Discrete Latent Variables

Art Sobolev

Research Scientist at Samsung AI Center
@art_sobolev | artem.sobolev.name

Deep|Bayes

1. Why Discreteness?
2. The Problem
3. Relaxations
4. Variance Reduction
5. Conclusion

Why Discreteness?

Motivation

- Easier to interpret discrete categories than continuous spectrum
  - **Example**: Discrete Variational Autoencoder
    - Assume observations can be described by some binary (or categorical) code
    - We want to learn both encoder and decoder for such code and observations
- Allow the model to make a discrete choice
  - **Example**: Hard Attention
    - An attention module generates binary mask of where to look at
    - The network classifies masked images
    - We want attention module to attend only important areas of the image
- Sometimes you need discrete predictions to have certain properties
  - **Example**: GANs for text
    - Generator outputs discrete text
    - Discriminator takes discrete text as input and classifies how real it is
    - We want the generator to output text that fools the discriminator

Motivation

Deep|Bayes

- Easier to interpret discrete categories than continuous spectrum
  - **Example:** Discrete Variational Autoencoder
    - Assume observations can be described by some binary (or categorical) code
    - We want to learn both encoder and decoder for such code and observations
- Allow the model to make a discrete choice
  - **Example:** Hard Attention
    - An attention module generates binary mask of where to look at
    - The network classifies masked images
    - We want attention module to attend only important areas of the image
- Sometimes you need discrete predictions to have certain properties
  - **Example:** GANs for text
    - Generator outputs discrete text
    - Discriminator takes discrete text as input and classifies how real it is
    - We want the generator to output text that fools the discriminator

- Easier to interpret discrete categories than continuous spectrum
  - **Example**: Discrete Variational Autoencoder
    - Assume observations can be described by some binary (or categorical) code
    - We want to learn both encoder and decoder for such code and observations
- Allow the model to make a discrete choice
  - **Example**: Hard Attention
    - An attention module generates binary mask of where to look at
    - The network classifies masked images
    - We want attention module to attend only important areas of the image
- Sometimes you need discrete predictions to have certain properties
  - **Example**: GANs for text
    - Generator outputs discrete text
    - Discriminator takes discrete text as input and classifies how real it is
    - We want the generator to output text that fools the discriminator

Motivation

Deep|Bayes

- Easier to interpret discrete categories than continuous spectrum
  - **Example**: Discrete Variational Autoencoder
    - Assume observations can be described by some binary (or categorical) code
    - We want to learn both encoder and decoder for such code and observations
- Allow the model to make a discrete choice
  - **Example**: Hard Attention
    - An attention module generates binary mask of where to look at
    - The network classifies masked images
    - We want attention module to attend only important areas of the image
- Sometimes you need discrete predictions to have certain properties
  - **Example**: GANs for text
    - Generator outputs discrete text
    - Discriminator takes discrete text as input and classifies how real it is
    - We want the generator to output text that fools the discriminator

- Easier to interpret discrete categories than continuous spectrum
  - **Example**: Discrete Variational Autoencoder
    - Assume observations can be described by some binary (or categorical) code
    - We want to learn both encoder and decoder for such code and observations
- Allow the model to make a discrete choice
  - **Example**: Hard Attention
    - An attention module generates binary mask of where to look at
    - The network classifies masked images
    - We want attention module to attend only important areas of the image
- Sometimes you need discrete predictions to have certain properties
  - **Example**: GANs for text
    - Generator outputs discrete text
    - Discriminator takes discrete text as input and classifies how real it is
    - We want the generator to output text that fools the discriminator

- Easier to interpret discrete categories than continuous spectrum
  - **Example**: Discrete Variational Autoencoder
    - Assume observations can be described by some binary (or categorical) code
    - We want to learn both encoder and decoder for such code and observations
- Allow the model to make a discrete choice
  - **Example**: Hard Attention
    - An attention module generates binary mask of where to look at
    - The network classifies masked images
    - We want attention module to attend only important areas of the image
- Sometimes you need discrete predictions to have certain properties
  - **Example**: GANs for text
    - Generator outputs discrete text
    - Discriminator takes discrete text as input and classifies how real it is
    - We want the generator to output text that fools the discriminator

Motivation

- Easier to interpret discrete categories than continuous spectrum
  - **Example**: Discrete Variational Autoencoder
    - Assume observations can be described by some binary (or categorical) code
    - We want to learn both encoder and decoder for such code and observations
- Allow the model to make a discrete choice
  - **Example**: Hard Attention
    - An attention module generates binary mask of where to look at
    - The network classifies masked images
    - We want attention module to attend only important areas of the image
- Sometimes you need discrete predictions to have certain properties
  - **Example**: GANs for text
    - Generator outputs discrete text
    - Discriminator takes discrete text as input and classifies how real it is
    - We want the generator to output text that fools the discriminator

The Problem

Typically problems boil down to optimizing an objective of the following form

$$\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \to \max_\phi$$

- We consider models where the objective is differentiable w.r.t. ϕ
  - Hence the gradient $\frac{\partial}{\partial \phi}\mathcal{L}(\phi)$ exists
- The expectation is expensive to compute due to large number of summands, turn to *Stochastic Optimization*
- Stochastic Optimization requires a stochastic (unbiased) estimate $g(\mathbf{z}, \phi)$ of the true gradient:

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} g(\mathbf{z}, \phi) = \frac{\partial}{\partial \phi}\mathcal{L}(\phi)$$

- No continuous reparametrization is possible for z
  - Because z takes finitely many different values

Optimizational Point of View

Typically problems boil down to optimizing an objective of the following form

$$\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \to \max_\phi$$

- We consider models where the objective is differentiable w.r.t. ϕ
  - Hence the gradient $\frac{\partial}{\partial \phi}\mathcal{L}(\phi)$ exists
- The expectation is expensive to compute due to large number of summands, turn to *Stochastic Optimization*
- Stochastic Optimization requires a stochastic (unbiased) estimate $g(\mathbf{z}, \phi)$ of the true gradient:

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} g(\mathbf{z}, \phi) = \frac{\partial}{\partial \phi}\mathcal{L}(\phi)$$

- No continuous reparametrization is possible for z
  - Because z takes finitely many different values

Typically problems boil down to optimizing an objective of the following form

$$\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \to \max_\phi$$

- We consider models where the objective is differentiable w.r.t. ϕ
  - Hence the gradient $\frac{\partial}{\partial \phi}\mathcal{L}(\phi)$ exists
- The expectation is expensive to compute due to large number of summands, turn to *Stochastic Optimization*
- Stochastic Optimization requires a stochastic (unbiased) estimate $g(\mathbf{z}, \phi)$ of the true gradient:

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} g(\mathbf{z}, \phi) = \frac{\partial}{\partial \phi}\mathcal{L}(\phi)$$

- No continuous reparametrization is possible for z
  - Because z takes finitely many different values

Optimizational Point of View

Typically problems boil down to optimizing an objective of the following form

$$\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \to \max_\phi$$

- We consider models where the objective is differentiable w.r.t. ϕ
  - Hence the gradient $\frac{\partial}{\partial \phi}\mathcal{L}(\phi)$ exists
- The expectation is expensive to compute due to large number of summands, turn to *Stochastic Optimization*
- Stochastic Optimization requires a stochastic (unbiased) estimate $g(\mathbf{z}, \phi)$ of the true gradient:

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} g(\mathbf{z}, \phi) = \frac{\partial}{\partial \phi}\mathcal{L}(\phi)$$

- No continuous reparametrization is possible for z
  - Because z takes finitely many different values

Typically problems boil down to optimizing an objective of the following form

$$\mathcal{L}(\phi) = \mathbb{E}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \to \max_\phi$$

