

Adversarial Variational Optimization of Non-Differentiable Simulators

Gilles Louppe¹ and Kyle Cranmer¹

¹*New York University*

Complex computer simulators are increasingly used across fields of science as generative models tying parameters of an underlying theory to experimental observations. Inference in this setup is often difficult, as simulators rarely admit a tractable likelihood function. In this note, we develop Adversarial Variational Optimization (AVO), a likelihood-free inference algorithm for fitting a non-differentiable generative model to continuous or discrete data. We adapt the training procedure of generative adversarial networks by replacing the differentiable generative network with a domain-specific simulator and solve the resulting non-differentiable minimax problem by minimizing variational upper bounds of the two adversarial objectives. Effectively, the procedure results in learning an arbitrarily tight proposal distribution over simulator parameters, such that the corresponding marginal distribution of the generated data matches the observations. We present results of the method with non-differentiable simulators producing discrete/continuous univariate/multi-dimensional data validate the proposed method.

I. INTRODUCTION

In many fields of science such as particle physics, climatology or population genetics, computer simulators are used to describe complex processes that tie parameters of an underlying theory to high dimensional observations. In most cases, these implicit generative models [15] are specified as procedural implementations of forward stochastic processes that generate discrete or continuous data. Because it is usually computationally intractable, most simulators do not provide a way to directly evaluate the likelihood function for a given observation, thereby making inference difficult. In addition, most scientific simulators are written using opaque low-level programming languages, hence raising the bar for likelihood-free inference algorithms relying e.g. on the simulator being a function with computable derivatives [7] or being a controllable probabilistic program [13].

In this note, we develop a likelihood-free inference algorithm for the point estimation of the parameters of a forward non-differentiable generative model. We adapt the adversarial training procedure of generative adversarial networks [6] by replacing the implicit generative network with a domain-based scientific simulator, and solve the resulting non-differentiable minimax problem by minimizing variational upper bounds [17, 21] of the adversarial objectives. The procedure results in learning a proposal distribution over simulator parameters, hence producing an arbitrarily tight family of models whose joint collection of generated samples matches the observed data.

II. PROBLEM STATEMENT

We consider a family of parameterized densities $p(\mathbf{x}|\boldsymbol{\theta})$ defined implicitly through the simulation of a stochastic generative process, where $\mathbf{x} \in \mathbb{R}^d$ is the data and $\boldsymbol{\theta}$ are the parameters of interest. The simulation may involve

some complicated latent process, such that

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} \quad (1)$$

where $\mathbf{z} \in \mathcal{Z}$ is a latent variable providing an external source of randomness. In particular, \mathbf{z} is not necessarily assumed to be a fixed-size vector (e.g., it can be a sequence of variable length) and its distribution $p(\mathbf{z}|\boldsymbol{\theta})$ may itself depend on $\boldsymbol{\theta}$ in some intricate way.

We assume that we already have an accurate simulation of the stochastic generative process that defines $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$, as specified through a highly regularized deterministic function $g(\cdot; \boldsymbol{\theta}) : \mathcal{Z} \rightarrow \mathbb{R}^d$ with usually few parameters. That is, we consider

$$\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta}) \equiv \mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta}), \mathbf{x} = g(\mathbf{z}; \boldsymbol{\theta}) \quad (2)$$

such that the likelihood $p(\mathbf{x}|\boldsymbol{\theta})$ can be considered as a non-differentiable reparameterization of the random variable \mathbf{z} . Importantly, the simulator g is assumed to be a non-invertible function, that can only be used to generate data in forward mode. For this reason, evaluating the integral in Eqn. 3 is intractable. As commonly found in science, we finally assume the lack of access to or existence of derivatives of g with respect to $\boldsymbol{\theta}$, e.g. as when g is specified as a computer program.

Given some observed data $\{\mathbf{x}_i | i = 1, \dots, N\}$ drawn from the (unknown) true distribution $p_r(\mathbf{x})$, our goal is the inference of the parameters of interest $\boldsymbol{\theta}^*$ that minimize the divergence between $p_r(\mathbf{x})$ and the modeled data distribution $p(\mathbf{x}|\boldsymbol{\theta})$ induced by $g(\cdot; \boldsymbol{\theta})$ over \mathbf{z} . That is,

$$\boldsymbol{\theta}^* = \arg \min_{\boldsymbol{\theta} \in \Theta} \rho(p_r(\mathbf{x}), p(\mathbf{x}|\boldsymbol{\theta})), \quad (3)$$

where ρ is some distance or divergence.

