Bridging Theory and Practice: An Empirical Analysis and Optimization of the GRU-ODE-Bayes Model

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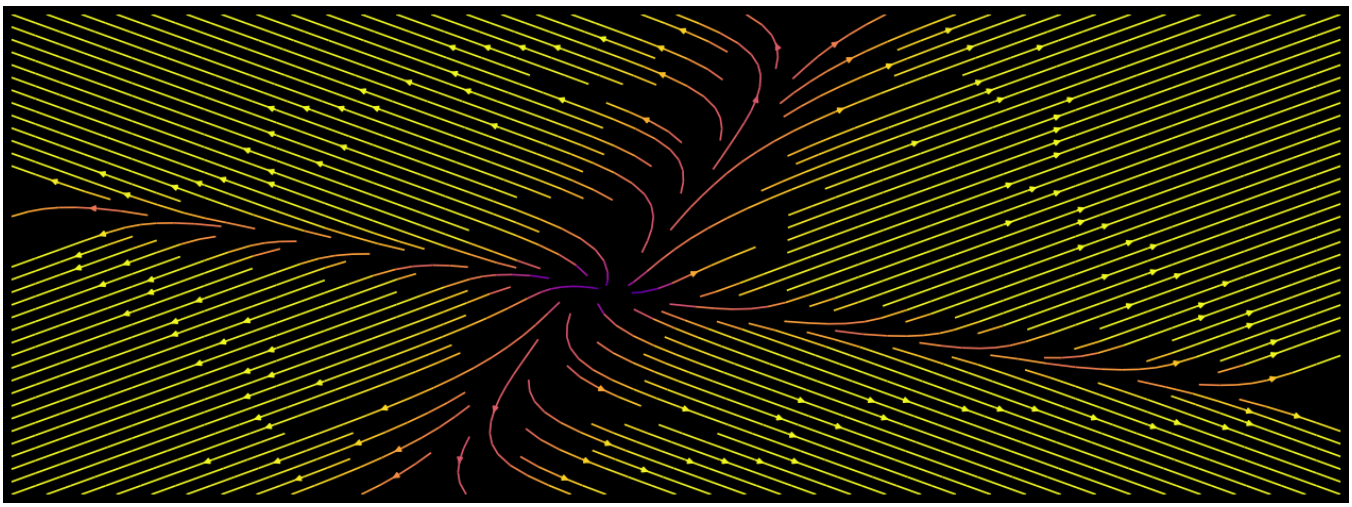

Figure 1: A stream plot visualizing the vector field of a simple Neural ODE (NODE) cell. The dynamics are defined by the equation $\frac{d\vec{y}}{dt} = \tanh(W \cdot \vec{y} + \vec{b})$ with randomly initialized weights W and biases $\vec{b}$. The arrows illustrate the flow of the learned dynamical system before any training.

Abstract

Continuous-time models based on Neural Ordinary Differential Equations (NODEs) offer a theoretically elegant solution for modeling sporadically-observed time series, a common challenge in fields like healthcare. The GRU-ODE-Bayes model represents a state-of-the-art approach, combining the continuous dynamics of an ODE solver with discrete updates inspired by Gated Recurrent Units (GRUs). This paper presents a deep, practical investigation into the implementation and performance of the GRU-ODE-Bayes model on real-world physiological datasets. We detail a systematic journey of optimization, from robust data engineering to vectorized implementation, to make the model trainable. Our investigation reveals two surprising findings. First, due to the significant overhead of the adjoint-based ODE solver for sequential, short-interval tasks, a CPU-based training pipeline significantly outperforms its GPU counterpart. Second, and more critically, a simpler baseline model that omits the ODE component entirely is not only orders of magnitude faster to train (30 seconds vs. 1 hour per epoch) but also achieves substantially higher classification accuracy (97.78% vs. 62%). These results challenge the practical utility of the added complexity of the GRU-ODE-Bayes architecture for classification tasks on this type of data, highlighting a crucial gap between theoretical promise and empirical performance.

