Reparameterization Gradient for Non-differentiable Models from Probabilistic Programming

Hongseok Yang
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Joint with Wonyeol Lee and Hangyeol Yu

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High-level message

$$\nabla_\theta \int H(\theta, x)\,\mathrm{d}x \;=\; \int \nabla_\theta H(\theta, x)\,\mathrm{d}x$$

- Careful when exchanging gradient and integration.

High-level message

$$\nabla_\theta \int H(\theta, x)\,\mathrm{d}x \neq \int \nabla_\theta H(\theta, x)\,\mathrm{d}x$$

- Careful when exchanging gradient and integration.
- May fail unexpectedly.

High-level message

$$\nabla_\theta \int H(\theta, x)\, \mathrm{d}x \;=\; \int \nabla_\theta H(\theta, x)\, \mathrm{d}x$$

$$+ \text{ CorrectionTerm}$$

- Careful when exchanging gradient and integration.
- May fail unexpectedly.
- May hold unexpectedly, but with correction.

Results informally with one simple example

```
(let
  [z (sample (normal 0 1))]
  (if (> z 0)
    (observe (normal 3 1) 0)
    (observe (normal -2 1) 0))
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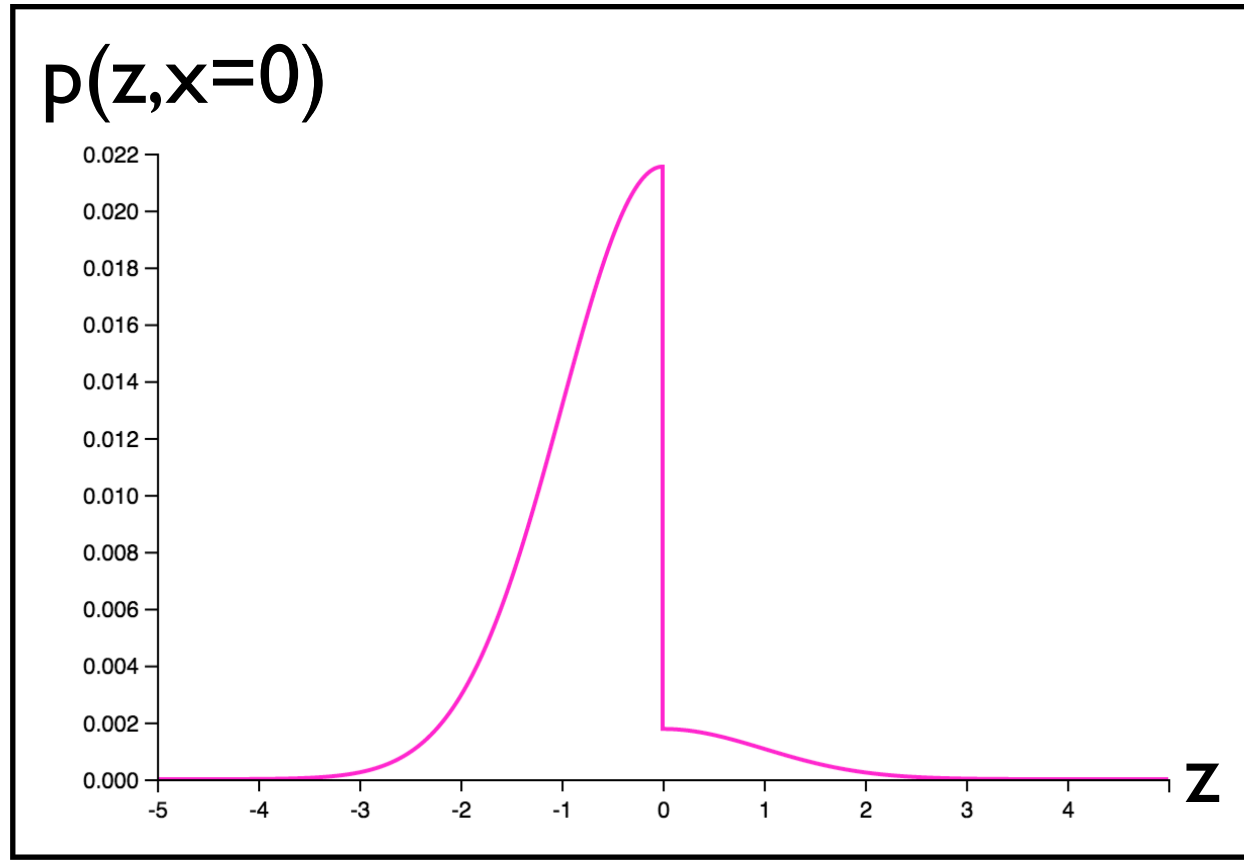

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$$\theta_{n+1} \leftarrow \theta_n + \eta \times \nabla_\theta \, \text{ELBO}_{\theta=\theta_n}$$

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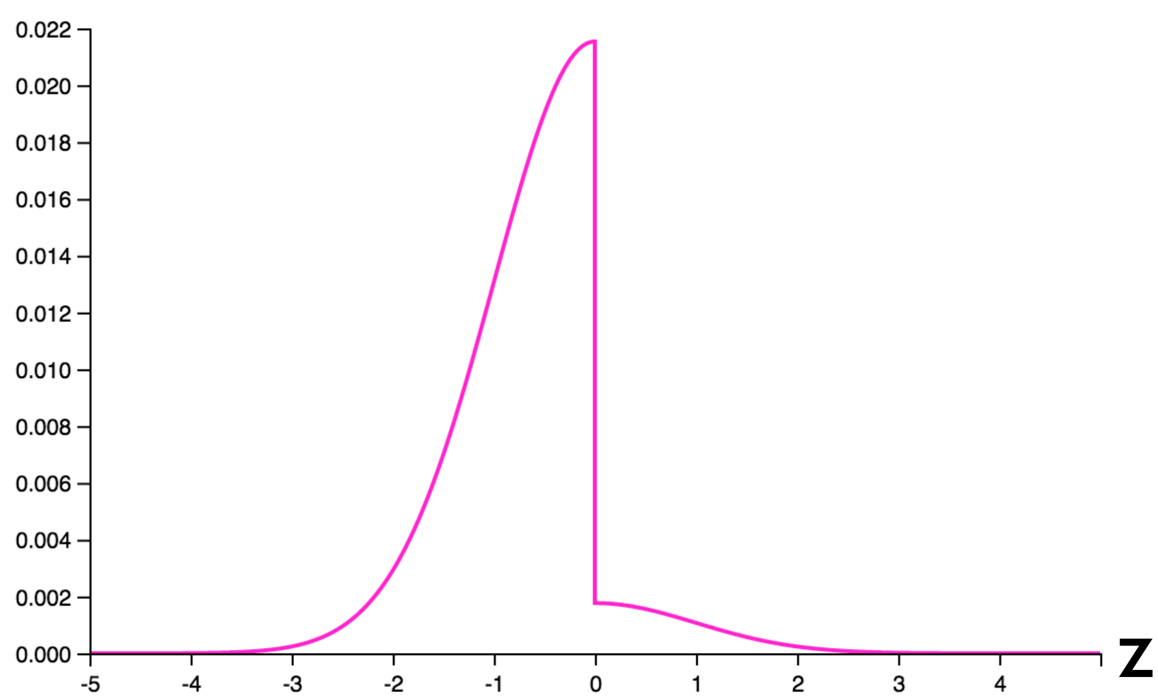
p(z,x=0)



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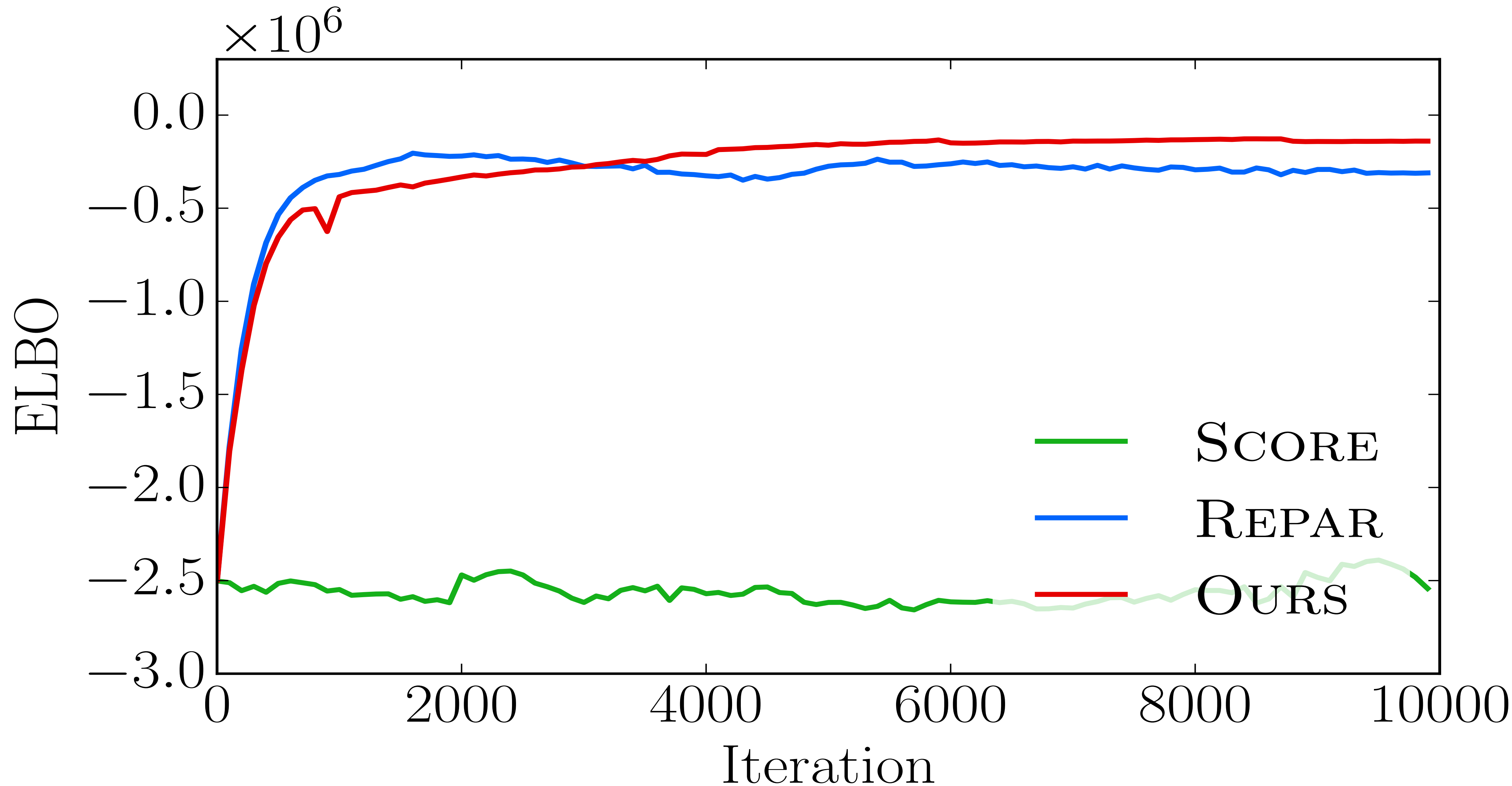
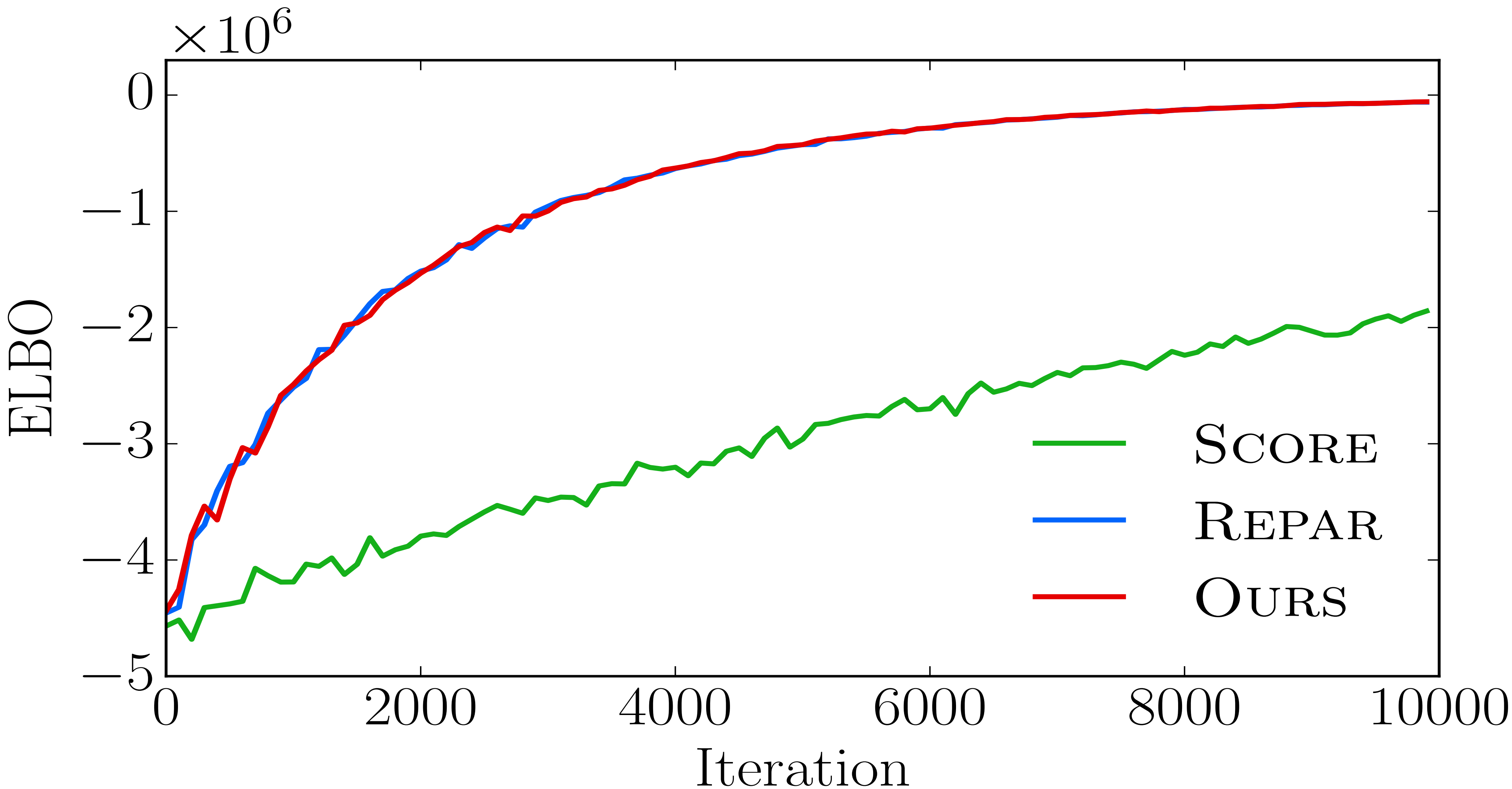


(a) `temperature` (stepsize = 0.001)



(e) `influenza` (stepsize = 0.001)

Results formally

Reparameterization gradient for non-differentiable models

Model $\quad p(z, x^0) = \sum_k [z \in A_k] \times r_k(z)$