III. BACKGROUND

A. Generative adversarial networks

Generative adversarial networks (GANs) were first proposed by [6] as a way to build an implicit genera-

tive model capable of producing samples from random noise \mathbf{z} . More specifically, a generative model $g(\cdot; \boldsymbol{\theta})$ is pit against an adversarial classifier $d(\cdot; \phi) : \mathbb{R}^d \rightarrow [0, 1]$ with parameters ϕ and whose antagonistic objective is to recognize real data \mathbf{x} from generated data $\tilde{\mathbf{x}} = g(\mathbf{z}; \boldsymbol{\theta})$. Both models g and d are trained simultaneously, in such a way that g learns to fool its adversary d (which happens when g produces samples comparable to the observed data), while d continuously adapts to changes in g . When d is trained to optimality before each parameter update of the generator, it can be shown that the original adversarial learning procedure [6] amounts to minimizing the Jensen-Shannon divergence $\text{JSD}(p_r(\mathbf{x}) \parallel p(\mathbf{x}|\boldsymbol{\theta}))$ between $p_r(\mathbf{x})$ and $p(\mathbf{x}|\boldsymbol{\theta})$.

As thoroughly explored in [1], GANs remain remarkably difficult to train because of vanishing gradients as d saturates, or because of unreliable updates when the training procedure is relaxed. As a remedy, Wasserstein GANs [2] reformulate the adversarial setup in order to minimize the Wasserstein-1 distance $W(p_r(\mathbf{x}), p(\mathbf{x}|\boldsymbol{\theta}))$ by replacing the adversarial classifier with a 1-Lipschitz adversarial critic $d(\cdot; \phi) : \mathbb{R}^d \rightarrow \mathbb{R}$.

$$W(p_r(\mathbf{x}), p(\mathbf{x}|\boldsymbol{\theta})) = \mathcal{L}_W = \sup_f \mathbb{E}_{p(\tilde{\mathbf{x}}|\boldsymbol{\theta})}[f(\tilde{\mathbf{x}})] - \mathbb{E}_{p_r(\mathbf{x})}[f(\mathbf{x})] \quad (4)$$

Under the WGAN-GP formulation of [8] for stabilizing the optimization procedure, training d and g results in alternating gradient updates on ϕ and $\boldsymbol{\theta}$ in order to respectively minimize

$$\mathcal{L}_d = \mathcal{L}_W + \lambda \mathbb{E}_{\tilde{\mathbf{x}} \sim p(\tilde{\mathbf{x}})}[(\|\nabla_{\tilde{\mathbf{x}}} d(\tilde{\mathbf{x}}; \phi)\|_2 - 1)^2] \quad (5)$$

$$\mathcal{L}_g = -\mathcal{L}_W \quad (6)$$

where $\hat{\mathbf{x}} := \epsilon \mathbf{x} + (1 - \epsilon)\tilde{\mathbf{x}}$, for $\epsilon \sim U[0, 1]$, $\mathbf{x} \sim p_r(\mathbf{x})$ and $\tilde{\mathbf{x}} \sim p(\mathbf{x}|\boldsymbol{\theta})$.

B. Variational optimization

Variational optimization [17, 18] and evolution strategies [21] are general optimization techniques that can be used to form a differentiable bound on the optima of a non-differentiable function. Given a function f to minimize, these techniques are based on the simple fact that

$$\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} f(\boldsymbol{\theta}) \leq \mathbb{E}_{\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})}[f(\boldsymbol{\theta})] = U(\boldsymbol{\psi}), \quad (7)$$

where $q(\boldsymbol{\theta}|\boldsymbol{\psi})$ is a proposal distribution with parameters $\boldsymbol{\psi}$ over input values $\boldsymbol{\theta}$. That is, the minimum of a set of function values is always less than or equal to any of their average. Provided that the proposal is flexible enough, the parameters $\boldsymbol{\psi}$ can be updated to place its mass arbitrarily tight around the optimum $\boldsymbol{\theta}^* = \min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} f(\boldsymbol{\theta})$.

Under mild restrictions outlined in [17], the bound $U(\boldsymbol{\psi})$ is differentiable with respect to $\boldsymbol{\psi}$, and using the

log-likelihood trick it comes:

$$\begin{aligned} \nabla_{\boldsymbol{\psi}} U(\boldsymbol{\psi}) &= \nabla_{\boldsymbol{\psi}} \mathbb{E}_{\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})}[f(\boldsymbol{\theta})] \\ &= \int f(\boldsymbol{\theta}) \nabla_{\boldsymbol{\psi}} q(\boldsymbol{\theta}|\boldsymbol{\psi}) d\boldsymbol{\theta} \\ &= \int [f(\boldsymbol{\theta}) \nabla_{\boldsymbol{\psi}} \log q(\boldsymbol{\theta}|\boldsymbol{\psi})] q(\boldsymbol{\theta}|\boldsymbol{\psi}) d\boldsymbol{\theta} \\ &= \mathbb{E}_{\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})}[f(\boldsymbol{\theta}) \nabla_{\boldsymbol{\psi}} \log q(\boldsymbol{\theta}|\boldsymbol{\psi})] \end{aligned} \quad (8)$$