Keywords

Neural Ordinary Differential Equations, GRU-ODE, Time Series, Adjoint Method, Performance Analysis, Computational Bottlenecks, Physiological Data

1 Introduction

Modeling time series data with irregular and sporadic observations is a persistent challenge in machine learning, with critical applications in domains such as healthcare, finance, and climate science. Traditional Recurrent Neural Networks (RNNs) and their variants, like LSTMs and GRUs, are designed for sequences with fixed, regular time steps and struggle to naturally handle the continuous-time nature of real-world processes.

Neural Ordinary Differential Equations (NODEs) [2] emerged as a powerful paradigm to address this limitation. By parameterizing the derivative of a hidden state with a neural network, NODEs learn a continuous-time dynamical system directly from data, allowing for evaluation at any point in time. The GRU-ODE-Bayes model

[1] builds upon this foundation, proposing a sophisticated architecture that propagates a system's hidden state using an ODE solver between observations and applies discrete, GRU-inspired updates at the moments observations are available.

While theoretically elegant, the practical implementation and performance characteristics of such complex models are not widely documented. The journey from a research paper's mathematical formulation to a working, efficient implementation is often fraught with non-trivial engineering challenges. This paper presents a deep dive into this process for the GRU-ODE-Bayes model. We document our journey from a naive implementation to a robust, vectorized model, tackling issues of data imbalance and computational bottlenecks.

Our investigation, conducted on three real-world physiological time series datasets, yields surprising and critical insights. We find that the computational overhead of the core ODE solver component makes the model train significantly faster on a CPU than on a high-end GPU. More importantly, we demonstrate that a simplified baseline model, which removes the continuous-time ODE dynamic entirely, is not only orders of magnitude faster but also dramatically more accurate for the task of arrhythmia classification. This work aims to bridge the gap between theory and practice, providing a critical analysis of the GRU-ODE-Bayes model's effectiveness and highlighting the crucial need to benchmark complex architectures against strong, simple baselines.

2 Theoretical Background

To understand our work, we first review the two core concepts upon which the GRU-ODE-Bayes model is built.

2.1 Neural Ordinary Differential Equations

A Neural ODE models the continuous evolution of a hidden state vector $\vec{z}(t)$ by defining its derivative with a neural network f:

$$\frac{d\vec{z}(t)}{dt} = f(\vec{z}(t), t, \theta) \tag{1}$$

Given an initial state $\vec{z}(t_0)$, the state at any later time t_1 can be found by integrating this differential equation:

$$\vec{z}(t_1) = \vec{z}(t_0) + \int_{t_0}^{t_1} f(\vec{z}(t), t, \theta)dt \tag{2}$$

This integration is performed by a numerical ODE solver. A key challenge is backpropagation through the solver. The adjoint sensitivity method [2] provides a highly memory-efficient solution by solving a second, augmented ODE backwards in time to compute gradients. This allows for training with constant memory cost with respect to depth. A full derivation of the adjoint method is provided in Appendix A and its generalization using a Hamiltonian formulation is in Appendix B.

2.2 The GRU-ODE-Bayes Model

The GRU-ODE-Bayes model [1] adapts the NODE framework for sporadically-observed time series. The core idea is twofold:

(1) **Between observations**, the hidden state $\vec{h}(t)$ evolves continuously according to an ODE solver.
(2) **At an observation** x_i at time t_i, the hidden state is updated using a mechanism analogous to a GRU cell, incorporating the new information.

The model also incorporates a Bayesian framework to quantify uncertainty, which involves minimizing the Evidence Lower Bound (ELBO). This objective function includes a reconstruction loss and a KL-divergence term that regularizes the latent space. The derivation for the KL divergence between two Gaussian distributions, a key component of the ELBO, is provided in Appendix C.

3 Implementation and Optimization

We implemented the GRU-ODE-Bayes model in PyTorch, using the `torchdiffeq` library for its implementation of the adjoint method. Our goal was to classify cardiac conditions from physiological data.

