Backpropagation
Through

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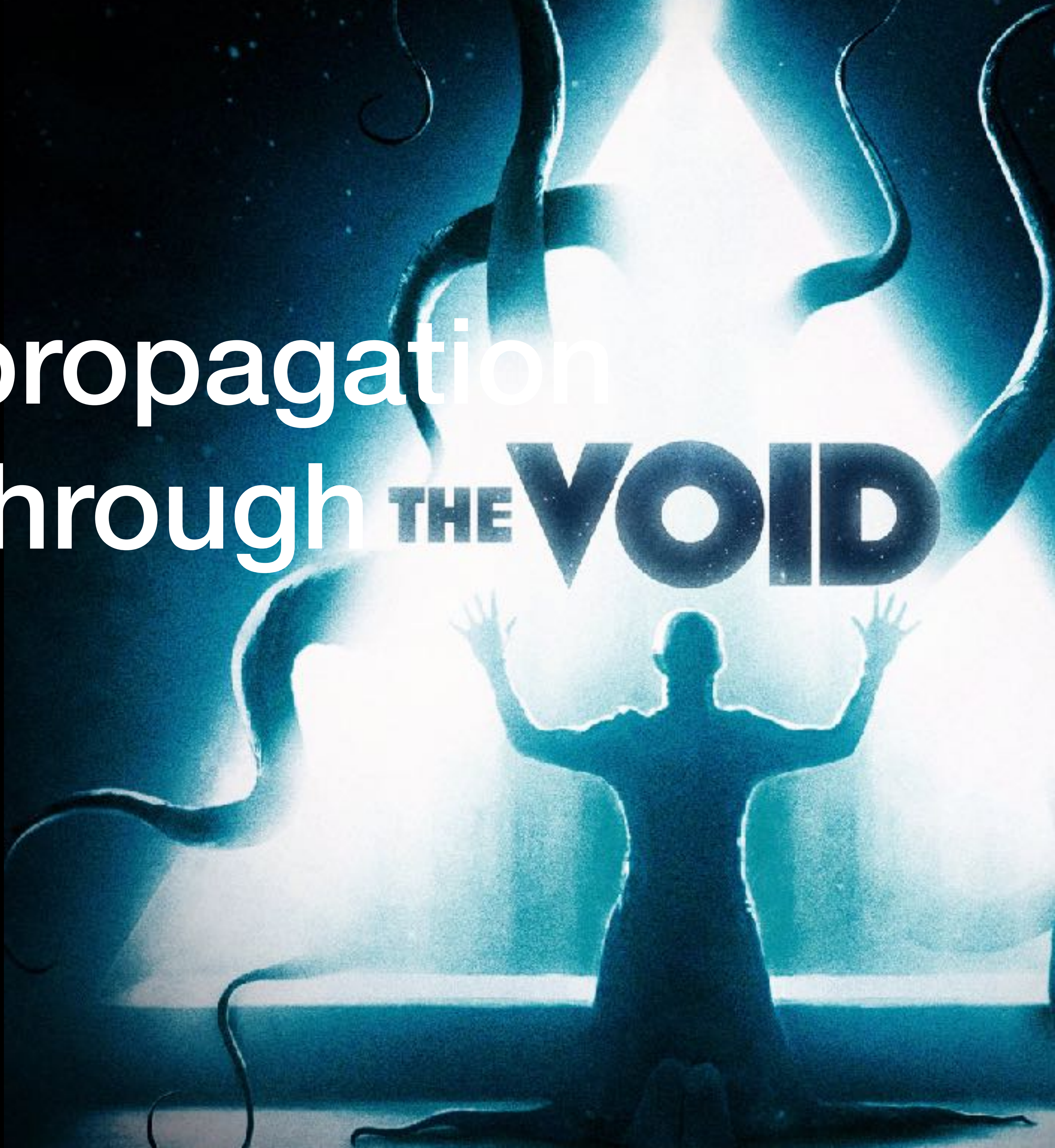


Backpropagation Through

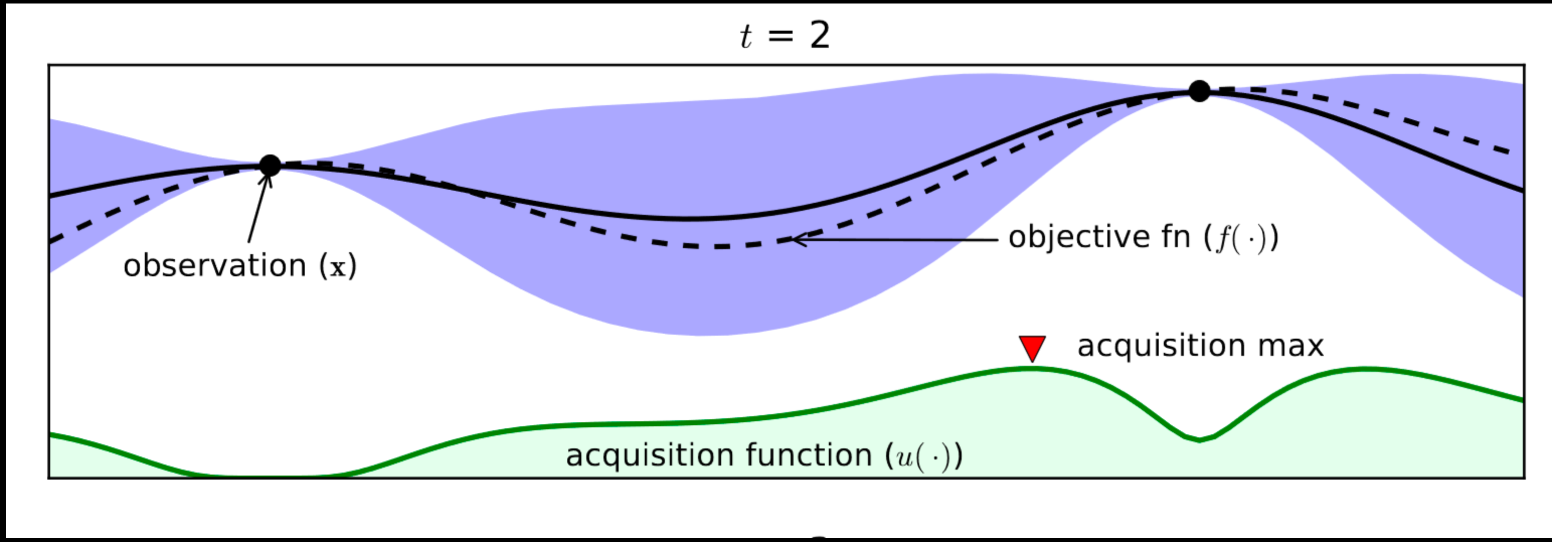
Will Grathwohl
Dami Choi
Yuhuai Wu
Geoff Roeder
David Duvenaud

Where do we see this guy?

$$\mathcal{L}(\theta) = \mathbb{E}_{p(b|\theta)}[f(b)]$$

- Variational Inference
- Hamiltonian Monte Carlo
- Policy Optimization
- Hard Attention