Effectively, this means that provided that the score function $\nabla_{\boldsymbol{\psi}} \log q(\boldsymbol{\theta}|\boldsymbol{\psi})$ of the proposal is known and that one can evaluate $f(\boldsymbol{\theta})$ for any $\boldsymbol{\theta}$, then one can construct empirical estimates of Eqn. 9, which can in turn be used to minimize $U(\boldsymbol{\psi})$ with stochastic gradient descent (or a variant thereof, like Adam [12] or the Natural Evolution Strategy algorithm [21], for scaling invariance and robustness to noisy gradients).

IV. ADVERSARIAL VARIATIONAL OPTIMIZATION

The alternating stochastic gradient descent on \mathcal{L}_d and \mathcal{L}_g in GANs (Section III A) inherently assumes that the generator g is a differentiable function. In the setting where we are interested in the inference of the parameters of a fixed non-differentiable simulator (Section II), rather than in learning the generative model itself, gradients $\nabla_{\boldsymbol{\theta}} g$ either do not exist or cannot be accessed. As a result, gradients $\nabla_{\boldsymbol{\theta}} \mathcal{L}_g$ cannot be constructed and the optimization procedure cannot be carried out.

In this work, we propose to rely on variational optimization to minimize \mathcal{L}_d and \mathcal{L}_g , thereby bypassing the non-differentiability of g . More specifically, we consider a proposal distribution $q(\boldsymbol{\theta}|\boldsymbol{\psi})$ over the parameters of g and $p(\mathbf{x}|\boldsymbol{\theta})$ and minimize in alternation the variational upper bounds

$$U_d = \mathbb{E}_{\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})}[\mathcal{L}_d] \quad (9)$$

$$U_g = \mathbb{E}_{\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})}[\mathcal{L}_g] \quad (10)$$

respectively over ϕ and $\boldsymbol{\psi}$. When updating ϕ , unbiased estimates of $\nabla_{\phi} U_d$ can be obtained by evaluating the exact and known gradient of U_d over mini-batches of true and generated data, as ordinarily done in stochastic gradient descent. When updating $\boldsymbol{\psi}$, estimates of $\nabla_{\boldsymbol{\psi}} U_g$ can be derived with forward simulations, as described in the previous section. That is,

$$\nabla_{\boldsymbol{\psi}} U_g = \mathbb{E}_{\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi}), \mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta})}[-d(g(\mathbf{z}; \boldsymbol{\theta}); \phi) \nabla_{\boldsymbol{\psi}} \log q(\boldsymbol{\theta}|\boldsymbol{\psi})], \quad (11)$$

which we can approximate with mini-batches of generated data

$$\nabla_{\boldsymbol{\psi}} U_g \approx \frac{1}{M} \sum_{m=1}^M -d(g(\mathbf{z}_m; \boldsymbol{\theta}_m); \phi) \nabla_{\boldsymbol{\psi}} \log q(\boldsymbol{\theta}_m|\boldsymbol{\psi}) \quad (12)$$

for $\boldsymbol{\theta}_m \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})$ and $\mathbf{z}_m \sim p(\mathbf{z}|\boldsymbol{\theta}_m)$. For completeness, Algorithm 1 outlines the proposed adversarial variational optimization (AVO) procedure, as built on top of

Algorithm 1 Adversarial variational optimization (AVO).

Inputs: observed data $\{\mathbf{x}_i \sim p_r(\mathbf{x})\}_{i=1}^N$, simulator g .

Outputs: proposal distribution $q(\boldsymbol{\theta}|\boldsymbol{\psi})$, such that $q(\mathbf{x}|\boldsymbol{\psi}) \approx p_r(\mathbf{x})$.

Hyper-parameters: The number n_{critic} of training iterations of d ; the size M of a mini-batch; the gradient penalty coefficient λ ; the entropy penalty coefficient γ .

