On the Reparameterisation Gradient for Non-Differentiable but Continuous Models

Dominik Wagner Luke Ong



LAFI 2023 15 January 2023

frame posterior inference as (deterministic) optimisation problem

frame posterior inference as (deterministic) optimisation problem

Posit: variational family of "simpler" guide distributions

frame posterior inference as (deterministic) optimisation problem

Posit: variational family of "simpler" guide distributions

Aim: find guide is "closest" to (true) posterior

frame posterior inference as (deterministic) optimisation problem

Posit: variational family of "simpler" guide distributions

Aim: find guide is *"closest"* to (true) posterior KL divergence

 $\operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\mathsf{z} \sim q_{\boldsymbol{\theta}}} \left[f(\boldsymbol{\theta}, \mathsf{z}) \right]$

$$\operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\mathsf{z} \sim q_{\boldsymbol{\theta}}} \left[f(\boldsymbol{\theta}, \mathsf{z}) \right]$$

use Stochastic Gradient Descent

 $\operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\theta}}} \left[f(\boldsymbol{\theta}, \mathbf{z}) \right]$

use Stochastic Gradient Descent

Key ingredient: estimation of gradient of expectation

 $\operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{z} \sim q_{\boldsymbol{\theta}}} \left[f(\boldsymbol{\theta}, \boldsymbol{z}) \right]$

use Stochastic Gradient Descent

Key ingredient: estimation of gradient of expectation

Score Estimator:

 $\operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\mathsf{z} \sim q_{\boldsymbol{\theta}}} \left[f(\boldsymbol{\theta}, \mathsf{z}) \right]$

use Stochastic Gradient Descent

Key ingredient: estimation of gradient of expectation

 Score Estimator: widely applicable but *high variance*

$$\operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\theta}}} \left[f(\boldsymbol{\theta}, \mathbf{z}) \right]$$

use Stochastic Gradient Descent

Key ingredient: estimation of gradient of expectation

 Score Estimator: widely applicable but *high variance*

Reparametrisation Estimator:

$$\boxed{\operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\theta}}}[f(\boldsymbol{\theta}, \mathbf{z})]}_{\left(\begin{array}{c} \uparrow \\ \uparrow \end{array} \right)}$$

expressed in PL with conditionals, may *not* be *differentiable/continuous*

use Stochastic Gradient Descent

Key ingredient: estimation of gradient of expectation

 Score Estimator: widely applicable but *high variance*

Reparametrisation Estimator:

better in practice but may be biased! [Lee et al., NeurIPS 2018]

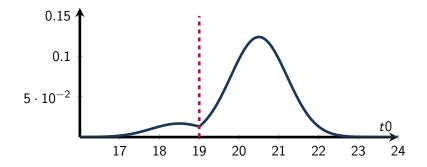
let t0 = sample normal(20,1)

let t0 = sample normal(20,1)mu = t0 + if t0 >= 19 then 0

let
$$t0 = sample normal(20,1)$$

 $mu = t0 + if t0 >= 19 then 0$
else 2 * (19-t0)

```
let t0 = sample normal(20,1)
    mu = t0 + if t0 >= 19 then 0
        else 2 * (19-t0)
        observe 21 from normal(mu, 1)
in t0
```



Is the Reparametrisation Gradient Estimator biased for continuous but possibly non-differentiable programs? *Is the Reparametrisation Gradient Estimator biased for continuous but possibly non-differentiable programs?*

No!

simply typed $\lambda\text{-calculus}$ with $\mathbb R$ and primitive operations + sample + observe

simply typed λ -calculus with \mathbb{R} and primitive operations + sample + observe + branching simply typed λ -calculus with \mathbb{R} and primitive operations + sample + observe + branching + *smoothed* branching

denotational version of weight/density semantics

- denotational version of weight/density semantics
- beyond measuarability: capture piecewise definition and continuity

- denotational version of weight/density semantics
- beyond measuarability: capture piecewise definition and continuity
- complication: smoothed conditionals at higher-order [ESOP23]

- denotational version of weight/density semantics
- beyond measuarability: capture piecewise definition and continuity
- complication: smoothed conditionals at higher-order [ESOP23]

Generalise construction of Frölicher spaces

- denotational version of weight/density semantics
- beyond measuarability: capture piecewise definition and continuity
- complication: smoothed conditionals at higher-order [ESOP23]

Generalise construction of Frölicher spaces

Unbiasedness for terms without conditionals

- denotational version of weight/density semantics
- beyond measuarability: capture piecewise definition and continuity
- complication: smoothed conditionals at higher-order [ESOP23]

Generalise construction of Frölicher spaces

Unbiasedness for terms without conditionals

Example. Rephrase conditional via non-differentiable primitive:

 $c \cdot (\underline{\operatorname{ReLU}}(19 - t_0))$

naive check intractable!

naive check intractable!

For analytic primitives f and g,

if
$$x - y < 0$$
 then $\underline{f} x y$ else $g x y$ is continuous

naive check intractable!

For analytic primitives f and g,

$$if x - y < 0 then \underline{f} x y else \underline{g} x y$$
$$\iff (f - g)_{|U} = 0$$

is continuous where $U \coloneqq \{(x, y) \mid x = y\}$

naive check intractable!

For analytic primitives f and g,

$$if x - y < 0 then \underline{f} x y else \underline{g} x y$$

$$\iff (f - g)|_{U} = 0$$

$$\iff f(x, y) = g(x, y)$$
* with probability 1

is continuous where $U := \{(x, y) \mid x = y\}$ $(x, y) \sim U$

naive check intractable!

For analytic primitives f and g,

$$if x - y < 0 then \underline{f} x y else \underline{g} x y$$

$$\iff (f - g)|_{U} = 0$$

$$\iff^{*} f(x, y) = g(x, y)$$

$$^{*} with \ probability \ 1$$

is continuous where $U := \{(x, y) \mid x = y\}$ $(x, y) \sim U$

Restrict guards to affine terms:

naive check intractable!

For analytic primitives f and g,

$$if x - y < 0 then \underline{f} x y else \underline{g} x y$$

$$\iff (f - g)|_{U} = 0$$

$$\iff^{*} f(x, y) = g(x, y)$$

$$^{*} with \ probability \ 1$$

is continuous where $U := \{(x, y) \mid x = y\}$ $(x, y) \sim U$

Restrict guards to affine terms:

efficiently sample from boundary

naive check intractable!

For analytic primitives f and g,

$$if x - y < 0 then \underline{f} x y else \underline{g} x y$$

$$\iff (f - g)_{|U} = 0$$

$$\iff f(x, y) = g(x, y)$$
* with probability 1

is continuous where $U := \{(x, y) \mid x = y\}$ $(x, y) \sim U$

Restrict guards to affine terms:

- efficiently sample from boundary
- efficiently check guard's consistency (linear arithmetic solvers)

Contributions

The Reparametrisation Gradient Estimator is unbiased for *continuous* but possibly *non-differentiable* programs

Contributions

The Reparametrisation Gradient Estimator is unbiased for *continuous* but possibly *non-differentiable* programs

categorical models

- prove unbiasedness in continuous setting
- establish continuity in languages with conditionals compositionally
 - for affine guards: efficient *randomised* check employing *linear arithmetic solvers*

Contributions

The Reparametrisation Gradient Estimator is unbiased for *continuous* but possibly *non-differentiable* programs

categorical models

- prove unbiasedness in continuous setting
- establish continuity in languages with conditionals compositionally
 - for affine guards: efficient *randomised* check employing *linear arithmetic solvers*

Foundation for *fast yet correct* (variational) inference for probabilistic programming