Bayesian optimization doesn’t scale yet



Shahriari et al., 2016

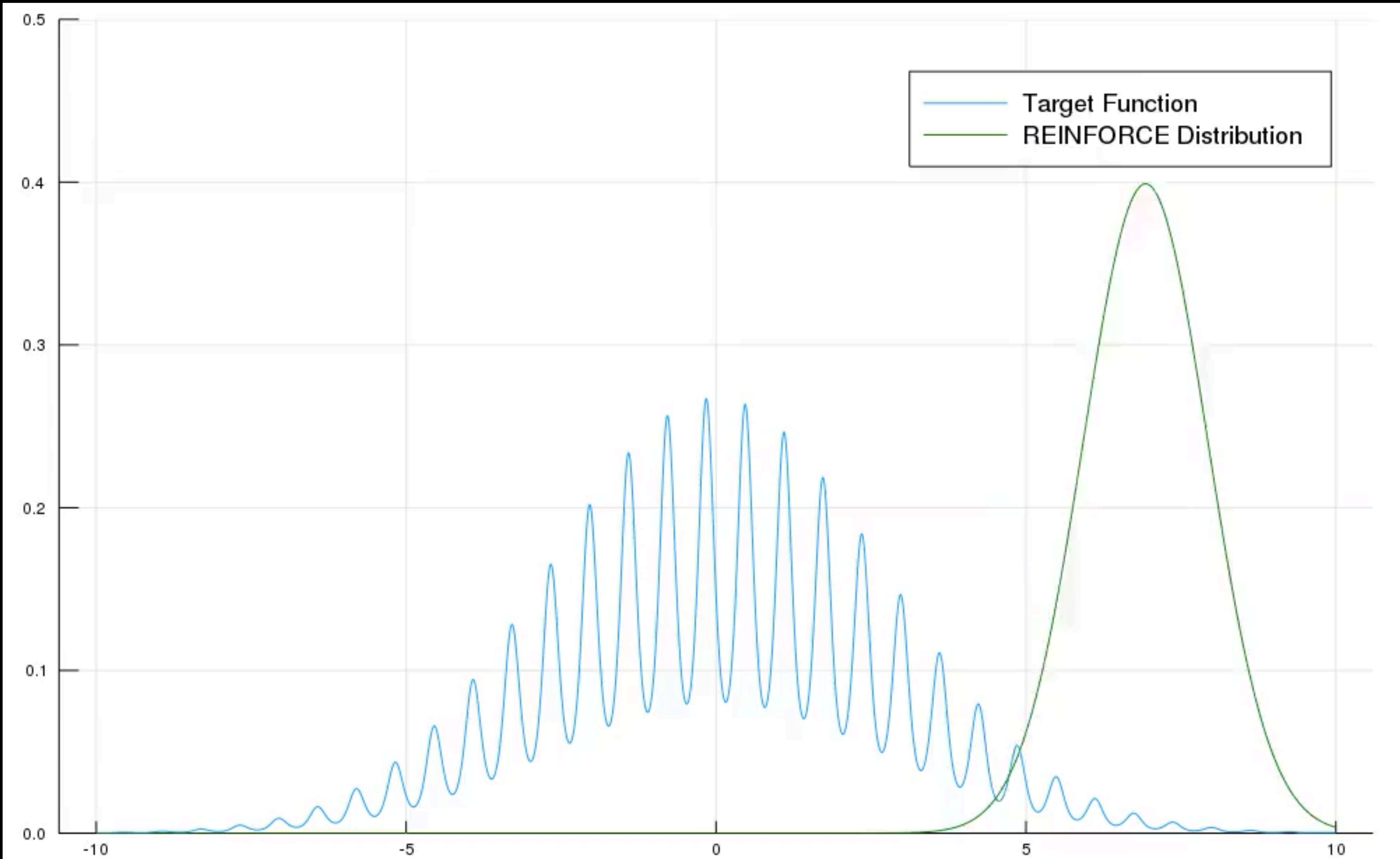
- Bayesopt is usually expensive, relative to model evals
- Global surrogate models not good enough in high dim.
- Even for expensive black-box functions, gradient-based optimization is embarrassingly competitive
- Can we add some cheap model-based optimization to REINFORCE?

REINFORCE (Williams, 1992)

$$\hat{g}_{\text{REINFORCE}}[f] = f\,(b)\,\frac{\partial}{\partial\theta}\log p(b|\theta), \qquad b \sim p(b|\theta)$$

- Unbiased
- Works for any f, not differentiable or even unknown
- high variance

$$\hat{g}_{\text{REINFORCE}}[f] = f\,(b)\,\frac{\partial}{\partial\theta}\log p(b|\theta), \qquad b \sim p(b|\theta)$$



Reparameterization Trick:

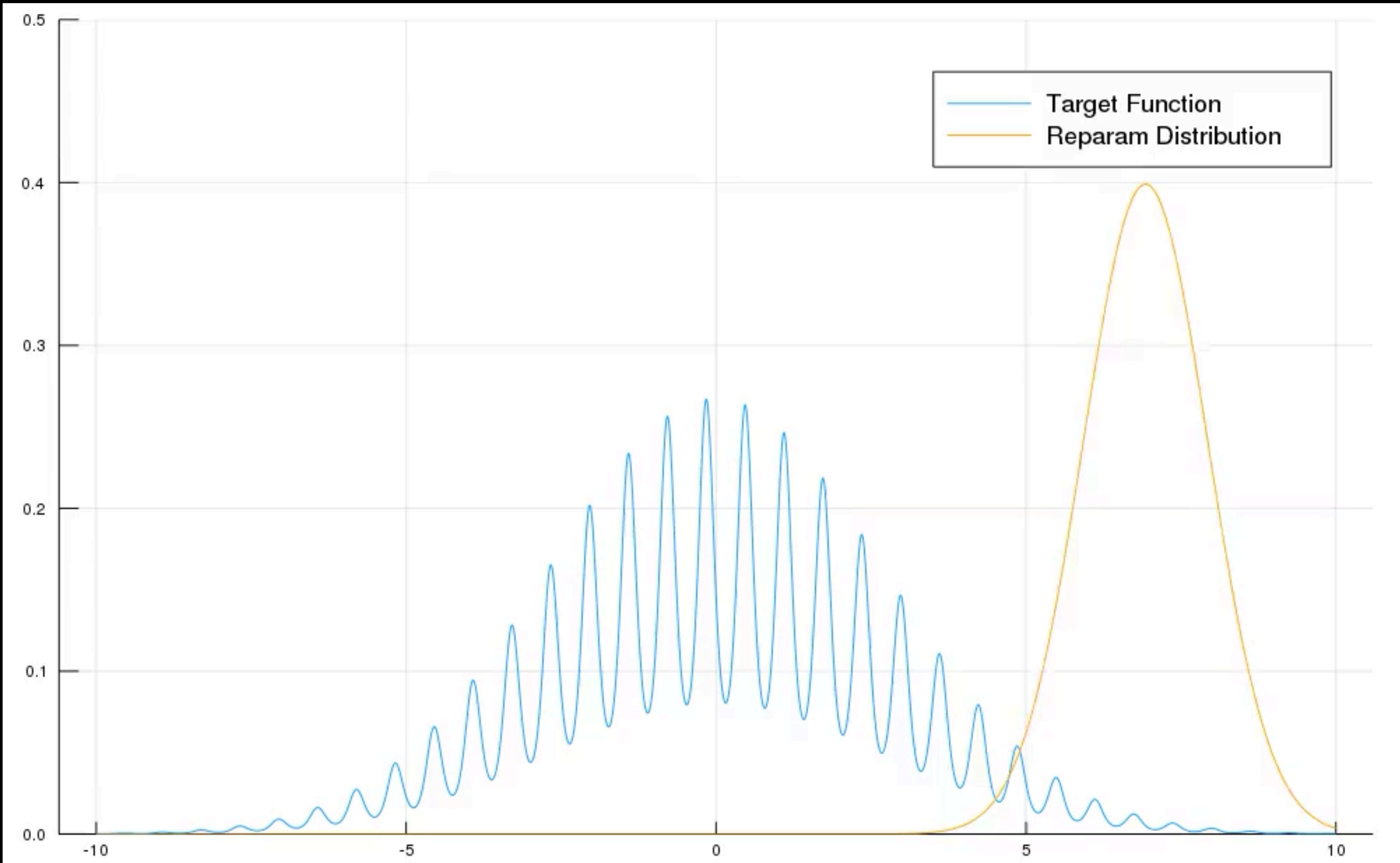
$$\hat{g}_{\mathrm{reparam}}[f] = \frac{\partial f}{\partial b}\frac{\partial b}{\partial \theta}$$

$$b = T(\theta, \epsilon), \epsilon \sim p(\epsilon)$$

- Usually lower variance
- Unbiased
- Gold standard, allowed huge continuous models

- Requires $f(b)$ to be known and differentiable
- Requires $p(b|\theta)$ to be differentiable

$$\hat{g}_{\text{reparam}}[f] = \frac{\partial f}{\partial b}\frac{\partial b}{\partial \theta} \qquad b = T(\theta, \epsilon), \epsilon \sim p(\epsilon)$$



Concrete/Gumbel-softmax

$$\hat{g}_{\text{concrete}}[f] = \frac{\partial f}{\partial \sigma(z/t)} \frac{\partial \sigma(z/t)}{\partial \theta} \qquad z = T(\theta, \epsilon), \epsilon \sim p(\epsilon)$$

- Tune variance vs bias
- Works well in practice for discrete models

- Biased
- $f(b)$ must be known and differentiable
- $p(z|\theta)$ must be differentiable
- Uses undefined behavior of $f(b)$