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1:  $q(\boldsymbol{\theta}|\boldsymbol{\psi}) \leftarrow$  prior on  $\boldsymbol{\theta}$  (with differentiable and known density)
2: while  $\boldsymbol{\psi}$  has not converged do
3:   for  $i = 1$  to  $n_{\text{critic}}$  do ▷ Update  $d$ 
4:     Sample a mini-batch  $\{\mathbf{x}_m \sim p_r(\mathbf{x}), \boldsymbol{\theta}_m \sim q(\boldsymbol{\theta}|\boldsymbol{\psi}), \mathbf{z}_m \sim p(\mathbf{z}|\boldsymbol{\theta}_m), \epsilon_m \sim U[0, 1]\}_{m=1}^M$ .
5:     for  $m = 1$  to  $M$  do
6:        $\tilde{\mathbf{x}}_m \leftarrow g(\mathbf{z}_m; \boldsymbol{\theta}_m)$ 
7:        $\hat{\mathbf{x}}_m \leftarrow \epsilon_m \mathbf{x}_m + (1 - \epsilon_m) \tilde{\mathbf{x}}_m$ 
8:        $U_d^{(m)} \leftarrow d(\tilde{\mathbf{x}}_m; \phi) - d(\mathbf{x}_m; \phi) + \lambda(\|\nabla_{\tilde{\mathbf{x}}_m} d(\tilde{\mathbf{x}}_m; \phi)\|_2 - 1)^2$ 
9:     end for
10:     $\phi \leftarrow \text{Adam}(\nabla_{\phi} \frac{1}{M} \sum_{m=1}^M U_d^{(m)})$ 
11:  end for
12:  Sample a mini-batch  $\{\boldsymbol{\theta}_m \sim q(\boldsymbol{\theta}|\boldsymbol{\psi}), \mathbf{z}_m \sim p(\mathbf{z}|\boldsymbol{\theta}_m)\}_{m=1}^M$ . ▷ Update  $q(\boldsymbol{\theta}|\boldsymbol{\psi})$ 
13:   $\nabla_{\boldsymbol{\psi}} U_g \leftarrow \frac{1}{M} \sum_{m=1}^M -d(g(\mathbf{z}_m; \boldsymbol{\theta}_m)) \nabla_{\boldsymbol{\psi}} \log q_{\boldsymbol{\psi}}(\boldsymbol{\theta}_m)$ 
14:   $\nabla_{\boldsymbol{\psi}} H(q_{\boldsymbol{\psi}}) \leftarrow \frac{1}{M} \sum_{m=1}^M \nabla_{\boldsymbol{\psi}} q_{\boldsymbol{\psi}}(\boldsymbol{\theta}_m) \log q_{\boldsymbol{\psi}}(\boldsymbol{\theta}_m)$ 
15:   $\boldsymbol{\psi} \leftarrow \text{Adam}(\nabla_{\boldsymbol{\psi}} U_g + \gamma \nabla_{\boldsymbol{\psi}} H(q_{\boldsymbol{\psi}}))$ 
16: end while

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WGAN-GP. Obviously, the variational relaxation could similarly be coupled with other variants of GANs and/or of evolution strategies.

Practically, the variational objectives 10-11 have the effect of replacing the modeled data distribution of Eqn. 2 with a distribution parameterized in terms of $\boldsymbol{\psi}$:

$$\mathbf{x} \sim q(\mathbf{x}|\boldsymbol{\psi}) \equiv \boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi}), \mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta}), \mathbf{x} = g(\mathbf{z}; \boldsymbol{\theta}). \quad (13)$$

Intuitively, this corresponds to a family of simulators, each configured with randomly sampled parameters $\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})$, whose joint collection of generated samples is optimized with adversarial training to approach the real data distribution $p_r(\mathbf{x})$. More formally, the learned model therefore corresponds to the marginal distribution of the generated data. That is,

$$q(\mathbf{x}|\boldsymbol{\psi}) = \int p(\mathbf{x}|\boldsymbol{\theta}) q(\boldsymbol{\theta}|\boldsymbol{\psi}) d\boldsymbol{\theta}. \quad (14)$$

In consequence, the proposed inference algorithm does not necessarily guarantee that the proposal distribution $q(\boldsymbol{\theta}|\boldsymbol{\psi})$ will place its mass arbitrarily tight around the parameters of interest, which might be an issue when one is rather interested in point estimates $\boldsymbol{\theta}^*$. For this purpose, we augment Eqn. 11 with a regularization term corresponding to the differential entropy H of the proposal distribution. That is,

$$U_g = \mathbb{E}_{\boldsymbol{\theta} \sim q(\boldsymbol{\theta}|\boldsymbol{\psi})} [\mathcal{L}_g] + \gamma H(q(\boldsymbol{\theta}|\boldsymbol{\psi})) \quad (15)$$

where $\gamma \in \mathbb{R}^+$ is a hyper-parameter controlling the trade-off between the generator objective and the tightness of the proposal distribution. For small values of γ , proposal distributions with large entropy are not penalized, which

may result in learning a smeared variation of the original simulator. On the other hand, for large values of γ , the procedure is constrained to fit a proposal distribution with low entropy, which has the effect of concentrating its density tightly around one or a few $\boldsymbol{\theta}$ values. A too large penalty may however eventually make the optimization unstable, as the variance of $\nabla_{\boldsymbol{\psi}} \log q(\boldsymbol{\theta}_m|\boldsymbol{\psi})$ typically increases as the entropy of the proposal decreases.

