace=True)
        (18): Linear(in_features=16, out_features=8, bias=True)
        (19): ReLU(inplace=True)
        (20): Linear(in_features=8, out_features=4, bias=True)
        (21): ReLU(inplace=True)
        (22): Linear(in_features=4, out_features=2, bias=True)
        (23): ReLU(inplace=True)
        (24): Linear(in_features=2, out_features=1, bias=True)
    )
)
------------------------

Loading dataset from ../A4_test_data.pt...
```

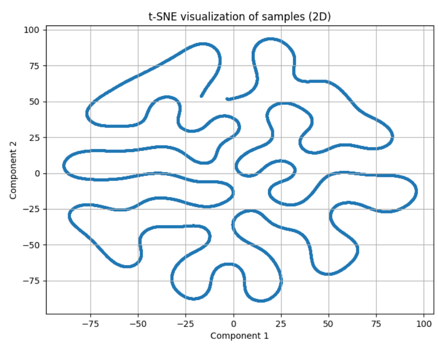
```
Dataset loaded in 0.17s. Shape: x=torch.Size([100000, 784]), energy=torch.Size([100000, 1])

--- Test Results ---
Loss: 288.1554
--- Script Finished ---
```

2 Task 1

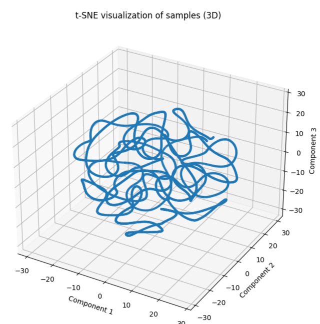
10000 samples were taken using each algorithm.

Sampling Algorithm	**Burn-in time (s)**	**Sampling time (s)**	**Total time (s)**
Algorithm 1	19.37	71.23	90.60
Algorithm 2	8.19	32.53	40.72

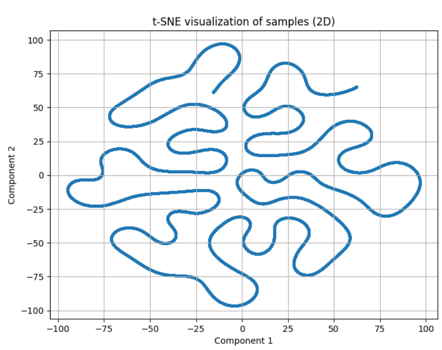
Table 1: Performance comparison of sampling algorithms for 10,000 samples.



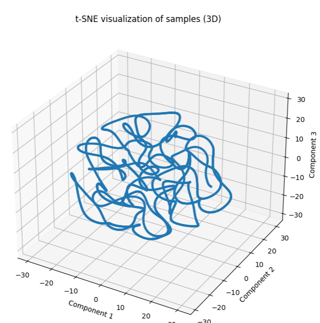
Algorithm 1 t-SNE 2d



Algorithm 1 t-SNE 3d



Algorithm 2 t-SNE 2d

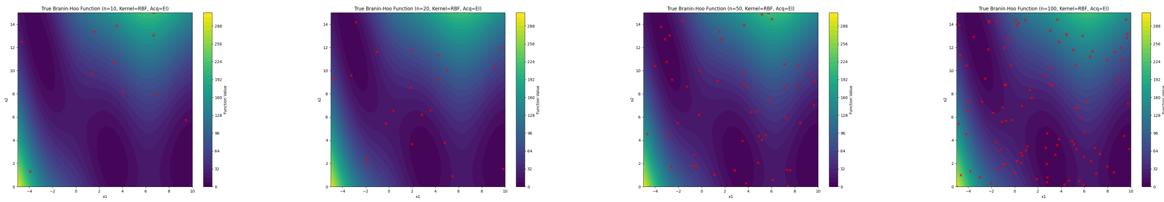


Algorithm 2 t-SNE 3d

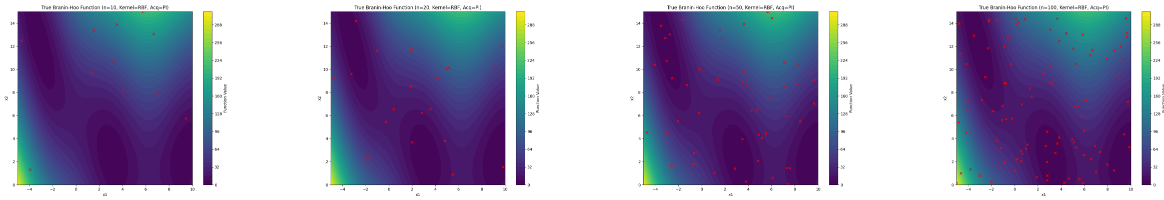
Figure 1: t-SNE plots for the two sampling algorithms.