3.1 Datasets and Preprocessing

We used three publicly available ECG databases: the BIDMC Congestive Heart Failure Database, the MIT-BIH Arrhythmia Database, and the MIT-BIH Normal Sinus Rhythm Database. The raw signals were preprocessed by:

(1) Filtering the signal to remove noise.
(2) Detecting R-peaks to identify heartbeats.
(3) Extracting QRS timings around each R-peak.
(4) Segmenting the long recordings into uniform, overlapping "chunks" of 512 observations to create a dataset of manageable, equally-sized samples. This step was critical to prevent GPU out-of-memory errors and stabilize training.

3.2 From Naive Loop to Vectorized Model

A naive implementation of the GRU-ODE-Bayes model involves a Python `for` loop that iterates through each observation in a sequence, alternating between an ODE solve and a discrete update. This approach proved to be a major performance bottleneck due to high overhead from many small, sequential operations.

To overcome this, we re-architected the forward pass to be fully vectorized. Instead of looping, our final implementation performs:

(1) **A single, batched `odeint` call** to compute a "base trajectory" for the hidden state over all required time points in the batch.
(2) **Vectorized tensor operations** (e.g., `gather`, `index_add_`) to apply the effects of all discrete updates simultaneously to the base trajectory.

This significantly reduced Python overhead and shifted the computation to a few large tensor operations, the ideal workload for modern deep learning frameworks.

4 Experimental Results and Analysis

Our experiments were designed to evaluate both the performance and the predictive accuracy of our optimized GRU-ODE-Bayes model against a strong baseline.

4.1 The GPU Performance Anomaly

Despite our vectorization efforts, we observed a baffling performance characteristic: the model trained significantly slower on a high-end GPU than on a CPU.

- **CPU Training Time (batch size 1):** ~1 hour / epoch.
- **GPU Training Time (batch size 64):** ~5 hours / epoch.

Systematic profiling revealed that the bottleneck was the `odeint_adjoint` function itself. For this model's specific workload—solving many short ODE segments back-to-back—the fixed overhead of launching CUDA kernels and managing the adjoint state on the GPU dominated the actual computation. The CPU, with its lower call overhead for sequential tasks, proved more efficient for this particular operational pattern.

4.2 Model Accuracy and Baseline Comparison

The most critical part of our analysis was comparing the full GRU-ODE-Bayes model against a simple but powerful baseline. This baseline uses the exact same architecture but **removes the ODE solver**, replacing it with a simple identity function that carries the last hidden state forward. The results were stark, as shown in Table 1.

Table 1: Performance and Accuracy Comparison.

Metric	GRU-ODE-Bayes	Baseline (No ODE)
Validation Accuracy	62.0%	**97.78%**
Training Time / Epoch	~1 hour (CPU)	~30 seconds

The complex, theoretically-motivated GRU-ODE-Bayes model was not only 120 times slower but also drastically less accurate than the simple baseline. The continuous dynamics modeled by the ODE solver did not provide a useful inductive bias for this classification task; instead, it appears to have hindered learning, possibly by introducing numerical instability or an overly complex loss landscape.

4.3 A Successful Application: Learning Dynamical Systems

To isolate and demonstrate the power of the NODE concept for its intended purpose, we conducted a supplementary experiment on a classic dynamical systems problem: learning the dynamics of the Lotka-Volterra (prey-predator) model. Here, the task is not classification, but to learn the underlying vector field from sparse trajectory data.

We first compare the ground truth dynamics to the output of a standard Multi-Layer Perceptron (MLP) with a similar number of parameters. As shown in Figure 2, the standard MLP is unable to learn the rotational structure of the system, demonstrating its lack of an appropriate inductive bias for this task.