A. Operator Variational Optimization

Original OPVI [16]

$$\lambda^* = \inf_{\lambda} \sup_{\phi} \mathbb{E}_{z \sim q(z|\lambda)} [(O^{p,q} f)_{\lambda}] \quad (16)$$

with

$$(O^{p,q} f) = \log q(z) - \log p(z|x) \forall f \in \mathcal{F} \quad (17)$$

To get into OPVI formalism

$$\boldsymbol{\psi}^* = \inf_{\boldsymbol{\psi}} \sup_{\phi} \mathbb{E}_{x \sim p_r(x)} [f(x)] - \mathbb{E}_{x \sim p(x|\boldsymbol{\psi})} [f(x)] \quad (18)$$

$$= \inf_{\boldsymbol{\psi}} \sup_{\phi} \mathbb{E}_{x \sim p(x|\boldsymbol{\psi})} [(O^{p_r, p_{\boldsymbol{\psi}}} f)_{\phi}] \quad (19)$$

with

$$(O^{p,q} f) = \left(\frac{p_r(x)}{p(x|\boldsymbol{\psi})} - 1 \right) f(x) \quad (20)$$

We can think of $p(x|\boldsymbol{\psi})$ as a *variational program* as described in [16], though more complicated than the a

simple reparametrization of normally distributed noise ϵ through a differentiable function $R(\epsilon, \psi)$. In our case, the variational program is a marginalized non-differentiable simulator simulator. Nevertheless, it can generate samples for x , is differentiable with respect to ϕ , and its density is be intractable.

V. EXPERIMENTS

A. Univariate discrete data

As a first illustrative experiment, we evaluate inference for a discrete Poisson distribution with unknown mean λ . We artificially consider the distribution as a parameterized simulator, from which we can only generate data.

The observed data is sampled from a Poisson with mean $\lambda^* = 7$. Algorithm 1 is run for 300 epochs with mini-batches of size $M = 64$ and the following configuration. For the critic d , we use a 3-layer MLP with 10 hidden nodes per layer and ReLU activations. At each epoch, Adam is run for $n_{\text{critic}} = 100$ iterations with a step size $\alpha = 0.01$, decay rates $\beta_1 = \beta_2 = 0.5$ and its inner first and second moment vectors reset at each outer epoch in order to avoid building momentum in staled directions. For estimating λ^* , we parameterize θ as $\log(\lambda)$ and use a univariate Gaussian proposal distribution $q(\theta|\psi)$ initialized with a mean at $\log(5)$ and unit variance. At each epoch, parameters ψ are updated by taking one Adam step, with $\alpha = 0.01$ and $\beta_1 = \beta_2 = 0.5$. The gradient penalty coefficient is set to $\lambda = 0.025$, and the entropy penalty is evaluated at both $\gamma = 0$ and $\gamma = 5$.

The top left plot in Figure 1 illustrates the resulting proposal distributions $q(\theta|\psi)$ after AVO. For both $\gamma = 0$ and $\gamma = 5$, the proposal distributions correctly concentrate their density around the true parameter value $\log(\lambda^*) = 1.94$. Under the effect of the positive entropy penalty $H(q(\theta|\psi))$, the proposal distribution for $\gamma = 5$ concentrates its mass more tightly, yielding in this case a more precise inference. The top right plot compares the model distributions to the true distribution. As theoretically expected from adversarial training, we see that the resulting distributions closely match the true distribution, with in this case visually slightly better results for the penalized model. The bottom plot of Figure 1 shows empirical estimates of $-U_d$ with respect to the epoch number. For both $\gamma = 0$ and $\gamma = 5$, the curves quickly fall towards 0, which indicates that $\mathbb{E}_{\tilde{\mathbf{x}} \sim p(\mathbf{x}|\theta)}[d(\tilde{\mathbf{x}}; \phi)] \approx \mathbb{E}_{\mathbf{x} \sim p_r(\mathbf{x})}[d(\mathbf{x}; \phi)]$ and that the critic cannot distinguish between true and model data. Despite the discreteness and the non-differentiability of the underlying generator, this confirms that inference with adversarial variational optimization works.