Control Variates

- Allow us to reduce variance of a Monte Carlo estimator

$$\hat{g}_{\mathrm{new}}(b) = \hat{g}(b) - c(b) + \mathbb{E}_{p(b)}[c(b)]$$

- Variance is reduced if $\mathrm{corr}(g, c) > 0$

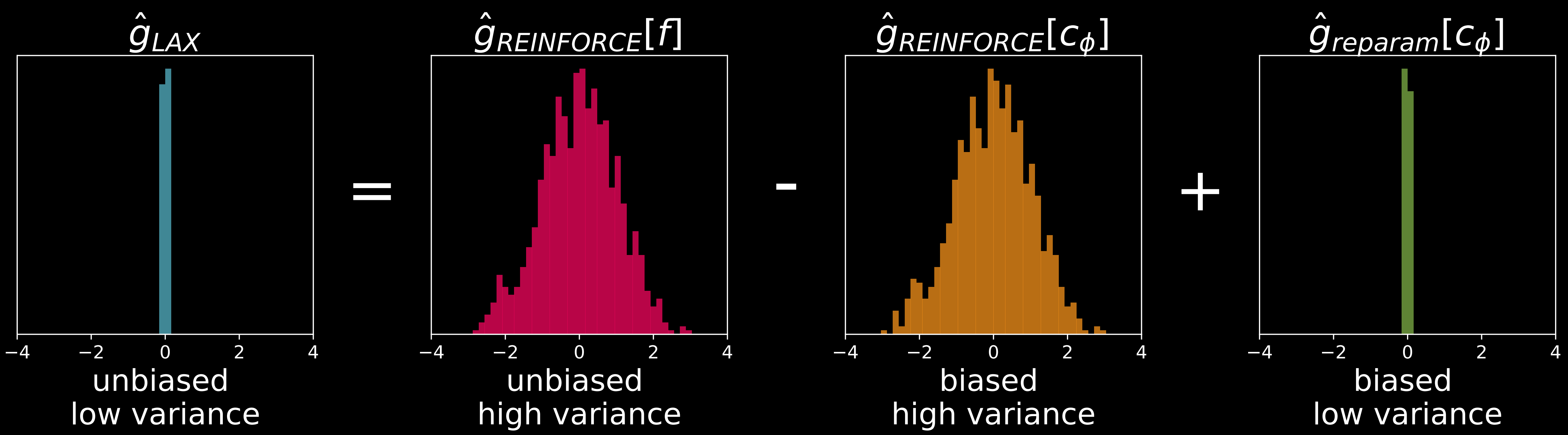
- Need to adapt g as problem changes during optimization

Our Approach

$$\begin{aligned}\hat{g}_{\mathrm{LAX}} &= g_{\mathrm{REINFORCE}}[f] - g_{\mathrm{REINFORCE}}[c_\phi] + g_{\mathrm{reparam}}[c_\phi] \\ &= [f(b) - c_\phi(b)] \frac{\partial}{\partial\theta} \log p(b|\theta) + \frac{\partial}{\partial\theta} c_\phi(b)\end{aligned}$$

Our Approach

$$\hat{g}_{\text{LAX}} = g_{\text{REINFORCE}}[f] - g_{\text{REINFORCE}}[c_\phi] + g_{\text{reparam}}[c_\phi]$$



Optimizing the Control Variate

$$\boxed{\frac{\partial}{\partial \phi}\text{Variance}(\hat{g}) = \mathbb{E}\left[\frac{\partial}{\partial \phi}\hat{g}^2\right]}$$

- For any unbiased estimator we can get Monte Carlo estimates for the gradient of the variance of $\hat{g}$
- Use to optimize c_ϕ
- Got trick from Ruiz et al. and REBAR paper

A self-tuning gradient estimator

- Jointly optimize original problem and surrogate together with stochastic optimization
- Requires higher-order derivatives

Algorithm 1 LAX: Optimizing parameters and a gradient control variate simultaneously.

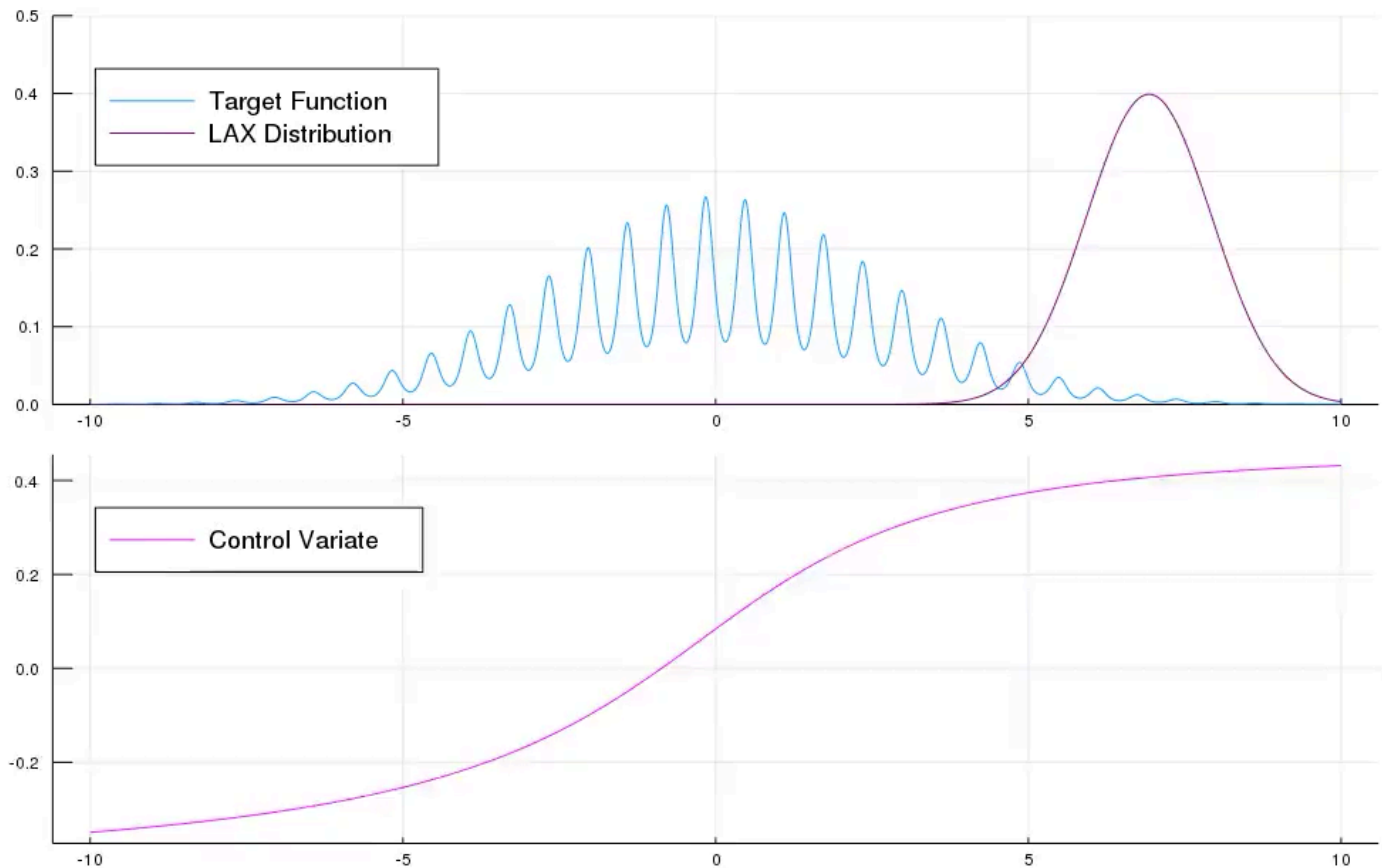
Require: $f(\cdot)$, $\log p(b|\theta)$, reparameterized sampler $b = T(\theta, \epsilon)$, neural network $c_\phi(\cdot)$, step sizes α_1, α_2

while not converged **do**
- $\epsilon \sim p(\epsilon)$ ▷ Sample noise
- $b \leftarrow T(\epsilon, \theta)$ ▷ Compute input
- $\hat{g}_\theta \leftarrow [f(b) - c_\phi(b)] \nabla_\theta \log p(b|\theta) + \nabla_\theta c_\phi(b)$ ▷ Estimate gradient of objective
- $\hat{g}_\phi \leftarrow \partial \hat{g}_\theta^2 / \partial \phi$ ▷ Estimate gradient of variance of gradient
- $\theta \leftarrow \theta - \alpha_1 \hat{g}_\theta$ ▷ Update parameters
- $\phi \leftarrow \phi - \alpha_2 \hat{g}_\phi$ ▷ Update control variate

end while

return θ

$$\hat{g}_{\mathrm{LAX}} = [f(b) - c_\phi(b)]\,\frac{\partial}{\partial\theta}\log p(b|\theta) + \frac{\partial}{\partial\theta}c_\phi(b)$$



What about discrete variables?

