Lecture 2: Gradient Estimators

CSC 2547 Spring 2018
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Based mainly on slides by Will Grathwohl, Dami Choi, Yuhuai Wu and Geoff Roeder

Where do we see this guy?

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

- Just about everywhere!
- Variational Inference
- Reinforcement Learning
- Hard Attention
- And so many more!

Gradient based optimization

- Gradient based optimization is the standard method used today to optimize expectations

- Necessary if models are neural-net based

- Very rarely can this gradient be computed analytically

Otherwise, we estimate…

- A number of approaches exist to estimate this gradient
- They make varying levels of assumptions about the distribution and function being optimized
- Most popular methods either make strong assumptions or suffer from high variance

REINFORCE (Williams, 1992)

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

- Unbiased
- Has few requirements
- Easy to compute

- Suffers from high variance

Reparameterization (Kingma & Welling, 2014)

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

- Lower variance empirically
- Unbiased

- Makes stronger assumptions
- Requires $f(b)$ is known and differentiable
- Requires $p(b|\theta)$ is reparameterizable

Concrete (Maddison et al., 2016)

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

- Works well in practice
- Low variance from reparameterization

- Biased
- Adds temperature hyper-parameter
- Requires that $f(b)$ is known, and differentiable
- Requires $p(z|\theta)$ is reparameterizable
- Requires $f(b)$ behaves predictably outside of domain

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 $\mathrm{corr}(g, c) > 0$

- Does not change bias

Putting it all together

- We would like a general gradient estimator that is
    - unbiased
    - low variance
    - usable when $f(b)$ is unknown
    - useable when $p(b|\theta)$ is discrete

Backpropagation Through

Backpropagation Through

Backpropagation Through

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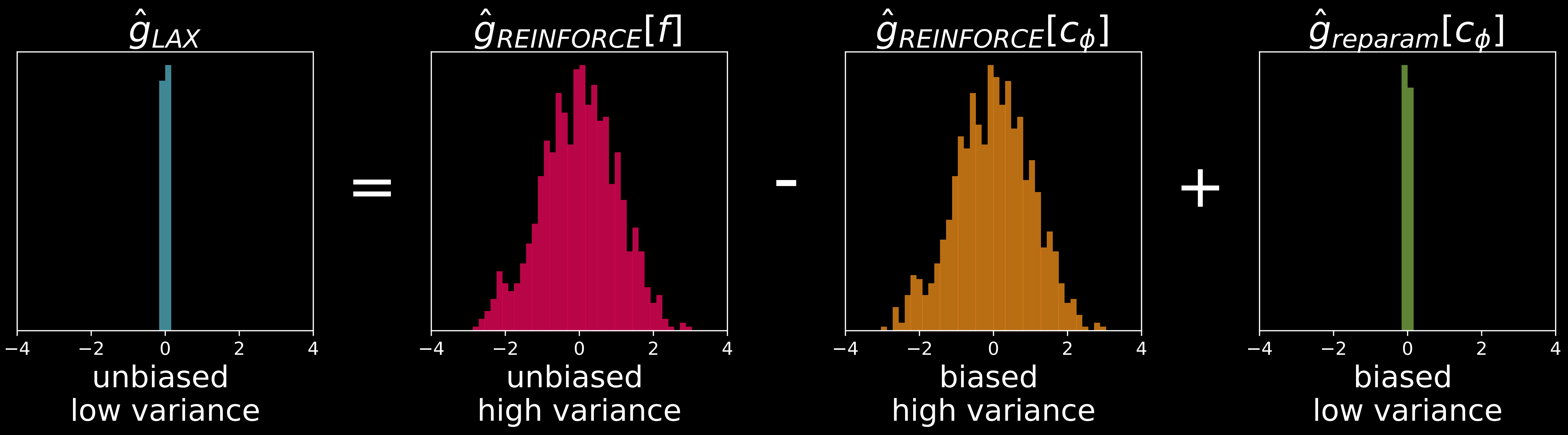
Our Approach

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



Our Approach

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

- Start with the reinforce estimator for $f(b)$
- We introduce a new function $c_\phi(b)$
- We subtract the reinforce estimator of its gradient and add the reparameterization estimator
- Can be thought of as using the reinforce estimator of $c_\phi(b)$ as a control variate

Optimizing the Control Variate

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

- For any unbiased estimator we can get Monte Carlo estimates for the gradient of the variance of $\hat{g}$
- Use to optimize c_ϕ

What about discrete b?