Next, we evaluate two NODE-based models, differing only in their activation function. The results in Figures 4 and 5 are striking. The Tanh-based NODE captures a distorted sense of rotation but fails to accurately model the system. In contrast, the ReLU-based NODE almost perfectly reconstructs the vector field. This result confirms that NODEs possess a powerful inductive bias for learning continuous vector fields, but their success is highly dependent on both the problem domain and key architectural choices.

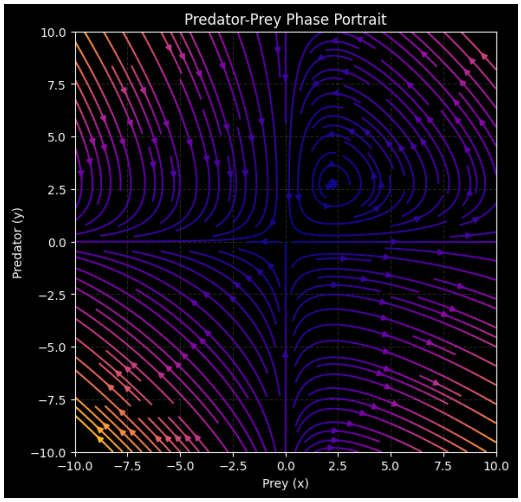

Figure 2: The ground truth vector field of the Lotka-Volterra dynamical system, showing its characteristic stable cycle.

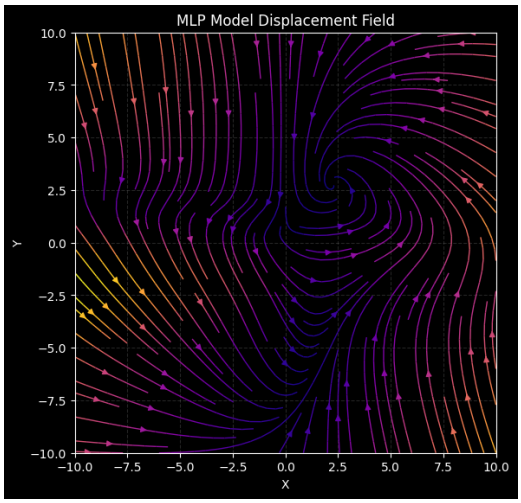

Figure 3: The vector field learned by a standard MLP. It fails to capture the rotational dynamics of the true system.

5 Discussion

Our findings present a cautionary tale about the application of complex models. The GRU-ODE-Bayes architecture, while theoretically compelling, failed to deliver on its promise for the practical task of arrhythmia classification on our datasets. The significant computational overhead and inferior performance compared to a simple baseline suggest that the model's core assumption—that modeling the continuous dynamics between heartbeats is beneficial—does not hold true for this problem. The classification task may depend more on the sequence of discrete QRS events rather than the subtle continuous evolution between them.

The performance anomaly where a CPU outperforms a GPU also serves as a critical reminder that hardware acceleration is not a universal solution. The nature of the computational workload is

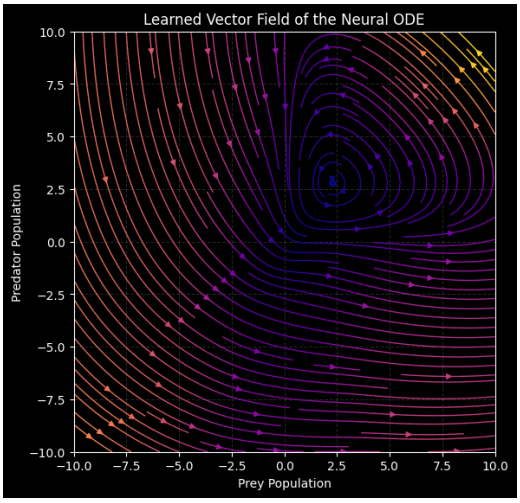

Figure 4: The learned vector field from a NODE with a Tanh activation function. The dynamics are distorted and inaccurate.