Extension to discrete $p(b|\theta)$

$$\hat{g}_{\text{DLAX}} = f(b)\frac{\partial}{\partial\theta}\log p(b|\theta) - c_\phi(z)\frac{\partial}{\partial\theta}\log p(z|\theta) + \frac{\partial}{\partial\theta}c_\phi(z)$$

$$b = H(z), z \sim p(z|\theta)$$

$$H(z) = b \sim p(b|\theta)$$

- Unbiased for all c_ϕ

Extension to discrete $p(b|\theta)$

$$\hat{g}_{\text{RELAX}} = [f(b) - c_\phi(\tilde{z})] \frac{\partial}{\partial\theta} \log p(b|\theta) + \frac{\partial}{\partial\theta} c_\phi(z) - \frac{\partial}{\partial\theta} c_\phi(\tilde{z})$$

$$b = H(z), z \sim p(z|\theta), \tilde{z} \sim p(z|b, \theta)$$

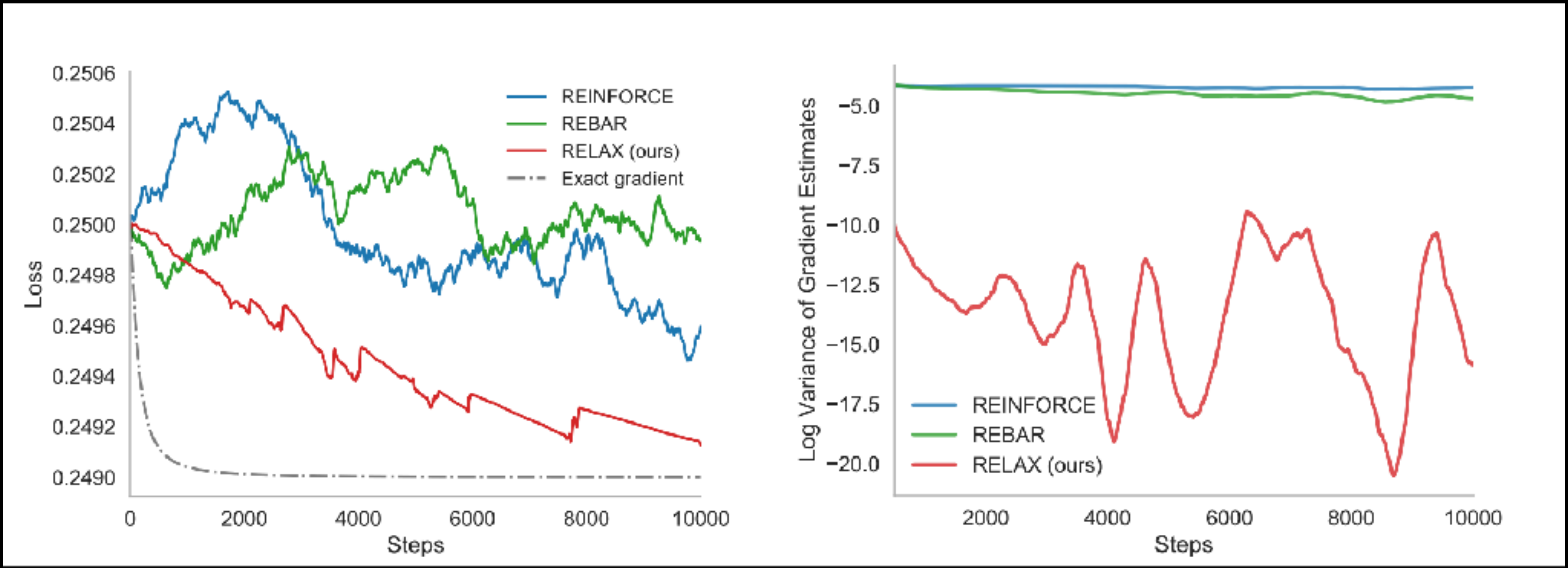
- Main trick introduced in REBAR (Tucker et al. 2017).
- We just noticed it works for any c()
- REBAR is special case of RELAX where c is concrete relaxation
- We use autodiff to tune entire surrogate, not just temperature

Toy Example

$$\boxed{\mathbb{E}_{p(b|\theta)}[(t-b)^2]}$$

- Used to validate REBAR (used t = .45)
- We use t = .499
- REBAR, REINFORCE extremely slow in this case
- Can RELAX improve?

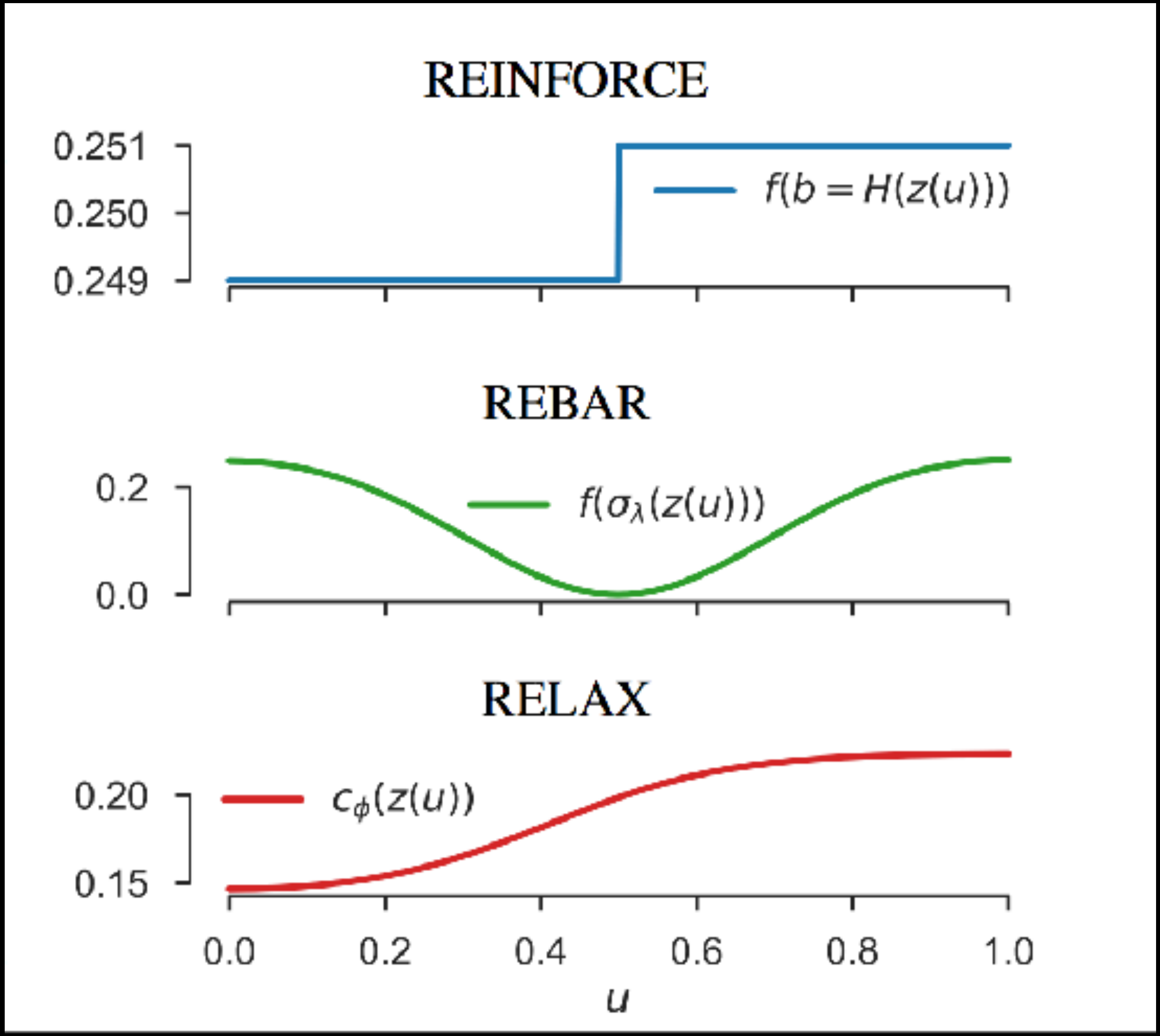
Toy Example



- massively reduced variance
- Surrogate needs time to catch up

Analyzing the Surrogate

- REBAR's fixed surrogate only adapts temperature param.
- RELAX surrogate balances REINFORCE variance and reparameterization variance
- Optimal surrogate is always smooth