- We consider models where the objective is differentiable w.r.t. ϕ
  - Hence the gradient $\frac{\partial}{\partial \phi}\mathcal{L}(\phi)$ exists
- The expectation is expensive to compute due to large number of summands, turn to *Stochastic Optimization*
- Stochastic Optimization requires a stochastic (unbiased) estimate $g(\mathbf{z}, \phi)$ of the true gradient:

$$\mathbb{E}_{q_\phi(\mathbf{z})} g(\mathbf{z}, \phi) = \frac{\partial}{\partial \phi}\mathcal{L}(\phi)$$

- No continuous reparametrization is possible for z
  - Because z takes finitely many different values

$$\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

$$\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

$$\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

$$\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

REINFORCE Estimator

$$\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

$$\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

$$\frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathbb{E}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

REINFORCE Estimator

$$\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) = \frac{\partial}{\partial \phi} \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z}) = \sum_{\mathbf{z}} \frac{\partial}{\partial \phi} q_\phi(\mathbf{z}) f(\mathbf{z})$$

Now note that $q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} q_\phi(\mathbf{z})$ (log-derivative trick)

$$= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) = \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} \left[\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) f(\mathbf{z}) \right]$$

In practice this expectation is intractable, thus we resort to Monte Carlo estimation:

$$g(\mathbf{z}_{1:M}, \phi) := \frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

This g is called the **REINFORCE** (aka log-derivative trick or score-function) estimator.

$$\frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

- Works for our case, discreteness does not get in the way
  - f is not even required to be continuous
- Typically has large variance
- Requires sophisticated *Variance Reduction* methods
  - Just taking bigger M gives only a modest improvement

$$\text{Var}\left[\frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m)\right] = \frac{1}{M} \text{Var}\left[f(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})\right]$$

  - Hence the "typical error" would decrease in proportion to $1/\sqrt{M}$.
  - In practice a single sample ($M = 1$) is often used.

$$\frac{1}{M}\sum_{m=1}^{M} f(\mathbf{z}_m)\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

- Works for our case, discreteness does not get in the way
    - f is not even required to be continuous
- Typically has large variance
- Requires sophisticated *Variance Reduction* methods
    - Just taking bigger M gives only a modest improvement

$$\text{Var}\left[\frac{1}{M}\sum_{m=1}^{M} f(\mathbf{z}_m)\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z}_m)\right] = \frac{1}{M}\text{Var}\left[f(\mathbf{z})\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z})\right]$$

- Hence the "typical error" would decrease in proportion to $1/\sqrt{M}$.
- In practice a single sample ($M = 1$) is often used.

REINFORCE

$$\frac{1}{M}\sum_{m=1}^{M} f(\mathbf{z}_m)\frac{\partial}{\partial \phi}\log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

- Works for our case, discreteness does not get in the way
  - f is not even required to be continuous
- Typically has large variance
- Requires sophisticated *Variance Reduction* methods
  - Just taking bigger M gives only a modest improvement

$$\text{Var}\left[\frac{1}{M}\sum_{m=1}^{M} f(\mathbf{z}_m)\frac{\partial}{\partial \phi}\log q_\phi(\mathbf{z}_m)\right] = \frac{1}{M}\text{Var}\left[f(\mathbf{z})\frac{\partial}{\partial \phi}\log q_\phi(\mathbf{z})\right]$$

  - Hence the "typical error" would decrease in proportion to $1/\sqrt{M}$.
  - In practice a single sample ($M = 1$) is often used.

$$\frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m), \qquad \mathbf{z}_m \sim q_\phi(\mathbf{z})$$

- Works for our case, discreteness does not get in the way
  - f is not even required to be continuous
- Typically has large variance
- Requires sophisticated *Variance Reduction* methods
  - Just taking bigger M gives only a modest improvement

$$\text{Var}\left[\frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}_m) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m)\right] = \frac{1}{M} \text{Var}\left[f(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})\right]$$

  - Hence the "typical error" would decrease in proportion to $1/\sqrt{M}$.
  - In practice a single sample ($M = 1$) is often used.

Consider 1-sample estimate

$$g^{\text{REINFORCE}}(\mathbf{z}, \phi) = \underbrace{f(\mathbf{z})}_{\text{scalar}} \underbrace{\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})}_{\text{vector}}, \qquad \mathbf{z} \sim q_\phi(\mathbf{z})$$

- Gradient estimate points in the direction of increasing probability of a given sample $\mathbf{z}$
  - Increases probability of $\mathbf{z}$ if it happened to be good
- The target function f only enters as a scaling coefficient, and no gradient $\frac{\partial f}{\partial z}$ is used (unlike the reparametrization trick)
  - Has no idea where to move probability mass *systematically*
  - $f(z) + c$ will give a different estimator
- **Random search in disguise!** [Rec18]

A wild random search appears

Consider 1-sample estimate

$$g^{\text{REINFORCE}}(\mathbf{z}, \phi) = \underbrace{f(\mathbf{z})}_{\text{scalar}} \overbrace{\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})}^{\text{vector}}, \qquad \mathbf{z} \sim q_\phi(\mathbf{z})$$

- Gradient estimate points in the direction of increasing probability of a given sample $\mathbf{z}$
  - Increases probability of $\mathbf{z}$ if it happened to be good
- The target function f only enters as a scaling coefficient, and no gradient $\frac{\partial f}{\partial z}$ is used (unlike the reparametrization trick)
  - Has no idea where to move probability mass *systematically*
  - $f(z) + c$ will give a different estimator
- **Random search in disguise!** [Rec18]

Consider 1-sample estimate

$$g^{\text{REINFORCE}}(\mathbf{z}, \phi) = \underbrace{f(\mathbf{z})}_{\text{scalar}} \overbrace{\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})}^{\text{vector}}, \qquad \mathbf{z} \sim q_\phi(\mathbf{z})$$

- Gradient estimate points in the direction of increasing probability of a given sample $\mathbf{z}$
  - Increases probability of $\mathbf{z}$ if it happened to be good
- The target function f only enters as a scaling coefficient, and no gradient $\frac{\partial f}{\partial z}$ is used (unlike the reparametrization trick)
  - Has no idea where to move probability mass *systematically*
  - $f(z) + c$ will give a different estimator
- **Random search in disguise!** [Rec18]

A wild random search appears

Deep|Bayes

Consider 1-sample estimate

$$g^{\text{REINFORCE}}(\mathbf{z}, \phi) = \underbrace{f(\mathbf{z})}_{\text{scalar}} \overbrace{\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})}^{\text{vector}}, \qquad \mathbf{z} \sim q_\phi(\mathbf{z})$$

- Gradient estimate points in the direction of increasing probability of a given sample $\mathbf{z}$
  - Increases probability of $\mathbf{z}$ if it happened to be good
- The target function f only enters as a scaling coefficient, and no gradient $\frac{\partial f}{\partial \mathbf{z}}$ is used (unlike the reparametrization trick)
  - Has no idea where to move probability mass *systematically*
  - $f(z) + c$ will give a different estimator
- **Random search in disguise!** [Rec18]

A wild random search appears

Consider 1-sample estimate

$$g^{\text{REINFORCE}}(\mathbf{z}, \phi) = \underbrace{f(\mathbf{z})}_{\text{scalar}} \overbrace{\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})}^{\text{vector}}, \qquad \mathbf{z} \sim q_\phi(\mathbf{z})$$

- Gradient estimate points in the direction of increasing probability of a given sample $\mathbf{z}$
  - Increases probability of $\mathbf{z}$ if it happened to be good
- The target function f only enters as a scaling coefficient, and no gradient $\frac{\partial f}{\partial \mathbf{z}}$ is used (unlike the reparametrization trick)
  - Has no idea where to move probability mass *systematically*
  - $f(z) + c$ will give a different estimator
- **Random search in disguise!** [Rec18]

Relaxations

Idea: Relax the objective over discrete random samples $\mathbf{z}$ into an objective oven continuous random samples $\tilde{\mathbf{z}}$ during training and use the reparametrization trick:

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \approx \mathop{\mathbb{E}}_{q_\phi(\tilde{\mathbf{z}})} f(\tilde{\mathbf{z}}) = \mathop{\mathbb{E}}_{p(\gamma)} f(\tilde{\mathbf{z}}(\gamma, \phi))$$

Keep the discrete testing phase model

Limitation: $f(F)$ has to be differentiable w.r.t. its input.

