# Gaussian Process Bandit Optimization of the Thermodynamic Variational Objective

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# Abstract

Achieving the full promise of the Thermodynamic Variational Objective (TVO), a recently proposed variational lower bound on the log evidence involving a onedimensional Riemann integral approximation, requires choosing a "schedule" of sorted discretization points. This paper introduces a bespoke Gaussian process bandit optimization method for automatically choosing these points. Our approach not only automates their one-time selection, but also dynamically adapts their positions over the course of optimization, leading to improved model learning and inference. We provide theoretical guarantees that our bandit optimization converges to the regret-minimizing choice of integration points. Empirical validation of our algorithm is provided in terms of improved learning and inference in Variational Autoencoders and Sigmoid Belief Networks.

# 1 Introduction

The Variational Autoencoder (VAE) framework has formed the basis for a number of recent advances in unsupervised representation learning [18, 36, 42]. Assuming a generative model involving latent variables, VAEs perform maximum likelihood parameter estimation by optimizing the tractable Evidence Lower Bound (ELBO) on the logarithm of the model evidence. In doing so, the VAE framework introduces an inference network, which seeks to approximate the true posterior over latent variables. While the ELBO is a common choice of variational inference objective, recent work has sought to improve the model learning [7, 39, 31, 26] or inference aspects [35, 19, 8, 13] of this task.

In this work, we build upon the recent Thermodynamic Variational Objective (TVO), which frames log-likelihood estimation as a one-dimensional integral over the unit interval [27]. The integral is estimated using a Riemann sum approximation, as visualized in Figure 1, yielding a natural family of variational inference objectives which generalize and tighten the ELBO.

The choice of a *d*-dimensional vector of points  $\boldsymbol{\beta} = [\beta_0, \beta_1, ..., \beta_{d-1}]^T$  at which to construct this numerical approximation is an important hyperparameter for the TVO, which we refer to as an "integration schedule" throughout this work. Previous work [27] uses a static integration schedule, and requires grid search over the choice of initial  $\beta_1$ . However, since the shape of the integrand reflects the quality of the inference network (§2), recent work [6] suggests that this scheduling procedure may be improved by dynamically choosing  $\boldsymbol{\beta}$  over the course of training. Our proposed approach also allows the TVO to be adapted to different model architectures and schedule dimensionality without the need for grid search.

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Figure 1: The TVO objective frames log likelihood estimation as a Riemann sum approximation to a 1-d integral, with the ELBO as a special case for a single  $\beta_0 = 0$ . The TVO (area in blue) bounds the integral more tightly than the ELBO (area within dotted lines).

Our primary contribution is to automate the choice of integration schedules using a Gaussian process bandit optimization. We first demonstrate that maximizing the TVO objective as a function of  $\beta$  is equivalent to a regret-minimization problem, where the black-box reward function reflects improvement in the objective for a given choice of schedule. We model this reward function over the course of training epochs using a time-varying Gaussian process (GP). Our entire procedure amounts to 1) choosing  $\beta$  to maximize an acquisition function in our surrogate GP model, 2) observing the reward function as the improvement in the TVO objective over one or more epochs of training with the chosen schedule, and 3) using these observations to update the GP model and select a new  $\beta$ . Our bandit algorithm is optimal in the sense of converging to a global regret-minimizing solution, as in the time-varying GP bandit optimization approach [5]. By choosing  $\beta$  to maximize an acquisition function that balances exploration and performance, our algorithm achieves global guarantees despite the non-convexity of the reward function. Further, our approach is directly aligned with the goal of improved model learning and inference, as the bandit reward function tracks the variational objective over the course of training.

We review the TVO framework in §2, before presenting our bandit optimization approach in §3. We provide details of our time-varying Gaussian process model and discuss its convergence properties in §4. Finally, we demonstrate that our method can improve both model learning and inference in Variational Autoencoders and Sigmoid Belief Networks, in §5.

# 2 The Thermodynamic Variational Objective (TVO)

Assuming a generative model  $p_{\theta}(\mathbf{x}, \mathbf{z})$ , we are interested in maximizing the log-likelihood  $\log p_{\theta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$  over parameters  $\theta$ , given the empirical data  $\mathbf{x}$ . However, this is intractable due to the integral over the latent variables  $\mathbf{z}$ . Variational inference methods [4] often seek to maximize the tractable ELBO instead, obtained by introducing an approximate posterior  $q_{\phi}(\mathbf{z} | \mathbf{x})$  and optimizing the objective

$$\mathsf{ELBO}(\theta, \phi, \mathbf{x}) = \log p_{\theta}(\mathbf{x}) - D_{\mathsf{KL}}[q_{\phi}(\mathbf{z} \mid \mathbf{x}) \mid \mid p_{\theta}(\mathbf{z} \mid \mathbf{x})] = \mathbb{E}_{q_{\phi}(\mathbf{z} \mid \mathbf{x})} \left[ \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z} \mid \mathbf{x})} \right].$$
(1)

Thermodynamic Integration (TI) [33, 10, 11] is a common technique for estimating (ratios of) partition functions in statistical physics, which instead frames estimating  $\log p_{\theta}(\mathbf{x})$  as a one-dimensional integral over a geometric mixture curve parameterized by  $\beta$ .<sup>1</sup> In particular, for the TVO, this curve interpolates between the approximate posterior  $q_{\phi}(\mathbf{z} | \mathbf{x})$  and true posterior  $p_{\theta}(\mathbf{z} | \mathbf{x})$ . Following [6]

<sup>&</sup>lt;sup>1</sup>Here  $\beta$  is a scalar to be consistent with notation in [27] In the remainder of the paper, we let  $\beta$  hold the sorted vector of discretization points  $\boldsymbol{\beta} = [\beta_0, \beta_1, ..., \beta_{d-1}]^T$ , so that each  $\beta_j$  specifies a  $\pi_{\beta_j}(\mathbf{z} \mid \mathbf{x})$  in (2).

this mixture curve can be interpreted as an exponential family of distributions over z given x

$$\pi_{\beta}(\mathbf{z} \mid \mathbf{x}) = q_{\phi}(\mathbf{z} \mid \mathbf{x}) \exp\{\beta \cdot \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z} \mid \mathbf{x})} - \log Z_{\beta}(\mathbf{x})\}$$
(2)  
where  $Z_{\beta}(\mathbf{x}) = \int q_{\phi}(\mathbf{z} \mid \mathbf{x})^{1-\beta} p_{\theta}(\mathbf{x}, \mathbf{z})^{\beta} d\mathbf{z}$ .