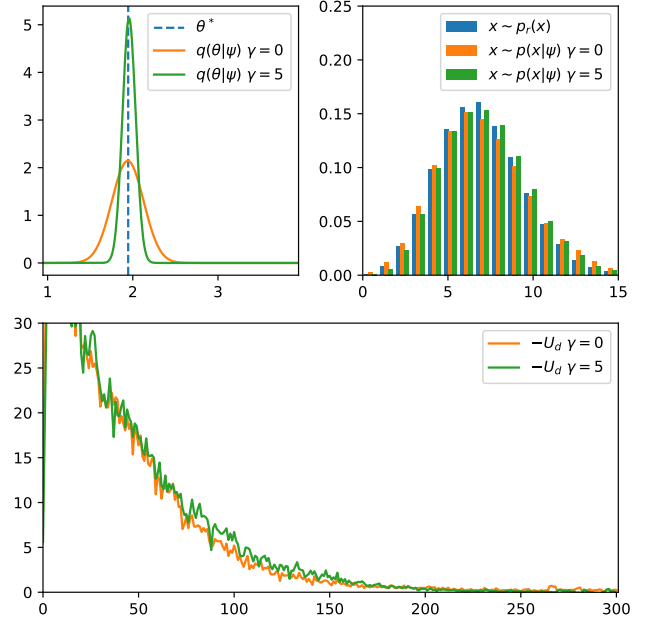


FIG. 1. Discrete Poisson model with unknown mean. (Top left) Proposal distributions $q(\theta|\psi)$ after adversarial variational optimization. For both $\gamma = 0$ and $\gamma = 5$, the distributions correctly concentrate their density around the true value $\log(\lambda^*)$. Penalizing the entropy of the proposal distribution ($\gamma = 5$) results in a tighter density. (Top right) Model distributions $q(\mathbf{x}|\psi)$ after training. This plot shows that the resulting parameterizations of the simulator closely reproduce the true distribution. (Bottom) Empirical estimates of the variational upper bound U_d as optimization progresses.

B. Multidimensional continuous data

As a second toy example, we evaluate parameter inference for a generator producing 5-dimensional continuous data, as originally specified in Section 4.2. of [3]. More specifically, we consider the following generative process:

- $\mathbf{z} = (z_0, z_1, z_2, z_3, z_4)$, such that $z_0 \sim \mathcal{N}(\mu = \alpha, \sigma = 1)$, $z_1 \sim \mathcal{N}(\mu = \beta, \sigma = 3)$, $z_2 \sim \text{Mixture}(\frac{1}{2}\mathcal{N}(\mu = -2, \sigma = 1), \frac{1}{2}\mathcal{N}(\mu = 2, \sigma = 0.5))$, $z_3 \sim \text{Exponential}(\lambda = 3)$, and $z_4 \sim \text{Exponential}(\lambda = 0.5)$;
- $\mathbf{x} = R\mathbf{z}$, where R is a fixed semi-positive definite 5×5 matrix defining a fixed projection of \mathbf{z} into the observed space.

We consider observed data generated at the nominal values $\theta^* = (\alpha^* = 1, \beta^* = -1)$. The simulator parameters are modeled with a factored Gaussian proposal distribution $q(\theta|\psi) = q(\alpha|\psi)q(\beta|\psi)$, where each component is initialized with zero mean and unit variance. Hyperparameters are set to $M = 64$, $n_{\text{critic}} = 100$, $\lambda = 0.025$, $\gamma = 10$ and Adam configured with $\alpha = 0.01$, $\beta_1 = 0.9$ and $\beta_2 = 0.999$. The network architecture of the critic is the same as in the previous example.

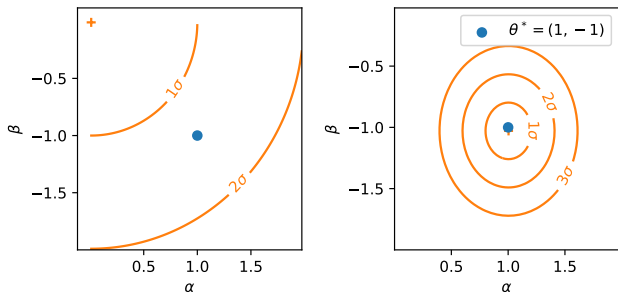


FIG. 2. Multidimensional continuous data. (Left) Density $q(\theta|\psi)$ at the beginning of the procedure, for a proposal distribution initialized with zero mean and unit variance. (Right) Density $q(\theta|\psi)$ after adversarial variational optimization ($\gamma = 10$). The proposal density correctly converges towards a distribution whose density concentrates around $\theta^* = (1, -1)$.