Define functions, not computation graphs

```
def relax(params, est_params, noise_u, noise_v, func_vals):
    samples = bernoulli_sample(params, noise_u)
    log_temperature, nn_params = est_params

    def surrogate(relaxed_samples):
        return nn_predict(nn_params, relaxed_samples)

    def surrogate_cond(params):
        cond_noise = conditional_noise(params, samples, noise_v)  # z tilde
        return concrete(params, log_temperature, cond_noise, surrogate)

    grad_surrogate = elementwise_grad(concrete)(params, log_temperature, noise_u, surrogate)
    surrogate_cond, grad_surrogate_cond = value_and_grad(surrogate_cond)(params)
    return reinforce(params, noise_u, func_vals - surrogate_cond) + \
           grad_surrogate - grad_surrogate_cond

def relax_all(params, est_params, noise_u, noise_v, f):
    # Returns objective, gradients, and gradients of variance of gradients.
    func_vals = f(bernoulli_sample(params, noise_u))
    var_vjp, grads = make_vjp(relax, argnum=1)(params, est_params, noise_u, noise_v, func_vals)
    d_var_d_est = var_vjp(2 * grads / grads.shape[0])
    return func_vals, grads, d_var_d_est
```

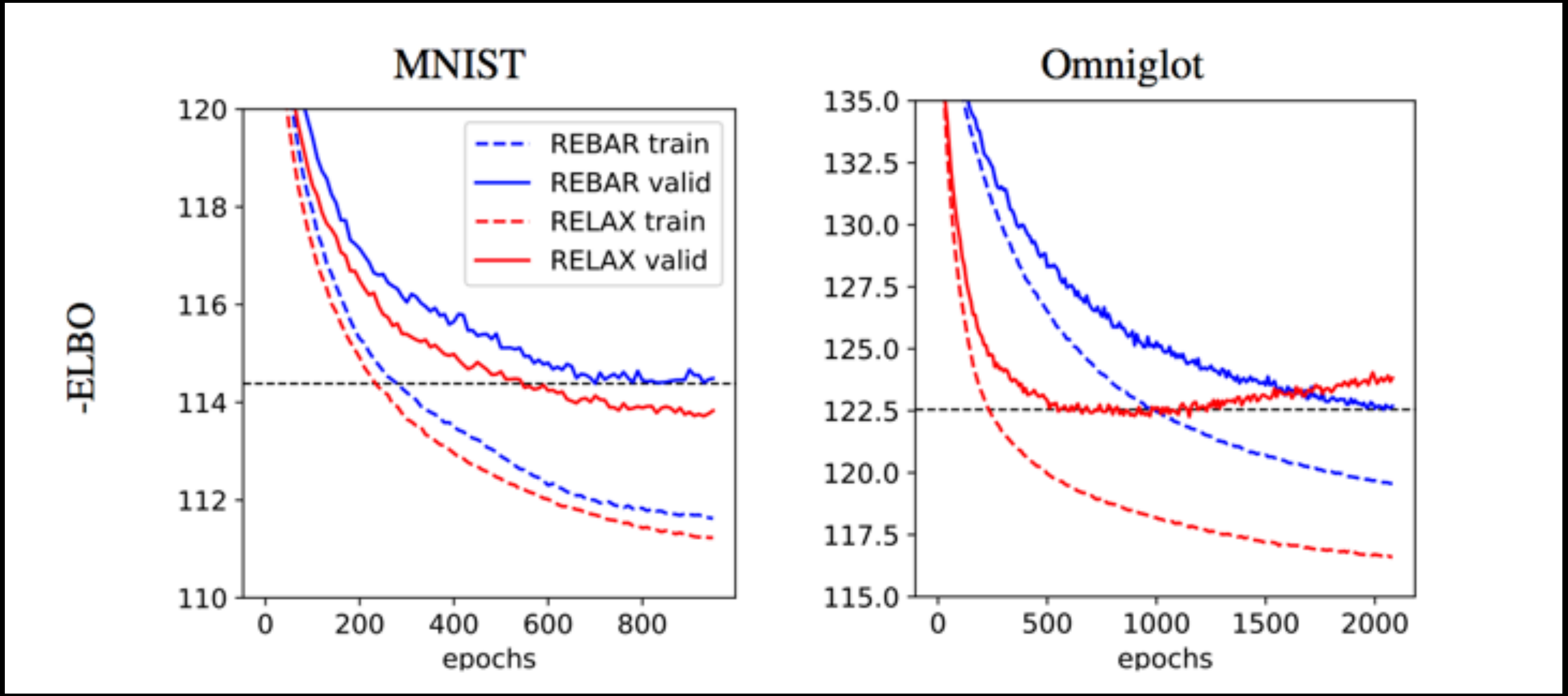
Discrete VAEs

$$\boxed{\log p(x) \geq \mathcal{L}(\theta) = \mathbb{E}_{q(b|x)}[\log p(x|b) + \log p(b) - \log q(b|x)]}$$

- Latent state is 200 Bernoulli variables
- Can't use reparameterization trick
- Can still use our knowledge of structure of model, combining REBAR and RELAX:

$$\boxed{c_\phi(z) = f(\sigma_\lambda(z)) + r_\rho(z)}$$

Bernoulli VAE Results



Dataset	Model	Concrete	NVIL	MuProp	REBAR	RELAX
MNIST	Nonlinear	-102.2	-101.5	-101.1	-81.01	**-78.13**
	linear one-layer	-111.3	-112.5	-111.7	-111.6	**-111.20**
	linear two-layer	-99.62	-99.6	-99.07	-98.22	**-98.00**
Omniglot	Nonlinear	-110.4	-109.58	-108.72	-56.76	**-56.12**
	linear one-layer	-117.23	-117.44	-117.09	-116.63	**-116.57**
	linear two-layer	-109.95	-109.98	-109.55	-108.71	**-108.54**

Table 1: Highest training ELBO for discrete variational autoencoders.

Rederiving Actor-Critic

$$\hat{g}_{\mathrm{AC}} = \sum_{t=1}^{T} \frac{\partial \log \pi(a_t|s_t,\theta)}{\partial\theta} \left[\sum_{t'=t}^{T} r_{t'} - c_\phi(s_t) \right]$$