Noting that  $\log Z_0(\mathbf{x}) = 0$  and  $\log Z_1(\mathbf{x}) = \log p_{\theta}(\mathbf{x})$ , TI now applies the fundamental theorem of calculus to write the model evidence as an integral

$$\log p_{\theta}(\mathbf{x}) - 0 = \int_{0}^{1} \frac{\partial}{\partial \beta} \log Z_{\beta}(\mathbf{x}) d\beta = \int_{0}^{1} \mathbb{E}_{\pi_{\beta}} \left[ \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z} \mid \mathbf{x})} \right] d\beta,$$
(3)

where we have used the known property of exponential families [44] that the derivative of  $\log Z_{\beta}(\mathbf{x})$  with respect to  $\beta$  matches the expected sufficient statistics [27, 6]. Masrani et al. [27] use self-normalized importance sampling (SNIS) to estimate each term in the integrand, with S importance samples and  $q_{\phi}(\mathbf{z} | \mathbf{x})$  as the proposal for each  $\beta$ 

$$\mathbb{E}_{\pi_{\beta}}[\cdot] \approx \sum_{\ell=1}^{S} \frac{w_{\ell}^{\beta}}{\sum_{\ell} w_{\ell}^{\beta}}[\cdot], \quad w_{\ell} = \frac{p_{\theta}(\mathbf{x}, \mathbf{z}_{\ell})}{q_{\phi}(\mathbf{z}_{\ell} \mid \mathbf{x})}, \ \mathbf{z}_{\ell} \sim q_{\phi}(\mathbf{z} \mid \mathbf{x}).$$
(4)

Since  $\log Z_{\beta}(\mathbf{x})$  is convex [44], we know that the integrand in (3) is an increasing function of  $\beta$ . Thus, we can obtain lower and upper bounds using left- and right-Riemann sums, respectively, over a discrete partition  $\beta$  of the unit interval. The left-Riemann sum then defines the TVO lower bound

$$\operatorname{TVO}(\theta, \phi, \boldsymbol{\beta}, \mathbf{x}) := \sum_{j=0}^{d-1} (\beta_{j+1} - \beta_j) \mathbb{E}_{\pi_{\beta_j}} \left[ \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z} \mid \mathbf{x})} \right],$$
(5)

where  $\beta = [\beta_j]_{j=0}^{d-1}$  with  $\beta_0 = 0$  and  $\beta_j < \beta_{j+1}$ . Note that the single-term left-Riemann sum with  $\beta = \beta_0 = 0$  matches the ELBO in (1), since  $\pi_0(\mathbf{z} | \mathbf{x}) = q_\phi(\mathbf{z} | \mathbf{x})$ . However, how to choose intermediate  $\beta_j$  for d > 1 remains an interesting question, which we proceed to frame as a bandit problem.

#### **3** From Evidence Maximization to Regret Minimization

We view the vector  $\beta \in [0,1]^d$  as an arm [1] to be pulled in a continuous space, given a fixed resource of T training epochs. After each round, we receive an estimate of the log evidence  $\mathcal{L}$ , from which we will construct a reward function. An important feature of our problem is that the integrand in Figure 1 changes between rounds as training progresses. Thus, our multi-armed bandit problem is said to be *time-varying*, in that the optimal arm and reward function depend on round t.

More formally, we define the time-varying reward function  $f_t : [0,1]^d \to \mathbb{R}$  which takes an input  $\beta_t$  and produces reward  $f_t(\beta_t)$ . At each round we get access to a noisy reward  $y_t = f_t(\beta_t) + \epsilon_t$  where we assume Gaussian noise  $\epsilon_t \sim \mathcal{N}(0, \sigma_f^2)$ . We aim to maximize the cumulative reward  $\sum_{t=1}^{T/w} f_t(\beta_t)$  across T/w rounds, where w is a divisor of T and will later control the ratio of bandit rounds t to training epochs *i*.

Maximizing the cumulative reward is equivalent to minimizing the cumulative regret

$$R_{T/w} := \sum_{t=1}^{T/w} f_t(\beta_t^*) - f_t(\beta_t),$$
(6)

where  $r_t := f_t(\beta_t^*) - f_t(\beta_t)$  is the *instantaneous regret* defined by the difference between the received reward  $f_t(\beta_t)$  and maximum reward attainable  $f_t(\beta_t^*)$  at round t. The regret, which is non-negative and monotonic, is more convenient to work with than the cumulative reward and will allow us to derive upper bounds in §4.3.

In order to translate the problem of maximizing the log evidence as a function of  $\beta$  into the bandits framework, we define a time-varying reward function  $f_t(\beta_t)$ . We construct this reward in such a way

Algorithm 1 GP-bandit for TVO (high level)

Input: schedule dimension d, reward function  $f_t(\beta_t)$  where  $\beta_t \in [0,1]^d$ , update frequency w 1: for t = 1...T do

- 2: Train  $\theta$ ,  $\phi$  for one epoch using TVO and previously  $\beta_{t-1}$ , evaluate  $\mathcal{L}_t$  from Eq. (5)
- 3: if mod(t, w) = 0: time to update  $\beta_t$  then
- 4: Estimate the utility  $y_t = \mathcal{L}_t \mathcal{L}_{t-w}$  and augment  $(\beta_{t-1}, t, y_t)$  into training data  $D_t$
- 5: Fit a time-varying, permutation invariant GP to  $D_t$
- 6: Estimate GP predictive mean  $\mu_t(\beta)$  and uncertainty  $\sigma_t(\beta)$  from Eqs. (15,16)
- 7: Select  $\beta_t = \arg \max \mu_t(\beta) + \sqrt{\kappa_t} \sigma_t(\beta)$  where  $\kappa_t$  is from Theorem 1
- 8: **end if**
- 9: end for

that minimizing the cumulative regret is equivalent to maximizing the final log evidence estimate  $\mathcal{L}_T := \log p_{\theta_T}(\mathbf{x})$ , i.e., such that  $\min R_{T/w} = \max \mathcal{L}_T$ .

Such a reward function can be defined by partitioning the T training epochs into windows of equal length w, and defining the reward for each window  $t \in \{0, 1, ..., T/w - 1\}$ 

$$f_t(\boldsymbol{\beta}_t) := \mathcal{L}_{w(t+1)} - \mathcal{L}_{wt} \tag{7}$$

as the difference between the TVO log evidence estimate one window-length in the future  $\mathcal{L}_{w(t+1)}$ and the present estimate  $\mathcal{L}_{wt}$ . Then, the cumulative reward is given by a telescoping sum over windows

$$\sum_{t=0}^{T/w - 1} f_t(\beta_t) = \left(\mathcal{L}_w - \mathcal{L}_0\right) + \left(\mathcal{L}_{2w} - \mathcal{L}_w\right) + \dots + \left(\mathcal{L}_{(T/w)w} - \mathcal{L}_{(T/w - 1)w}\right)$$
(8)

$$=\mathcal{L}_T - \mathcal{L}_0,\tag{9}$$

where  $\mathcal{L}_0$  is the initial (i.e. untrained) loss. Recalling the definition of cumulative regret in Eq. (6),

$$\min R_{T/w} = \min \left( \sum_{t=0}^{T/w - 1} f_t(\beta_t^*) \right) - \left( \sum_{t=0}^{T/w - 1} f_t(\beta_t) \right)$$
(10)

$$= \min\left(\left(\mathcal{L}_T^* - \mathcal{L}_0\right) - \left(\mathcal{L}_T - \mathcal{L}_0\right)\right)$$
(11)

$$= \min\left(\operatorname{const} - \mathcal{L}_T\right) \tag{12}$$

$$= \max \mathcal{L}_T. \tag{13}$$

Therefore minimizing the cumulative regret for the reward function defined by Eq. (7) is equivalent to maximizing the log evidence on the final epoch. Next, we describe how to design an optimal decision mechanism to minimize the cumulative regret  $R_{T/w}$  using Gaussian processes.

