

Computational Statistics

Hyperspherical VAE

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2. Sampling method
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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
- Various experiments, where the \mathcal{S} -VAE (von Mises-Fisher distributions) often outperforms the \mathcal{N} -VAE (Gaussian distributions) in low dimensions



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Algorithm 1 Overview of the sampling method from $\mathcal{S}(\mu, \kappa)$

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

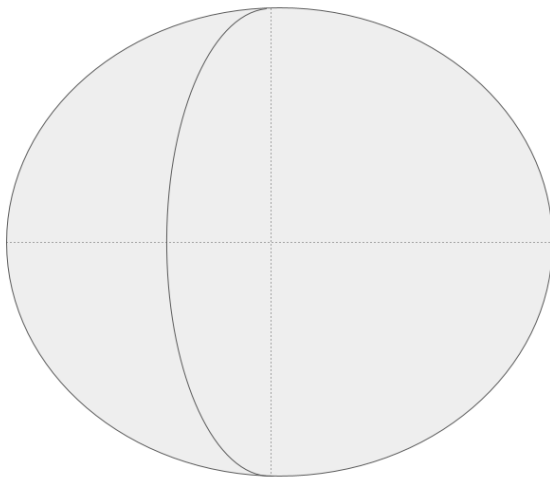


Algorithm 2 Overview of the sampling method from $\mathcal{S}(\mu, \kappa)$

- 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})
 - 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** $z' = U(\mu)z \sim q(z'|\mu, \kappa)$
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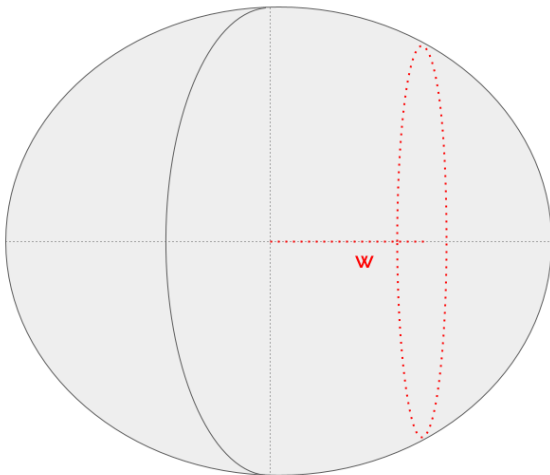
Sampling w from $g(w|\kappa, \theta)$



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

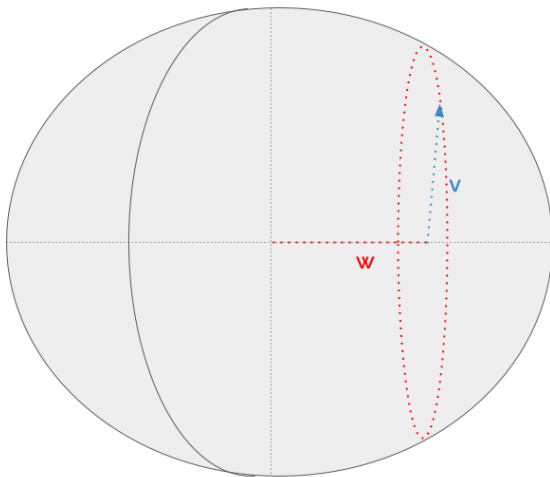


Sampling w from $g(w|\kappa)$

- Case $d = 3$
- Case $d > 3$



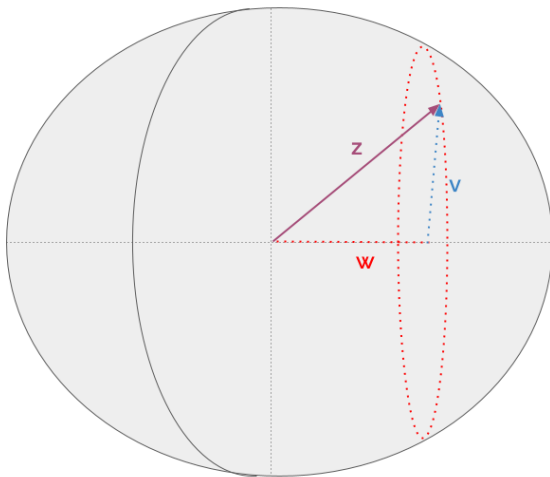
Sampling w from $g(w|\kappa)$



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



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



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



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

Algorithm 3 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  $\varepsilon_i$ 
```



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

$$\nabla_{\theta} \mathbb{E}_{g(\varepsilon|\theta)}[\dots] = \mathbb{E}_{\pi(\varepsilon|\theta)}[\dots] = \mathbb{E}_{(\varepsilon_i, U_i)_i}[\dots]$$

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

- 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



reproduire l'experience

- data (Inès)
- ~~implémenter les modèles~~ (Victor VGAE)
- gradients pour le hyperspherical VAE (Inès)
- courbes d'entraînement dans le cas normal (Victor)
- entraînement et evaluation



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Conclusion and Discussion

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








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-  Thomas N. Kipf and Max Welling.
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-  Andriy Mnih and Karol Gregor.
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-  Andrew Kachites McCallum, Kamal Nigam, Jason Rennie, and Kristie Seymore.
Automating the construction of internet portals with machine learning.
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-  Christian A. Naesseth, Francisco J. R. Ruiz, Scott W. Linderman, and David M. Blei.
Reparameterization gradients through acceptance-rejection sampling algorithms, 2020.



References

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