

Discrete Latent Variable Models

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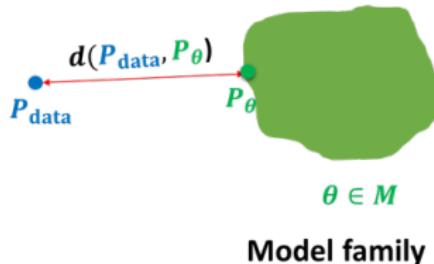
Stanford University

Lecture 17

Summary



$$\mathbf{x}_i \sim P_{\text{data}} \\ i = 1, 2, \dots, n$$



Major themes in the course

- Representing probability distributions
 - Probability density/mass functions: autoregressive models, flow models, variational autoencoders, energy-based models.
 - Sampling process: Generative adversarial networks.
 - Score function: Score-based generative models
- Distances between distributions: two sample test, maximum likelihood training, score matching, noise contrastive estimation.
- Evaluation of generative models

Plan for today: Discrete Latent Variable Modeling

Why should we care about discreteness?

- Discreteness is all around us!
 - Decision Making: Should I attend CS 236 lecture or not?
 - Structure learning

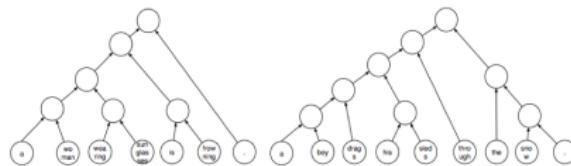


Figure 2: Examples of tree structures learned by our model which show that the model discovers simple concepts such as noun phrases and verb phrases.

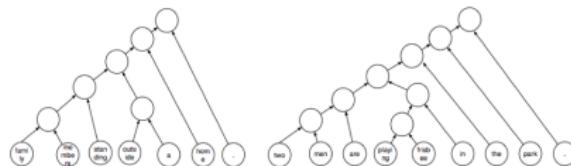
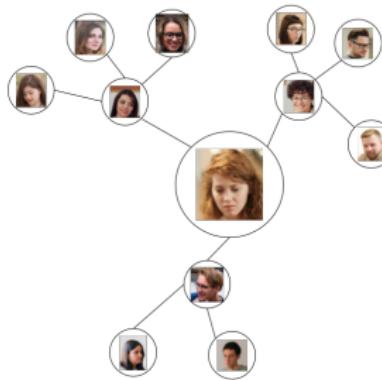


Figure 3: Examples of unconventional tree structures.

Source: Yogatama et al., 2017

Why should we care about discreteness?

- Many data modalities are inherently discrete
 - Graphs



- Text, DNA Sequences, Program Source Code, Molecules, and lots more

Stochastic Optimization

- Consider the following optimization problem

$$\max_{\phi} E_{q_{\phi}(z)}[f(z)]$$

- Recap example: Think of $q(\cdot)$ as the inference distribution for a VAE

$$\max_{\theta, \phi} E_{q_{\phi}(z|x)} \left[\log \frac{p_{\theta}(x, z)}{q_{\phi}(z|x)} \right].$$

- Gradients w.r.t. θ can be derived via linearity of expectation

$$\begin{aligned} \nabla_{\theta} E_{q_{\phi}(z|x)} [\log p_{\theta}(x, z) - \log q_{\phi}(z | x)] &= E_{q_{\phi}(z|x)} [\nabla_{\theta} \log p_{\theta}(x, z)] \\ &\approx \frac{1}{k} \sum_k \nabla_{\theta} \log p_{\theta}(x, z^k) \end{aligned}$$

- If z is continuous, $q_{\phi}(\cdot)$ is reparameterizable, and $f(\cdot)$ is differentiable, then we can use reparameterization to compute gradients w.r.t. ϕ

Stochastic Optimization with Reparameterization

Consider the following optimization problem

$$\max_{\phi} E_{q_{\phi}(\mathbf{z})}[f(\mathbf{z})]$$

Reparameterization trick:

- $\epsilon \sim p(\epsilon)$
- $\mathbf{z} = g_{\phi}(\epsilon) \sim q_{\phi}(\mathbf{z})$
- $E_{q_{\phi}(\mathbf{z})}[f(\mathbf{z})] = E_{\epsilon \sim p(\epsilon)}[f(g_{\phi}(\epsilon))]$
- Gradient ascent:

$$\begin{aligned}\nabla_{\phi} E_{q_{\phi}}(\mathbf{z})[f(\mathbf{z})] &= \nabla_{\phi} E_{\epsilon \sim p(\epsilon)}[f(g_{\phi}(\epsilon))] \\ &= E_{\epsilon \sim p(\epsilon)}[\nabla_{\phi} f(g_{\phi}(\epsilon))] \\ &= E_{\epsilon \sim p(\epsilon)}[\nabla_{\mathbf{z}} f(\mathbf{z}) \nabla_{\phi} g_{\phi}(\epsilon)]\end{aligned}$$

Assumptions: $f(\mathbf{z})$ is differentiable, and $q_{\phi}(\mathbf{z})$ is reparameterizable.