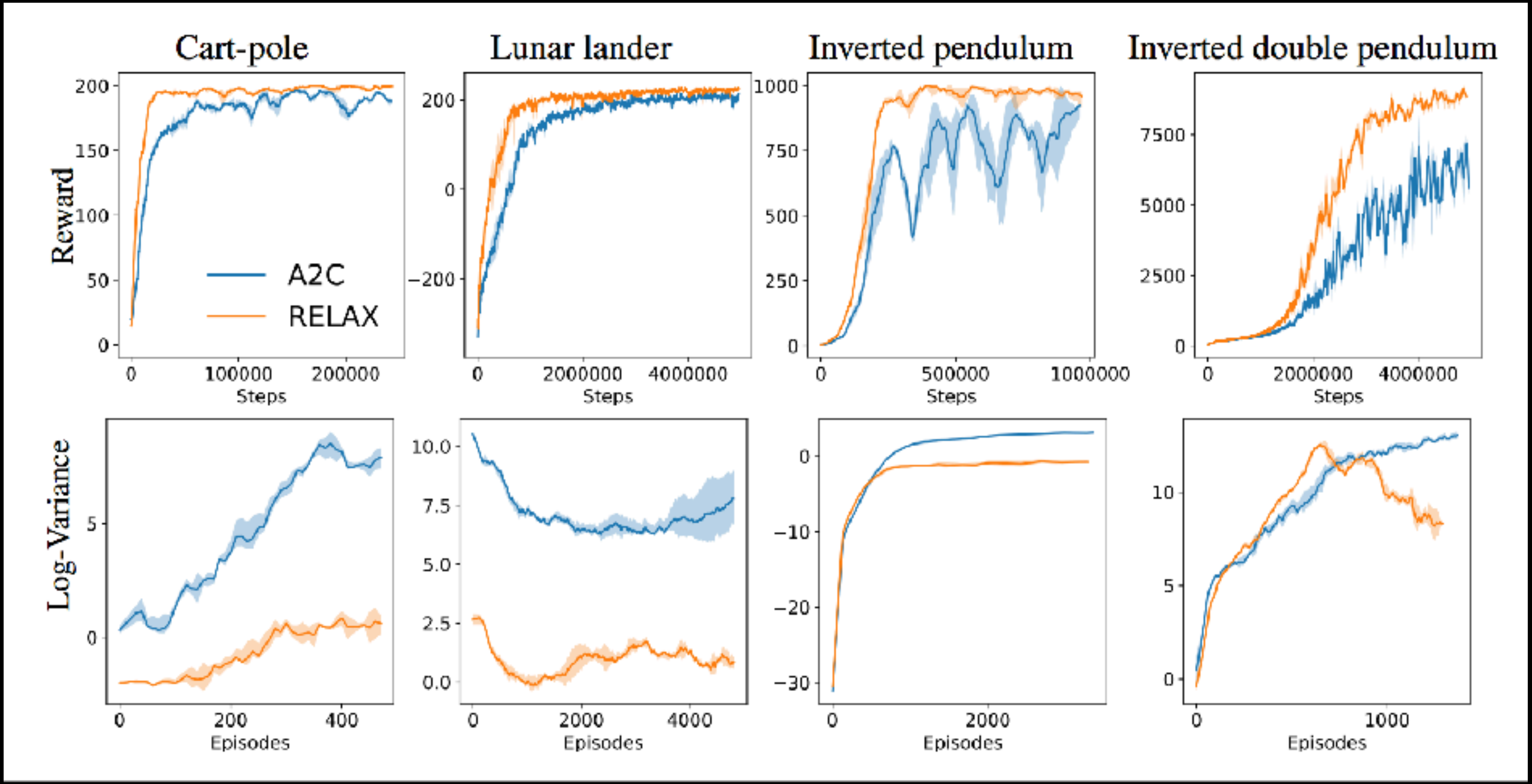
- c_ϕ is an estimate of the value function
- This is exactly the REINFORCE estimator using an estimate of the value function as a control variate
- Why not use action in control variate?
- Dependence on action would add bias

LAX for RL

$$\boxed{\hat{g}_{\mathrm{LAX}} = \sum_{t=1}^{T} \frac{\partial \log \pi(a_t|s_t,\theta)}{\partial \theta} \left[\sum_{t'=t}^{T} r_{t'} - c_\phi(s_t,a_t) \right] + \frac{\partial}{\partial \theta} c_\phi(s_t,a_t)}$$

- Action-dependence in control variate
- unbiased for policy, and unbiased for baseline
- Standard baseline optimization methods minimize squared error from reward or value function. We directly minimize variance.

Model-Free RL "Results"



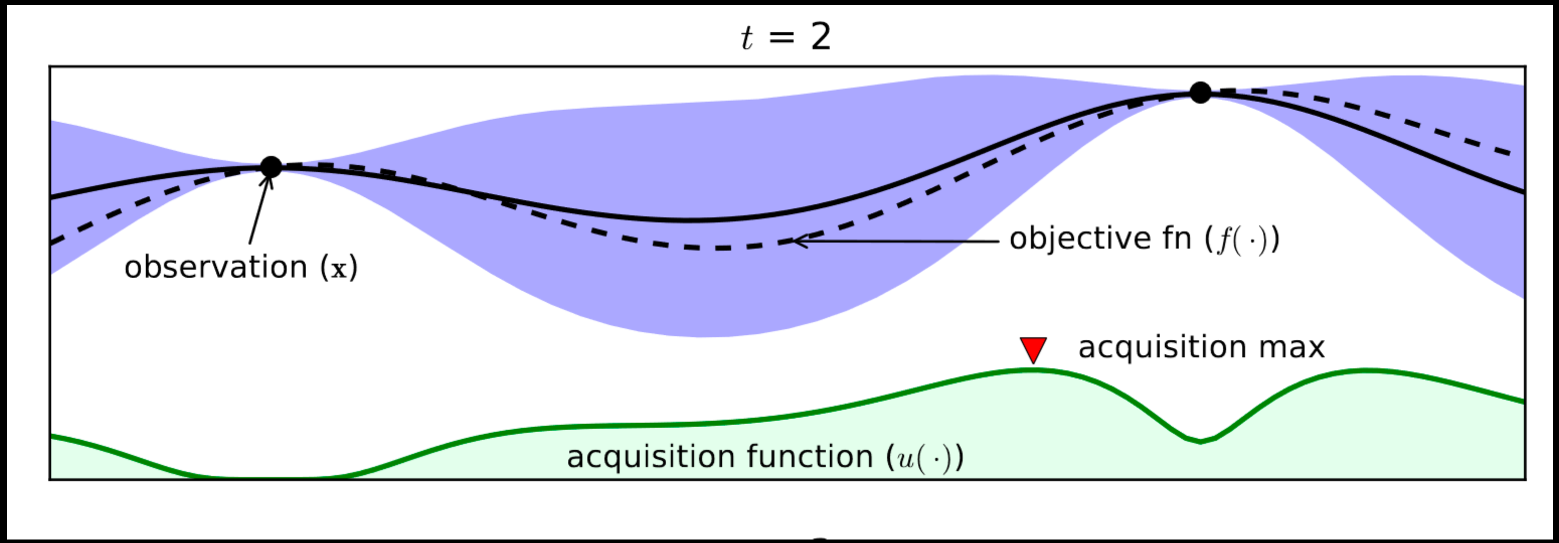
- Faster convergence, but real story is unbiased critic updates.

- Excellent criticism of experimental setup in "The Mirage of Action-Dependent Baselines in Reinforcement Learning" (Tucker et al. 2018). Better experiments would examine high-dimensional action regime.

RELAX Properties

- Pros:
  - unbiased
  - low variance (after tuning)
  - usable when $f(b)$ is unknown, or not differentiable
  - useable when $p(b|\theta)$ is discrete
- Cons:
  - need to define surrogate
  - when progress is made, need to wait for surrogate to adapt
  - Higher-order derivatives still awkward in TF and PyTorch

Local surrogates are a nice compromise



Shahriari et al., 2016

- Global surrogate models not good enough in high dim.
- Local surrogates are less demanding to construct
- Local minima less of a problem in high dim.
- Want low variance? Take gradient of variance

