Computational Statistics

Hyperspherical VAE

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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 $vMF(\mu, \kappa)$

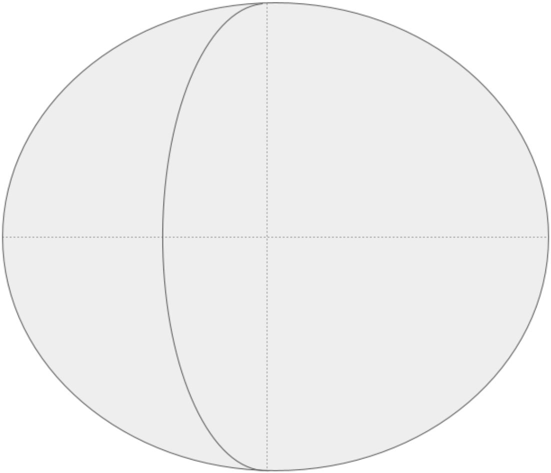
1: Sample $z \sim q(z|e_1, \kappa)$ where $e_1 = (1, 0, \ldots, 0)$
2: Compute Householder reflection $U(\mu)$ so that $U(\mu)e_1 = \mu$
3: **return** $z' = U(\mu)z$

Sampling z from vMF

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

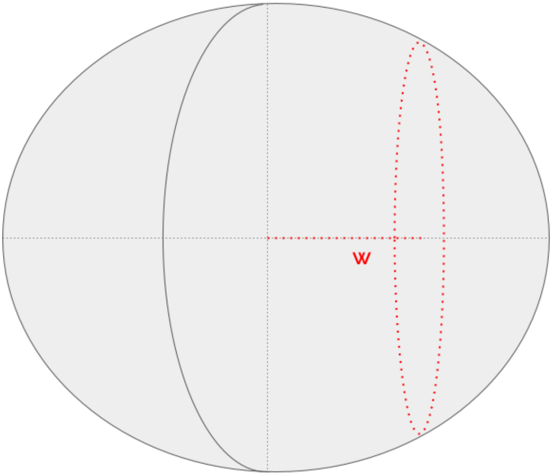
1: Sample $z \sim q(z|e_1, \kappa)$ where $e_1 = (1, 0, \dots, 0)$
2: Sample $w \in \mathbb{R} \sim g(w|\kappa)$ by acceptance rejection sampling
3: Sample $v \in \mathbb{R}^{d-1} \sim \mathcal{U}(S^{d-2})$ (uniform on the hypersphere S^{d-2} independent of w)
4: $z \leftarrow (w, \sqrt{1-w^2}v^T)^T$
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

- **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

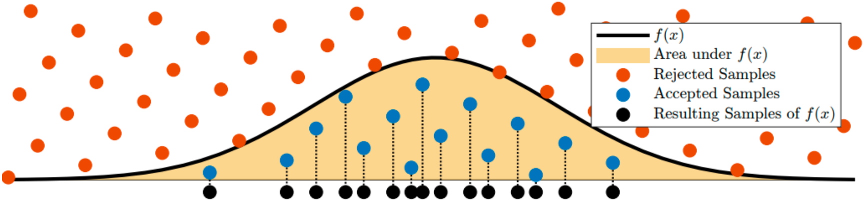


Illustration from [FH]

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

- 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 $v \sim \mathcal{S}^2$ and $w \in [-1, 1]$ has density

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

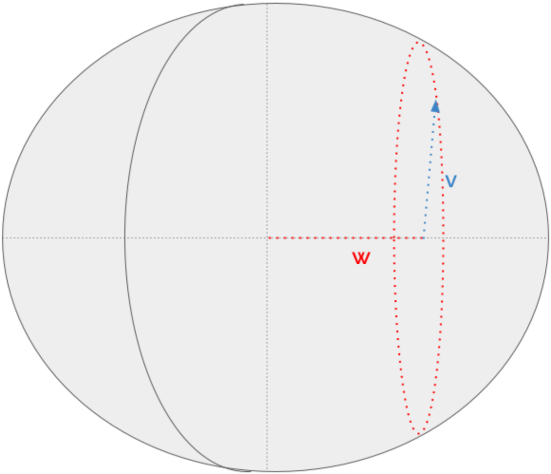
  - We compute its cumulative distribution function $F_W(w)$ and its inverse