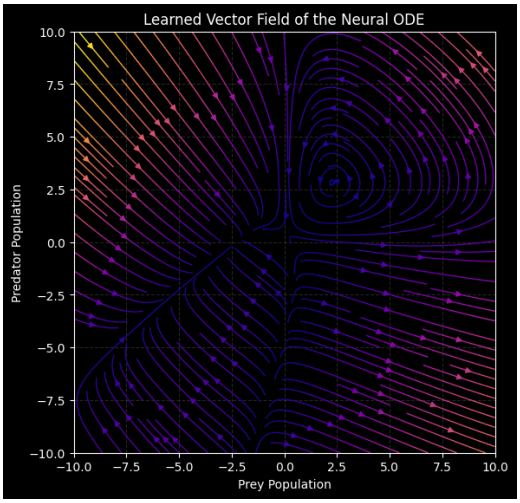

Figure 5: The learned vector field from a NODE with a ReLU activation function. The model accurately reconstructs the true dynamics.

paramount, and algorithms involving many small, sequential steps may not benefit from a GPU's massively parallel architecture.

6 Conclusion

In this paper, we documented the implementation, optimization, and critical evaluation of the GRU-ODE-Bayes model. Through a rigorous process, we successfully trained the model on real-world physiological data, but discovered that its complexity was its downfall. A simpler baseline without the continuous-time ODE component was vastly superior in both speed and accuracy. Our work underscores the importance of empirical validation and the principle of Occam's razor in machine learning: a simpler model that performs better is the better model. While Neural ODEs remain a powerful tool, particularly for learning physical dynamics, their application requires careful consideration of the problem's nature and a thorough comparison against strong, simpler baselines.

Acknowledgments

To Robert, for the bagels and explaining CMYK and color spaces.

References

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A Derivation of the Adjoint Method for Neural ODEs

This appendix provides a detailed derivation of the adjoint method as presented in Appendix B of the paper [2]. The derivation here is presented in a more intuitive manner, aiming to deduce the result from first principles rather than starting with the definition of the adjoint state.

A.1 Context

In a standard Recurrent Neural Network (RNN), a sequence of hidden states is generated, where each state carries information to the next:

$$\vec{h}_{t+1} = \vec{h}_t + f(\vec{h}_t, \theta_t) \tag{3}$$

The Neural Ordinary Differential Equation (NODE) model extends this concept to the continuous-time domain. As the time steps approach zero, the sequence of hidden states can be modeled as a continuous trajectory, $\vec{z}(t)$, governed by an ordinary differential equation (ODE):

$$\frac{d\vec{z}(t)}{dt} = \dot{\vec{z}} = f(\vec{z}(t), \theta, t) \tag{4}$$

We wish to find the gradient of a loss function L with respect to the parameters θ. Typically, L depends directly only on the state at the final time, $L(\vec{z}(t_1))$. To find this gradient, we use the method of Lagrange multipliers to construct a new functional, $\mathcal{J}$, which incorporates the dynamic constraint of the ODE.

$$\mathcal{J}(\vec{z}, \vec{\lambda}, \theta) = L(\vec{z}(t_1)) + \int_{t_0}^{t_1} \vec{\lambda}^T(t) \left[f(\vec{z}(t), \theta, t) - \dot{\vec{z}}(t) \right] \, dt \tag{5}$$

By construction, the value of $\mathcal{J}$ is identical to L whenever the dynamic constraint is satisfied. We analyze the first variation of $\mathcal{J}$, denoted $\delta\mathcal{J}$, by considering the contributions from each of its arguments:

$$\delta\mathcal{J} = \frac{\delta\mathcal{J}}{\delta\vec{z}} \, \delta\vec{z} + \frac{\delta\mathcal{J}}{\delta\theta} \, \delta\theta + \frac{\delta\mathcal{J}}{\delta\vec{\lambda}} \, \delta\vec{\lambda} \tag{6}$$