Idea: Relax the objective over discrete random samples $\mathbf{z}$ into an objective oven continuous random samples $\tilde{\mathbf{z}}$ during training and use the reparametrization trick:

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \approx \mathop{\mathbb{E}}_{q_\phi(\tilde{\mathbf{z}})} f(\tilde{\mathbf{z}}) = \mathop{\mathbb{E}}_{p(\gamma)} f(\tilde{\mathbf{z}}(\gamma, \phi))$$

Keep the discrete testing phase model

Limitation: $f(F)$ has to be differentiable w.r.t. its input.

Idea: Relax the objective over discrete random samples $\mathbf{z}$ into an objective oven continuous random samples $\tilde{\mathbf{z}}$ during training and use the reparametrization trick:

$$\mathbb{E}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \approx \mathbb{E}_{q_\phi(\tilde{\mathbf{z}})} f(\tilde{\mathbf{z}}) = \mathbb{E}_{p(\gamma)} f(\tilde{\mathbf{z}}(\gamma, \phi))$$

Keep the discrete testing phase model

Limitation: $f(\cdot)$ has to be differentiable w.r.t. its input.

Idea: Relax the objective over discrete random samples $\mathbf{z}$ into an objective oven continuous random samples $\tilde{\mathbf{z}}$ during training and use the reparametrization trick:

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \approx \mathop{\mathbb{E}}_{q_\phi(\tilde{\mathbf{z}})} f(\tilde{\mathbf{z}}) = \mathop{\mathbb{E}}_{p(\gamma)} f(\tilde{\mathbf{z}}(\gamma, \phi))$$

Keep the discrete testing phase model

Limitation: $f(F)$ has to be differentiable w.r.t. its input.

Gumbel-Max Trick

Deep|Bayes

An old trick to sample Categorical random variables

$$z \sim \text{Categorical}(\pi_1, \dots, \pi_K),$$

Minimum of independent exponential distributions with carefully chosen probabilities has the same distribution:

$$z \overset{d}{=} \underset{k}{\text{argmin}} \frac{\xi_k}{\pi_k}, \qquad \xi_k \sim \text{Exp}(1)$$

Equivalently (applying $-\log$)

$$z \overset{d}{=} \underset{k}{\text{argmax}} \left[\log \pi_k \overbrace{- \log \xi_k}^{\gamma_k} \right], \qquad \xi_k \sim \text{Exp}(1)$$

Converts sampling K-ary discrete random variable into optimization of noise-perturbed logits, $\gamma := -\log \xi$ has standard Gumbel$(0, 1)$ distribution.

- Gives a reparametrization, but not a continuous one!

An old trick to sample Categorical random variables

$$z \sim \text{Categorical}(\pi_1, \dots, \pi_K),$$

Minimum of independent exponential distributions with carefully chosen probabilities has the same distribution:

$$z \stackrel{d}{=} \operatorname*{argmin}_k \frac{\xi_k}{\pi_k}, \qquad \xi_k \sim \text{Exp}(1)$$

Equivalently (applying $-\log$)

$$z \stackrel{d}{=} \operatorname*{argmax}_k \left[\log \pi_k \overbrace{- \log \xi_k}^{\gamma_k} \right], \qquad \xi_k \sim \text{Exp}(1)$$

Converts sampling K-ary discrete random variable into optimization of noise-perturbed logits, $\gamma := -\log \xi$ has standard Gumbel$(0, 1)$ distribution.

- Gives a reparametrization, but not a continuous one!

An old trick to sample Categorical random variables

$$z \sim \text{Categorical}(\pi_1, \dots, \pi_K),$$

Minimum of independent exponential distributions with carefully chosen probabilities has the same distribution:

$$z \overset{d}{=} \underset{k}{\text{argmin}} \frac{\xi_k}{\pi_k}, \qquad \xi_k \sim \text{Exp}(1)$$

Equivalently (applying $-\log$)

$$z \overset{d}{=} \underset{k}{\text{argmax}} \left[\log \pi_k \overbrace{- \log \xi_k}^{\gamma_k} \right], \qquad \xi_k \sim \text{Exp}(1)$$

Converts sampling K-ary discrete random variable into optimization of noise-perturbed logits, $\gamma := -\log \xi$ has standard Gumbel$(0, 1)$ distribution.

- Gives a reparametrization, but not a continuous one!

Gumbel-Max Trick

An old trick to sample Categorical random variables

$$z \sim \text{Categorical}(\pi_1, \dots, \pi_K),$$

Minimum of independent exponential distributions with carefully chosen probabilities has the same distribution:

$$z \stackrel{d}{=} \underset{k}{\text{argmin}} \frac{\xi_k}{\pi_k}, \qquad \xi_k \sim \text{Exp}(1)$$

Equivalently (applying $-\log$)

$$z \stackrel{d}{=} \underset{k}{\text{argmax}} \left[\log \pi_k \overbrace{- \log \xi_k}^{\gamma_k} \right], \qquad \xi_k \sim \text{Exp}(1)$$

Converts sampling K-ary discrete random variable into optimization of noise-perturbed logits, $\gamma := -\log \xi$ has standard Gumbel$(0, 1)$ distribution.

- Gives a reparametrization, but not a continuous one!

Gumbel-Softmax Trick [JGP17], [MMT17]

Approximate argmax with softmax (with temperature)

$$\text{softmax}_\tau(x)_j := \frac{\exp(x_j/\tau)}{\sum_{k=1}^K \exp(x_k/\tau)}$$

Temperature controls "sharpness" of the softmax:

- $\tau = 0$ recovers argmax $=$ softmax$_0$
- $\tau = \infty$ leads to uniform distribution that ignores any disparities

Then assume the discrete $\mathbf{z}$ is a one-hot vector and replace with a continuous relaxation $\tilde{\mathbf{z}}$

$$\tilde{\mathbf{z}}\,(\gamma, \pi) := \text{softmax}_\tau\,(\log \pi_1 + \gamma_1, \dots, \log \pi_K + \gamma_K)$$

Where each $\gamma_k \sim \text{Gumbel}(0, 1)$ is a standard Gumbel random variable, and can be generated from uniform noise u_k as

$$\gamma_k \overset{d}{=} -\log(-\log u_k), \qquad u_k \sim \text{Uniform}(0, 1)$$

Approximate argmax with softmax (with temperature)

$$\text{softmax}_\tau(x)_j := \frac{\exp(x_j/\tau)}{\sum_{k=1}^K \exp(x_k/\tau)}$$

Temperature controls "sharpness" of the softmax:

- $\tau = 0$ recovers argmax $= \text{softmax}_0$
- $\tau = \infty$ leads to uniform distribution that ignores any disparities

Then assume the discrete $\mathbf{z}$ is a one-hot vector and replace with a continuous relaxation $\tilde{\mathbf{z}}$

$$\tilde{\mathbf{z}}\,(\gamma, \pi) := \text{softmax}_\tau\,(\log \pi_1 + \gamma_1, \dots, \log \pi_K + \gamma_K)$$