Starting with a proposal distribution $q(\theta|\psi)$ largely spread over the parameter space, as illustrated in the left plot of Figure 2, inference quickly converges towards a proposal distribution whose density concentrates around the nominal values θ^* , as shown in the right plot of Figure 2. Overall, this example further illustrates and confirms the ability of adversarial variational optimization for inference with multiple parameters and multidimensional data, where reliable approximations of $p(\mathbf{x}|\theta)$ in a traditional MLE setting would otherwise be difficult to construct.

C. Electron-positron annihilation

As a more challenging example, we now consider a (simplified) simulator from particle physics for electron-positron collisions resulting in muon-antimuon pairs ($e^+e^- \rightarrow \mu^+\mu^-$). The simulator approximates the distribution of observed measurements $\mathbf{x} = \cos(A) \in [-1, 1]$, where A is the polar angle of the outgoing muon with respect to the originally incoming electron. This random variable is approximately distributed as

$$p(\mathbf{x}|E_{\text{beam}}, G_f) = \frac{1}{Z} [(1 + \mathbf{x}^2) + c(E_{\text{beam}}, G_f)\mathbf{x}] \quad (21)$$

where Z is a known normalization constant and c is an asymmetry coefficient function. Due to the linear term in the expression, the density $p(\mathbf{x}|E_{\text{beam}}, G_f)$ exhibits a so-called *forward-backward* asymmetry. Its size depends on the values of the parameters E_{beam} (the beam energy) and G_f (the Fermi constant) through the coefficient function c . Given the known analytic form of the probability density function, a simulator for \mathbf{x} can be implemented with rejection sampling [20]. As an arbitrary number of random drawings may be required before passing the acceptance threshold, this illustrates how the latent variable \mathbf{z} does not necessarily need to be fixed-sized vector,

and how its density $p(\mathbf{z}|\theta)$ may depend on θ in some complicated way (Section II).

In this example, we consider observed data generated with $\theta^* = (E_{\text{beam}}^* = 42, G_f^* = 0.9)$. The simulator parameters are modeled with a factored Gaussian proposal distribution $q(\theta|\psi) = q(E_{\text{beam}}|\psi)q(G_f|\psi)$, where each component is respectively initialized with mean 45 and 1 and variance 1 and 0.01. Hyper-parameters are set to $M = 64$, $n_{\text{critic}} = 100$, $\lambda = 0.0025$ and Adam configured with $\alpha = 0.01$, $\beta_1 = 0.9$ and $\beta_2 = 0.999$. As for the first example, we compare entropy penalties $\gamma = 0$ and $\gamma = 5$.

The top left plot in Figure 3 illustrates the resulting proposal distributions $q(\theta|\psi)$ for $\gamma = 0$ and $\gamma = 5$ after AVO. We see that the distributions both arrive in the neighborhood of θ^* , with a density more highly concentrated for $\gamma = 5$ than for $\gamma = 0$. Despite these differences and the relative distance with θ^* , both models closely match the observed data, as shown in the top right plot of Figure 3, with again slightly better results for the entropy penalized model. This suggests either a relatively flat landscape around θ^* or that the observed data can in this case also be reproduced with a smeared variation $q(\mathbf{x}|\psi)$ of the simulator. Finally, the bottom plot of Figure 3 shows that for both $\gamma = 0$ and $\gamma = 5$ the variational upper bound $-U_d$ quickly fall towards 0, which indicates convergence towards a distribution that the critic cannot distinguish from the true distribution. In summary, despite the intricate relation between the observations \mathbf{x} , the latent variable \mathbf{z} and the parameters θ , this example demonstrates the efficacy of AVO for parameter inference on a black box simulator.

VI. RELATED WORKS

As reviewed in [15], likelihood-free inference is intimately tied to a class of algorithms that can be framed as density estimation-by-comparison. In most cases, these inference algorithms are formulated as an iterative two-step process where the model distribution is first compared to the true data distribution and then updated to make it more comparable to the latter.

Closest to our work are procedures that rely on a classifier to estimate the discrepancy between the true and the model distributions. For example, [10] uses non linear logistic regression for fitting unnormalized differentiable statistical models, while [6] exploits an adversarial neural network for learning a differentiable implicit generative model. In the likelihood-free setup, [3–5] estimate likelihood ratios through supervised classification, which can in turn be used for parameter inference in combination with a gradient-free optimization algorithm. Similarly, [9] makes use of classification accuracy as a summary statistics for approximate Bayesian computation.