What if either of the above assumptions fails?

Stochastic Optimization with the log derivative trick

- Consider the following optimization problem

$$\max_{\phi} E_{q_{\phi}(z)}[f(z)]$$

- For many class of problem scenarios, reparameterization trick is infeasible
- Scenario 1:** $f(\cdot)$ is non-differentiable in z e.g., optimizing a black box reward function in reinforcement learning
- Scenario 2:** $q_{\phi}(z)$ cannot be reparameterized as a differentiable function of ϕ with respect to a fixed base distribution e.g., discrete distributions
- The log derivative trick gives a general-purpose solution to both these scenarios
- We will first analyze it in the context of **bandit problems** and then extend it to **latent variable models** with discrete latent variables

Multi-armed bandits



- Example: Pulling arms of slot machines—which arm to pull?
- Set A of possible actions. E.g., pull arm 1, arm 2, . . . , etc.
- Each action $\mathbf{z} \in A$ has a reward $f(\mathbf{z})$
- Randomized policy for choosing actions $q_\phi(\mathbf{z})$ parameterized by ϕ .
For example, ϕ could be the parameters of a categorical distribution
- **Goal:** Learn the parameters ϕ that maximize our earnings (in expectation)

$$\max_{\phi} E_{q_\phi(\mathbf{z})}[f(\mathbf{z})]$$

Log derivative trick for gradient estimation

- Want to compute a gradient with respect to ϕ of the expected reward

$$E_{q_\phi(\mathbf{z})}[f(\mathbf{z})] = \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z})$$

$$\begin{aligned} \frac{\partial}{\partial \phi_i} E_{q_\phi(\mathbf{z})}[f(\mathbf{z})] &= \sum_{\mathbf{z}} \frac{\partial q_\phi(\mathbf{z})}{\partial \phi_i} f(\mathbf{z}) = \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{1}{q_\phi(\mathbf{z})} \frac{\partial q_\phi(\mathbf{z})}{\partial \phi_i} f(\mathbf{z}) \\ &= \sum_{\mathbf{z}} q_\phi(\mathbf{z}) \frac{\partial \log q_\phi(\mathbf{z})}{\partial \phi_i} f(\mathbf{z}) = E_{q_\phi(\mathbf{z})} \left[\frac{\partial \log q_\phi(\mathbf{z})}{\partial \phi_i} f(\mathbf{z}) \right] \end{aligned}$$

Log derivative trick for gradient estimation

- Want to compute a gradient with respect to ϕ of

$$E_{q_\phi(z)}[f(z)] = \sum_z q_\phi(z) f(z)$$

- The log derivative trick gives

$$\nabla_\phi E_{q_\phi(z)}[f(z)] = E_{q_\phi(z)} [f(z) \nabla_\phi \log q_\phi(z)]$$

- We can now construct a Monte Carlo estimate
- Sample z^1, \dots, z^K from $q_\phi(z)$ and estimate

$$\nabla_\phi E_{q_\phi(z)}[f(z)] \approx \frac{1}{K} \sum_k f(z^k) \nabla_\phi \log q_\phi(z^k)$$

- Assumption: The distribution $q(\cdot)$ is easy to sample from and evaluate probabilities
- Works for both discrete and continuous distributions

Variational Learning of Latent Variable Models

- To learn the variational approximation we need to compute the gradient with respect to ϕ of

$$\begin{aligned}\mathcal{L}(\mathbf{x}; \theta, \phi) &= \sum_{\mathbf{z}} q_{\phi}(\mathbf{z}|\mathbf{x}) \log p_{\theta}(\mathbf{x}, \mathbf{z}) + H(q_{\phi}(\mathbf{z}|\mathbf{x})) \\ &= E_{q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x}, \mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x})]\end{aligned}$$

