Computational Statistics Hyperspherical VAE

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- 1. Introduction
- 2. Sampling method
- 3. Reparameterization Trick
- 4. Experiments on link prediction
- 5. Conclusion and Discussion





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Introduction

2018 paper from Tim R. Davidson et al. [DFDC+]

- Replacing the Gaussian prior and approximate posterior distributions with a von Mises-Fisher distribution
- Goal: better model data with a hyperspherical latent structure
- ullet Various experiments, where the $\mathcal{S}\text{-VAE}$ (von Mises-Fisher distributions) often outperforms the $\mathcal{N}\text{-VAE}$ (Gaussian distributions) in low dimensions





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Ines

Démontrer que la méthode de sampling marche





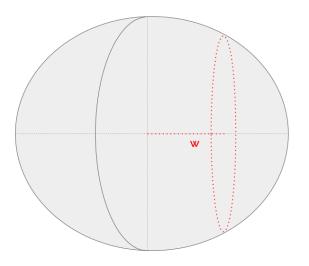
Sampling w from $g(w|\kappa, \theta)$



 S^2 : unit sphere in \mathbb{R}^3

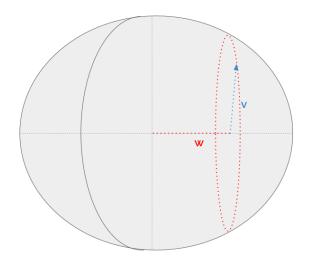


Sampling w



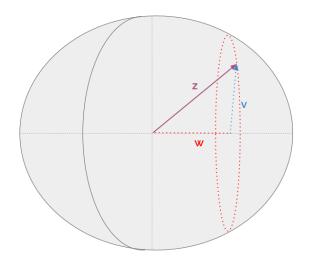


Sampling w





Sampling w





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Reparameterization Trick

The authors use a reparameterization trick that has been extended to distributions that can be sampled using rejection sampling [NRLB20].

Algorithm 1 Reparameterized Rejection Sampling (from [NRLB20])

- 1: $i \leftarrow 0$
- 2: repeat
- 3: $i \leftarrow i + 1$
- 4: Propose $\varepsilon_i \sim s(\varepsilon)$
- 5: Simulate $u_i \sim \mathcal{U}[0,1]$
- 6: **until** $u_i < \frac{g(h(\varepsilon_i,\theta);\bar{\theta})}{r(h(\varepsilon_i,\theta);\theta)}$
- 7: **return** ε_i



Monte Carlo estimation

By noting $\pi(\varepsilon|\theta)$ the distribution of the resulting ε , we have

$$abla_{ heta} \mathbb{E}_{g(arepsilon| heta)}[...] = \mathbb{E}_{\pi(arepsilon| heta)}[...] \ " = \mathbb{E}_{(arepsilon_i,U_i)_i}[...]"$$

Problem: $(\varepsilon_i, U_i)_{i \in \mathbb{N}}$ is not a random variable (it is a stochastic process) No reference to a convergence proof in [DFDC⁺, NRLB20, PBJ12, MG14]





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Experiments on link prediction

- Expliquer l'expérience (tâche à faire, données, negative sampling) reproduire l'experience
- data (Ines)
- implementer les modèles (Victor VGAE)
- gradients pour le hyperspherical VAE
- courbes d'entraînement dans le cas normal
- entrainement et evaluation





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Conclusion and Discussion

- Quite meaningful contribution in low dimensions
- \bullet Algorithm not really useful in high dimensions, due to vanishing surface problem and soap bubble effect of the $\mathcal{N}\textsc{-VAE}$
- Much less variance parameters (1 vs. d for $\mathcal{N}\text{-VAE}$), so possibly less expressivity
- vérifier différentes dimensions de l'espace latent
- et algo vraiment utile en petite ou moyenne dimension ?



References

Tim R. Davidson, Luca Falorsi, Nicola De Cao, Thomas Kipf, and Jakub M. Tomczak.

Hyperspherical variational auto-encoders.

- Andriy Mnih and Karol Gregor.

 Neural variational inference and learning in belief networks, 2014.
- Christian A. Naesseth, Francisco J. R. Ruiz, Scott W. Linderman, and David M. Blei.

Reparameterization gradients through acceptance-rejection sampling algorithms, 2020.

John Paisley, David Blei, and Michael Jordan. Variational bayesian inference with stochastic search, 2012.