# 4 Minimizing Regret with Gaussian Processes

There are two unresolved problems with the reward function defined in Eq. (7) which still must be addressed. The first is that it is not in fact computable, due to its use of future observations. The second is that it ignores the ordering constraint required for  $\beta$  to be a valid Riemann partition.

We can handle both by problems by using a permutation-invariant Gaussian process to form a surrogate for the reward function  $f_t(\beta_t)$ . The surrogate model will be updated by past rewards, and used in place of  $f_t(\beta_t)$  to select the next schedule at the current round, as described in Algorithm 1.

In §4.1 we formally define how to use (time-varying) Gaussian processes in bandit optimization, before describing how our permutation-invariant kernel can be used to solve the problem of ordering constraints on  $\beta$  in §4.2. Finally in §4.3 we provide a theoretical guarantee that our bandit optimization will converge to the regret-minimizing choice of  $\beta$ .

#### 4.1 Time-varying Gaussian processes for Bandit Optimization

A popular design in handling time-varying functions [21, 41, 20, 32] such as  $f_t(\beta_t)$  is to jointly model the spatial and temporal dimensions using a product of covariance functions  $k = k_\beta \otimes k_T$ , where  $k_\beta : [0,1]^d \times [0,1]^d \to \mathbb{R}$  is a spatial covariance function over actions,  $k_T : \mathbb{N} \times \mathbb{N} \to \mathbb{R}$  is a temporal covariance function, and  $k : \mathbb{R}^{d+1}_+ \times \mathbb{R}^{d+1}_+ \to \mathbb{R}$ .

Under this joint modeling framework, the GP is defined as follows. At round t we have the history of rewards  $y_t = [y_0, ..., y_t]^T$  and sample points  $X_t = \{x_0, ..., x_t\}$ , where we define  $x_t \in \mathbb{R}^{d+1}$  to be the concatenation of  $\beta_t$  and timestep t, i.e  $x_t := [\beta_t, t]^T$ . Then the time-varying reward function is GP-distributed according to

$$f_t \sim GP(0, k(\boldsymbol{x}, \boldsymbol{x}')) \qquad \text{where } k(\boldsymbol{x}, \boldsymbol{x}') := k_\beta(\boldsymbol{\beta}, \boldsymbol{\beta}') \times k_T(t, t'), \tag{14}$$

where we have assumed zero prior mean for simplicity. For theoretical convenience we follow [5] and choose  $k_T(t,t') = (1-\omega)^{\frac{|t-t'|}{2}}$ , where  $\omega$  is a "forgetting-remembering" trade-off parameter learned from data. We describe  $k_\beta(\beta, \beta')$  in §4.2.

Using standard Gaussian identities [3, 34], the posterior predictive is also GP distributed, with mean and variance given by

$$\mu_t(\boldsymbol{\beta}_*) = \boldsymbol{k}_t(\boldsymbol{\beta}_*)^T \left( \boldsymbol{K}_t + \sigma_f^2 \boldsymbol{I} \right)^{-1} \boldsymbol{y}_t$$
(15)

$$\sigma_t^2(\boldsymbol{\beta}_*) = \boldsymbol{k}_t(\boldsymbol{\beta}_*, \boldsymbol{\beta}_*) - \boldsymbol{k}_t(\boldsymbol{\beta}_*)^T \left(\boldsymbol{K}_t + \sigma_f^2 \boldsymbol{I}\right)^{-1} \boldsymbol{k}_t(\boldsymbol{\beta}_*)$$
(16)

where  $k_t(\beta) = [k(x_0, x), ..., k(x_t, x)]^T$  and  $K_t = [k(x, x')]_{x, x' \in X_t}$ . Using this permutationinvariant, time-varying GP we can select  $\beta_{t+1}$  by maximizing a linear combination of the GP posterior mean and variance w.r.t  $\beta_t$ 

$$\boldsymbol{\beta}_{t+1} = \operatorname*{arg\,max}_{\boldsymbol{\beta}_t} \mu_t(\boldsymbol{\beta}_t) + \sqrt{\kappa_t} \sigma_t(\boldsymbol{\beta}_t), \tag{17}$$

where Eq. (17) is referred to as an *acquisition function* and  $\kappa_t$  is its exploration-exploitation trade-off parameter. We note that there are other acquisition functions available [16, 14, 15]. Our acquisition function, Eq. (17), is the time-varying version of GP-UCB [40, 5], which allows us to obtain convergence results in §4.3 and set  $\kappa_t$  in Theorem 1.

## 4.2 Ordering Constraints and Permutation Invariance

Recall that the vector  $\boldsymbol{\beta} = [\beta_0, ..., \beta_{d-1}]^T$  holds the locations of the left Riemann integral approximation in Eq. (5). In order for the left Riemann approximation to the TVO to be sensible, there must be an ordering constraint imposed on  $\boldsymbol{\beta}$  such that  $0 < \beta_1 < ... < \beta_{d-1} < 1$ . We model this in our GP using a projection operator  $\Phi$  which imposes the constraint by sorting the vector  $\boldsymbol{\beta}$ . Applying  $\Phi$  within the spatial kernel, we obtain

$$k_{\beta}(\boldsymbol{\beta}, \boldsymbol{\beta}') := k_{S}(\Phi(\boldsymbol{\beta}), \Phi(\boldsymbol{\beta}')).$$
(18)

This projection does not change the value of our acquisition function, and maintains the positive definite for any covariance function for the spatial  $k_s$ , e.g., Matern, Polynomial. We then optimize the acquisition function via a projected-gradient approach. If a  $\beta_t$  iterate leaves the feasible set after taking a gradient step, we project it back into the feasible set using  $\Phi$  and continue. We note that existing work in the GP literature has considered such projection operations in various contexts [38, 43].

#### 4.3 Convergence Analysis

In Eq. (10), we showed that maximizing the TVO objective function  $\mathcal{L}_{\mathcal{T}}$  as a function of  $\beta_t$  is equivalent to minimizing the cumulative regret  $R_{T/w}$  by sequential optimization within the bandit framework. Here, the subscript T/w refers to the number of bandit updates given the maximum epochs T and the update frequency w where  $w \ll T$ .