- The function inside the brackets also depends on ϕ (and θ, \mathbf{x}). Want to compute a gradient with respect to ϕ of

$$E_{q_{\phi}(\mathbf{z}|\mathbf{x})} [f(\phi, \theta, \mathbf{z}, \mathbf{x})] = \sum_{\mathbf{z}} q_{\phi}(\mathbf{z}|\mathbf{x}) f(\phi, \theta, \mathbf{z}, \mathbf{x})$$

- The log derivative trick yields

$$\nabla_{\phi} E_{q_{\phi}(\mathbf{z}|\mathbf{x})} [f(\phi, \theta, \mathbf{z}, \mathbf{x})] = E_{q_{\phi}(\mathbf{z}|\mathbf{x})} [f(\phi, \theta, \mathbf{z}, \mathbf{x}) \nabla_{\phi} \log q_{\phi}(\mathbf{z}|\mathbf{x}) + \nabla_{\phi} f(\phi, \theta, \mathbf{z}, \mathbf{x})]$$

- We can now construct a Monte Carlo estimate of $\nabla_{\phi} \mathcal{L}(\mathbf{x}; \theta, \phi)$

The log derivative trick has high variance

- Want to compute a gradient with respect to ϕ of

$$E_{q_\phi(\mathbf{z})}[f(\mathbf{z})] = \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z})$$

- The log derivative trick is

$$\nabla_\phi E_{q_\phi(\mathbf{z})}[f(\mathbf{z})] = E_{q_\phi(\mathbf{z})} [f(\mathbf{z}) \nabla_\phi \log q_\phi(\mathbf{z})]$$

- Monte Carlo estimate: Sample $\mathbf{z}^1, \dots, \mathbf{z}^K$ from $q_\phi(\mathbf{z})$

$$\nabla_\phi E_{q_\phi(\mathbf{z})}[f(\mathbf{z})] \approx \frac{1}{K} \sum_k f(\mathbf{z}^k) \nabla_\phi \log q_\phi(\mathbf{z}^k) := f_{\text{MC}}(\mathbf{z}^1, \dots, \mathbf{z}^K)$$

- Monte Carlo estimates of gradients are unbiased

$$E_{\mathbf{z}^1, \dots, \mathbf{z}^K \sim q_\phi(\mathbf{z})} [f_{\text{MC}}(\mathbf{z}^1, \dots, \mathbf{z}^K)] = \nabla_\phi E_{q_\phi(\mathbf{z})}[f(\mathbf{z})]$$

- Almost never used in practice because of high variance
- Variance can be reduced via carefully designed control variates

Control Variates

- The log derivative trick gives

$$\nabla_{\phi} E_{q_{\phi}(\mathbf{z})}[f(\mathbf{z})] = E_{q_{\phi}(\mathbf{z})}[f(\mathbf{z}) \nabla_{\phi} \log q_{\phi}(\mathbf{z})]$$

- Given any constant B (a control variate)

$$\nabla_{\phi} E_{q_{\phi}(\mathbf{z})}[f(\mathbf{z})] = E_{q_{\phi}(\mathbf{z})}[(f(\mathbf{z}) - B) \nabla_{\phi} \log q_{\phi}(\mathbf{z})]$$

- To see why,

$$\begin{aligned} E_{q_{\phi}(\mathbf{z})}[B \nabla_{\phi} \log q_{\phi}(\mathbf{z})] &= B \sum_{\mathbf{z}} q_{\phi}(\mathbf{z}) \nabla_{\phi} \log q_{\phi}(\mathbf{z}) = B \sum_{\mathbf{z}} \nabla_{\phi} q_{\phi}(\mathbf{z}) \\ &= B \nabla_{\phi} \sum_{\mathbf{z}} q_{\phi}(\mathbf{z}) = B \nabla_{\phi} 1 = 0 \end{aligned}$$

- Monte Carlo gradient estimates of both $f(\mathbf{z})$ and $f(\mathbf{z}) - B$ have same expectation
- These estimates can however have different variances

Control variates

- Suppose we want to compute

$$E_{q_\phi(\mathbf{z})}[f(\mathbf{z})] = \sum_{\mathbf{z}} q_\phi(\mathbf{z}) f(\mathbf{z})$$

- Define

$$\hat{f}(\mathbf{z}) = f(\mathbf{z}) + a(h(\mathbf{z}) - E_{q_\phi(\mathbf{z})}[h(\mathbf{z})])$$

