Evaluating different approaches of implementing Bayesian Neural Networks in the context of Bioprocesses

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Scope: Internship
Skills: Strong ML background, Python/PyTorch, Critical thinking
                  (Bioprocess knowledge not crucial)
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Executive Summary

The primary goal of this project is to explore different ways of implementing efficient Bayesian Neural Networks (Bayesian NNs) for bioprocess applications. These models will be developed and evaluated for a variety of datasets (in-silico and potentially real processes) and benchmarked against our current implementation of the Bayesian NN.

Background

Brief introduction / Context

Bioprocesses relies on the use of living organisms to produce various products, presenting a dynamic system with complex interactions. Modeling is crucial for design, optimization, monitoring and control of these processes. The complexity of these systems prevents the development of pure knowledge–based models while the expense of collecting data limits the application of purely data-driven machine learning (ML) model. Hybrid models are a paradigm of models that augment ML models with a knowledge backbone, available in the form of system of differential equations.

$$\frac{dX_i}{dt} = f(X, Z) + \text{In}_i - \text{Out}_i$$

$$f(X, Z) = NN(X, Z)$$

Current approaches / State of the art

The straightforward augmentation into the ML framework can be realized by discretizing the differential equations and learning a mapping between the current time to a future time point.

$$X_{i,t+1} = X_{i,t} + \Delta t \times (f(X_t, Z) + \text{In}_i - \text{Out}_i)$$

We have an existing implementation with a recurrent neural network, specifically, an LSTM to learn the function f(X,Z). This implementation already encodes a Bayesian feature by learning a variance head by minimizing the negative log likelihood loss.

Challenges

While this framework already presents promising results, as part of this project, we would like to extensively characterize the avenue of Bayesian NNs.

Project rationale / Approach

Particularly, we would like to characterize the impact of different loss functions, sampling procedure to compute probability distributions, incorporating data uncertainties in the model in the context of our existing framework. In addition, we would like to test an alternative approach of implementing Bayesian NNs by defining priors on the NN weights and learning the relevant posterior distribution of weight space, based on data.

Objectives

1. **Design choice Assessment in the current framework:** Get familiarized with the current framework. Then evaluate the impact of modulating different parameters: Losses, sampling techniques, incorporation of data noises etc., on the predicative performance and confidence interval generation capabilities. Test on in-silico datasets and confirm trends on benchmark datasets from real processes.

2. **Alternative Bayesian NN framework:** Implement the alternative Bayesian NN framework along with relevant losses, sampling procedures, training-validation-test pipelines and capabilities to obtain confidence interval.

3. **Predictive Performance assessment:** Study the performance of the model for base predictive capabilities and benchmark against current Bayesian NN for different datasets. Computational time and memory-efficiency are important parameter to monitor.

4. **Capability assessment:** Evaluate the pro-cons of both frameworks and determine a pragmatic choice to carry forward.

Methods and Work Plan

Data and Resources

- Datasets: Existing in-silico bioprocess datasets with varying noise and sampling; selected de-identified real processes for external validity (subject to availability).

- Software: Python, PyTorch

Timeline

Timeline subject to the scope. Preference: Longer the better.

Phase	Tasks	Target Dates
Exploration	Literature review, baseline reproduction.	Wk 1–3
Assess	Impact of design choices in current framework.	Wk 4–6
Benchmark	Build the alternative Bayesian NN; Establish benchmarks.	Wk 7–10
Stress Tests	Pros-cons evaluation of frameworks.	Wk 11
Wrap-up	Documentation; presentation; next steps.	Wk 12

Expected Outcome

At the end of this project, we hope to have a clear assessment of the abilities of two different reasonably characterized implementation of Bayesian NN for application to bioprocesses.

References

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