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

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

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

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



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

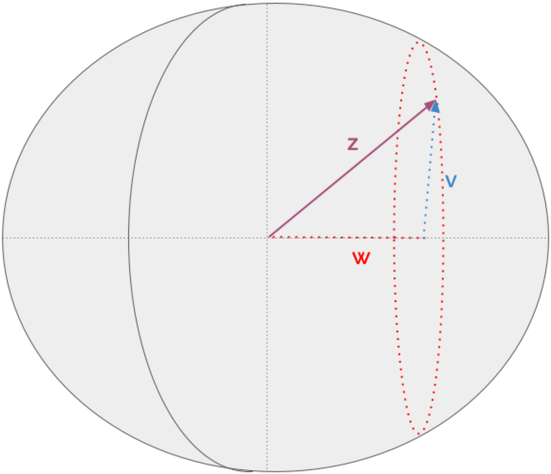
Sampling v from $\mathcal{U}(S^{d-2})$

- $\mathcal{N}(0, I_{d-1})$ is rotationally symmetric around the origin
- $f_{Y_1,\dots,Y_{d-1}} = \frac{1}{\sqrt{2\pi}^{d-1}} exp(-(Y_1^2 + \cdots + Y_{d-1}^2)/2) = \frac{1}{\sqrt{2\pi}^{d-1}} exp(-1^2/2)$ 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: $Y_i \leftarrow \frac{X_i}{\sqrt{X_1^1 + \cdots + X_{d-1}^2}}$
3: **return** $(Y_i)_{i=1,\dots,d-1} \sim \mathcal{U}(S^{d-2})$

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



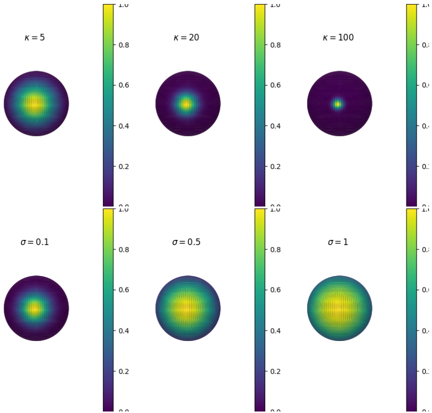
$$z = (w, \sqrt{1 - w^2} v^T)^T$$

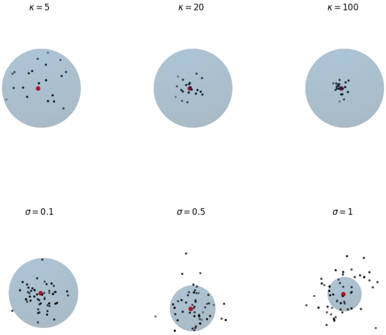
Algorithm 4 Overview of the sampling method from $vMF(\mu, \kappa)$

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

1: Sample $z \sim q(z|e_1, \kappa)$ where $e_1 = (1, 0, \ldots, 0)$
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: $\quad i \leftarrow i + 1$
4: $\quad$ Propose $\varepsilon_i \sim s(\varepsilon)$
5: $\quad$ 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** ε_i

Monte Carlo estimation

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

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

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

- Reconstruction loss
  - $$\mathcal{L}_{recon} = -\mathbb{E}_{q_\psi}(log\ \ p_\phi(x|z))$$
  - $$-\nabla_\kappa \mathcal{L}_{recon} \approx g_{recon} + g_{cor}$$
- KL Divergence
  - $$\mathcal{L}_{\mathcal{KL}} = \mathcal{KL}(q(z|\mu,\kappa)||p(z))$$
  - $$\nabla_\kappa \mathcal{L}_{\mathcal{KL}}$$

The formulas were explicity computed in the article.

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- 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 ?

References

Tim R. Davidson, Luca Falorsi, Nicola De Cao, Thomas Kipf, and Jakub M. Tomczak.
Hyperspherical variational auto-encoders.

Daniel Frisch and Uwe Hanebeck.
Rejection sampling from arbitrary multivariate distributions using generalized fibonacci lattices.

Thomas N. Kipf and Max Welling.
Variational graph auto-encoders.

Andriy Mnih and Karol Gregor.
Neural variational inference and learning in belief networks, 2014.

Andrew Kachites McCallum, Kamal Nigam, Jason Rennie, and Kristie Seymore.
Automating the construction of internet portals with machine learning.
Information Retrieval, 3(2):127–163, 2000.