Adversarial Variational Optimization of Non-Differentiable Simulators

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Complex computer simulators are increasingly used across fields of science to describe generative models tying parameters of an underlying theory to experimental observations. Inference in this setup is often difficult, as simulators rarely provide a way to directly evaluate the likehood function for a given observation. In this note, we develop a likelihood-free inference algorithm for fitting a forward non-differentiable generative model to observed data. We adapt the adversarial training procedure of generative adversarial networks by replacing the implicit generative network with a domain-based scientific simulator, and solve the resulting non-differentiable minimax problem by minimizing variationial upper bounds of the 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. [GL: Mention experimental results.] [GL: Add 'so what?' conclusion.]

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 [12] are specified as procedural implementations of forward stochastic processes that generate 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 [6] or being a controllable probabilistic program [11].

In this note, we develop a likelihood-free inference algorithm for the point estimation from observed data of the parameters of a forward non-differentiable generative model. We propose to adapt the adversarial training procedure of generative adversarial networks [5] 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 [13, 14] of the adversarial objectives. The procedure results in learning a proposal distribution over simulator parameters, hence producing an abitrarily tight family of models whose joint collection of generated samples matches the observed data.

II. PROBLEM STATEMENT

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

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

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 $p(\mathbf{z}|\theta)$ may itself depend on θ in some intricated way.

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

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

such that the likelihood $p(\mathbf{x}|\theta)$ can be rewritten as

$$p(\mathbf{x}|\theta) = \frac{\partial}{\partial x_1} \dots \frac{\partial}{\partial x_d} \int_{\{\mathbf{z}: g(\mathbf{z};\theta) \leq \mathbf{x}\}} p(\mathbf{z}|\theta) \mu(d\mathbf{z}), \tag{3}$$

where μ is a probability measure. 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 θ, 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 θ^* that minimize the divergence between $p_r(\mathbf{x})$ and the modeled data distribution $p(\mathbf{x}|\theta)$ induced by $g(\cdot; \theta)$ over $\mathbf{z}$. That is,

$$\theta^* = \arg\min_{\theta \in \Theta} \rho(p_r(\mathbf{x}), p(\mathbf{x}|\theta)), \tag{4}$$

where ρ is some distance or divergence.

III. BACKGROUND

A. Generative adversarial networks

Generative adversarial networks (GANs) were first proposed by [5] as a way to build an implicit generative model capable of producing samples from random noise $\mathbf{z}$. More specifically, a generative model $g(\cdot;\theta)$ is pit against an adversarial classifier $d(\cdot;\phi) : \mathbb{R}^d \to [0,1]$ with parameters ϕ and whose antagonistic objective is to recognize real data $\mathbf{x}$ from generated data $\tilde{\mathbf{x}} = g(\mathbf{z};\theta)$. 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 amounts to minimizing the Jensen-Shannon divergence $\text{JSD}(p_r(\mathbf{x}) \parallel p(\mathbf{x}|\theta))$ between $p_r(\mathbf{x})$ and $p(\mathbf{x}|\theta)$.

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 $W(p_r(\mathbf{x}), p(\mathbf{x}|\theta))$ by replacing the adversarial classifier with a 1-Lipschitz adversarial critic $d(\cdot;\phi) : \mathbb{R}^d \to \mathbb{R}$. Under the WGAN-GP formulation of [7] for stabilizing the optimization procedure, training d and g results in alternating gradient updates on ϕ and θ in order to respectively minimize

$$\begin{aligned}\mathcal{L}_d = &\mathbb{E}_{\tilde{\mathbf{x}}\sim p(\mathbf{x}|\theta)}[d(\tilde{\mathbf{x}};\phi)] - \mathbb{E}_{\mathbf{x}\sim p_r(\mathbf{x})}[d(\mathbf{x};\phi)] \\ &+ \lambda \mathbb{E}_{\hat{\mathbf{x}}\sim p(\hat{\mathbf{x}})}[(||\nabla_{\hat{\mathbf{x}}} d(\hat{\mathbf{x}};\phi)||_2 - 1)^2] \qquad (5)\\ \mathcal{L}_g = &- \mathbb{E}_{\tilde{\mathbf{x}}\sim p(\mathbf{x}|\theta)}[d(\tilde{\mathbf{x}};\phi)] \qquad (6)\end{aligned}$$

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 $\tilde{\mathbf{x}} \sim p(\mathbf{x}|\theta)$.

B. Variational optimization

Evolution strategies [14] and variational optimization [13] 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

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

where $q(\theta|\psi)$ is a proposal distribution with parameters ψ over input values θ. 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 ψ can be updated to place its mass arbitrarily tight around the optimum $\theta^* = \min_{\theta\in\Theta} f(\theta)$.

Under mild restrictions outlined in [13], the bound $U(\psi)$ is differentiable with respect to ψ, and using the log-likelihood trick it comes:

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

Effectively, this means that provided that the score function $\nabla_\psi \log q(\theta|\psi)$ of the proposal is known and that one can evaluate $f(\theta)$ for any θ, then one can construct empirical estimates of Eqn. 8, which can in turn be used to minimize $U(\psi)$ with stochastic gradient descent (or a variant thereof, like Adam [10] or the Natural Evolution Strategy algorithm [14], 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 not interested in learning the implicit model itself but are rather interested in the inference of parameters of a fixed non-differentiable simulator (Section II), gradients $\nabla_\theta g$ either do not exist or cannot be accessed. As a result, gradients $\nabla_\theta \mathcal{L}_g$ 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 $q(\theta|\psi)$ over the parameters of g and $p(\mathbf{x}|\theta)$ and minimize in alternation the variational upper bounds

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

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

respectively over ϕ and ψ. When updating d, unbiased gradient 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 g, estimates of $\nabla_\psi U_g$ can be derived with forward simulations, as described in the previous section. That is,

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

which we can approximate with mini-batches of generated data

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

Algorithm 1 Adversarial variational optimization.