In this context, the proposed method can be considered as a direct adaptation of generative adversarial networks [6] to non-differentiable simulators. It also constitutes an approximate gradient descent alternative to

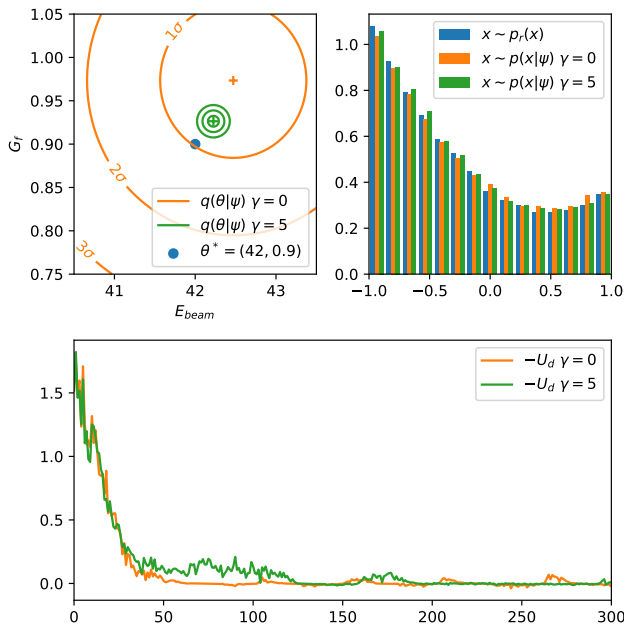


FIG. 3. Electron-positron annihilation. (*Top left*) Proposal distributions $q(\theta|\psi)$ after adversarial variational optimization. The density of the penalized distribution ($\gamma = 5$) is here highly concentrated, resulting in the green mass near θ^* . (*Top right*) Model distributions $q(\mathbf{x}|\psi)$ after training. Despite the differences between their respective proposal distributions, both models closely match the observed data. (*Bottom*) Empirical estimates of the variational upper bound U_d as optimization progresses.

likelihood-free inference based on bayesian optimization and approximated density ratios [3, 4] or to classifier ABC [9].

This work has many connections to variational inference, in which the goal is to optimize the recognition model $q(\theta|\psi)$ so that it is close to the true posterior $p(\theta|x)$. This is slightly different from variational optimization (or variational learning), where the goal is to find θ^* such that $p(x|\theta^*) \approx p_r(x)$. Typically in variational inference the model $p(x|\theta)$ admits a density, so that the likelihood is known. Thus, assuming the prior also admits a density, it is tractable to evaluate the posterior is (up to a constant factor). In Adversarial Variational Bayes [14] and, equivalently, the PC-Adv algorithm of [11], the authors use an adversarial setup, but assume a known density $p(x|\theta)$ that is differentiable with respect to θ .

In [19], the authors consider Variational Bayes with an intractable likelihood. In that approach “The only requirement is that the intractable likelihood can be estimated unbiasedly.” In the case of most simulators it is not clear how one would obtain the unbiased estimator $\hat{p}(x|\theta)$.

In [11] the author defines implicit distributions to be “probability models whose probability density function may be intractable, but there is a way to 1) sample from them exactly and/or calculate and approximate expectations under them, and 2) calculate or estimate gradients of such expectations with respect to model parameters.” This notion of implicit model does not include most scientific simulators as 2) is not satisfied. The JC-Adv and JC-Den algorithm defined there applies to implicit models, but, as the author points out, is aimed at variational inference and “does not provide a direct way to learn model parameters θ ”.

VII. SUMMARY

In this note, we develop a likelihood-free inference algorithm for fitting a forward non-differentiable simulator to continuous or discrete observed data. The algorithm combines adversarial training with variational optimization to minimize variational upper bounds on the otherwise non-differentiable adversarial objectives. Effectively, the procedure results in learning an arbitrarily tight proposal distribution over the simulator parameters, such that corresponding the marginal distribution of the generated data matches the observations. Preliminary results with non-differentiable discrete or continuous simulators validate the proposed method.

While the obtained results are encouraging, the complete validation of the method remains to be carried out in real conditions on a full fledged scientific simulator – which we plan to achieve for a next version of this work. In terms of method, several components need to be further investigated. First, we need to better study the interplay between the entropy penalty and the adversarial objectives. Second, we should better understand the dynamics of the optimization procedure, in particular when combined with momentum-based optimizers like Adam. Third, we need to consider whether less noisy estimates of the gradients $\nabla_\psi U_g$ can be computed, in particular by exploiting the fact in the composition $d(g(\mathbf{z}; \theta); \psi)$ the derivatives of d are known exactly.

KC: could also use this to tune non-differentiable fast simulator to slower full simulator. Then fixed data size not an issue

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