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

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

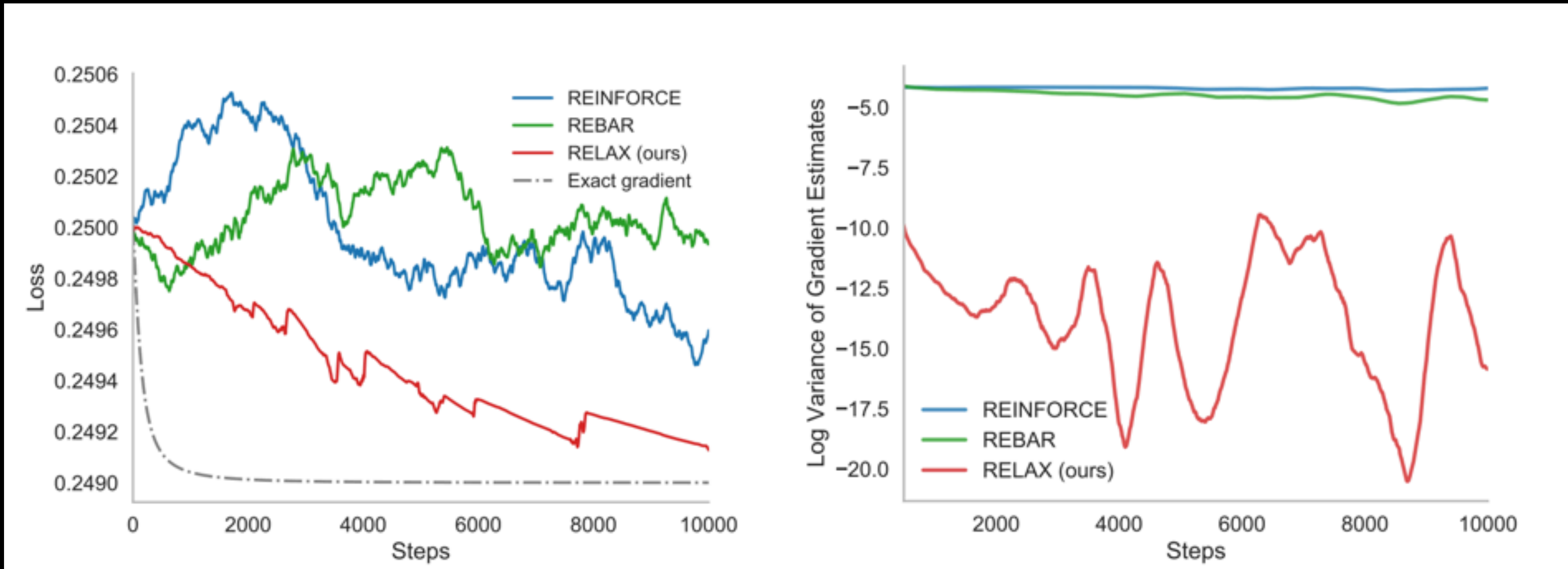
$$b = H(z), z \sim p(z|\theta), \tilde{z} \sim p(z|b, \theta)$$

- When b is discrete, we introduce a relaxed distribution $p(z|\theta)$ and a function H where $H(z) = b \sim p(b|\theta)$
- We use the conditioning scheme introduced in REBAR (Tucker et al. 2017)
- Unbiased for all c_ϕ