Inputs: observed data $\{\mathbf{x}_i \sim p_r(\mathbf{x})\}_{i=1}^N$, simulator g.
Outputs: proposal distribution $q(\theta|\psi)$, such that $p_r(\mathbf{x}) \approx p(\mathbf{x}|\psi)$.
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.

$q(\theta|\psi) \leftarrow$ prior on θ (with differentiable and known density)
while ψ has not converged **do**
  for $i = 1$ to n_{critic} **do** ▷ Update d
    Sample a mini-batch $\{\mathbf{x}_m \sim p_r(\mathbf{x}), \theta_m \sim q(\theta|\psi), \mathbf{z}_m \sim p(\mathbf{z}|\theta_m), \epsilon_m \sim U[0,1]\}_{m=1}^M$.
    for $m = 1$ to M **do**
      $\tilde{\mathbf{x}}_m \leftarrow g(\mathbf{z}_m; \theta_m)$
      $\hat{\mathbf{x}}_m \leftarrow \epsilon_m \mathbf{x}_m + (1 - \epsilon_m)\tilde{\mathbf{x}}_m$
      $U_d^{(m)} \leftarrow d(\tilde{\mathbf{x}}_m; \phi) - d(\mathbf{x}_m; \phi) + \lambda(||\nabla_{\hat{\mathbf{x}}_m} d(\hat{\mathbf{x}}_m; \phi)||_2 - 1)^2$
    end for
    $\phi \leftarrow \text{Adam}(\nabla_\phi \frac{1}{M} \sum_{m=1}^M U_d^{(m)})$
  end for
  Sample a mini-batch $\{\theta_m \sim q(\theta|\psi), \mathbf{z}_m \sim p(\mathbf{z}|\theta_m)\}_{m=1}^M$. ▷ Update q_ψ
  $\nabla_\psi U_g \leftarrow \frac{1}{M} \sum_{m=1}^M -d(g(\mathbf{z}_m; \theta_m)) \nabla_\psi \log q_\psi(\theta_m)$
  $\nabla_\psi H(q_\psi) \leftarrow \frac{1}{M} \sum_{m=1}^M \nabla_\psi q_\psi(\theta_m) \log q_\psi(\theta_m)$
  $\psi \leftarrow \text{Adam}(\nabla_\psi U_g + \gamma \nabla_\psi H(q_\psi))$
end while

for $\theta_m \sim q(\theta|\psi)$ and $\mathbf{z}_m \sim p(\mathbf{z}|\theta_m)$ and . [GL: Can we exploit the fact that $\nabla_{\mathbf{x}} d(\mathbf{x})$ is known exactly for building better estimates $\hat{\nabla}_\psi U_g$?] For completeness, Algorithm 1 outlines the proposed adversarial variational optimization procedure, as built on top of WGAN-GP. Obviously, the variational relaxation could similarly be coupled with other variants of GANs and/or of evolution strategies.

Practically, the variational objectives 9-10 have the effect of replacing the modeled data distribution of Eqn. 2 with a distribution parameterized in terms of ψ:

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

Intuitively, this corresponds to a family of simulators, each configured with randomly sampled parameters $\theta \sim q(\theta|\psi)$, 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 $p(\mathbf{x}|\psi)$ therefore corresponds to the marginal distribution $\int q(\theta|\psi)p(\mathbf{x}|\theta)d\theta$ of the generated data. [GL: Connection with variational bayes?]

In consequence, the proposed inference algorithm does not necessarily guarantee that the proposal distribution $q(\theta|\psi)i$ will place its mass arbitrarily tight around the parameters of interest, which might be an issue when one is rather interested in point estimates θ^*. For this purpose, we augment Eqn. 10 with a regularization term corresponding to the differential entropy H of the proposal distribution. That is,

$$U_g = \mathbb{E}_{\theta \sim q(\theta|\psi)}[\mathcal{L}_g] + \gamma H(q(\theta|\psi)) \quad (14)$$

where $\gamma \in \mathbb{R}^+$ is a hyperparameter controlling the trade-off between the generator objective and the tightness of the proposal distribution. 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 θ values. On the other hand, for small values of γ, proposal distributions with larger entropy are not penalized, which may result in learning a smeared variation of the original simulator. [GL: Add note on minimum entropy, otherwise it degenerates back to a non-differentiable function.]

V. EXPERIMENTS

A. Gaussian mixture model

B. Plinko

C. Physics example

VI. RELATED WORKS

As reviewed in [12], 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 generated data distributions. For example, [9] uses non linear logistic regression for fitting unnormalized differentiable statistical models, while [5] exploits an adversarial neural network for learning a differentiable implicit generative model. In the likelihood-free setup, [3, 4] estimate likeli-

hood ratios through supervised classification, which can in turn be used for parameter inference in combination with a gradient-free optimization algorithm. Similarly, [8] makes use of classification accuracy as a summary statistics for approximate Bayesian computation. [GL: Explain what's new about the proposed work.]

VII. SUMMARY

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