A.2 First Variation of the Functional

A.2.1 Variation with Respect to $\vec{\lambda}$. Setting the variation with respect to the Lagrange multiplier $\vec{\lambda}$ to zero recovers the original

dynamic constraint:

$$\frac{\delta \mathcal{J}}{\delta \vec{\lambda}} = f(\vec{z}, \theta, t) - \dot{\vec{z}} = 0 \quad \Longrightarrow \quad \dot{\vec{z}} = f(\vec{z}, \theta, t) \tag{7}$$

A.2.2 Variation with Respect to θ. The contribution from the explicit dependence on the parameter θ is:

$$\frac{\delta \mathcal{J}}{\delta \theta}\, \delta\theta = \int_{t_0}^{t_1} \vec{\lambda}^T(t)\, \frac{\partial f}{\partial \theta}\, \delta\theta\, dt \tag{8}$$

A.2.3 Variation with Respect to $\vec{z}$. The variation of $\mathcal{J}$ with respect to the trajectory $\vec{z}(t)$ is:

$$\frac{\delta \mathcal{J}}{\delta \vec{z}}\, \delta\vec{z} = \frac{\partial L}{\partial \vec{z}(t_1)}\, \delta\vec{z}(t_1) + \int_{t_0}^{t_1} \vec{\lambda}^T(t) \left[\frac{\partial f}{\partial \vec{z}}\, \delta\vec{z} - \delta\dot{\vec{z}} \right] dt \tag{9}$$

We apply integration by parts to the term containing $\delta\dot{\vec{z}}$:

$$-\int_{t_0}^{t_1} \vec{\lambda}^T \delta\dot{\vec{z}}\, dt = \int_{t_0}^{t_1} \dot{\vec{\lambda}}^T \delta\vec{z}\, dt - \left[\vec{\lambda}^T \delta\vec{z} \right]_{t_0}^{t_1} \tag{10}$$

Substituting this back and rearranging terms yields:

$$\begin{aligned} \frac{\delta \mathcal{J}}{\delta \vec{z}}\, \delta\vec{z} = &\left(\frac{\partial L}{\partial \vec{z}(t_1)} - \vec{\lambda}^T(t_1) \right) \delta\vec{z}(t_1) \\ &+ \vec{\lambda}^T(t_0)\, \delta\vec{z}(t_0) + \int_{t_0}^{t_1} \left[\vec{\lambda}^T\, \frac{\partial f}{\partial \vec{z}} + \dot{\vec{\lambda}}^T \right] \delta\vec{z}\, dt \end{aligned} \tag{11}$$

Since the initial condition $\vec{z}(t_0)$ is fixed, its variation $\delta\vec{z}(t_0)$ is zero. To nullify the remaining arbitrary variations, we strategically define the **adjoint state** $\vec{\lambda}(t)$ by enforcing two conditions:

(1) **Boundary Condition at Final Time (t_1):**

$$\vec{\lambda}^T(t_1) = \frac{\partial L}{\partial \vec{z}(t_1)} \tag{12}$$

(2) **Differential Equation of the Adjoint State:**

$$\dot{\vec{\lambda}}^T(t) = -\vec{\lambda}^T(t)\, \frac{\partial f}{\partial \vec{z}} \tag{13}$$

By imposing these conditions, the entire variation with respect to $\vec{z}$ vanishes.

A.3 Final Result

With the variations with respect to $\vec{z}$ and $\vec{\lambda}$ being zero, the total variation $\delta L = \delta \mathcal{J}$ simplifies to only the explicit contribution from θ:

$$\frac{dL}{d\theta}\, \delta\theta = \int_{t_0}^{t_1} \vec{\lambda}^T(t)\, \frac{\partial f}{\partial \theta}\, \delta\theta\, dt \tag{14}$$

This gives the final expression for the gradient of the loss function:

$$\frac{dL}{d\theta} = \int_{t_0}^{t_1} \vec{\lambda}^T(t)\, \frac{\partial f}{\partial \theta}\, dt \tag{15}$$

B Generalized Adjoint Method via Hamiltonian Formalism

Building upon the previous derivation, we can generalize the adjoint method for more complex models by employing a Hamiltonian framework, inspired by optimal control theory. This is particularly useful for models like GRU-ODE-Bayes that may include a running loss term.