Where each $\gamma_k \sim \text{Gumbel}(0, 1)$ is a standard Gumbel random variable, and can be generated from uniform noise u_k as

$$\gamma_k \overset{d}{=} -\log(-\log u_k), \qquad u_k \sim \text{Uniform}(0, 1)$$

Approximate argmax with softmax (with temperature)

$$\text{softmax}_\tau(x)_j := \frac{\exp(x_j/\tau)}{\sum_{k=1}^{K} \exp(x_k/\tau)}$$

Temperature controls "sharpness" of the softmax:

- $\tau = 0$ recovers argmax $= \text{softmax}_0$
- $\tau = \infty$ leads to uniform distribution that ignores any disparities

Then assume the discrete $\mathbf{z}$ is a one-hot vector and replace with a continuous relaxation $\tilde{\mathbf{z}}$

$$\tilde{\mathbf{z}}\,(\gamma, \pi) := \text{softmax}_\tau\,(\log \pi_1 + \gamma_1, \dots, \log \pi_K + \gamma_K)$$

Where each $\gamma_k \sim \text{Gumbel}(0, 1)$ is a standard Gumbel random variable, and can be generated from uniform noise u_k as

$$\gamma_k \stackrel{d}{=} -\log(-\log u_k), \qquad u_k \sim \text{Uniform}(0, 1)$$

Gumbel-Softmax Trick: Implementation Details

Now we can rewrite the expectation w.r.t. independent noise $\gamma_1, \ldots, \gamma_K$

$$\mathcal{L}(\phi) = \mathbb{E}_{\gamma} f(\tilde{\mathbf{z}}\,(\gamma, \phi)), \qquad \gamma_k \sim \text{Gumbel}(0, 1)$$

Gradient estimate is obtained simply by exchanging $\frac{\partial}{\partial \phi}$ and $\mathbb{E}$:

$$g^{\text{Rep}}(\gamma, \phi) = \frac{\partial}{\partial \phi} f(\tilde{\mathbf{z}}\,(\gamma, \pi(\phi)))$$

Similar to stochastic discrete nodes replaced by their expectation (softmax), but has **noise injected into log-probabilities**

- Noise helps exploration and regularizes
- Right kind of noise makes $\tilde{\mathbf{z}}$ similar to one-hot vectors
  - Reducing the train-test mismatch

Gumbel-Softmax Trick: Implementation Details

Now we can rewrite the expectation w.r.t. independent noise $\gamma_1, \dots, \gamma_K$

$$\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{\gamma} f(\tilde{\mathbf{z}}\,(\gamma, \phi)), \qquad \gamma_k \sim \text{Gumbel}(0, 1)$$

Gradient estimate is obtained simply by exchanging $\frac{\partial}{\partial \phi}$ and $\mathbb{E}$:

$$g^{\text{Rep}}(\gamma, \phi) = \frac{\partial}{\partial \phi} f(\tilde{\mathbf{z}}\,(\gamma, \pi(\phi)))$$

Similar to stochastic discrete nodes replaced by their expectation (softmax), but has **noise injected into log-probabilities**

- Noise helps exploration and regularizes
- Right kind of noise makes $\tilde{\mathbf{z}}$ similar to one-hot vectors
  - Reducing the train-test mismatch

Gumbel-Softmax Trick: Implementation Details

Now we can rewrite the expectation w.r.t. independent noise $\gamma_1, \dots, \gamma_K$

$$\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{\gamma} f(\tilde{\mathbf{z}}(\gamma, \phi)), \qquad \gamma_k \sim \text{Gumbel}(0, 1)$$

Gradient estimate is obtained simply by exchanging $\frac{\partial}{\partial \phi}$ and $\mathbb{E}$:

$$g^{\text{Rep}}(\gamma, \phi) = \frac{\partial}{\partial \phi} f(\tilde{\mathbf{z}}(\gamma, \pi(\phi)))$$

Similar to stochastic discrete nodes replaced by their expectation (softmax), but has **noise injected into log-probabilities**

- Noise helps exploration and regularizes
- Right kind of noise makes $\tilde{\mathbf{z}}$ similar to one-hot vectors
    - Reducing the train-test mismatch

In a special case of $K = 2$ we can write a bit more sample-efficient scheme:

$$\tilde{z} = \sigma_\tau\left(\log \frac{p}{1-p} + \upsilon\right), \qquad \upsilon \sim \text{Logistic}(0, 1)$$

where Logistic(0, 1) is the distribution of difference of two Gumbels:

$$\upsilon \stackrel{d}{=} \gamma_1 - \gamma_2$$

You can easily see this by yourself by simplifying the formula of the softmax over 2 classes.

In a special case of $K = 2$ we can write a bit more sample-efficient scheme:

$$\tilde{z} = \sigma_\tau\left(\log \frac{p}{1-p} + \upsilon\right), \qquad \upsilon \sim \text{Logistic}(0, 1)$$

where Logistic(0, 1) is the distribution of difference of two Gumbels:

$$\upsilon \overset{d}{=} \gamma_1 - \gamma_2$$

You can easily see this by yourself by simplifying the formula of the softmax over 2 classes.

Gumbel-Softmax Trick: Binary Case

In a special case of $K = 2$ we can write a bit more sample-efficient scheme:

$$\tilde{z} = \sigma_\tau \left(\log \frac{p}{1-p} + \upsilon \right), \qquad \upsilon \sim \text{Logistic}(0, 1)$$

where Logistic(0, 1) is the distribution of difference of two Gumbels:

$$\upsilon \overset{d}{=} \gamma_1 - \gamma_2$$

You can easily see this by yourself by simplifying the formula of the softmax over 2 classes.

Gumbel-Softmax Trick: Binary Case

In a special case of $K = 2$ we can write a bit more sample-efficient scheme:

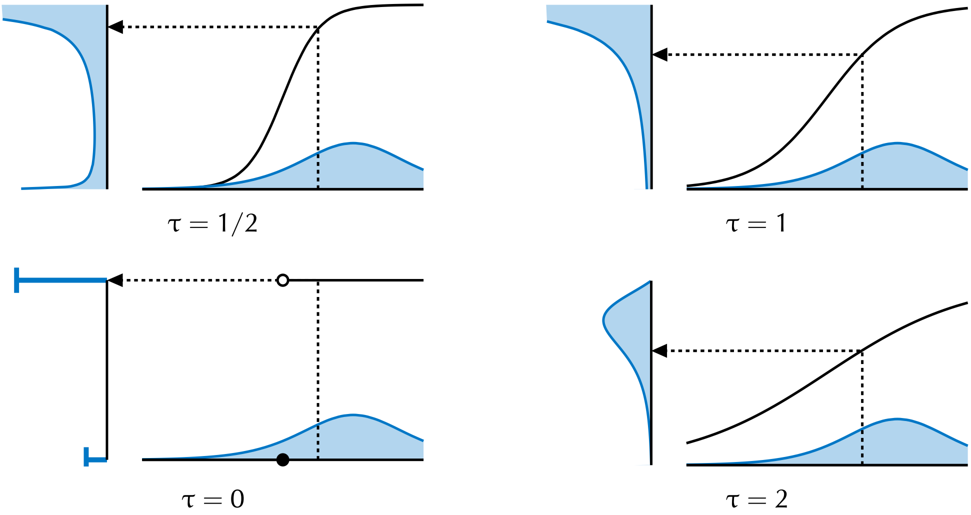
$$\tilde{z} = \sigma_\tau \left(\log \tfrac{p}{1-p} + \upsilon \right), \qquad \upsilon \sim \text{Logistic}(0, 1)$$

where Logistic(0, 1) is the distribution of difference of two Gumbels:

$$\upsilon \stackrel{d}{=} \gamma_1 - \gamma_2$$

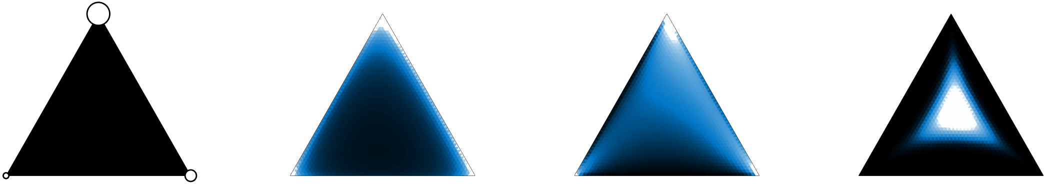
You can easily see this by yourself by simplifying the formula of the softmax over 2 classes.