- $h(\mathbf{z})$ is referred to as a control variate
- Assumption: $E_{q_\phi(\mathbf{z})}[h(\mathbf{z})]$ is known
- Monte Carlo gradient estimates of $f(\mathbf{z})$ and $\hat{f}(\mathbf{z})$ have the same expectation

$$E_{\mathbf{z}^1, \dots, \mathbf{z}^K \sim q_\phi(\mathbf{z})}[\hat{f}_{\text{MC}}(\mathbf{z}^1, \dots, \mathbf{z}^K)] = E_{\mathbf{z}^1, \dots, \mathbf{z}^K \sim q_\phi(\mathbf{z})}[f_{\text{MC}}(\mathbf{z}^1, \dots, \mathbf{z}^K)]$$

but different variances

- Can try to learn and update the control variate during training

Control variates

- Deriving an alternate Monte Carlo estimate for log derivative gradients based on control variates
- Sample $\mathbf{z}^1, \dots, \mathbf{z}^K$ from $q_\phi(\mathbf{z})$

$$\begin{aligned}& \nabla_\phi E_{q_\phi(\mathbf{z})}[f(\mathbf{z})] \\&= \nabla_\phi E_{q_\phi(\mathbf{z})}[f(\mathbf{z}) + a(h(\mathbf{z}) - E_{q_\phi(\mathbf{z})}[h(\mathbf{z})])] \\&\approx \frac{1}{K} \sum_k f(\mathbf{z}^k) \nabla_\phi \log q_\phi(\mathbf{z}^k) + a \left(\frac{1}{K} \sum_{k=1}^K h(\mathbf{z}^k) - E_{q_\phi(\mathbf{z})}[h(\mathbf{z})] \right) \\&:= f_{\text{MC}}(\mathbf{z}^1, \dots, \mathbf{z}^K) + a \left(h_{\text{MC}}(\mathbf{z}^1, \dots, \mathbf{z}^K) - E_{q_\phi(\mathbf{z})}[h(\mathbf{z})] \right) \\&:= \hat{f}_{\text{MC}}(\mathbf{z}^1, \dots, \mathbf{z}^K)\end{aligned}$$

- What is $\text{Var}(\hat{f}_{\text{MC}})$ vs. $\text{Var}(f_{\text{MC}})$?

Control variates

- Comparing $\text{Var}(\hat{f}_{\text{MC}})$ vs. $\text{Var}(f_{\text{MC}})$

$$\begin{aligned}\text{Var}(\hat{f}_{\text{MC}}) &= \text{Var}(f_{\text{MC}} + a \left(h_{\text{MC}} - E_{q_\phi(\mathbf{z})}[h(\mathbf{z})] \right)) \\ &= \text{Var}(f_{\text{MC}} + ah_{\text{MC}}) \\ &= \text{Var}(f_{\text{MC}}) + a^2 \text{Var}(h_{\text{MC}}) + 2a \text{Cov}(f_{\text{MC}}, h_{\text{MC}})\end{aligned}$$

- To get the optimal coefficient a^* that minimizes the variance, take derivatives w.r.t. a and set them to 0

$$a^* = -\frac{\text{Cov}(f_{\text{MC}}, h_{\text{MC}})}{\text{Var}(h_{\text{MC}})}$$

Control variates

- Comparing $\text{Var}(\hat{f}_{\text{MC}})$ vs. $\text{Var}(f_{\text{MC}})$

$$\text{Var}(\hat{f}_{\text{MC}}) = \text{Var}(f_{\text{MC}}) + a^2 \text{Var}(h_{\text{MC}}) + 2a \text{Cov}(f_{\text{MC}}, h_{\text{MC}})$$

- Setting the coefficient $a = a^* = -\frac{\text{Cov}(f_{\text{MC}}, h_{\text{MC}})}{\text{Var}(h_{\text{MC}})}$

$$\begin{aligned}\text{Var}(\hat{f}_{\text{MC}}) &= \text{Var}(f_{\text{MC}}) - \frac{\text{Cov}(f_{\text{MC}}, h_{\text{MC}})^2}{\text{Var}(h_{\text{MC}})} \\ &= \text{Var}(f_{\text{MC}}) - \frac{\text{Cov}(f_{\text{MC}}, h_{\text{MC}})^2}{\text{Var}(h_{\text{MC}})\text{Var}(f_{\text{MC}})} \text{Var}(f_{\text{MC}}) \\ &= (1 - \rho(f_{\text{MC}}, h_{\text{MC}})^2) \text{Var}(f_{\text{MC}})\end{aligned}$$