A Simple Example

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

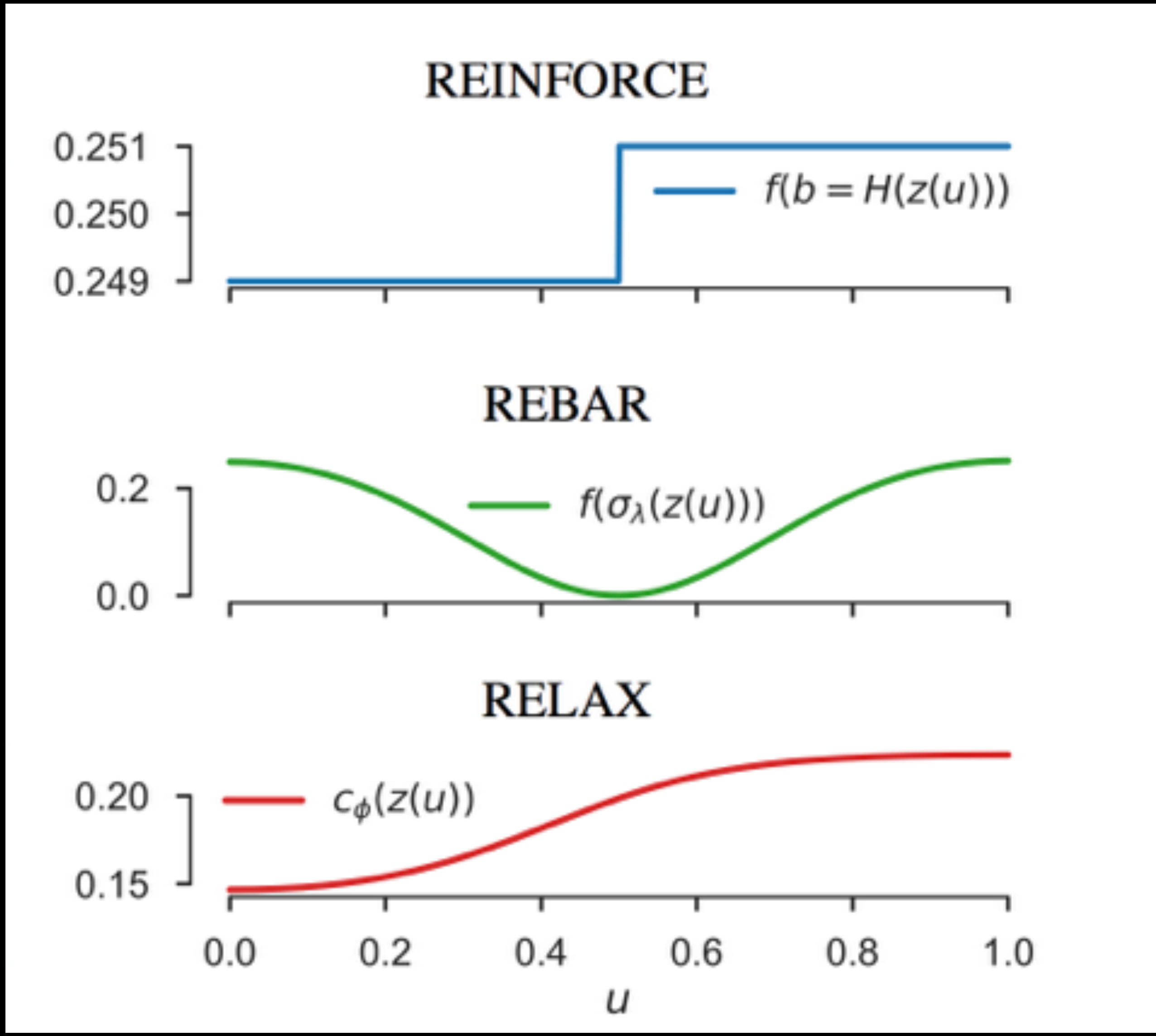
- Used to validate REBAR (used t = .45)
- We use t = .499
- REBAR, REINFORCE fail due to noise outweighing signal
- Can RELAX improve?