Gumbel-Softmax Trick: Temperature



Gumbel-Softmax Trick: Temperature

For K-ary categorical r.v. it has been shown that for $\tau \leqslant \frac{1}{K-1}$ there are no modes in the interior of the probability simplex



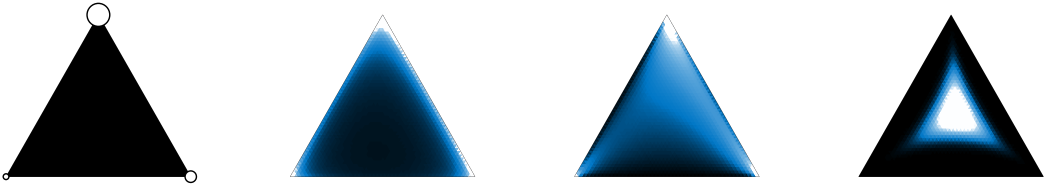
$\tau = 0$ $\tau = 1/2$ $\tau = 1$ $\tau = 2$

How to choose a specific temperature?

- Small temperature leads to high variances, but resembles discrete case well
- Large temperatures have lower variance, but deviates away from the discrete case
- In practice grid search over a couple possible values

Gumbel-Softmax Trick: Temperature

For K-ary categorical r.v. it has been shown that for $\tau \leqslant \frac{1}{K-1}$ there are no modes in the interior of the probability simplex



$\tau = 0$ $\qquad$ $\tau = 1/2$ $\qquad$ $\tau = 1$ $\qquad$ $\tau = 2$

How to choose a specific temperature?

- Small temperature leads to high variances, but resembles discrete case well
- Large temperatures have lower variance, but deviates away from the discrete case
- In practice grid search over a couple possible values

Consider 4-way categorical r.v. $z \sim q(z) = \text{Categorical}(z|\pi_1, \pi_2, \pi_3, \pi_4)$ where $\pi_j = \text{softmax}(\theta)_j$ and $\theta \in \mathbb{R}^4$ is a parameter vector. We seek to estimate the gradient of the following objective:

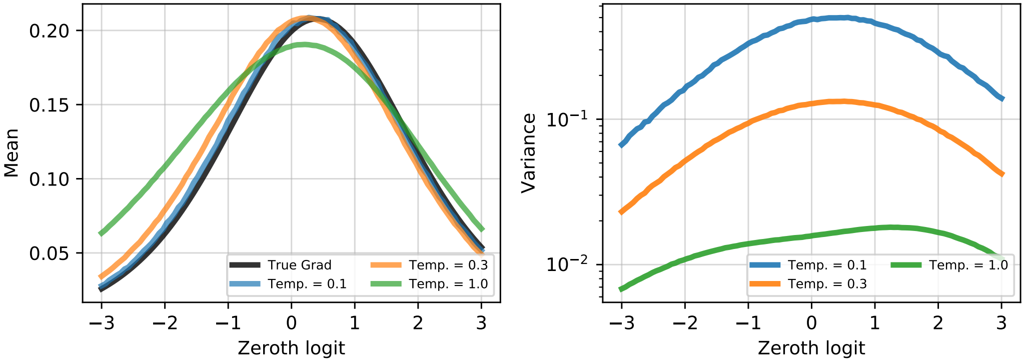
$$\mathbb{E}_{q(z)} \cos(z) \to \min_{\theta}$$

It's relaxed version is

$$\mathbb{E}_{p(\gamma_{1:4})} \cos\left(\text{softmax}_\tau(\theta + \gamma)^T [0, 1, 2, 3]\right) \to \min_{\theta}$$

Now we can use the reparametrization trick to estimate the gradient w.r.t. θ

Toy Example contd.



Gumbel-Softmax Trick: Conclusions

- Gumbel-Softmax relaxes discrete random variables into continuous, enabling the reparametrization trick
- Relaxations change the objective, yet no theory on how good the relaxation is
  - Relaxation introduces bias
- Temperature τ is a hyperparameter that needs to be tuned

There exist other relaxations, however they are

- Less mathematically elegant
- Do not seem to work better empirically
- Sometimes heuristic in nature

Gumbel-Softmax Trick: Conclusions

DeepBayes

- Gumbel-Softmax relaxes discrete random variables into continuous, enabling the reparametrization trick
- Relaxations change the objective, yet no theory on how good the relaxation is
  - Relaxation introduces bias
- Temperature τ is a hyperparameter that needs to be tuned

There exist other relaxations, however they are

- Less mathematically elegant
- Do not seem to work better empirically
- Sometimes heuristic in nature

Gumbel-Softmax Trick: Conclusions

DeepBayes

- Gumbel-Softmax relaxes discrete random variables into continuous, enabling the reparametrization trick
- Relaxations change the objective, yet no theory on how good the relaxation is
  - Relaxation introduces bias
- Temperature τ is a hyperparameter that needs to be tuned

There exist other relaxations, however they are

- Less mathematically elegant
- Do not seem to work better empirically
- Sometimes heuristic in nature

Gumbel-Softmax Trick: Conclusions

- Gumbel-Softmax relaxes discrete random variables into continuous, enabling the reparametrization trick
- Relaxations change the objective, yet no theory on how good the relaxation is
  - Relaxation introduces bias
- Temperature τ is a hyperparameter that needs to be tuned

There exist other relaxations, however they are

- Less mathematically elegant
- Do not seem to work better empirically
- Sometimes heuristic in nature

Gumbel-Softmax Trick: Conclusions

- Gumbel-Softmax relaxes discrete random variables into continuous, enabling the reparametrization trick
- Relaxations change the objective, yet no theory on how good the relaxation is
  - Relaxation introduces bias
- Temperature τ is a hyperparameter that needs to be tuned

There exist other relaxations, however they are

- Less mathematically elegant
- Do not seem to work better empirically
- Sometimes heuristic in nature

Variance Reduction

Consider some $b(\mathbf{z})$ with **tractable** expectation $\mu := \mathbb{E}_{q(\mathbf{z})} b(\mathbf{z})$. Then

$$\mathbb{E}_{q(\mathbf{z})} f(\mathbf{z}) = \mathbb{E}_{q(\mathbf{z})} \left[(f(\mathbf{z}) - b(\mathbf{z})) + \mu \right]$$

■ might be a lower-variance estimate if $f(\mathbf{z})$ and $b(\mathbf{z})$ are positively correlated:

$$\text{Var}\left[\blacksquare\right] = \text{Var}\left[f(\mathbf{z}) - b(\mathbf{z})\right] = \text{Var}\left[f(\mathbf{z})\right] + \text{Var}\left[b(\mathbf{z})\right] - 2\text{Cov}\left[f(\mathbf{z}), b(\mathbf{z})\right]$$

- Unbiased estimator
- $b(\mathbf{z})$ is called *Control Variate*
- Convenient if $b(\mathbf{z})$ is zero-mean
- We can choose any $b(\mathbf{z})$ we want
- Can take several samples M to reduce the variance further

Intuitively, we extract some tractable part $b(\mathbf{z})$ of the $f(\mathbf{z})$ and estimate the rest with Monte Carlo.