- Correlation coefficient $\rho(f_{\text{MC}}, h_{\text{MC}})$ is between -1 and 1. For maximum variance reduction, we want f_{MC} and h_{MC} to be highly correlated

Neural Variational Inference and Learning (NVIL)

- Latent variable models with discrete latent variables are often referred to as belief networks
- Variational learning objective is same as ELBO

$$\begin{aligned}\mathcal{L}(\mathbf{x}; \theta, \phi) &= \sum_{\mathbf{z}} q_{\phi}(\mathbf{z}|\mathbf{x}) \log p_{\theta}(\mathbf{x}, \mathbf{z}) + H(q_{\phi}(\mathbf{z}|\mathbf{x})) \\ &= E_{q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}, \mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x})] \\ &:= E_{q_{\phi}(\mathbf{z}|\mathbf{x})}[f(\phi, \theta, \mathbf{z}, \mathbf{x})]\end{aligned}$$

- Here, \mathbf{z} is discrete and hence we cannot use reparameterization

Neural Variational Inference and Learning (NVIL)

- NVIL (Mnih&Gregor, 2014) learns belief networks via the log derivative trick + control variates
- **Control Variate 1:** Constant baseline B
- **Control Variate 2:** Input dependent baseline $h_\psi(\mathbf{x})$
- Gradient ascent w.r.t. ϕ with the log derivative trick + control variates

$$\nabla_\phi \mathcal{L}(\mathbf{x}; \theta, \phi, \psi, B)$$

$$= E_{q_\phi(\mathbf{z}|\mathbf{x})} [(f(\phi, \theta, \mathbf{z}, \mathbf{x}) - h_\psi(\mathbf{x}) - B) \nabla_\phi \log q_\phi(\mathbf{z}|\mathbf{x}) + \nabla_\phi f(\phi, \theta, \mathbf{z}, \mathbf{x})]$$

- Gradient ascent w.r.t. θ
- Optimize ψ, B to minimize $E_{q_\phi(\mathbf{z}|\mathbf{x})} [(f(\phi, \theta, \mathbf{z}, \mathbf{x}) - h_\psi(\mathbf{x}) - B)^2]$

Towards reparameterized, continuous relaxations

- Consider the following optimization problem

$$\max_{\phi} E_{q_{\phi}(z)}[f(z)]$$

- Reparameterization trick is not directly applicable for discrete z
- The log derivative trick is a general-purpose solution, but needs careful design of control variates
- Next:** Relax z to a continuous random variable with a reparameterizable distribution

Gumbel Distribution

- Setting: We are given i.i.d. samples y_1, y_2, \dots, y_n from some underlying distribution. How can we model the distribution of

$$g = \max\{y_1, y_2, \dots, y_n\}$$

- E.g., predicting maximum water level in a river based on historical data to detect flooding
- The **Gumbel distribution** is very useful for modeling extreme, rare events, e.g., natural disasters, finance
- CDF for a Gumbel random variable g is parameterized by a location parameter μ and a scale parameter β

$$F(g; \mu, \beta) = \exp \left(-\exp \left(-\frac{g - \mu}{\beta} \right) \right)$$

Categorical Distributions

- Let \mathbf{z} denote a k -dimensional categorical random variable with distribution q parameterized by class probabilities $\pi = \{\pi_1, \pi_2, \dots, \pi_k\}$. We will represent \mathbf{z} as a one-hot vector
- Gumbel-Max reparameterization trick** for sampling from categorical random variables

$$\mathbf{z} = \text{one_hot} \left(\arg \max_i (g_i + \log \pi_i) \right)$$

where g_1, g_2, \dots, g_k are i.i.d. samples drawn from $\text{Gumbel}(0, 1)$

- In words, we can sample from $\text{Categorical}(\pi)$ by taking the $\arg \max$ over k Gumbel perturbed log-class probabilities $g_i + \log \pi_i$;
- Reparametrizable since randomness is transferred to a fixed $\text{Gumbel}(0, 1)$ distribution!
- Problem: $\arg \max$ is non-differentiable w.r.t. π

Relaxing Categorical Distributions to Gumbel-Softmax

- Gumbel-Max Sampler (non-differentiable w.r.t. π):

$$\mathbf{z} = \text{one_hot} \left(\arg \max_i (g_i + \log \pi) \right)$$

- **Key idea:** Replace $\arg \max$ with soft max to get a Gumbel-Softmax random variable $\hat{\mathbf{z}}$
- Output of softmax is differentiable w.r.t. π
- Gumbel-Softmax Sampler (differentiable w.r.t. π):

$$\hat{\mathbf{z}} = \text{soft max}_i \left(\frac{g_i + \log \pi}{\tau} \right)$$

