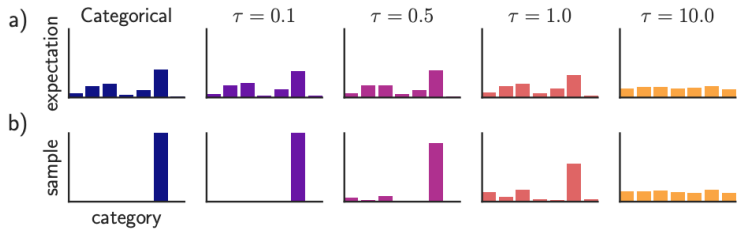
TECHNISCHE UNIVERSITÄT DARMSTADT

Relaxed continuous time Markov chains

Deep generative models such as the variational autoencoder [1] have led to breakthroughs in generating synthetic data from complicated distributions, e.g. natural images. The key ingredient of this success story is a new way of parameter learning via sampling-based variational inference [2]. Suppose one is interested in an intractable Bayesian posterior $p(x \mid y)$ for given data y. The goal is to approximate $p(x \mid y)$ by a tractable parametric family $q_\phi(x)$ where ϕ are variational parameters. To find the best value of ϕ one generates samples for a given ϕ_i. These samples are used to estimate the dissimilarity between $p(x \mid y)$ and $q_{\phi_i}(x)$ as well as the corresponding gradient. This allows to improve the estimate of ϕ via stochastic gradient descent.

The approach sketched above is particularly effective for reparametrizeable distributions. This means that there exists a random variable Z and a function g such that $X := g(Z, \phi)$ has the density $q_\phi(x)$. A simple example would be a normally distributed random variable $X \sim \mathcal{N}(\mu, \sigma^2)$ that can be written as $X = \mu + \sigma Z$ for $Z \sim \mathcal{N}(0, 1)$. The main advantage of reparametrizaion is that it separates the model from the source of randomness. This allows to use standard deep learning libraries such as PyTorch or Tensorflow for automatic gradient computation [3]. Initially, reparametrization has been limited to continuous distributions. Recently, relaxation techniques such as the Gumbel-Softmax approach have been developed that approximate a discrete distribution by a continuous one. The relaxed distribution is then accessible to reparametrization [4, 5].



Continuous relaxation of a categorical distribution. Image rom [4].

Continuous time Markov chains (CTMCs) are stochastic processes with discrete states and exponentially distributed waiting times between the jumps. In systems biology, they are routinely used to describe the time evolution of molecule counts within a cell. Due to their discrete nature and the large number of states, learning CTMCs from biological data is still challenging [6]. The goal of this project is to explore relaxation techniques for CTMC simulation. This may pave the way for powerful simulation-based inference techniques and combinations of CTMCs with deep learning architectures.

Requirements:

- Background in statistical machine learning or probabilistic modeling
- Basic Python programming

For further information, please contact Christian Wildner.

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