3 Task 2

n is the number of samples taken from the Branin-Hoo function.

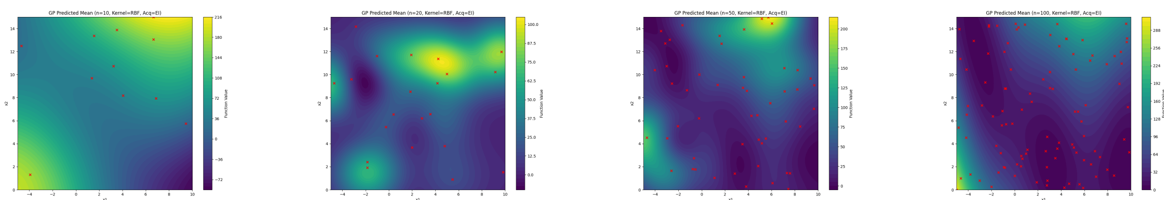


n=10 with EI n=20 with EI n=50 with EI n=100 with EI

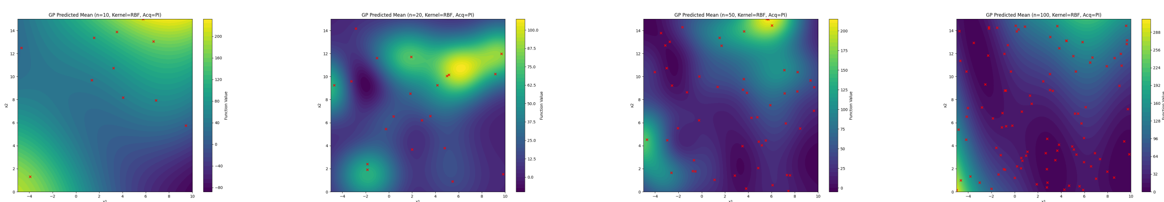


n=10 with PI n=20 with PI n=50 with PI n=100 with PI

Figure 2: RBF kernel true function with different acquisition functions.

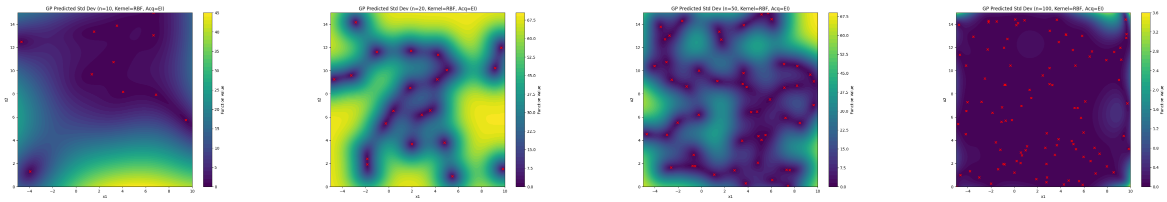


n=10 with EI n=20 with EI n=50 with EI n=100 with EI

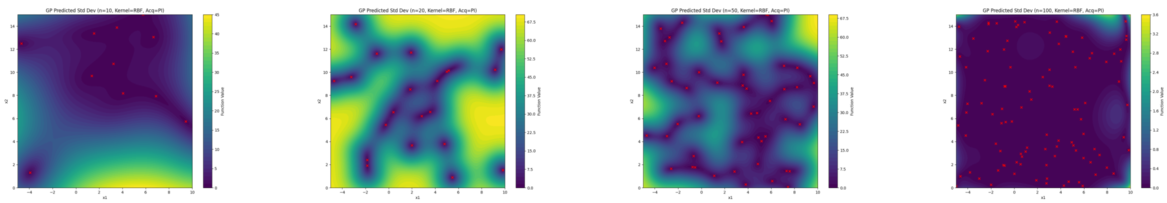


n=10 with PI n=20 with PI n=50 with PI n=100 with PI

Figure 3: RBF kernel GP mean with different acquisition functions.