We now derive an upper bound on the cumulative regret, and show that it asymptotically goes to zero as T increases, i.e.,  $\lim_{T\to\infty} \frac{R_{T/w}}{T} = 0$ . Thus, our bandit will converge to choosing  $\beta_T$  which yields the optimal value of the TVO objective  $\mathcal{L}_T^*$  for model parameters at step T.



Figure 2: Time-varying reward function  $f_t(\beta_t)$  after 2k, 3k, and 10k training epochs, with bandit choices of a single intermediate  $\beta_1$  (i.e.  $\beta = [0, \beta_1]$ ) colored by timestep. Scattered  $\beta_1$  in neighboring epochs indicate 'exploration', while similarly colored values of  $\beta_1$  in regions where the GP mean, or predicted reward, is high indicate 'exploitation'.

We present the main theoretical result in Theorem 1. Our TVO framework mirrors the standard timevarying GP bandit optimization, and thus inherits convergence guarantees from Bogunovic et al. [5]. However, as discussed in Appendix §C, we provide a tighter bound on the mutual information gain  $\gamma_{T/w}$  which may be of wider interest.

**Theorem 1.** Let the domain  $\mathcal{D} \subset [0,1]^d$  be compact and convex. Let  $L_t \geq 0$  be the Lipschitz constant for the reward function at time t. Assume that the covariance function k is almost surely continuously differentiable, with  $f \sim GP(0,k)$ . Further, for  $t \leq T$  and  $j \leq d$ , we assume

$$Pr\left(\sup\left|\partial f_t(\boldsymbol{\beta}_t)/\partial \boldsymbol{\beta}_t^{(j)}\right| \ge L_t\right) \le ae^{-(L_t/b)^2}$$

for appropriate choice of a and b corresponding to  $L_t$ .

For  $\delta \in (0, 1)$ , we write  $\kappa_{T/w} = 2 \log \frac{\pi^2 T^2}{2\delta w^2} + 2d \log db \frac{T^2}{w^2} \sqrt{\log \frac{da\pi^2 T^2}{2\delta w^2}}$  and  $C_1 = 8/\log(1+\sigma_f^2)$ . Then, after T/w time steps, our algorithm satisfies

$$R_{T/w} = \sum_{t=1}^{T/w} f_t(\boldsymbol{\beta}_t^*) - f_t(\boldsymbol{\beta}_t) \le \sqrt{\gamma_{T/w} \cdot C_1 \cdot \kappa_{T/w} \cdot T/w} + 2$$

with probability at least  $1 - \delta$ , where  $\gamma_{T/w}$  is the maximum information gain for the time-varying covariance function (see below).

In the above theorem, the quantity  $\gamma_{T/w}$  measures the maximum information gain obtained about the reward function after pulling T/w arms [40, 5]. In the Appendix §C, we show that  $\gamma_{T/w} \leq$  $\left(1+T/\left[w\tilde{N}\right]\right)\left(\gamma_{\tilde{N}}^{\boldsymbol{\beta}}+\sigma_{f}^{-2}\tilde{N}^{5/2}\omega\right)$ , where  $\tilde{N} \in \{1,...,T/w\}$  denotes a time-varying block length, and  $\gamma^{\beta}_{\tilde{N}}$  is defined with respect to the covariance kernel for  $\beta$ . For our particular choice of exponentiated-quadratic kernel, the maximum information gain scales as  $\gamma_{\tilde{N}}^{\beta} \leq \mathcal{O}(\log \tilde{N}^{d+1})$ [40]. Compared with [5], our proof tightens the upper bound on  $\gamma_{T/w}$  from  $\mathcal{O}(\tilde{N}^3)$  to  $\mathcal{O}(\tilde{N}^{5/2})$ . the bound as  $R_{T/w}$ write Combining  $\lesssim$ these terms. we can then  $\mathcal{O}(\sqrt{\left[\log \tilde{N}^{d+1} + \sigma_f^{-2} \tilde{N}^{5/2} \omega\right] T/w})$ , which is sublinear in T when the function f becomes time-invariant, i.e.,  $\omega \to 0$ . In contrast, the sublinear guarantee does not hold when the time-varying function is non-correlated, i.e.,  $\omega = 1$ , in which case the time covariance matrix becomes identity matrix. The bound is tighter for lower schedule dimension d.

# **5** Experiments

We demonstrate the effectiveness of our method for training VAEs [18] on MNIST and Fashion MNIST, and a Sigmoid Belief Network [28] on binarized MNIST and binarized Omniglot, using the TVO objective. In Appendix D, we explore learning and inference in a discrete probabilistic context-free grammar [24], showing that the TVO objective and our bandit optimization can translate to other

learning settings. In addition, we run ablation studies using random choices of  $\beta$  and a GP without permutation invariance, and compare the runtime and performance of our method with grid search. Our code is available at http://github.com/ntienvu/tvo\_gp\_bandit.

**Experimental Setup:** We evaluate our GPbandit for  $S \in \{10, 50\}$  and  $d \in \{2, 5, 10, 15\}$ and, for each configuration, train until convergence using 5 random seeds. Note that, for each setting of d, we implicitly include  $\beta_0 = 0$  and append 1 to the vector  $\beta$  to perform the integration in Eq. (5).

For each S, d configuration, we compare against three baseline integration schedules: loguniform spacing in the interval  $[\beta_1, 1]$ , linearuniform spacing in the interval [0, 1], and the moments schedule of [6, 12], which corresponds to uniform spacing along the y-axis. For log/linear-uniform spacing, we set  $\beta_1 = 0.025$ for all experiments, reflecting the results of grid search in [27]. We use a fixed model architecture for all experiments, which we describe in Appendix A.

To obtain the bandit feedback in Eq. (7), we use a fixed, linear schedule with d = 50 for calculating  $\mathcal{L}_t$  with Eq. (5). This yields a tighter  $\log p_{\theta}(\mathbf{x})$  bound, decouples reward function evaluation from model training and schedule selection in each round, and is still efficient using SNIS in Eq. (4). We limit the value of dfor TVO training following observations of deteriorating performance in [27].

#### Selecting $\beta_t$ by GP Bandit Selecting $\beta_t$ by GP Bandit $\beta_t$

Figure 3: Bandit-chosen  $\beta$  over time on MNIST using d = 5. We can interpret the  $\beta$  selection process in 3 phases: (blue) random selection in initial epochs; (orange) focusing on small values  $\beta_i < 0.5$  as training progresses; (green) moving toward  $\beta_i = 1$  as learning approaches convergence. The bottom panel illustrates a hypothetical integrand curve and  $\beta$  selections at intermediate (left) and later (right) epochs.