Consider some $b(\mathbf{z})$ with **tractable** expectation $\mu := \mathbb{E}_{q(\mathbf{z})} b(\mathbf{z})$. Then

$$\mathbb{E}_{q(\mathbf{z})} f(\mathbf{z}) = \mathbb{E}_{q(\mathbf{z})} \left[\color{red}{(f(\mathbf{z}) - b(\mathbf{z})) + \mu} \right]$$

$\color{red}{\blacksquare}$ might be a lower-variance estimate if $f(\mathbf{z})$ and $b(\mathbf{z})$ are positively correlated:

$$\text{Var}\left[\color{red}{\blacksquare}\right] = \text{Var}\left[f(\mathbf{z}) - b(\mathbf{z})\right] = \text{Var}\left[f(\mathbf{z})\right] + \color{blue}{\text{Var}\left[b(\mathbf{z})\right] - 2\text{Cov}\left[f(\mathbf{z}), b(\mathbf{z})\right]}$$

- Unbiased estimator
- $b(\mathbf{z})$ is called *Control Variate*
- Convenient if $b(\mathbf{z})$ is zero-mean
- We can choose any $b(\mathbf{z})$ we want
- Can take several samples M to reduce the variance further

Intuitively, we extract some tractable part $b(\mathbf{z})$ of the $f(\mathbf{z})$ and estimate the rest with Monte Carlo.

Control Variates

Consider some $b(\mathbf{z})$ with **tractable** expectation $\mu := \mathbb{E}_{q(\mathbf{z})} b(\mathbf{z})$. Then

$$\mathop{\mathbb{E}}_{q(\mathbf{z})} f(\mathbf{z}) = \mathop{\mathbb{E}}_{q(\mathbf{z})} \left[(f(\mathbf{z}) - b(\mathbf{z})) + \mu \right]$$

$\blacksquare$ might be a lower-variance estimate if $f(\mathbf{z})$ and $b(\mathbf{z})$ are positively correlated:

$$\text{Var}\left[\blacksquare\right] = \text{Var}\left[f(\mathbf{z}) - b(\mathbf{z})\right] = \text{Var}\left[f(\mathbf{z})\right] + \text{Var}\left[b(\mathbf{z})\right] - 2\text{Cov}\left[f(\mathbf{z}), b(\mathbf{z})\right]$$

- Unbiased estimator
- $b(\mathbf{z})$ is called *Control Variate*
- Convenient if $b(\mathbf{z})$ is zero-mean

- We can choose any $b(\mathbf{z})$ we want
- Can take several samples M to reduce the variance further

Intuitively, we extract some tractable part $b(\mathbf{z})$ of the $f(\mathbf{z})$ and estimate the rest with Monte Carlo.

Consider some $b(\mathbf{z})$ with **tractable** expectation $\mu := \mathbb{E}_{q(\mathbf{z})} b(\mathbf{z})$. Then

$$\mathbb{E}_{q(\mathbf{z})} f(\mathbf{z}) = \mathbb{E}_{q(\mathbf{z})} \left[(f(\mathbf{z}) - b(\mathbf{z})) + \mu \right]$$

■ might be a lower-variance estimate if $f(\mathbf{z})$ and $b(\mathbf{z})$ are positively correlated:

$$\text{Var}\left[\blacksquare\right] = \text{Var}\left[f(\mathbf{z}) - b(\mathbf{z})\right] = \text{Var}\left[f(\mathbf{z})\right] + \text{Var}\left[b(\mathbf{z})\right] - 2\text{Cov}\left[f(\mathbf{z}), b(\mathbf{z})\right]$$

- Unbiased estimator
- $b(\mathbf{z})$ is called *Control Variate*
- Convenient if $b(\mathbf{z})$ is zero-mean
- We can choose any $b(\mathbf{z})$ we want
- Can take several samples M to reduce the variance further

Intuitively, we extract some tractable part $b(\mathbf{z})$ of the $f(\mathbf{z})$ and estimate the rest with Monte Carlo.

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z}_{1:M})} \left[\frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \right] + \mu(\phi)$$

It's REINFORCE gradient is

$$g_b^{\text{REINFORCE}}(\mathbf{z}, \phi) = \frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m) + \frac{\partial}{\partial \phi} \mu(\phi)$$

- $b(\mathbf{z})$ is typically called *baseline*
- Essentially a control variate of the form $b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})$
  - Other CVs are possible, but this is convenient as it approximates the function itself
- Unbiased estimate of the true gradient since $\mathbb{E}_{q_\phi(\mathbf{z})} b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} \mu(\phi)$
- For right $b(\mathbf{z})$ might have much lower variance

$$\mathbb{E}_{q_\phi(\mathbf{z}_{1:M})}\left[\frac{1}{M}\sum_{m=1}^{M}(f(\mathbf{z}_m) - b(\mathbf{z}_m))\right] + \mu(\phi)$$

It's REINFORCE gradient is

$$g_b^{\text{REINFORCE}}(\mathbf{z}, \phi) = \frac{1}{M}\sum_{m=1}^{M}(f(\mathbf{z}_m) - b(\mathbf{z}_m))\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z}_m) + \frac{\partial}{\partial\phi}\mu(\phi)$$

- $b(\mathbf{z})$ is typically called *baseline*
- Essentially a control variate of the form $b(\mathbf{z})\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z})$
  - Other CVs are possible, but this is convenient as it approximates the function itself
- Unbiased estimate of the true gradient since $\mathbb{E}_{q_\phi(\mathbf{z})} b(\mathbf{z})\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z}) = \frac{\partial}{\partial\phi}\mu(\phi)$
- For right $b(\mathbf{z})$ might have much lower variance

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z}_{1:M})} \left[\frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \right] + \mu(\phi)$$

It's REINFORCE gradient is

$$g_b^{\text{REINFORCE}}(\mathbf{z}, \phi) = \frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m) + \frac{\partial}{\partial \phi} \mu(\phi)$$

- $b(\mathbf{z})$ is typically called *baseline*
- Essentially a control variate of the form $b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})$
    - Other CVs are possible, but this is convenient as it approximates the function itself
- Unbiased estimate of the true gradient since $\mathbb{E}_{q_\phi(\mathbf{z})} b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} \mu(\phi)$
- For right $b(\mathbf{z})$ might have much lower variance

$$\mathop{\mathbb{E}}_{q_\phi(\mathbf{z}_{1:M})} \left[\frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \right] + \mu(\phi)$$

It's REINFORCE gradient is

$$g_b^{\text{REINFORCE}}(\mathbf{z}, \phi) = \frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m) + \frac{\partial}{\partial \phi} \mu(\phi)$$

- $b(\mathbf{z})$ is typically called *baseline*
- Essentially a control variate of the form $b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})$
  - Other CVs are possible, but this is convenient as it approximates the function itself
- Unbiased estimate of the true gradient since $\mathbb{E}_{q_\phi(\mathbf{z})} b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} \mu(\phi)$
- For right $b(\mathbf{z})$ might have much lower variance

$$\mathbb{E}_{q_\phi(\mathbf{z}_{1:M})} \left[\frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \right] + \mu(\phi)$$

It's REINFORCE gradient is

$$g_b^{\text{REINFORCE}}(\mathbf{z}, \phi) = \frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}_m) + \frac{\partial}{\partial \phi} \mu(\phi)$$

- $b(\mathbf{z})$ is typically called *baseline*
- Essentially a control variate of the form $b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})$
  - Other CVs are possible, but this is convenient as it approximates the function itself
- Unbiased estimate of the true gradient since $\mathbb{E}_{q_\phi(\mathbf{z})} b(\mathbf{z}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) = \frac{\partial}{\partial \phi} \mu(\phi)$
- For right $b(\mathbf{z})$ might have much lower variance