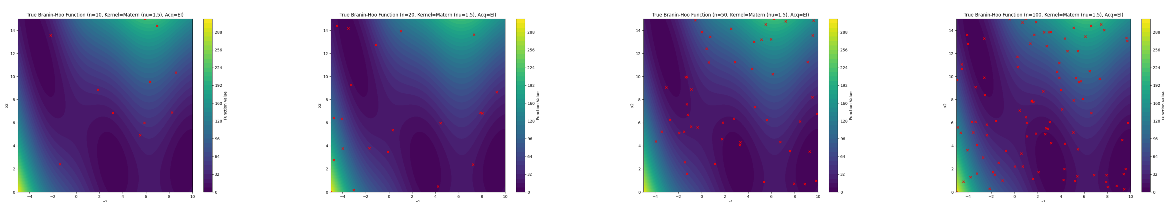


n=10 with EI n=20 with EI n=50 with EI n=100 with EI

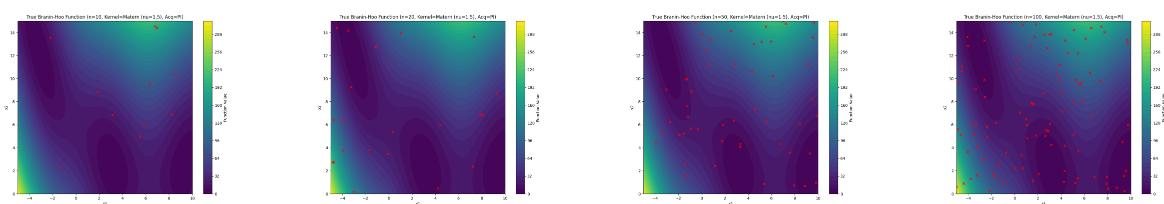


n=10 with PI n=20 with PI n=50 with PI n=100 with PI

Figure 4: RBF kernel GP standard deviation with different acquisition functions.

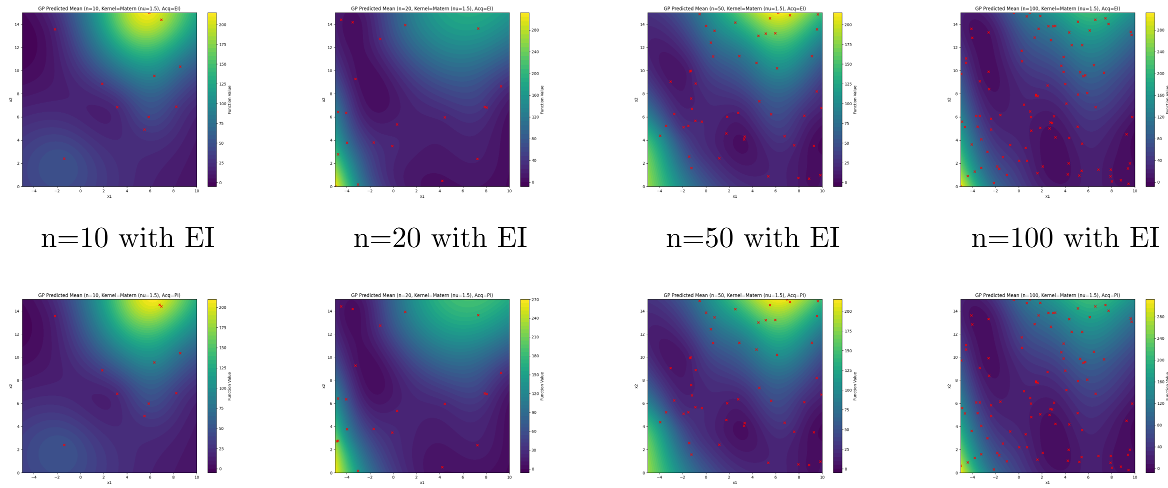


n=10 with EI n=20 with EI n=50 with EI n=100 with EI



n=10 with PI n=20 with PI n=50 with PI n=100 with PI

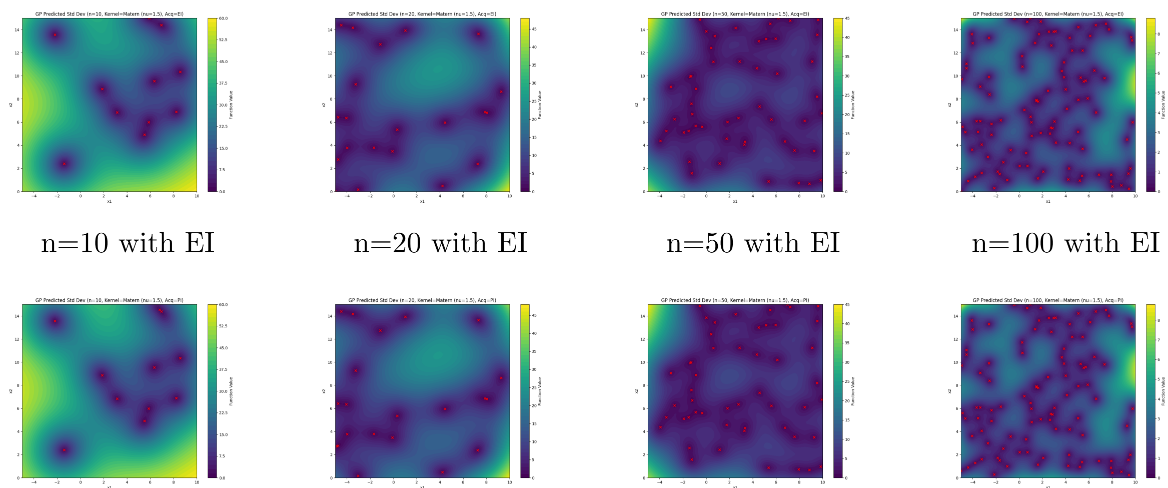
Figure 5: Matern kernel true function with different acquisition functions.