#### GP Implementation: For GP modeling, we

use an exponentiated quadratic covariance function for  $k_{\beta}$  and estimate hyperparameters via type II maximum likelihood estimation [34]. We use multi-start BFGS [9] to optimize the acquisition function in Eq. (17). We set the update frequency w = 6 initially and increment w by one after every 10 bandit iterations to account for smaller objective changes later in training, and update early if  $\mathcal{L}_t \leq -0.05$ . We found that selecting  $\beta_j$  too close to either 0 or 1 could negatively affect performance, and thus restrict  $\boldsymbol{\beta} \in [0.05, 0.95]^d$  in all experiments. We follow a common practice to standardize with the running average the utility score  $y \sim \mathcal{N}(0, 1)$  for robustness.

#### 5.1 Scheduling Behaviour

We first investigate the behaviour of our time-varying reward function and bandit scheduling. These experiments highlight the adaptive nature of our algorithm, as we inspect the choice of integration schedule across training epochs for both d = 2 and d = 5.

**Time-varying Reward Function:** In Figure 2, we visualize the mean and variance of our timevarying estimate of the utility function  $y_t = f_t(\beta_t) + \epsilon_t$  after 2000, 3000, and 10,000 epochs, respectively. We illustrate the choice of  $\beta$  for d = 2, so that  $\beta_0 = 0$  is fixed and we can write the reward as  $f_t(\beta_1)$ . Colored dots indicate values of  $\beta_1$  selected by our bandit algorithm in each round, with the vertical axis reflecting the observed reward  $f_t(\beta_1)$  as the change in model evidence  $\mathcal{L}$ .

In the first two panels, we observe instances where our bandit prioritizes exploitation, choosing similar, high-reward  $\beta_1$  values in neighboring rounds with the same color. However, note that these  $\beta_1$  may not match the highest GP predictive mean for  $f_t(\beta)$ , since the blue line is shown at the final training epoch in a window. In the final panel, we observe that our time-varying reward function has adapted to have very low variance, since the TVO objective changes only slightly near convergence and the choice of  $\beta_1$  has little impact.



Figure 4: Performance comparison for continuous VAE on MNIST and Fashion MNIST. *Top*: we compare model learning performance using test likelihood (higher is better). *Bottom*: We compare posterior inference as measured by the test KL divergence (lower is better) against the log and moments baselines. Although, in general, we find that models with worse  $\log p(\mathbf{x})$  tend to have lower  $D_{KL}$ , our GP-bandit schedule provides improvements in both learning and inference.



Figure 5: Performance comparison in discrete latent variable model using a Sigmoid Belief Network on the binarized MNIST dataset. Our GP-bandit achieves comparable results to the log and moments schedule in terms model learning (higher  $\log p(\mathbf{x})$ ), with better posterior inference (lower  $D_{KL}$ ).

 $\beta$  Across Training: In Figure 3, we visualize bandit choices of  $\beta$  with d = 5. In initial epochs (blue), the GP-bandit algorithm prioritizes exploration before focusing on  $\beta_j < 0.5$  in the second phase (orange). As the VAE converges, our algorithm begins to explore  $\beta_j$  further from zero (green).

Beyond avoiding the need for an expensive grid search, a primary motivation for our bandit approach is a lack of knowledge about the shape of the integrand. Using the intuition that  $\beta_j$  choices should be concentrated in regions where the integrand is changing quickly in order to obtain accurate Riemann approximations, we can still translate the observed bandit choices of  $\beta$  into example integrands in the middle (orange) and late (green) stages of training in the bottom panel of Fig. 3. An integrand that rises steeply away from  $\beta = 0$  indicates that  $q_{\phi}(\mathbf{z} | \mathbf{x})$  is mismatched to  $p_{\theta}(\mathbf{z} | \mathbf{x})$ , and the TVO might be improved by choosing small  $\beta_j$ . As the curve begins to smooth later in training, with a higher proportion of importance samples yielding high likelihood under the generative model, our bandit begins to explore  $\beta_j$  closer to 1.

#### 5.2 Model Learning and Inference

**Continuous VAE:** We present results of training a continuous VAE on the MNIST and Fashion MNIST dataset in Figure 4. We measure model learning performance using the test log evidence, as estimated by the IWAE bound [7] with 5000 samples per data point. We also compare inference performance using  $D_{\text{KL}}[q_{\phi}(\mathbf{z} | \mathbf{x}) || p_{\theta}(\mathbf{z} | \mathbf{x})]$ , which we calculate by subtracting the test ELBO from our estimate of log  $p_{\theta}(\mathbf{x})$ .

For most scenarios in Figure 4, our GP bandit optimization outperforms baselines with respect to both model learning and inference. In general, we observe that models with lower model evidence attain lower test KL divergence. Thus, in comparing inference performance in the bottom panel of Figure 4, we compare against the log and moment schedules, baselines with comparable test log

likelihoods. It is notable that our approach often achieves better results for both learning (higher  $\log p_{\theta}(\mathbf{x})$ ) and inference (lower  $D_{\text{KL}}$ ). We obtain the highest log evidence with d = 10 for MNIST and d = 15 for Fashion MNIST.

**Sigmoid Belief Network:** We present similar results for learning discrete latent variable models using a Sigmoid Belief Network [28]. We show results on binarized MNIST in Figure 5, with binarized Omniglot in Figure 7 in Appendix D.2. Our GP bandit optimization achieves competitive model learning performance with the log-uniform and moment schedules and better posterior inference across models with comparable  $\log p(\mathbf{x})$ , indicating our GP-bandit schedule can flexibly optimize the TVO for various model types.

# 6 Conclusion

We have presented a new approach for automated selection of the integration schedule for the Thermodynamic Variational Objective. Our bandit framework optimizes a reward function that is directly linked to improvements in the generative model evidence over the course of training the model parameters. We show theoretically that this procedure asymptotically minimizes the regret as a function of the choice of schedule. Finally, we demonstrated that the proposed approach empirically outperforms existing schedules in both model learning and inference for discrete and continuous generative models.

Our GP bandit optimization offers a general solution to choosing the integration schedule in the TVO. However, our algorithm, as well as all other existing schedules, still rely on the number of partitions d as a hyperparameter which is fixed over the course of the training. Incorporating the adaptive selection of d into our bandit optimization remains an interesting direction for future work.

# 7 Broader Impact

Our research can be widely applied for variational inference in deep generative models, including variational autoencoders with autoregressive decoders and normalizing flows. Variational inference, and Bayesian methods more generally, have broad applications spanning science and engineering, from epidemiology [45] to particle physics [2]. Our methodological contributions for variational inference may find broader impact through improved modelling in these disparate domains. However, our method is general in nature, so domain-specific applications should further consider implications for deployment in the real-world.

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# A Experimental Setup

**Dataset Description** The discrete and continuous VAE literature use slightly different training procedures. For continuous VAEs, we follow the sampling procedure described in footnote 2, page 6 of Burda et al. [7], and sample binary-valued pixels with expectation equal to the original gray scale  $28 \times 28$  image. We split MNIST [25] and Fashion MNIST [46] into 60k training examples and 10k testing examples across 10 classes.