We define a total loss functional T_L that includes both a final loss and an integrated loss over the trajectory:

$$T_L(\vec{q}_n, \theta, t_1, t_0) = L(\vec{q}_n(t_1)) + \int_{t_0}^{t_1} \mathcal{L}(\vec{q}_n(t), \theta, t)\, dt \tag{16}$$

The system is subject to the dynamic constraint $\dot{\vec{q}}_n(t) = f_n(\vec{q}_i(t), \theta, t)$, with a fixed initial state ($\delta\vec{q}_n(t_0) = 0$). We use the Einstein summation convention over repeated indices.

We define an augmented functional J with Lagrange multipliers $\vec{p}_n(t)$ (the co-state variables). We then define the **Hamiltonian**, H, for this system:

$$H(\vec{q}_n, \vec{p}_n, \theta, t) = \vec{p}_i(t) \cdot f_i(\vec{q}_i, \theta, t) - \mathcal{L}(\vec{q}_n, \theta, t) \tag{17}$$

This allows us to rewrite the augmented functional J compactly:

$$J(\vec{q}_n, \vec{p}_n, \theta) = L(\vec{q}_n(t_1)) + \int_{t_0}^{t_1} \left[\vec{p}_i(t) \cdot \dot{\vec{q}}_i(t) - H(\vec{q}_n, \vec{p}_n, \theta, t) \right] dt \tag{18}$$

B.1 First Variation of the Functional

B.1.1 Variation with respect to $\vec{q}_n$. After integrating by parts, the variation with respect to $\vec{q}_n$ is:

$$\delta J_{\vec{q}_n} = \left(\frac{\partial L}{\partial \vec{q}_n(t_1)} + \vec{p}_n(t_1) \right) \cdot \delta\vec{q}_n(t_1) - \int_{t_0}^{t_1} \left[\dot{\vec{p}}_i + \frac{\partial H}{\partial \vec{q}_i} \right] \cdot \delta\vec{q}_i\, dt \tag{19}$$

To make this variation zero, we define the **co-state equations** and terminal condition:

$$\dot{\vec{p}}_n(t) = -\frac{\partial H}{\partial \vec{q}_n} \tag{20}$$

$$\vec{p}_n(t_1) = -\frac{\partial L}{\partial \vec{q}_n(t_1)} \tag{21}$$

B.1.2 Variation with respect to $\vec{p}_n$. The variation with respect to $\vec{p}_n$ must also be zero, which recovers the **state equations**:

$$\delta J_{\vec{p}_n} = \int_{t_0}^{t_1} \delta\vec{p}_i \cdot \left[\dot{\vec{q}}_i - \frac{\partial H}{\partial \vec{p}_i} \right] dt = 0 \quad \Longrightarrow \quad \dot{\vec{q}}_n = \frac{\partial H}{\partial \vec{p}_n} \tag{22}$$

Note that $\frac{\partial H}{\partial \vec{p}_n} = f_n$, recovering the original system dynamics.

B.1.3 Variation with respect to θ. With all other variations being zero, the total variation $\delta T_L = \delta J$ depends only on the explicit variation of θ in the Hamiltonian:

$$\delta J_\theta = -\int_{t_0}^{t_1} \frac{\partial H}{\partial \theta}\, \delta\theta\, dt \tag{23}$$

This yields the final gradient for the total loss:

$$\frac{dT_L}{d\theta} = -\int_{t_0}^{t_1} \frac{\partial H}{\partial \theta}\, dt \tag{24}$$