- RELAX outperforms baselines
- Considerably reduced variance!
- RELAX learns reasonable surrogate

Analyzing the Surrogate

- REBAR's fixed surrogate cannot produce consistent and correct gradients
- RELAX learns to balance REINFORCE variance and reparameterization variance



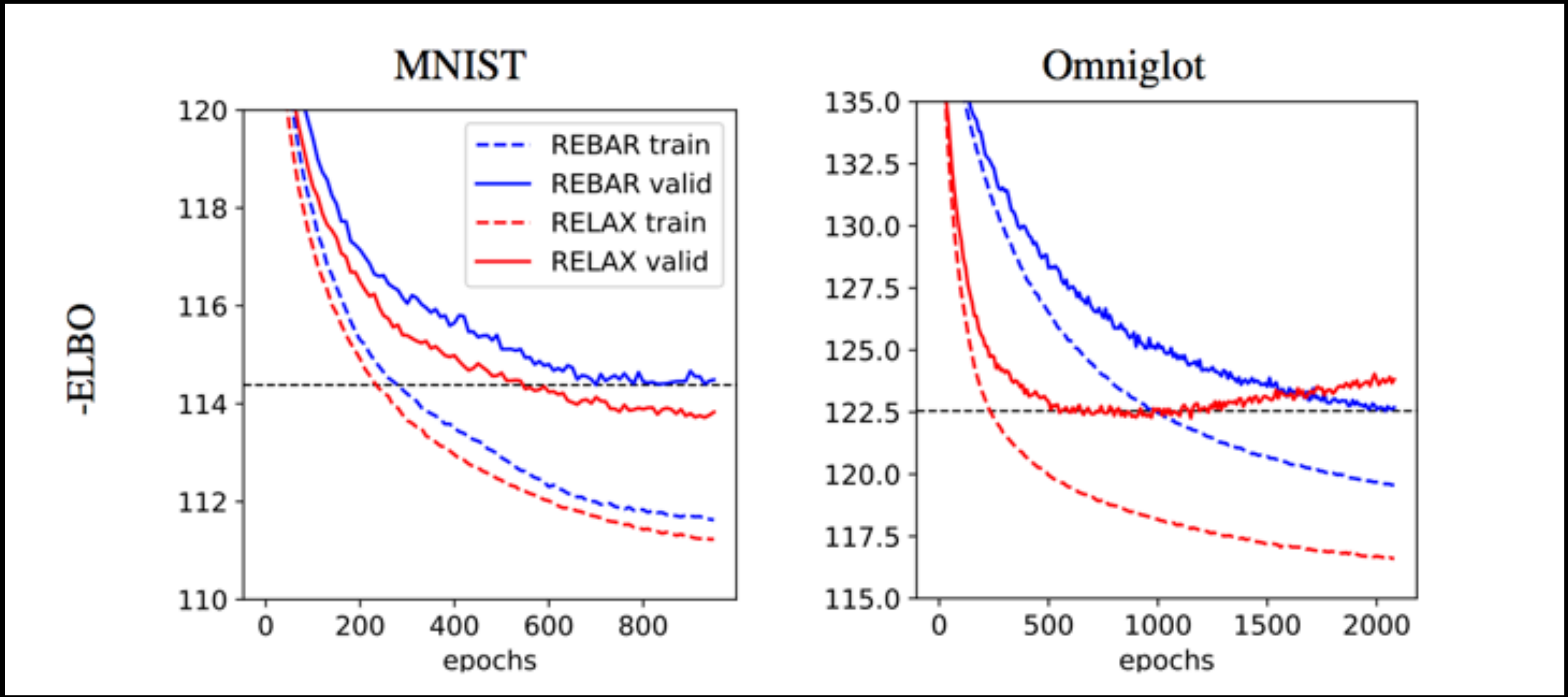
A More Interesting Application

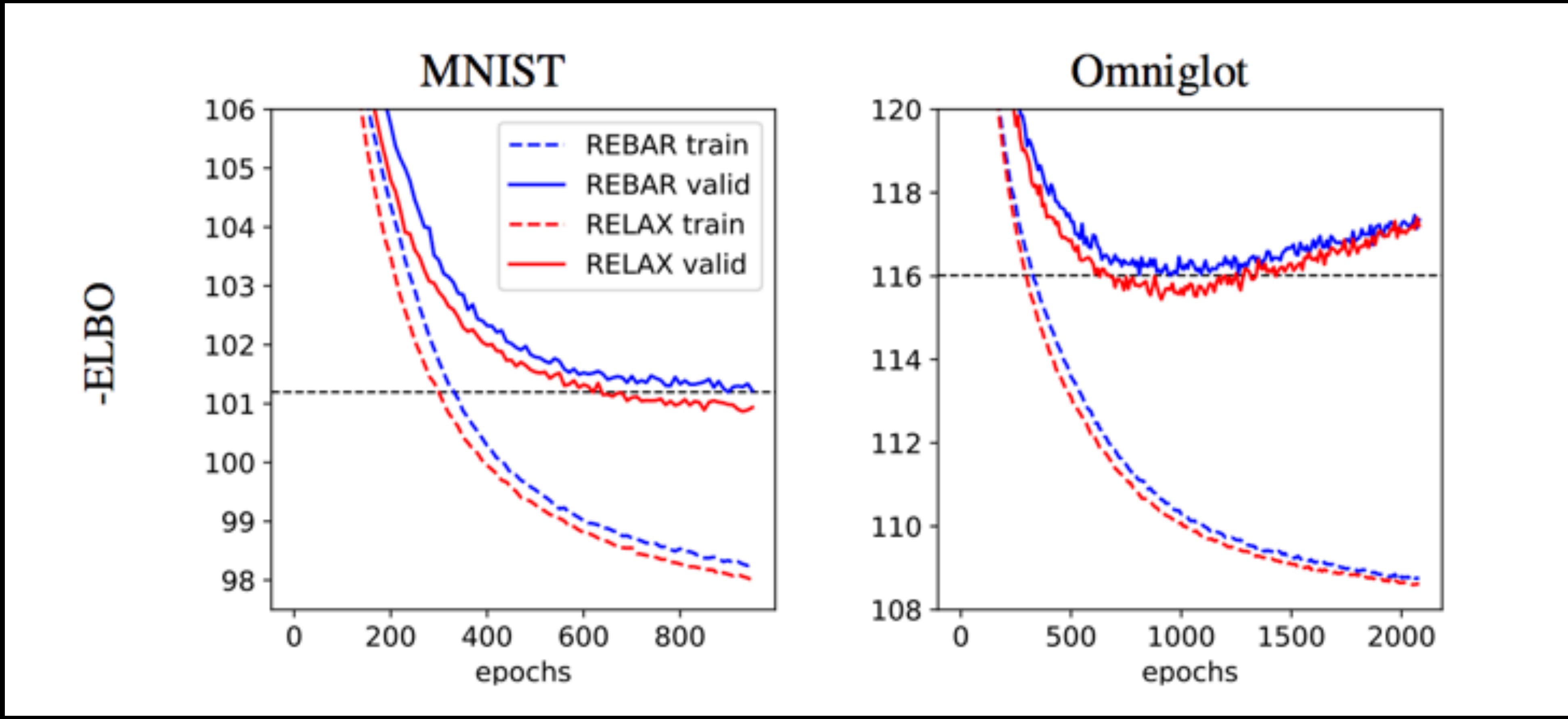
$$\log p(x) \geq \mathcal{L}(\theta) = \mathbb{E}_{q(b|x)}[\log p(x|b) + \log p(b) - \log q(b|x)]$$

- Discrete VAE
- Latent state is 200 Bernoulli variables
- Discrete sampling makes reparameterization estimator unusable

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

Results


MNIST
Omniglot
-ELBO
REBAR train
REBAR valid
RELAX train
RELAX valid
epochs
epochs


MNIST
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epochs
epochs

Reinforcement Learning

- Policy gradient methods are very popular today (A2C, A3C, ACKTR)
- Seeks to find $\mathrm{argmax}_\theta E_{\tau\sim\pi(\tau|\theta)}[R(\tau)]$
- Does this by estimating $\frac{\partial}{\partial\theta}E_{\tau\sim\pi(\tau|\theta)}[R(\tau)]$
- R is not known so many popular estimators cannot be used

