# 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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# Sampling z' from vMF

### **Algorithm 1** Overview of the sampling method from $vMF(\mu, \kappa)$

- 1: Sample  $z \sim q(z|e_1, \kappa)$  where  $e_1 = (1, 0, ..., 0)$
- 2: Compute Householder reflection  $U(\mu)$  so that  $U(\mu)e_1=\mu$
- 3: **return**  $z' = U(\mu)z$





## Sampling z from vMF

#### **Algorithm 2** Overview of the sampling method from $vMF(\mu, \kappa)$

- 1: Sample  $z \sim q(z|e_1, \kappa)$  where  $e_1 = (1, 0, \dots, 0)$
- 2: Sample  $w \in \mathbb{R} \sim g(w|\kappa)$  by acceptance rejection sampling
- 3: Sample  $v \in \mathbb{R}^{d-1} \sim \mathcal{U}(S^{d-2})$  (uniform on the hypersphere  $S^{d-2}$  independent of w)
- 4:  $z \leftarrow (w, \sqrt{1-w^2}v^T)^T$
- 5: Compute Householder reflection  $U(\mu)$  so that  $U(\mu)e_1=\mu$
- 6: **return**  $z' = U(\mu)z \sim q(z'|\mu,\kappa)$





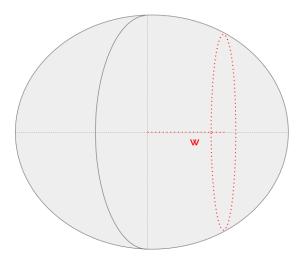
# Sampling w from $g(w|\kappa, \theta)$



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



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



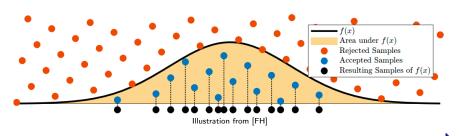
Sample  $w \in \mathbb{R} \sim g(w|\kappa,d)$  by acceptance rejection sampling



# Sampling w from $g(w|\kappa)$

#### Generale case

- Sample target distribution  $w \in \mathbb{R} \sim g(w|\kappa)$  by sampling a proposal  $w_{prop}$  of known density  $r(w|\kappa)$
- Perform backpropagation by reparameterizing  $r(w|\kappa)$  so that the sampling is independent of the parameters
- Note that r is not explicitly given in the article





# Sampling w from $g(w|\kappa)$

- $\blacksquare$  Case d=3: faster to use inverse transformation method
  - The vMF distribution explicity writes :

$$f_{vMF}(z) = \frac{\kappa}{4\pi \ sinh(\kappa)} exp(\kappa \mu^T z)$$

•  $(w, \sqrt{1-w^2}v^T)^T \sim vMF(e_1, \kappa)$  where  $v \sim S^2$  and  $w \in [-1, 1]$  has density

$$f_W(w) = \frac{\kappa}{2 \ sinh(\kappa)} exp(\kappa w)$$

• We compute its cumulative distribution function  $F_W(w)$  and its inverse

$$F_W^{-1}(u) = \frac{1}{\kappa} ln(\exp(-\kappa) + 2 \sinh(\kappa)u)$$

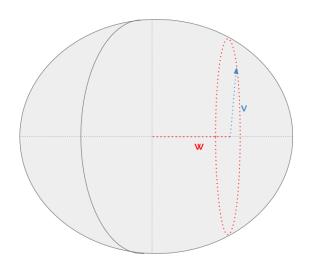
• As  $sinh(\kappa)$  is numerically instable, we rewrites

$$F_W^{-1}(u) = 1 + \frac{1}{\kappa} ln(u + (1 - u)exp(-2\kappa))$$





# Sampling $\nu$ from $\mathcal{U}(S^{d-2})$



Sample  $v \in \mathbb{R}^{d-1} \sim \mathcal{U}(S^{d-2})$ 



# Sampling v from $\mathcal{U}(S^{d-2})$

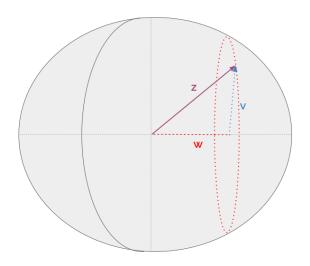
- $\mathcal{N}(0, I_{d-1})$  is rotationally symmetric around the origin
- $f_{Y_1,...,Y_{d-1}} = \frac{1}{\sqrt{2\pi}^{d-1}} exp(-(Y_1^2 + \cdots + Y_{d-1}^2)/2) = \frac{1}{\sqrt{2\pi}^{d-1}} exp(-1^2/2)$  which is constant in all of the angular variables.

### **Algorithm 3** Sampling v from $\mathcal{U}(S^{d-2})$

- 1: Generate d-1 iid variables  $(X_i)$  from  $\mathcal{N}(0,1)$
- 2:  $Y_i \leftarrow \frac{X_i}{\sqrt{X_1^1 + \dots + X_{d-1}^2}}$
- 3: **return**  $(Y_i)_{i=1,...,d-1} \sim \mathcal{U}(S^{d-2})$



# Sampling z from $q(z|e_1, \kappa)$



$$z = (w, \sqrt{1 - w^2}v^T)^T$$



### Transform z

### **Algorithm 4** Overview of the sampling method from $vMF(\mu, \kappa)$

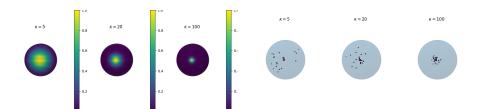
```
Require: \mu \in \mathbb{R}^d, \kappa \in \mathbb{R}_+
```

- 1: Sample  $z \sim q(z|e_1, \kappa)$  where  $e_1 = (1, 0, ..., 0)$
- 2: Compute Householder reflection  $U(\mu)$  so that  $U(\mu)e_1=\mu$
- 3:  $u \leftarrow Normalize(e_1 \mu)$
- 4:  $U \leftarrow I 2uu^T$
- 5: **return**  $z' = U(\mu)z$





# Sampling results







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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 5 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**  $u_i < \frac{g(h(\varepsilon_i,\theta);\theta)}{r(h(\varepsilon_i,\theta);\theta)}$
- 7: return  $\varepsilon_i$



### Monte Carlo estimation

By noting  $\pi(\varepsilon|\theta)$  the distribution of the resulting  $\varepsilon$ , 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<sup>+</sup>, NRLB20, PBJ12, MG14]





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### Experiments on link prediction

- Link prediction on a graph dataset: given a graph with some edges removed, predict the likelihood for each pair of nodes to be connected by an edge
- Cora dataset [MNRS00]: 2708 publications, 5429 links, 1433-dimensional feature vectors
- Using a Variational Graph Auto-Encoder [KW]: a variational encoder which uses a graph neural network (GNN) as encoder
- Reconstruction loss:

$$\mathbb{E}_{q(\mathbf{Z}|\mathbf{X},\mathbf{A})}(\log p(\mathbf{A}|\mathbf{Z})) \quad \text{where} p(\mathbf{A}|\mathbf{Z}) = \prod_{i=1}^{N} \prod_{j=1}^{N} p(A_{i,j}|\mathbf{z}_{i},\mathbf{z}_{j})$$

• Negative sampling: in the sum  $\sum_{i,j} \log p(A_{i,j}|\mathbf{z}_i,\mathbf{z}_j)$ , keep all positive edges and one randomly sampled negative edge per positive edge



### **TODO**

#### reproduire l'experience

- data (Ines)
- implementer les modèles (Victor VGAE)
- gradients pour le hyperspherical VAE (Inès)
- courbes d'entraînement dans le cas normal (Victor)
- 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



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