For Sigmoid Belief Networks, we follow the procedure described by Mnih and Rezende [29] and use 50k training examples and 10k testing examples (the remaining 10k validation examples are not used) with the binarized MNIST [37] dataset.

**Training Procedure** All models are written in PyTorch and trained on GPUs. For each scheduler, we train for 10,000 epochs using the Adam optimizer [17] with a learning rate of  $10^{-3}$ , and minibatch size of 1000. All weights are initialized with PyTorch's default initializer. For the neural network architecture, we use two hidden layers of [100, 25] nodes.

**Reward Evaluation** To obtain the bandit feedback in Eq. (7), we use a fixed, linear schedule with d = 50 for calculating  $\mathcal{L}_t$  with Eq. (5). This yields a tighter  $\log p_\theta(\mathbf{x})$  bound, decouples reward function evaluation from model training and schedule selection in each round, and is still efficient using SNIS in Eq. (4). We limit the value of d for TVO training following observations of deteriorating performance in [27].

## **B** GP kernels and treatment of GP hyperparameters

We present the GP kernels and treatment of GP hyperparameters for the black-box function f.

We use the exponentiated quadratic (or squared exponential) covariance function for input hyperparameter  $k_{\beta}(\beta, \beta') = \exp\left(-\frac{||\beta-\beta'||^2}{2\sigma_{\beta}^2}\right)$  and a time kernel  $k_T(t, t') = (1-\omega)^{\frac{|t-t'|}{2}}$  where the observation  $\beta$  and t are normalized to  $[0, 1]^d$  and the outcome y is standardized  $y \sim \mathcal{N}(0, 1)$  for robustness. As a result, our product kernel becomes

$$k\left([\boldsymbol{\beta},t],[\boldsymbol{\beta}',t']\right) = k(\boldsymbol{\beta},\boldsymbol{\beta}') \times k(t,t') = \exp\left(-\frac{||\boldsymbol{\beta}-\boldsymbol{\beta}'||^2}{2\sigma_{\boldsymbol{\beta}}^2}\right) (1-\omega)^{\frac{|t-t'|}{2}}.$$

The length-scales  $\sigma_{\beta}$  is estimated from the data indicating the variability of the function with regards to the hyperparameter input x and number of training iterations t. Estimating appropriate values for them is critical as this represents the GP's prior regarding the sensitivity of performance w.r.t. changes in the number of training iterations and hyperparameters. We note that previous works have also utilized the above product of spatial and temporal covariance functions for different settings [21, 5, 30].

We fit the GP hyperparameters by maximizing their posterior probability (MAP),  $p(\sigma_l, \omega | \boldsymbol{\beta}, \mathbf{t}, \mathbf{y}) \propto p(\sigma_l, \omega, \boldsymbol{\beta}, \mathbf{t}, \mathbf{y})$ , which, thanks to the Gaussian likelihood, is available in closed form as [34]

$$\ln p\left(\mathbf{y},\boldsymbol{\beta},\mathbf{t},\sigma_{l},\omega\right) = \frac{1}{2}\mathbf{y}^{T}\left(\boldsymbol{K}+\sigma^{2}\mathbf{I}_{N}\right)^{-1}\mathbf{y} - \frac{1}{2}\ln\left|\boldsymbol{K}+\sigma^{2}\mathbf{I}_{N}\right| + \ln p_{\text{hyp}}\left(\sigma_{x},\omega\right) + \text{const} \quad (19)$$

where  $\mathbf{I}_N$  is the identity matrix in dimension N (the number of points in the training set), and  $p_{\text{hyp}}(\sigma_l, \omega)$  is the prior over hyperparameters, described in the following.

We maximize the marginal likelihood in Eq. (19) to select the suitable lengthscale parameter  $\sigma_l$ , remembering-forgetting trade-off  $\omega$ , and noise variance  $\sigma_f^2$ .

Optimizing Eq. (19) involves taking the derivative w.r.t. each variable, such as  $\frac{\partial \ln p(\mathbf{y}, \boldsymbol{\beta}, \mathbf{t}, \sigma_l, \omega)}{\partial \omega} = \frac{\partial \ln p(\mathbf{y}, \boldsymbol{\beta}, \mathbf{t}, \sigma_l, \omega)}{\partial \mathbf{K}} \times \frac{\partial \mathbf{K}}{\partial k(t, t')} \times \frac{\partial k(t, t')}{\partial \omega}$ . While the derivatives of  $\sigma_l$  and  $\sigma_f^2$  are standard and can be found in [34], we present the derivative w.r.t.  $\omega$  as follows

$$\frac{\partial k(t,t')}{\partial \omega} = -v \left(1 - \omega\right)^{v-1} \text{ where } v = |t - t'|/2.$$
(20)

We optimize Eq. (19) with a gradient-based optimizer, providing the analytical gradient to the algorithm. We start the optimization from the previous hyperparameter values  $\theta_{prev}$ . If the optimization fails due to numerical issues, we keep the previous value of the hyperparameters.

# C Proof of Theorem 1

Our use of the TVGP within the TVO setting requires no problem specific modifications compared to the general formulation in Bogunovic. As such, the proof of Theorem 1 closely follows the proof of Theorem 4.3 in Bogunovic et al. [5] App. C. with time kernel  $k_{\rm T}(i,j) = (1-\omega)^{\frac{|i-j|}{2}}$ . At a high level, their proof proceeds by partitioning the *T* random functions into blocks of length  $\tilde{N}$ , and bounding each using Mirsky's theorem. Referring to Table 1 for notation, this results in a bound on the maximum mutual information

$$\tilde{\gamma}_{\tilde{N}} \le \left(\frac{T}{\tilde{N}} + 1\right) \left(\gamma_{\tilde{N}} + \tilde{N}^3 \omega\right),\tag{21}$$

which leads directly to their bound on the cumulative regret (cf. App C.2 in [5]). Our contribution is to recognize we can achieve a tighter bound on the maximum mutual information with an application Cauchy Schwarz and Jensen's inequality.

