Implicit Reparameterization Gradients

Michael Figurnov, Shakir Mohamed, Andriy Mnih

Poster: Room 210 #33

DeepMind

Reparameterization gradients

Core part of variational autoencoders, automatic variational inference, etc.

Backpropagation in graphs with continuous random variables

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$$\frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(z)}[f(z)] = \mathbb{E}_{q_\phi(z)} \underbrace{\left[\frac{\partial f(z)}{\partial z} \frac{\partial z}{\partial \phi}\right]}_{\text{backpropagation}}$$

continuous
(Normal, ...)

differentiable
(ELBO, …)

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requires a *tractable* inverse transformation!
Normal, Logistic, …

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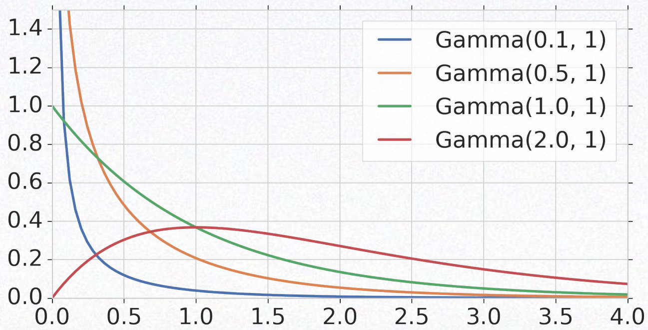
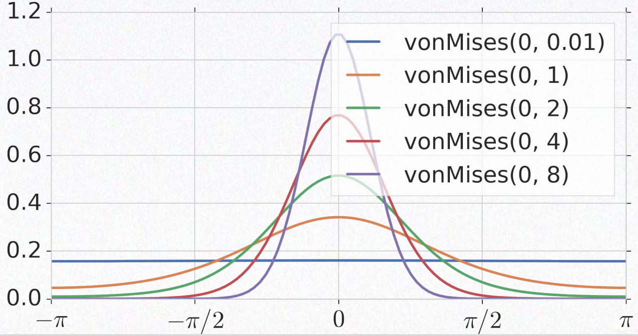
We show how to use *implicit differentiation* for reparameterization of other continuous random variables, such as Gamma and von Mises





Explicit and implicit reparameterization

Cumulative density function $F(z|\phi) \equiv \int_{-\infty}^{z} q_\phi(t)dt = u \sim \text{Uniform}(0,1)$

	Sampling (forward pass)	Gradients (backward pass)
Explicit		
Implicit		

Explicit and implicit reparameterization

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Derivation: implicit differentiation $\frac{dF(z|\phi)}{d\phi} = \frac{du}{d\phi}$

$$\underbrace{\frac{\partial F(z|\phi)}{\partial z}}_{q_\phi(z)} \frac{\partial z}{\partial \phi} + \frac{\partial F(z|\phi)}{\partial \phi} = 0$$

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often not implemented in numerical libraries

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How to compute $\frac{\partial F(z|\phi)}{\partial \phi}$?

Relative metrics (lower is better)

	Gamma		Von Mises	
Method	Error	Time	Error	Time
Automatic differentiation of the CDF code	**1x**	**1x**	**1x**	**1x**
Finite difference	832x	2x	514x	1.2x
Jankowiak & Obermeyer (2018) concurrent work; closed-form approximation	18x	5x	-	-

Jankowiak, Obermeyer "Pathwise Derivatives Beyond the Reparameterization Trick." ICML, 2018

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Knowles (2015) approximate *explicit* reparameterization	2840x	63x	-	-