Aside: Evolution Strategies optimize a linear surrogate

$$\hat{w} = (X^{\top}X)^{-1}X^{\top}y$$

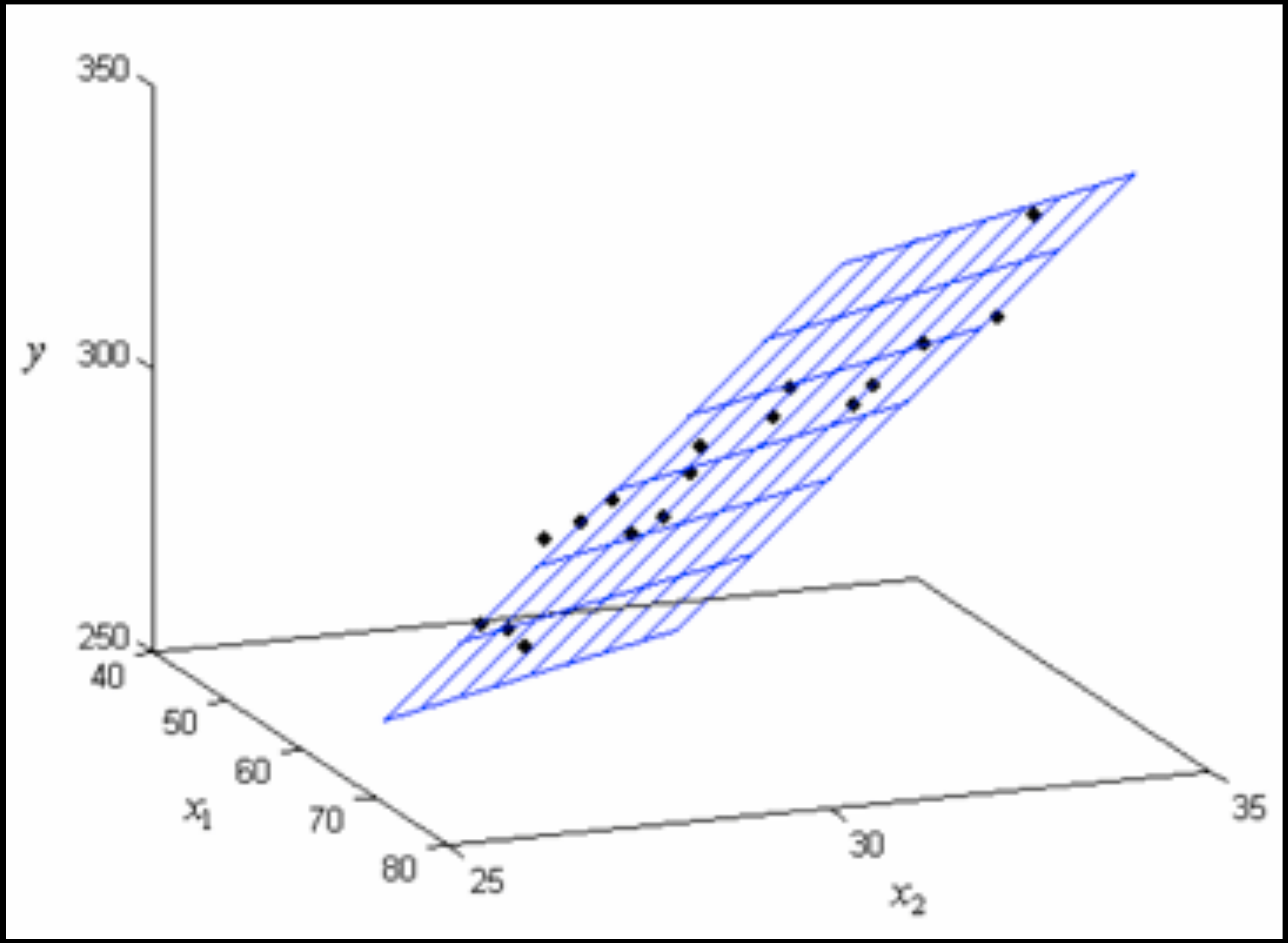
$$\approxeq \mathbb{E}\left[(X^{\top}X)\right]^{-1}X^{\top}y$$