Proof. Beginning from Bogunovic et al. [5] Eq. (58), we have

$$\tilde{\gamma}_{\tilde{N}} \le \gamma_{\tilde{N}} + \sum_{i=1}^{N} \log\left(1 + \Delta_i\right) \tag{22}$$

$$\tilde{\gamma}_{\tilde{N}} \le \gamma_{\tilde{N}} + \tilde{N} \log \left( 1 + \frac{1}{\tilde{N}} \sum_{i=1}^{\tilde{N}} \Delta_i \right)$$
 Jensen's inequality (23)

$$\tilde{\gamma}_{\tilde{N}} \leq \gamma_{\tilde{N}} + \tilde{N} \log \left( 1 + \frac{1}{\sqrt{\tilde{N}}} \sqrt{\sum_{i=1}^{\tilde{N}} \Delta_i^2} \right)$$
 Cauchy-Schwartz (24)  
$$\tilde{N}$$

$$\tilde{\gamma}_{\tilde{N}} \le \gamma_{\tilde{N}} + \tilde{N} \log \left( 1 + \tilde{N}^{3/2} \omega \right) \qquad \qquad \sum_{i=1}^{N} \Delta_i^2 \le \tilde{N}^4 \omega^2 \tag{25}$$

$$\tilde{\gamma}_{\tilde{N}} \le \gamma_{\tilde{N}} + \tilde{N}^{5/2}\omega \qquad \qquad \log(1+x) \le x \qquad (26)$$

This bound is tighter than [5] Eq. (60)  $(\tilde{N}^{5/2} \leq \tilde{N}^3)$ , where the latter was achieved via a simple constrained optimization argument. Using (26), Theorem 1 follows using identical arguments as in [5].

# **D** Additional Experiments and Ablation Studies

We present additional experiments on a Probabilistic Context Free Grammar (PCFG) model and Sigmoid Belief Networks in §D.1 and §D.2, a wall-clock time benchmark in §D.3, ablation studies in §D.4, and additional training curves in §D.5.

#### D.1 Training Probabilistic Context Free Grammar

In order to evaluate our method outside of the Variational Autoencoder framework, we consider model learning and amortized inference in the probabilistic context-free grammar setting described in Section 4.1 of Le et al. [24]. Here  $p_{\theta}(\mathbf{x}, \mathbf{z}) = p(\mathbf{x} | \mathbf{z})p_{\theta}(\mathbf{z})$ , where  $p_{\theta}(\mathbf{z})$  is a prior over parse trees  $\mathbf{z}$ ,  $p(\mathbf{x} | \mathbf{z})$  is a soft relaxation of the  $\{0, 1\}$  likelihood which indicates if sentence  $\mathbf{x}$  matches the set of terminals (i.e the sentence) produced by  $\mathbf{z}$ , and  $\theta$  is the set of probabilities associated with each production rule in the grammar. The inference network  $\phi$  is a recurrent neural network which outputs  $q_{\phi}(\mathbf{z} | \mathbf{x})$ , the conditional distribution of a parse tree given an input sentence. We use

Parameter	Domain	Meaning
ω	scalar, $(0, 1)$	Remembering-forgetting trade-off parameter ( $\epsilon$ in [5])
$\mathbf{f}_T$	vector, $\mathbb{R}^T$	Vector of T function evaluations from $f$ , $\mathbf{f_T} := [f(x_1),, f(x_T)]^T$ .
$ ilde{\mathbf{f}}_T$	vector, $\mathbb{R}^T$	( <i>time-varying case</i> ) Vector of T function evaluations from $f_{1:T}$ , $\mathbf{\tilde{f}}_T := [f_1(x_1),, f_T(x_T)]^T$
$I(\mathbf{y}_T; \mathbf{f}_T)$	scalar, $\mathbb{R}^+$	The mutual information in $\mathbf{f}_T$ after revealing $\mathbf{y}_T = \mathbf{f}_T + \epsilon$ . For a GP with covariance function $\mathbf{K}_T$ , $I(\mathbf{y}_T; \mathbf{f}_T) = \frac{1}{2} \log  \mathbf{I} + \sigma^{-2} \mathbf{K}_T $
$\tilde{I}(\mathbf{y}_T; \mathbf{\tilde{f}}_T)$	scalar, $\mathbb{R}^+$	( <i>time-varying case</i> ) Mutual information $\tilde{I}(\mathbf{y}_T; \mathbf{\tilde{f}}_T) = \frac{1}{2} \log  \mathbf{I} + \sigma^{-2} \mathbf{\tilde{K}}_T $ , where $\mathbf{\tilde{K}}_T$ is a covariance function that incorporates time kernel $k_T(i, j)$
$\gamma_T$	scalar, $\mathbb{R}^+$	The maximum information gain $\gamma_T := \max_{x_1,,x_T} I(\mathbf{y}_T; \mathbf{f}_T)$ after $T$ rounds
$\tilde{\gamma}_T$	scalar, $\mathbb{R}^+$	( <i>time-varying case</i> ) The analogous time-varying maximum information gain $\tilde{\gamma}_T := \max_{x_1,,x_T} \tilde{I}(\mathbf{y}_T; \mathbf{\tilde{f}}_T)$
$\tilde{N}$	scalar, $\mathbb{R}^+$	An artifact of the proof technique used by [5]. The T time steps are partitioned into blocks of length $\tilde{N}$

Table 1: Supporting notations in regret analysis. We use notation to similar to Appendix C of Bogunovic et al. [5] when possible.

the Astronomers PCFG considered by Le et al. [24], and therefore have access to the ground truth production probabilities  $\theta_{true}$ , which we will use to evaluate the quality of our learned model  $\theta$ .

We compare the TVO with GP-bandit and log schedules against REINFORCE, WAKE-WAKE, and WAKE-SLEEP, where WAKE-WAKE and WAKE-SLEEP use data from the true model  $\mathbf{x} \sim p_{\theta_{true}}(\mathbf{x})$  and learned model  $\mathbf{x} \sim p_{\theta}(\mathbf{x})$  respectively. For each run, we use a batch size of 2 and train for 2000 epochs with Adam using default parameters. For all KL divergences (see caption in Figure 6), we compute the median over 20 seeds and then plot the average over the last 100 epochs.

As observed by Le et al. [24], sleep- $\phi$  updates avoid the deleterious effects of the SNIS bias and is therefore preferable to wake- $\phi$  updates in this context. Therefore for all runs we use the TVO to update  $\theta$ , and use sleep- $\phi$  to update  $\phi$ . Sleep- $\phi$  is a special case of the TVO (cf. Masrani et al. [27] Appendix G.1).

In Figure 6 we see that both GP-bandits and log schedules have comparable performance in this setting, with TVO-log, S = 20 achieving the lowest  $\text{KL}[p_{\theta}||p_{\theta_{\text{true}}}]$  and  $\text{KL}[q_{\phi}(\mathbf{z} | \mathbf{x})||p_{\theta_{\text{true}}}(\mathbf{z} | \mathbf{x})]$  across all trials.  $\text{KL}[q_{\phi}||p_{\theta_{\text{true}}}]$  is a preferable metric to  $\text{KL}[q_{\phi}||p_{\theta}]$  because the former does not depend on the quality of the learned model. We also note that GP-bandits appears to be less sensitive to the number of partitions than the log schedule.

#### D.2 Training Sigmoid Belief Network on Binarized Omniglot

We train the Sigmoid Belief Network described in §5.2 on the binarized Omniglot dataset. Omniglot [22] has 1623 handwritten characters across 50 alphabets. We manually binarize the omniglot[23] dataset by sampling once according to procedure described in [7], and split the binarized omniglot dataset into 23,000 training and 8,070 test examples. Results are shown in Figure 7. At S = 50, GP-bandit achieves similar model learning but better inference compared to log scheduling.