Knowles, "Stochastic gradient variational Bayes for Gamma approximating distributions." arXiv, 2015
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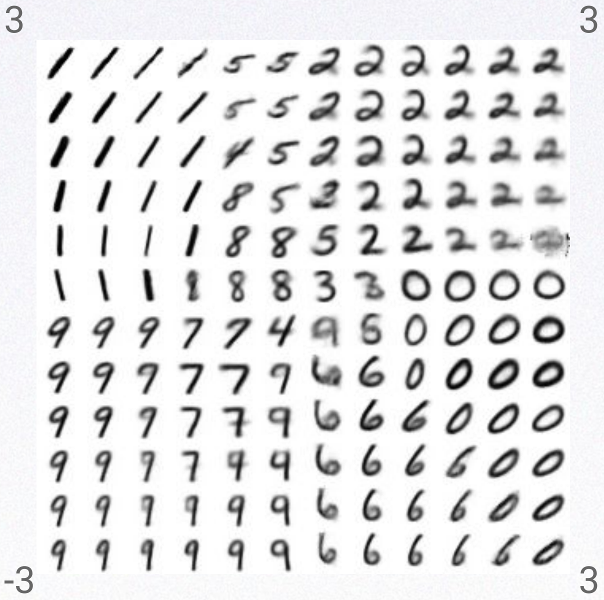
Variational Autoencoder

2D latent spaces for MNIST



Normal prior and posterior

Variational Autoencoder

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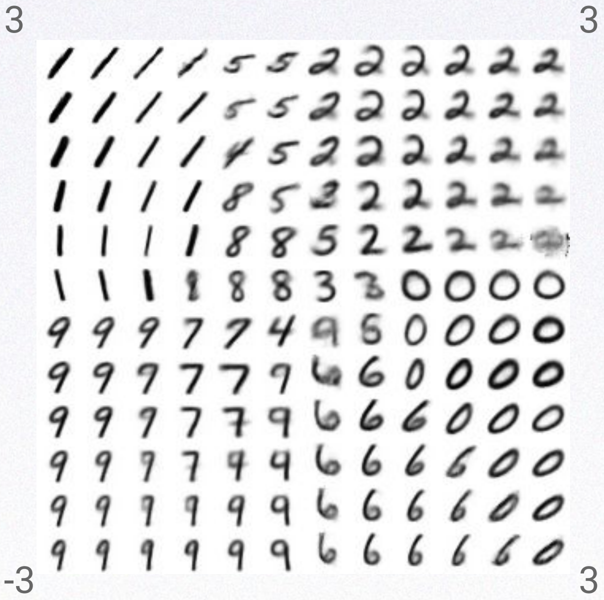

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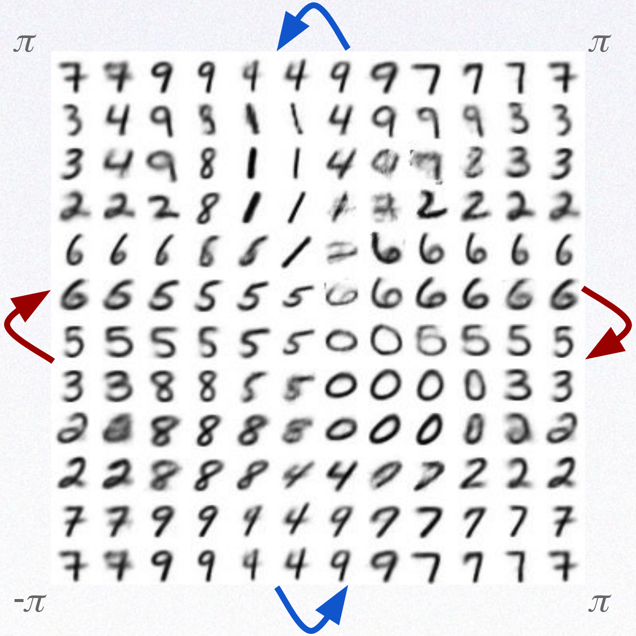