Actor Critic

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

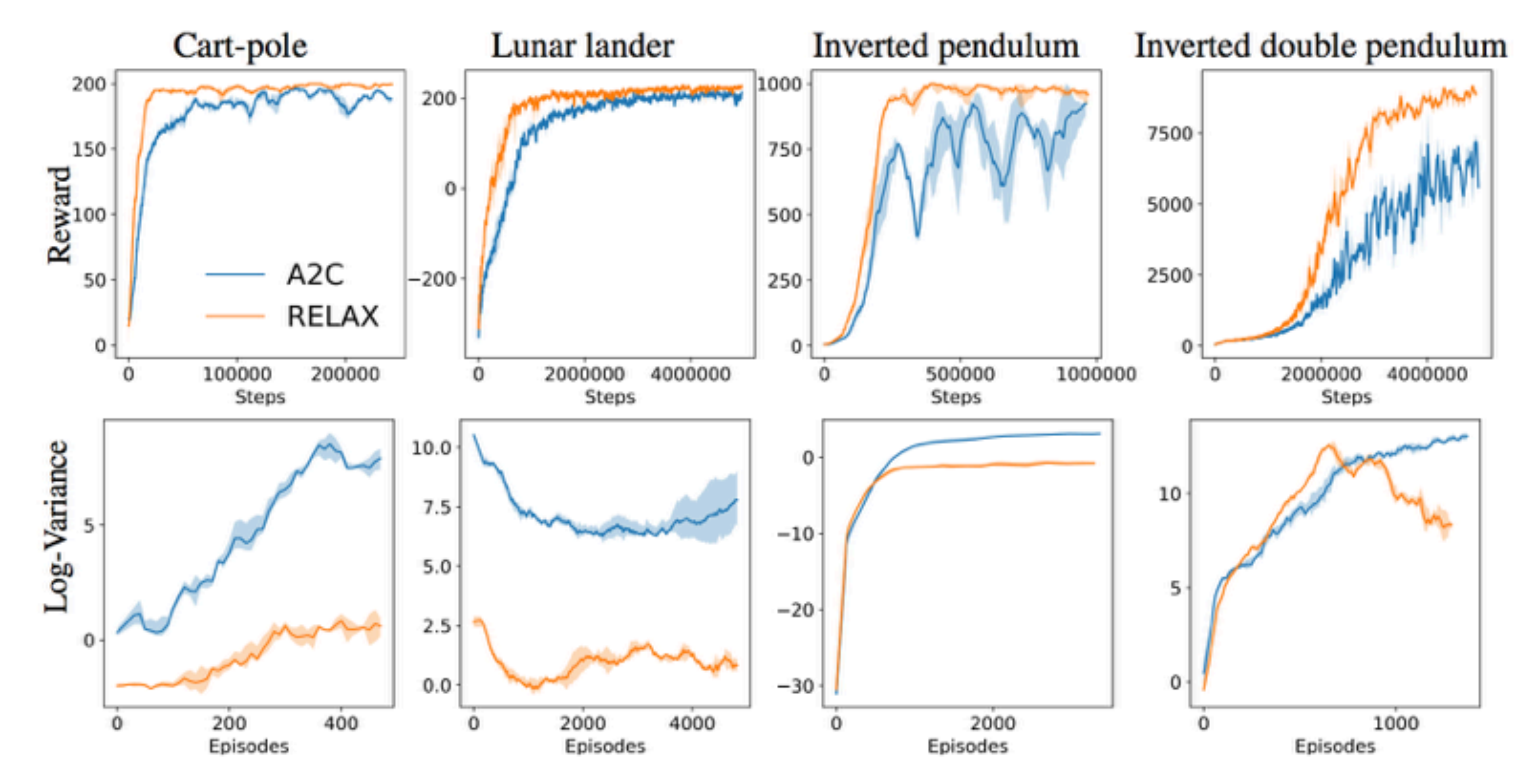
- c_ϕ is an estimate of the value function
- This is exactly the REINFORCE estimator using an estimate of the value function as a control variate
- Why not use action in control variate?
- Dependence on action would add bias

LAX for RL

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

- Allows for action dependence in control variate
- Remains unbiased
- Similar extension available for discrete action spaces