C Derivation of KL Divergence for Univariate Gaussians

C.1 The Definition

The Kullback-Leibler (KL) divergence between two continuous probability distributions, $P \sim \mathcal{N}(\mu_0, \sigma_0^2)$ and $Q \sim \mathcal{N}(\mu_1, \sigma_1^2)$, is defined as an expectation:

$$D_{\mathrm{KL}}(P \parallel Q) = \mathbb{E}_{x \sim P} \left[\log \left(\frac{p(x)}{q(x)} \right) \right] \tag{25}$$

Using the properties of logarithms, we can split this into two terms:

$$D_{\mathrm{KL}}(P \parallel Q) = \mathbb{E}_{x\sim P}\left[\log(p(x))\right] - \mathbb{E}_{x\sim P}\left[\log(q(x))\right] \tag{26}$$

C.2 Step 1: The Cross-Entropy Term

The natural logarithm of the PDF for $q(x)$ is:

$$\log(q(x)) = -\frac{1}{2}\log(2\pi\sigma_1^2) - \frac{(x-\mu_1)^2}{2\sigma_1^2} \tag{27}$$

We take the expectation of this expression with respect to $x \sim P$:

$$\mathbb{E}_P\left[\log(q(x))\right] = -\frac{1}{2}\log(2\pi\sigma_1^2) - \frac{1}{2\sigma_1^2}\mathbb{E}_P\left[(x-\mu_1)^2\right] \tag{28}$$

We evaluate the expectation $\mathbb{E}_P\left[(x-\mu_1)^2\right]$:

$$\begin{aligned}
\mathbb{E}_P\left[(x-\mu_1)^2\right] &= \mathbb{E}_P\left[((x-\mu_0)+(\mu_0-\mu_1))^2\right] \\
&= \mathbb{E}_P\left[(x-\mu_0)^2 + 2(x-\mu_0)(\mu_0-\mu_1) + (\mu_0-\mu_1)^2\right] \\
&= \mathbb{E}_P[(x-\mu_0)^2] + 2(\mu_0-\mu_1)\mathbb{E}_P[x-\mu_0] + (\mu_0-\mu_1)^2 \\
&= \sigma_0^2 + 0 + (\mu_0-\mu_1)^2 = \sigma_0^2 + (\mu_0-\mu_1)^2
\end{aligned}$$

Plugging this back gives the cross-entropy:

$$\mathbb{E}_P\left[\log(q(x))\right] = -\frac{1}{2}\log(2\pi) - \log(\sigma_1) - \frac{\sigma_0^2 + (\mu_0-\mu_1)^2}{2\sigma_1^2} \tag{29}$$

C.3 Step 2: The Entropy Term

The term $\mathbb{E}_P\left[\log(p(x))\right]$ is the negative of the differential entropy of a Gaussian, a standard result:

$$\mathbb{E}_P\left[\log(p(x))\right] = -\frac{1}{2}\log(2\pi\sigma_0^2) - \frac{1}{2} = -\frac{1}{2}\log(2\pi) - \log(\sigma_0) - \frac{1}{2} \tag{30}$$

C.4 Step 3: Assembling the Final Result

We compute $D_{\mathrm{KL}} = (30) - (29)$:

$$\begin{aligned}
D_{\mathrm{KL}} &= \left(-\frac{1}{2}\log(2\pi) - \log(\sigma_0) - \frac{1}{2}\right) \\
&\quad - \left(-\frac{1}{2}\log(2\pi) - \log(\sigma_1) - \frac{\sigma_0^2 + (\mu_0-\mu_1)^2}{2\sigma_1^2}\right) \\
&= -\log(\sigma_0) - \frac{1}{2} + \log(\sigma_1) + \frac{\sigma_0^2 + (\mu_0-\mu_1)^2}{2\sigma_1^2}
\end{aligned}$$

Rearranging the terms gives the final, conventional form:

$$D_{\mathrm{KL}}(P \parallel Q) = \log\left(\frac{\sigma_1}{\sigma_0}\right) + \frac{\sigma_0^2 + (\mu_0-\mu_1)^2}{2\sigma_1^2} - \frac{1}{2} \tag{31}$$