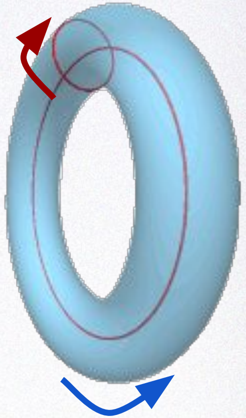

Uniform prior, von Mises posterior

Torus adapted from https://en.wikipedia.org/wiki/Torus#/media/File:Sphere-like_degenerate_torus.gif

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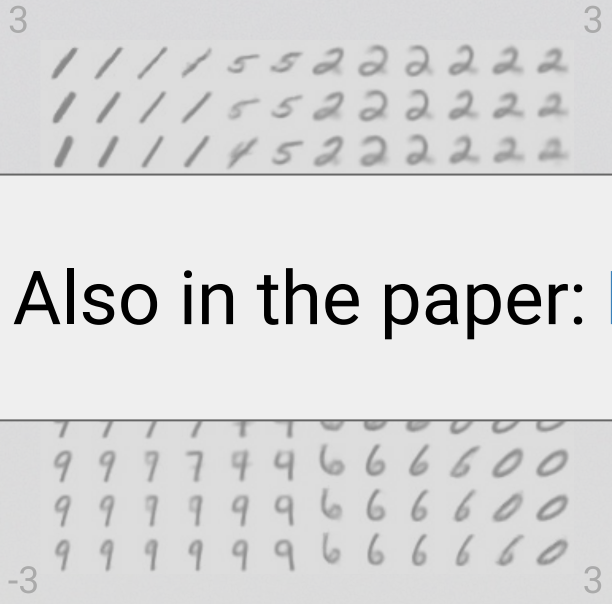
Also in the paper: **Latent Dirichlet Allocation**



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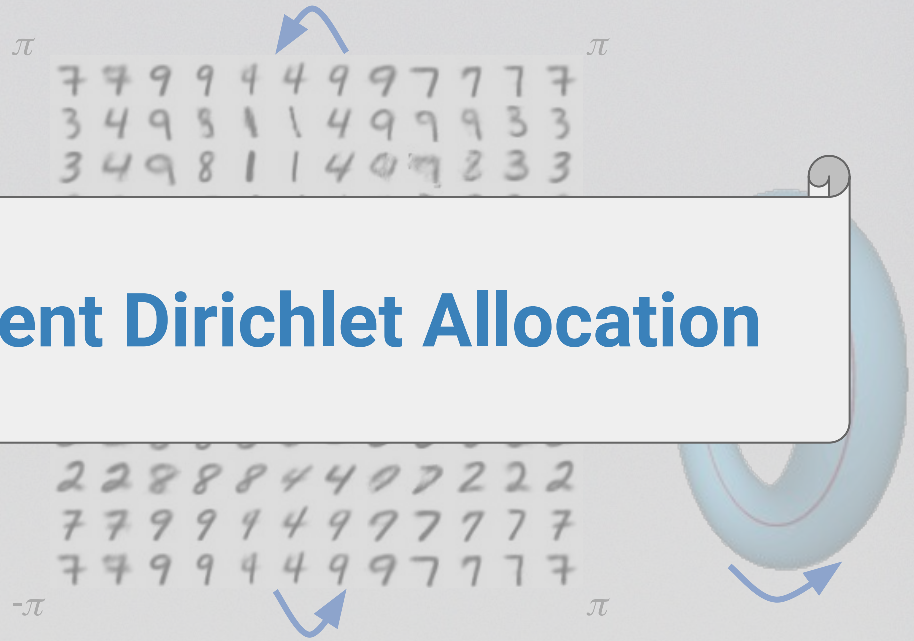

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Implicit Reparameterization Gradients

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- A more general view of the reparameterization gradients
  - Decouple sampling from gradient estimation
- Reparameterization gradients for Gamma, von Mises, Beta, Dirichlet, ...
  - Faster and more accurate than the alternatives
  - Implemented in TensorFlow Probability:
    `tfp.distributions.{Gamma,VonMises,Beta,Dirichlet,...}`
- Move away from making modelling choices for computational convenience

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