- **Constant baseline** $b(\mathbf{z}) = c$

$$(f(\mathbf{z}) - c)\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \overbrace{\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} c}^{=0}$$

  Just centers the learning signal, the optimal c is

$$c = \frac{\sum_{d=1}^{D} \text{Cov}\left[f(\mathbf{z})\frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z}), \frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z})\right]}{\sum_{d=1}^{D} \text{Var}\left[\frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z})\right]}$$

  Can be estimated using moving averages, but beware the variance!
- If some contextual observation is available (like x in VAE), the optimal constant baseline now depends on x. **NVIL** [MG14] proposes to learn the baseline network by minimizing the expected MSE:

$$\mathop{\mathbb{E}}_{p(x)} \mathop{\mathbb{E}}_{q_\phi(z|x)} (f(\mathbf{z}) - b(x))^2 \to \min_{b(x)}$$

- **Constant baseline** $b(\mathbf{z}) = c$

$$(f(\mathbf{z}) - c)\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \overbrace{\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} c}^{=0}$$

  Just centers the learning signal, the optimal c is

$$c = \frac{\sum_{d=1}^{D} \text{Cov}\left[f(\mathbf{z}) \frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z}), \frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z})\right]}{\sum_{d=1}^{D} \text{Var}\left[\frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z})\right]}$$

  Can be estimated using moving averages, but beware the variance!
- If some contextual observation is available (like x in VAE), the optimal constant baseline now depends on x. **NVIL** [MG14] proposes to learn the baseline network by minimizing the expected MSE:

$$\mathop{\mathbb{E}}_{p(x)} \mathop{\mathbb{E}}_{q_\phi(z|x)} (f(\mathbf{z}) - b(x))^2 \to \min_{b(x)}$$

- **Constant baseline** $b(\mathbf{z}) = c$

$$(f(\mathbf{z}) - c)\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \overbrace{\frac{\partial}{\partial \phi} \mathop{\mathbb{E}}_{q_\phi(\mathbf{z})} c}^{=0}$$

Just centers the learning signal, the optimal c is

$$c = \frac{\sum_{d=1}^{D} \operatorname{Cov}\left[f(\mathbf{z}) \frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z}), \frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z})\right]}{\sum_{d=1}^{D} \operatorname{Var}\left[\frac{\partial}{\partial \phi_d} \log q_\phi(\mathbf{z})\right]}$$

Can be estimated using moving averages, but beware the variance!

- If some contextual observation is available (like x in VAE), the optimal constant baseline now depends on x. **NVIL** [MG14] proposes to learn the baseline network by minimizing the expected MSE:

$$\mathop{\mathbb{E}}_{p(x)} \mathop{\mathbb{E}}_{q_\phi(z|x)} (f(\mathbf{z}) - b(x))^2 \to \min_{b(x)}$$

Let $b(\mathbf{z})$ be a first-order Taylor expansion of $f(\mathbf{z})$ at some point μ:

$$b(\mathbf{z}) = f(\mu) + \frac{\partial f}{\partial \mathbf{z}}(\mu)^T (\mathbf{z} - \mu)$$

We'll take $\mu := \mu(\phi) = \mathbb{E}_{q_\phi(\mathbf{z})} \mathbf{z}$. This leads to

$$g^{\mu\text{-prop}}(\mathbf{z}, \phi) = (f(\mathbf{z}) - b(\mathbf{z})) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \frac{\partial f(\mu(\phi))}{\partial \phi}$$

- Backpropagates through the mean, and then fine-tunes inaccuracies with REINFORCE
- One could use 2nd order Taylor expansion, but that is more computationally expensive

MuProp [GLSM16]

Let $b(\mathbf{z})$ be a first-order Taylor expansion of $f(\mathbf{z})$ at some point μ:

$$b(\mathbf{z}) = f(\mu) + \frac{\partial f}{\partial \mathbf{z}}(\mu)^T(\mathbf{z} - \mu)$$

We'll take $\mu := \mu(\phi) = \mathbb{E}_{q_\phi(\mathbf{z})}\, \mathbf{z}$. This leads to

$$g^{\mu\text{-prop}}(\mathbf{z}, \phi) = (f(\mathbf{z}) - b(\mathbf{z}))\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \frac{\partial f(\mu(\phi))}{\partial \phi}$$

- Backpropagates through the mean, and then fine-tunes inaccuracies with REINFORCE
- One could use 2nd order Taylor expansion, but that is more computationally expensive

MuProp [GLSM16]

Let $b(\mathbf{z})$ be a first-order Taylor expansion of $f(\mathbf{z})$ at some point μ:

$$b(\mathbf{z}) = f(\mu) + \frac{\partial f}{\partial \mathbf{z}}(\mu)^T (\mathbf{z} - \mu)$$

We'll take $\mu := \mu(\phi) = \mathbb{E}_{q_\phi(\mathbf{z})} \mathbf{z}$. This leads to

$$g^{\mu\text{-prop}}(\mathbf{z}, \phi) = (f(\mathbf{z}) - b(\mathbf{z})) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \frac{\partial f(\mu(\phi))}{\partial \phi}$$

- Backpropagates through the mean, and then fine-tunes inaccuracies with REINFORCE
- One could use 2nd order Taylor expansion, but that is more computationally expensive

Let $b(\mathbf{z})$ be a first-order Taylor expansion of $f(\mathbf{z})$ at some point μ:

$$b(\mathbf{z}) = f(\mu) + \frac{\partial f}{\partial \mathbf{z}}(\mu)^T (\mathbf{z} - \mu)$$

We'll take $\mu := \mu(\phi) = \mathbb{E}_{q_\phi(\mathbf{z})} \mathbf{z}$. This leads to

$$g^{\mu\text{-prop}}(\mathbf{z}, \phi) = (f(\mathbf{z}) - b(\mathbf{z})) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \frac{\partial f(\mu(\phi))}{\partial \phi}$$

- Backpropagates through the mean, and then fine-tunes inaccuracies with REINFORCE
- One could use 2nd order Taylor expansion, but that is more computationally expensive

Typically we seek low-variance estimators. Why not minimize the variance w.r.t. a baseline in the first place?

$$\text{Var}[g(\mathbf{z}, \phi)] = \mathbb{E}\, g(\mathbf{z}, \phi)^2 - (\mathbb{E}\, g(\mathbf{z}, \phi))^2$$

- In general minimizing variance leads to increase in bias
  - Estimators with control variates are **unbiased for any baseline**
- Use Stochastic Optimization to minimize the second moment of the gradient.

For example, for **NVIL** a better objective would be

$$\mathop{\mathbb{E}}_{p(x)} \mathop{\mathbb{E}}_{q_\phi(z|x)} \left((f(\mathbf{z}) - b(x)) \frac{\partial}{\partial \phi} \log q_\phi(z|x) \right)^2 \to \min_{b(x)}$$

Typically we seek low-variance estimators. Why not minimize the variance w.r.t. a baseline in the first place?

$$\text{Var}[g(\mathbf{z}, \phi)] = \mathbb{E}\, g(\mathbf{z}, \phi)^2 - (\mathbb{E}\, g(\mathbf{z}, \phi))^2$$

- In general minimizing variance leads to increase in bias
  - Estimators with control variates are **unbiased for any baseline**
- Use Stochastic Optimization to minimize the second moment of the gradient.