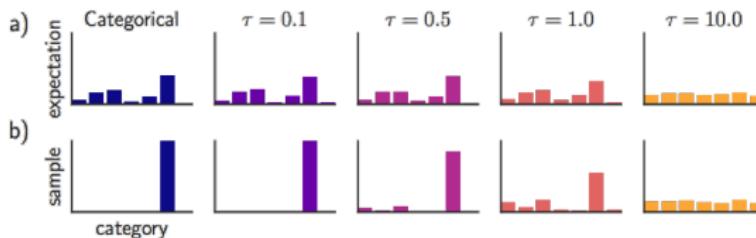
where $\tau > 0$ is a tunable parameter referred to as the temperature

Bias-variance tradeoff via temperature control

- Gumbel-Softmax distribution is parameterized by both class probabilities π and the temperature $\tau > 0$

$$\hat{\mathbf{z}} = \text{soft max}_i \left(\frac{g_i + \log \pi}{\tau} \right)$$

- Temperature τ controls the degree of the relaxation via a bias-variance tradeoff

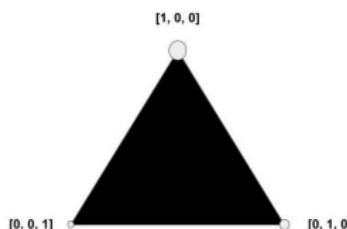


Source: Jang et al., 2017

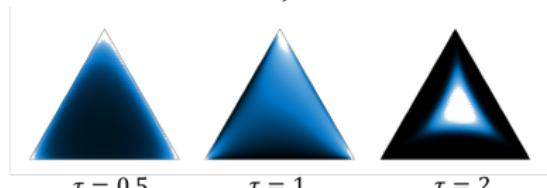
- As $\tau \rightarrow 0$, samples from $\text{Gumbel-Softmax}(\pi, \tau)$ are similar to samples from $\text{Categorical}(\pi)$
Pro: low bias in approximation **Con:** High variance in gradients
- As $\tau \rightarrow \infty$, samples from $\text{Gumbel-Softmax}(\pi, \tau)$ are similar to samples from $\text{Categorical}\left(\left[\frac{1}{k}, \frac{1}{k}, \dots, \frac{1}{k}\right]\right)$ (i.e., uniform over k categories)

Geometric Interpretation

- Consider a categorical distribution with class probability vector $\pi = [0.60, 0.25, 0.15]$
- Define a probability simplex with the one-hot vectors as vertices



- For a categorical distribution, all probability mass is concentrated at the vertices of the probability simplex
- Gumbel-Softmax samples points within the simplex (lighter color intensity implies higher probability)



Source: Maddison et al., 2018

Gumbel-Softmax in action

- Original optimization problem

$$\max_{\phi} E_{q_{\phi}(\mathbf{z})}[f(\mathbf{z})]$$

where $q_{\phi}(\mathbf{z})$ is a categorical distribution and $\phi = \pi$

- Relaxed optimization problem

$$\max_{\phi} E_{q_{\phi}(\hat{\mathbf{z}})}[f(\hat{\mathbf{z}})]$$

where $q_{\phi}(\hat{\mathbf{z}})$ is a Gumbel-Softmax distribution and $\phi = \{\pi, \tau\}$

- Usually, temperature τ is explicitly annealed. Start high for low variance gradients and gradually reduce to tighten approximation
Note that $\hat{\mathbf{z}}$ is not a discrete category. If the function $f(\cdot)$ explicitly requires a discrete \mathbf{z} , then we estimate **straight-through gradients**:
 - Use hard $\mathbf{z} \sim \text{Categorical}(\mathbf{z})$ for evaluating objective in forward pass
 - Use soft $\hat{\mathbf{z}} \sim \text{GumbelSoftmax}(\hat{\mathbf{z}}, \tau)$ for evaluating gradients in backward pass

Summary

- Discovering discrete latent structure e.g., categories, rankings, matchings etc. has several applications
- Stochastic Optimization w.r.t. parameterized discrete distributions is challenging
- The log derivative trick is the general purpose technique for gradient estimation, but suffers from high variance
- Control variates can help in controlling the variance
- Continuous relaxations to discrete distributions offer a biased, reparameterizable alternative with the trade-off in significantly lower variance