$$= \left[I\sigma^2\right]^{-1}X^{\top}y$$

$$= \left[I\sigma^2\right]^{-1}(\epsilon\sigma)^{\top}y$$

$$= \sum_i \frac{\epsilon_i y_i}{\sigma}$$

$$= \sum_i \frac{\epsilon_i f(\epsilon_i\sigma)}{\sigma}$$

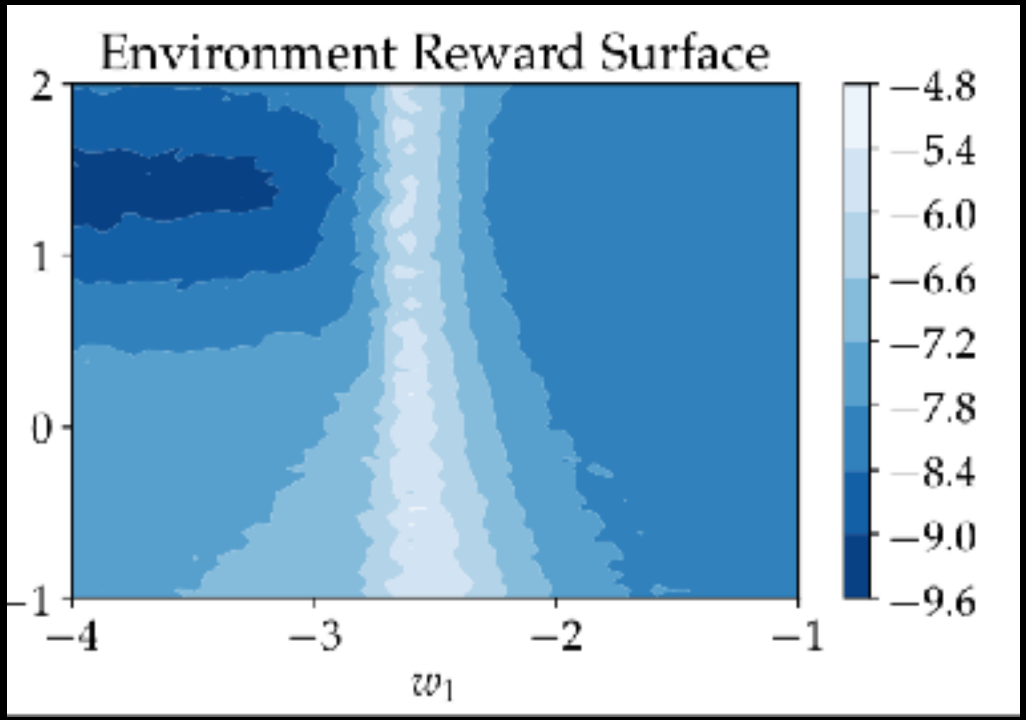


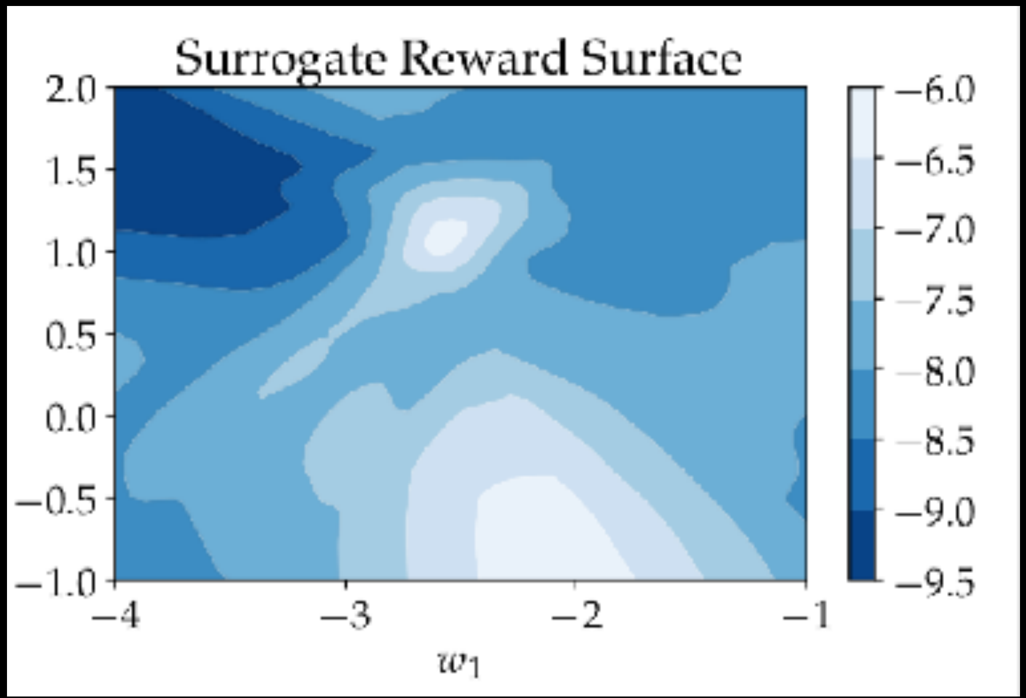
$$\epsilon \sim \mathcal{N}(0, I)$$

$$x = \epsilon\sigma$$

Aside: Evolution Strategies optimize a linear surrogate

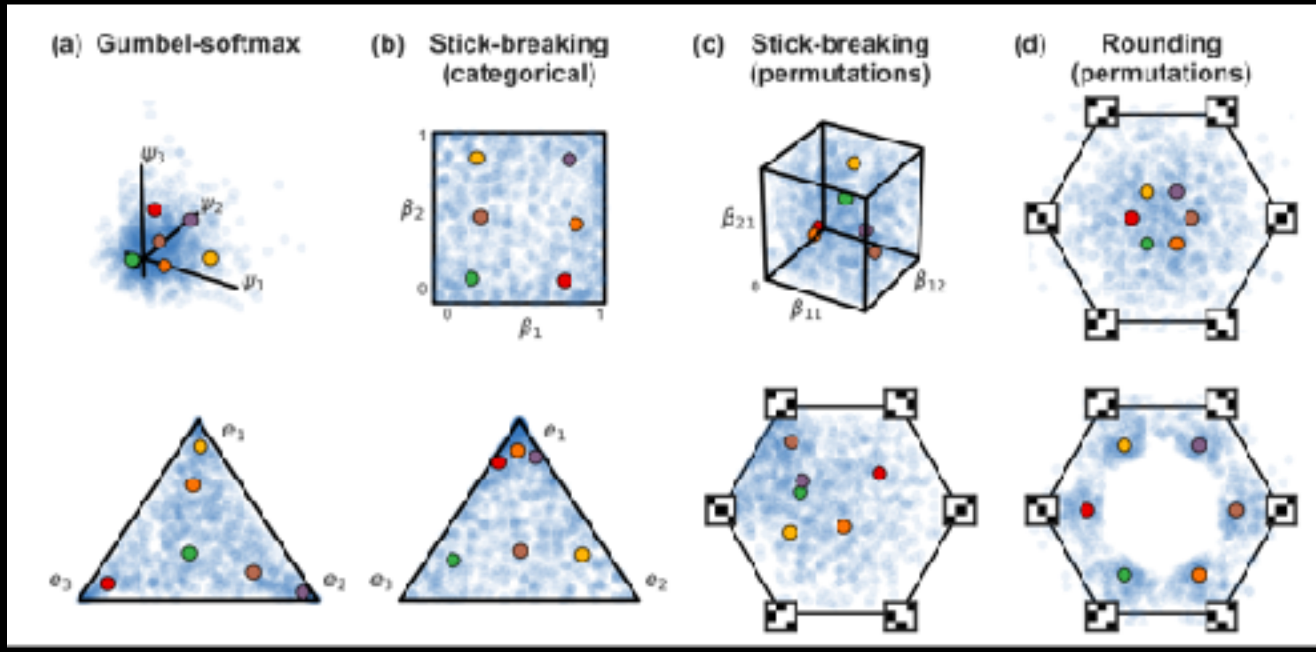
- Throws away all observations each step
- Use a neural net surrogate, and experience replay
- Distributed ES algorithm works for any gradient-free optimization algorithm
- w/ students Geoff Roeder, Yuhuai (Tony) Wu, Jaiming Song



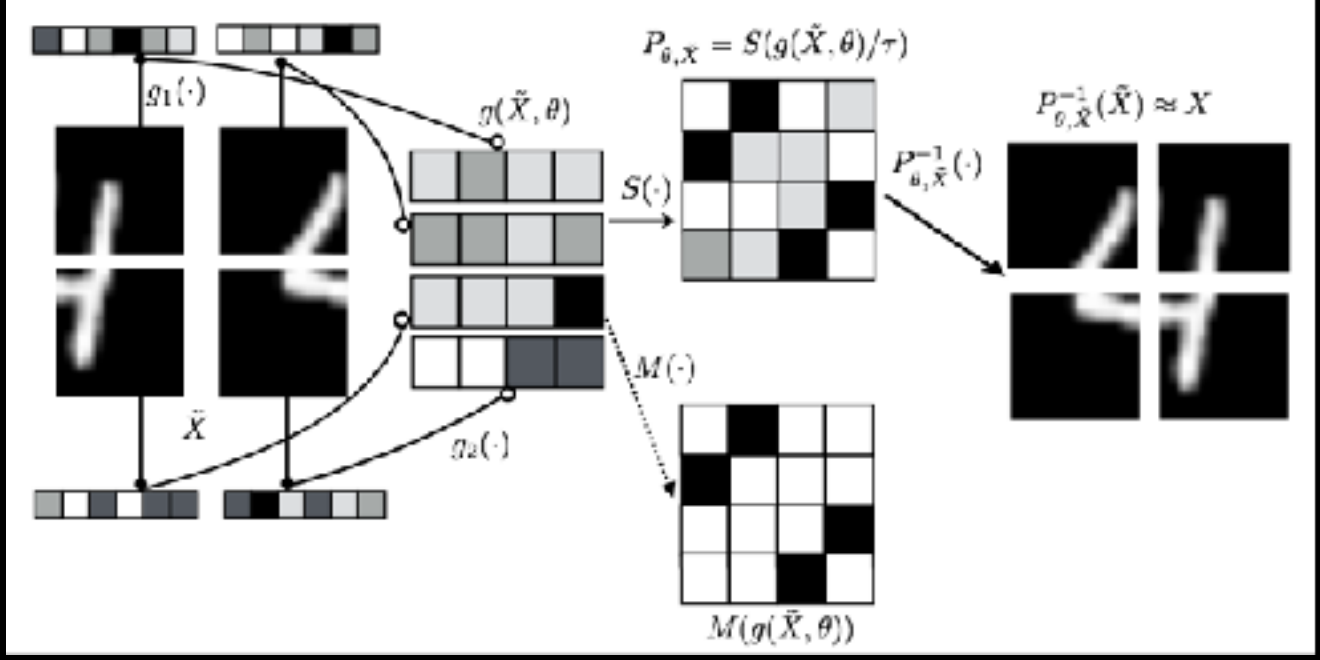


Future Work

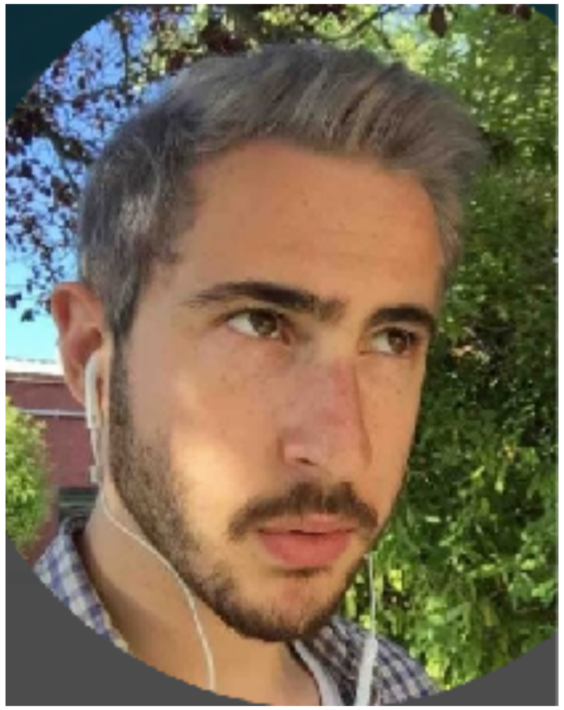
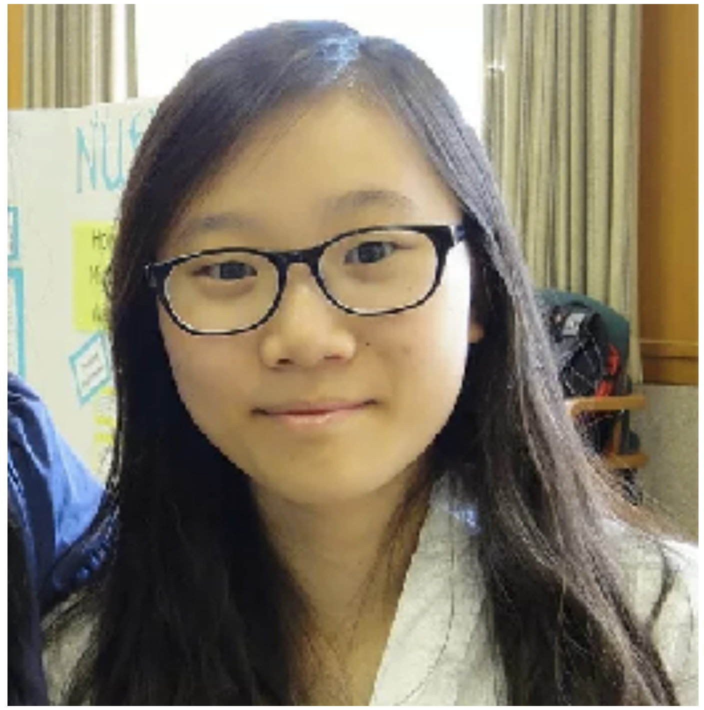
- What does the optimal surrogate look like? Use calculus of variations.
- Train the surrogate off-policy: $c_\phi(a, s, \pi)$
- REBAR, RELAX for more complicated discrete objects, e.g. trees
- Mostly open problem: Control variates for sequential discrete choices.



Linderman et al., 2017



Mena et al., 2018

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Geoffrey Roeder, Jesse Bettencourt,
David Duvenaud

Thanks!

https://github.com/duvenaud/relax

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Speed Comparison