n=10 with EI | n=20 with EI | n=50 with EI | n=100 with EI

n=10 with PI | n=20 with PI | n=50 with PI | n=100 with PI

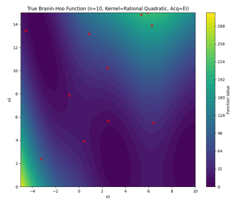
Figure 6: Matern kernel GP mean with different acquisition functions.



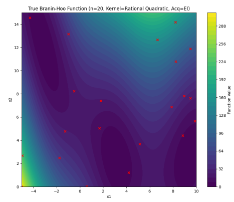
n=10 with EI | n=20 with EI | n=50 with EI | n=100 with EI

n=10 with PI | n=20 with PI | n=50 with PI | n=100 with PI

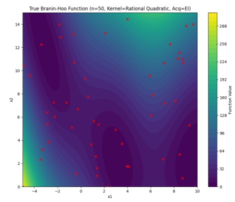
Figure 7: Matern kernel GP standard deviation with different acquisition functions.



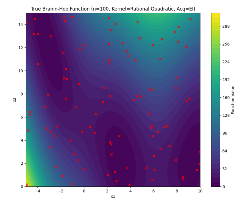
n=10 with EI



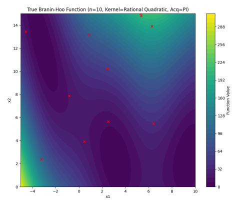
n=20 with EI



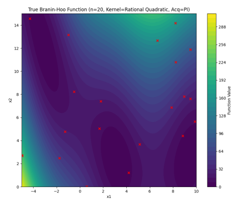
n=50 with EI



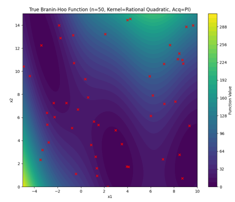
n=100 with EI



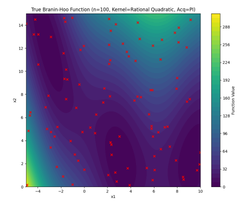
n=10 with PI



n=20 with PI

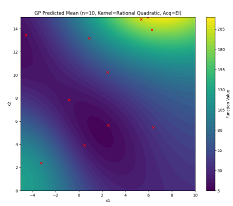


n=50 with PI

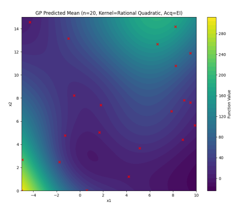


n=100 with PI

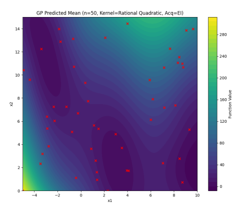
Figure 8: Rational Quadratic kernel true function with different acquisition functions.