Results



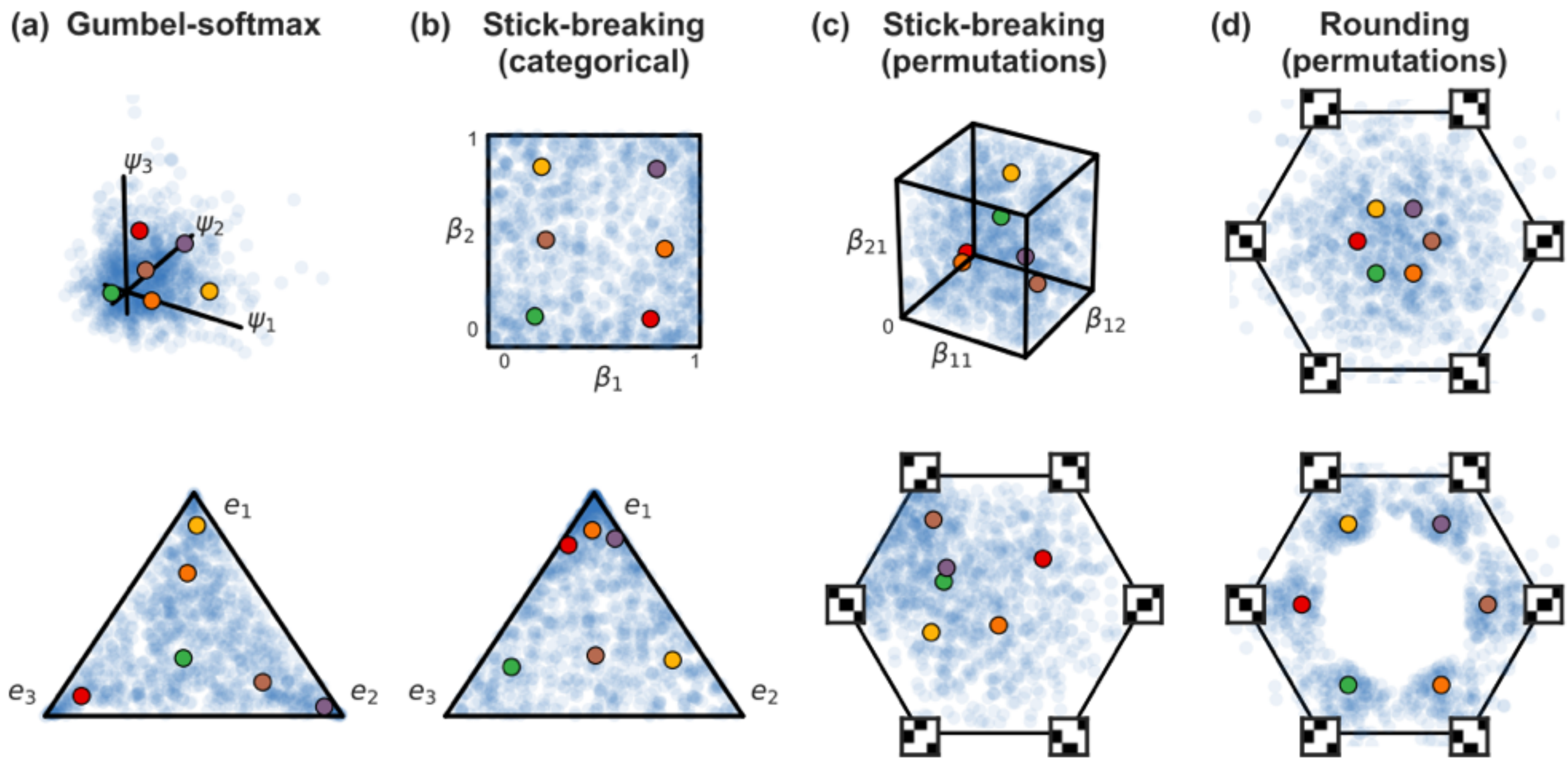
- Improved performance
- Lower variance gradient estimates