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$$\mathrm{ELBO}_\theta = \mathbb{E}_{q(\varepsilon)}\Big[\sum_k [\varepsilon \in f_\theta^{-1}(A_k)] \times H_k(\varepsilon, \theta) \Big]$$

$$\nabla_\theta \mathrm{ELBO}_\theta = \mathbb{E}_{q(\varepsilon)}\Big[\sum_k [\varepsilon \in f_\theta^{-1}(A_k)] \times \nabla_\theta H_k(\varepsilon, \theta) \Big]$$

$$+ \sum_k \text{surface integral over } \partial f_\theta^{-1}(A_k)$$

Accounts for the impact of moving the boundaries. Can be estimated by (optimised) manifold sampling when boundaries are affine.

$$\text{Model} \quad p(z, x^0) = \textstyle\sum_k [z \in A_k] \times r_k(z).$$

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Correction term for k

Surface integral over $\partial f_\theta^{-1}(A_k)$

$$= \int_{\partial f_\theta^{-1}(A_k)} \Big(q(\epsilon) H_k(\epsilon, \theta) \mathbf{V}(\epsilon, \theta) \Big) \cdot \mathrm{d}\boldsymbol{\Sigma}$$

- $\mathbf{V}(\varepsilon,\theta)_{ij} = (\partial f_\theta^{-1} / \partial \theta_i)_j$
- $\boldsymbol{\Sigma}$ is a normal vector of ∂A_k
- $\mathbf{V}(\varepsilon,\theta) \bullet \mathrm{d}\boldsymbol{\Sigma}$ is a matrix-vector product

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Two ingredients

- Differentiation under moving domain:

$$\nabla_\theta \int_{B_\theta} g(\epsilon, \theta)\, \mathrm{d}\epsilon = \int_{B_\theta} (\nabla_\theta g + \nabla_\epsilon \cdot (g\mathbf{V}))(\epsilon, \theta)\, \mathrm{d}\epsilon$$

- Divergence theorem:

$$\int_B \left(\nabla \cdot \mathbf{G} \right) \mathrm{d}V = \int_{\partial B} \mathbf{G} \cdot \mathrm{d}\mathbf{\Sigma}$$

Reference

- “Reparameterization gradient for non-differentiable models” by Lee, Yu and Yang. 2018.