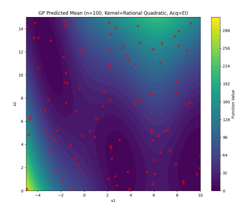
n=10 with EI



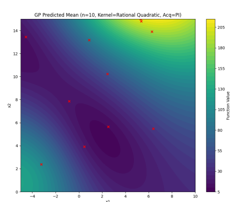
n=20 with EI



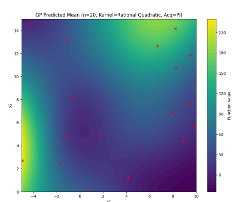
n=50 with EI



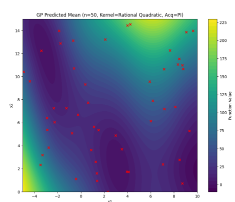
n=100 with EI



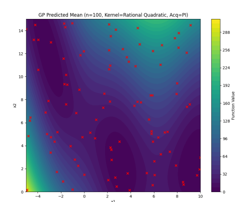
n=10 with PI



n=20 with PI

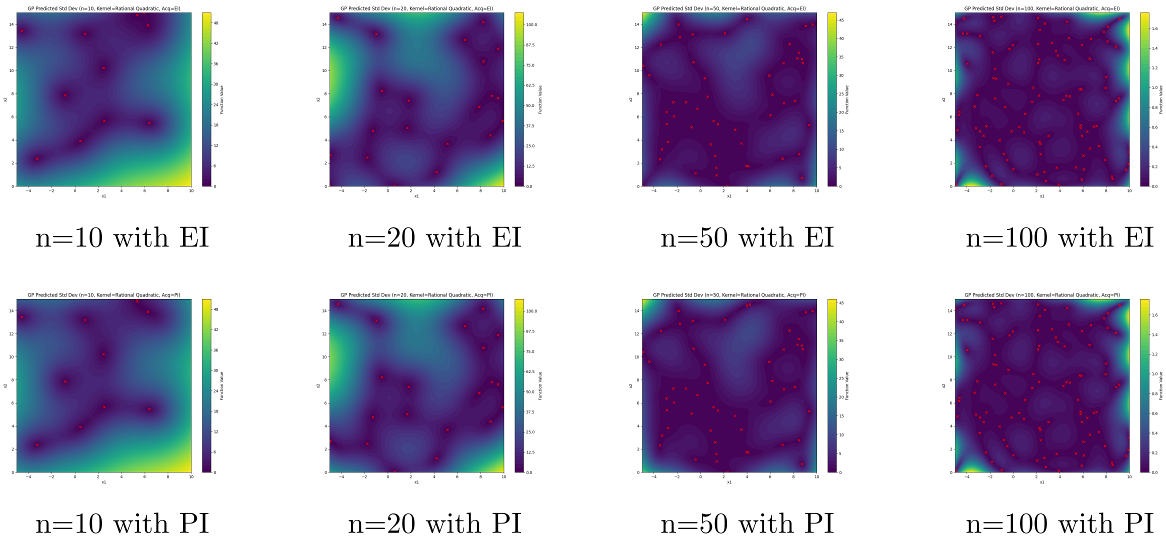


n=50 with PI



n=100 with PI

Figure 9: Rational Quadratic kernel GP mean with different acquisition functions.



n=10 with EI | n=20 with EI | n=50 with EI | n=100 with EI

n=10 with PI | n=20 with PI | n=50 with PI | n=100 with PI

Figure 10: Rational Quadratic kernel GP standard deviation with different acquisition functions.

Observations

1. **Effect of Sample Size (n):**
   - As n increases, the GP mean becomes more accurate and closely resembles the true function.
   - The standard deviation decreases, indicating improved confidence in predictions.
2. **EI vs. PI:**
   - **EI** promotes better exploration, especially at smaller n, by sampling more diverse regions.
   - **PI** is more exploitative and often clusters samples, potentially leading to suboptimal local solutions.
3. **Kernel Behavior:**
   - **RBF Kernel:** Produces smooth, globally consistent approximations. Performs well across all n.
   - **Matern Kernel:** Shows more localized variations; slower to converge but captures fine-grained features.
   - **Rational Quadratic Kernel:** Balances smoothness and local adaptability. Strong performance even at low n.
4. **Uncertainty Patterns:**
   - Higher uncertainty (GP std dev) is seen at the edges or unsampled regions.
   - These areas shrink as n increases, particularly with EI-based acquisition.

Contributions

- **Deeptanshu Malu**:
  1. Formulated the trie data structure design for Task 1.
  2. Coded the multi head decoding algorithm for Task 2.
- **Deevyanshu Malu**:
  1. Coded the trie data structure and the constrained decoding algorithm for Task 1.
  2. Coded the multi head decoding algorithm for Task 2.
- **Neel Rambhia**:
  1. Completed all decoding algorithms in Task 0.
  2. Coded the single head decoding algorithm for Task 2.

Acknowledgements

- We have also used Copilot for faster coding and not for direct logic.
- Used ChatGPT to generate the trie data structure but filled in the logic ourselves.