Future Work

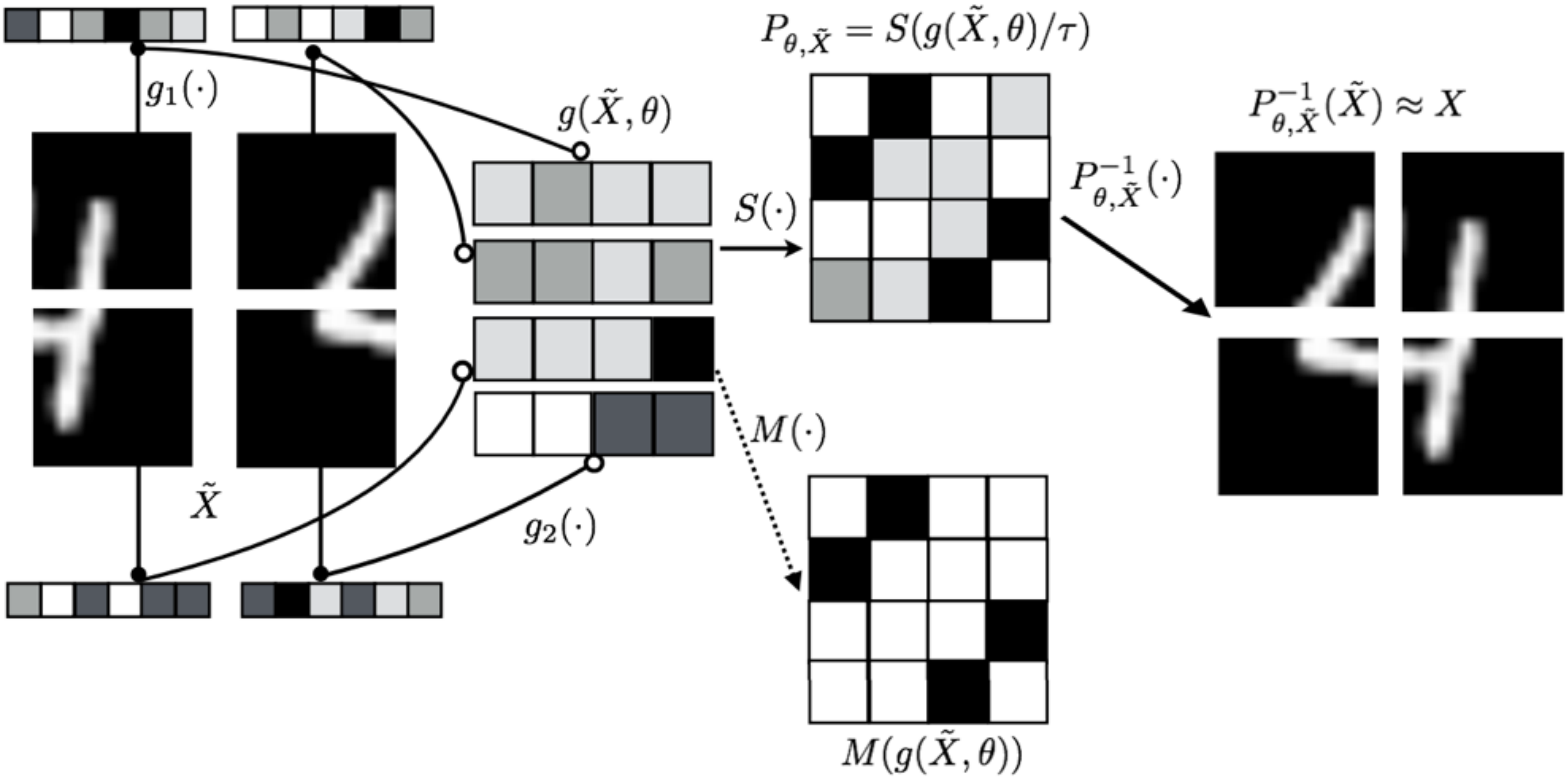
- What does the optimal surrogate look like?
- Many possible variations of LAX and RELAX
- Which provides the best tradeoff between variance, ease of implementation, scope of application, performance
- RL
    - Incorporate other variance reduction techniques (GAE, reward bootstrapping, trust-region)
    - Ways to train the surrogate off-policy
- Applications
    - Inference of graph structure (coming soon)
    - Inference of discrete neural network architecture components (coming soon)

Directions

- Surrogate can take any form
  - can rely on global information even if forward pass only uses local info
  - Can depend on order even if forward pass is invariant
- Reparameterization can take many forms, ongoing work on reparameterizing through rejection sampling, or distributions on permutations



Reparameterizing the Birkhoff Polytope for Variational Permutation Inference



Learning Latent Permutations with Gumbel-Sinkhorn Networks

Why are we optimizing policies anyways?

- Next week: Variational optimization