#### D.3 Wall-clock time Comparison

We benchmark the wall-clock time of our GP-bandit schedule against the cumulative wall-clock time of the grid-search log schedule. For both schedules we train a VAE on the Omniglot dataset for S = 10 and 5000 epochs. For the log schedule, we run the sweep ran by Masrani et al. [27] (cf. section 7.2), i.e.  $20 \beta_1$  linearly spaced between  $[10^{-2}, 0.9]$  for d = 2, ..., 6, for a total of 100 runs. For a fair comparison against the log schedule, we loop over d = 2, ..., 6 for our GP bandits because d is unlearned, for a total of five runs. We note that each run of the GP bandits schedule



Figure 6: Evaluation of model learning in a PCFG, where  $\theta$  is the set of probabilities associated with each production rule in the grammar, and  $\phi$  is an RNN which generates the conditional probability of a parse tree given a sentence. GP-bandits (ours) is comparable to the baseline log schedule and less sensitive to number of partitions, as evaluated by the KL divergence between learned and true model parameters (top row). Inference network learning is evaluated by the KL divergence between  $q_{\phi}(\mathbf{z} | \mathbf{x})$  and  $p_{\theta_{true}}(\mathbf{z} | \mathbf{x})$  (middle row) and  $p_{\theta}(\mathbf{z} | \mathbf{x})$  (bottom row). We compare against REINFORCE, WAKE-WAKE, and WAKE-SLEEP, where some baselines aren't shown due to being out of range. At S = 20, TVO with log and GP-bandits schedule outperforms REINFORCE, WAKE-WAKE, and WAKE-SLEEP both in terms of the quality of the generative model (top row, right) and inference network (middle row, right) for all  $S \in \{2, 5, 10, 20\}$ .



Figure 7: Performance of the Sigmoid Belief Network described in §5.2 on the binarized omniglot dataset. The GP-bandit schedule at d = 15, S = 50 outperforms all baselines in terms of model and inference network learning.

includes learning the GP hyperparameters as described in Appendix B. For both schedules, we take the best  $\log p(x)$  and corresponding KL divergence, and plot the cumulative run time across all runs. The results in Table 2 show that the GP-bandits schedule does comparable to the grid searched log schedule (log likelihood: -110.72 vs -110.99) while requiring significantly less cumulative wall-clock time (10 hrs vs 178 hrs).



Figure 8: We compare the performance between our GP-bandit against the Random search (Rand) baseline which uniformly generates the integration schedules  $\beta_t$ . The GP-bandit schedule outperforms the random counterpart by using information obtained from previous choices, as described in Algorithm 1.

Table 2: Wallclock time of the GP-bandit schedule compared to the grid-search of [27] for the log schedule. GP-bandit approach achieves a competitive test log likelihood and lower KL divergence compared with the grid-searched log schedule, but requires significantly lower cumulative run-time.

	best $\log p(x)$	best kl	number of runs	cumulative run time (hrs)
GP bandit (ours)	-110.995	7.655	5	10.99
grid-searched log	-110.722	8.389	100	177.01

#### **D.4** Ablation studies

**Ablation study between GP-bandit and random search.** To demonstrate that our model can leverage useful information from past data, we compare against the Random Search picks the integration schedule uniformly at random.

We present the results in Figure 8 using MNIST (left) and Fashion MNIST (right). We observe that our GP-bandit clearly outperforms the Random baseline. The gap is generally increasing with larger dimension d, e.g., d = 15 as the search space grows exponentially with the dimension.

**Ablation study between permutation invariant GPs.** We compare our GP-bandit model using two versions of (1) non-permutation invariant GP and (2) permutation invariant GP in Table 3.

Our permutation invariant GP does not need to add all permuted observations into the model, but is still capable of generalizing. The result in Table 3 confirms that if we have more samples to learn the GP, such as using larger epochs budget T, the two versions will result in the same performance. On the other hand, if we have limited number of training budgets, e.g., using lower number of epochs, the permutation invariant GP will be more favorable and outperforms the non-permutation invariant. In addition, the result suggests that for higher dimension d = 15 (number of partitions) our permutation invariant GP performs consistently better than the counterpart.

#### **D.5** Training Curves

We show example training curves for  $S = 10, d \in \{5, 15\}$  obtained using the linear, log, moment, and GP-bandit schedules in Figure 9. We can see sudden drops in the GP-bandit training curves indicating our model is exploring alternate schedules during training (cf. Section 4.1).

Table 3: Comparison between permutation invariant and non-permutation invariant in MNIST dataset using S=10 (top) and S=50 (bottom). The best scores are in bold. Given T used epochs, the number of bandit update and thus the number of sample for GP is T/w where w = 10 is the frequency update. The permutation invariant will be more favorable when we have less samples for fitting the GP, as indicated in less number of used epochs T = 1000, 2000. The performance is comparable when we collect sufficiently large number of samples, e.g., when T/w = 1000.

<b>S=</b> 10	Used Epoch $T$ / Bandit Iteration	1000/100	2000/200	5000/500	10000/1000
<b>d=</b> 5	Perm Invariant Non Perm Invariant	<b>-91.488</b> -91.554	<b>-90.129</b> -90.206	<b>-89.130</b> -89.262	-88.651 -88.552
d=10	Perm Invariant Non Perm Invariant	<b>-91.430</b> -91.553	<b>-90.219</b> -90.249	-89.159 <b>-89.110</b>	-88.603 <b>-88.466</b>
d=15	Perm Invariant Non Perm Invariant	<b>-91.386</b> -91.550	<b>-90.059</b> -90.224	<b>-88.957</b> -89.215	<b>-88.504</b> -88.564
<b>S=</b> 50	Used Epoch T/ Bandit Iteration	1000/100	2000/200	5000/500	10000/1000
S=50 d=5	Used Epoch T/ Bandit Iteration Permutation Invariant Non Permutation Invariant	1000/100 -90.071 -90.119	2000/200 -89.068 -89.142	5000/500 -88.163 -88.215	10000/1000 -87.979 - <b>87.860</b>
S=50 d=5 d=10	Used Epoch T/ Bandit Iteration Permutation Invariant Non Permutation Invariant Perm Invariant Non Permutation Invariant	1000/100 -90.071 -90.119 -90.125 -90.212	2000/200 -89.068 -89.142 -89.115 -89.225	5000/500 -88.163 -88.215 -88.187 -88.231	10000/1000 -87.979 -87.860 -87.859 -87.702



Figure 9: We plot  $\log p(\mathbf{x})$  on the training set throughout  $S = 10, d \in \{5, 15\}$  for each dataset using the experimental setup described in Appendix A. The final training log likelihoods are consistent with the test log likelihoods. Small drops in the GP-bandit training curves indicate the algorithm exploring the reward landscape (see Section 4.1).