For example, for **NVIL** a better objective would be

$$\mathop{\mathbb{E}}_{p(x)} \mathop{\mathbb{E}}_{q_\phi(z|x)} \left((f(\mathbf{z}) - b(x)) \frac{\partial}{\partial \phi} \log q_\phi(z|x) \right)^2 \to \min_{b(x)}$$

Typically we seek low-variance estimators. Why not minimize the variance w.r.t. a baseline in the first place?

$$\text{Var}[g(\mathbf{z}, \phi)] = \mathbb{E}\, g(\mathbf{z}, \phi)^2 - (\mathbb{E}\, g(\mathbf{z}, \phi))^2$$

- In general minimizing variance leads to increase in bias
  - Estimators with control variates are **unbiased for any baseline**
- Use Stochastic Optimization to minimize the second moment of the gradient.

For example, for **NVIL** a better objective would be

$$\mathop{\mathbb{E}}_{p(x)} \mathop{\mathbb{E}}_{q_\phi(z|x)} \left((f(\mathbf{z}) - b(x)) \frac{\partial}{\partial \phi} \log q_\phi(z|x) \right)^2 \to \min_{b(x)}$$

Variance Minimization

Typically we seek low-variance estimators. Why not minimize the variance w.r.t. a baseline in the first place?

$$\mathrm{Var}[g(\mathbf{z}, \phi)] = \mathbb{E}\, g(\mathbf{z}, \phi)^2 - (\mathbb{E}\, g(\mathbf{z}, \phi))^2$$

- In general minimizing variance leads to increase in bias
  - Estimators with control variates are **unbiased for any baseline**
- Use Stochastic Optimization to minimize the second moment of the gradient.

For example, for **NVIL** a better objective would be

$$\mathop{\mathbb{E}}_{p(x)} \mathop{\mathbb{E}}_{q_\phi(z|x)} \left((f(\mathbf{z}) - b(x)) \frac{\partial}{\partial \phi} \log q_\phi(z|x) \right)^2 \to \min_{b(x)}$$

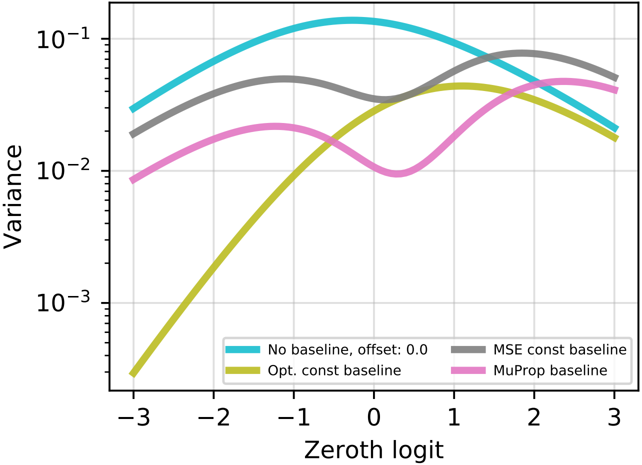
- REBAR [TMM+17] uses Gumbel-relaxed f as a baseline

$$g^{\text{REBAR}}(\mathbf{z}, \phi) := \big(f(\mathbf{z}) - \eta f(\tilde{\mathbf{z}}_\phi \mid \mathbf{z})\big) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \eta \frac{\partial}{\partial \phi} \big(f(\tilde{\mathbf{z}}_\phi) - f(\tilde{\mathbf{z}}_\phi \mid \mathbf{z})\big)$$

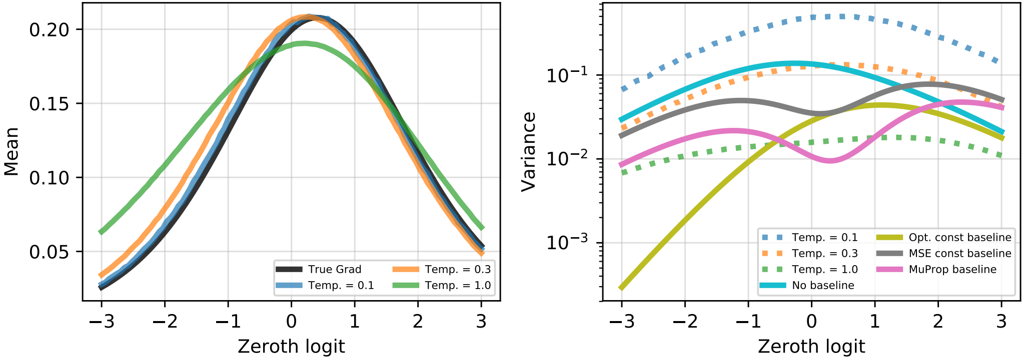
  - Efficiently reparametrizable
  - Hyperparameters τ and η can be learned using the variance minimization principle
  - Backpropagates through Gumbel-relaxed objective, but has additional corrections for the introduced bias
  - **The baseline's expectation is intractable, but reparametrizable**
- RELAX [GCW+18] learns the baseline $b(z)$ using variance minimization:

$$g^{\text{RELAX}}(\mathbf{z}, \phi) := \big(f(\mathbf{z}) - b(\tilde{\mathbf{z}}_\phi \mid \mathbf{z})\big) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}) + \frac{\partial}{\partial \phi} \big(b(\tilde{\mathbf{z}}_\phi) - b(\tilde{\mathbf{z}}_\phi \mid \mathbf{z})\big)$$

Toy Example Again



Toy Example Overall



Deep|Bayes

Conclusion

Conclusion

Relaxation-based methods

- Straightforward to implement
- Work well in practice
- Have hyperparameters to tune
- Have biased gradients aka introduce train-test mismatch

Variance Reduction methods

- Cumbersome
- Not clear if their results are worth added complexity
- Always unbiased
- Allow you to tune baseline to minimize variance
- **Random search on steroids**

Still ongoing research topic, many other approaches not covered

Relaxation-based methods

- Straightforward to implement
- Work well in practice
- Have hyperparameters to tune
- Have biased gradients aka introduce train-test mismatch

Variance Reduction methods

- Cumbersome
- Not clear if their results are worth added complexity
- Always unbiased
- Allow you to tune baseline to minimize variance
- **Random search on steroids**

Still ongoing research topic, many other approaches not covered

For more estimators for both discrete and continuous cases see my blog:

- http://artem.sobolev.name/tags/stochastic computation graphs series.html

For more in-depth treatment of the continuous case see "Monte Carlo Gradient Estimation in Machine Learning" by S. Mohamed, M. Rosca, M. Figurnov, A. Mnih:

- https://arxiv.org/abs/1906.10652

References I

- Will Grathwohl, Dami Choi, Yuhuai Wu, Geoff Roeder, and David Duvenaud, *Backpropagation through the void: Optimizing control variates for black-box gradient estimation*, International Conference on Learning Representations, 2018.
- Shixiang Gu, Sergey Levine, Ilya Sutskever, and Andriy Mnih, *Muprop: Unbiased backpropagation for stochastic neural networks*, International Conference on Learning Representations, 2016.
- Eric Jang, Shixiang Gu, and Ben Poole, *Categorical reparameterization with gumbel-softmax*, International Conference on Learning Representations, 2017.
- Andriy Mnih and Karol Gregor, *Neural variational inference and learning in belief networks*, Proceedings of the 31st International Conference on Machine Learning (ICML), 2014.

- Chris J. Maddison, Andriy Mnih, and Yee Whye Teh, *The concrete distribution: A continuous relaxation of discrete random variables*, International Conference on Learning Representations, 2017.
- Ben Recht, *arg min blog: The policy of truth*, `http://www.argmin.net/2018/02/20/reinforce/`, 2018.
- George Tucker, Andriy Mnih, Chris J Maddison, John Lawson, and Jascha Sohl-Dickstein, *Rebar: Low-variance, unbiased gradient estimates for discrete latent variable models*, Advances in Neural Information Processing Systems 30 (I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, eds.), Curran Associates, Inc., 2017, pp. 2627–2636.