Computational Statistics

Hyperspherical VAE

Victor Deng Inès Vati

École Normale Supérieure Paris-Saclay, Master MVA

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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
- 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 $\mathcal{S}(\mu, \kappa)$

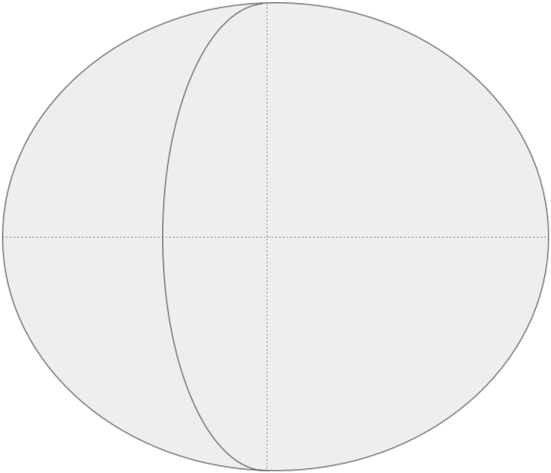
1: Sample $z \sim q(z|e_1, \kappa)$ where $e_1 = (1, 0, \dots, 0)$
2: Compute Householder reflection $U(\mu)$ so that $U(\mu)e_1 = \mu$
3: **return** $z' = U(\mu)z$

Sampling z from vMF

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

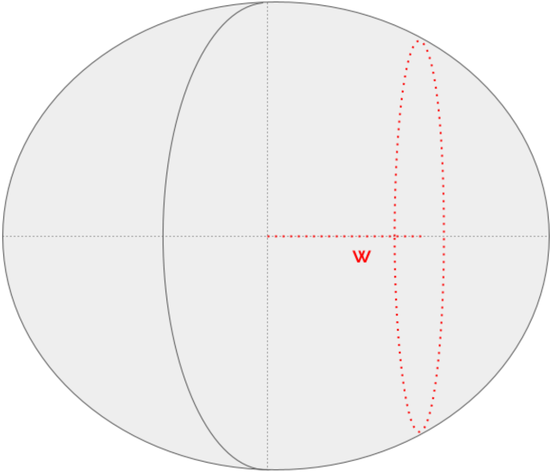
Sample $z \sim q(z|e_1, \kappa)$ where $e_1 = (1, 0, \ldots, 0)$
Sample $w \in \mathbb{R} \sim g(w|\kappa)$ by acceptance rejection sampling
Sample $v \in \mathbb{R}^{d-1} \sim \mathcal{U}(S^{d-2})$ (uniform on the hypersphere S^{d-2})
$z \leftarrow (w, \sqrt{1-w^2}v^T)^T$
Compute Householder reflection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

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



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

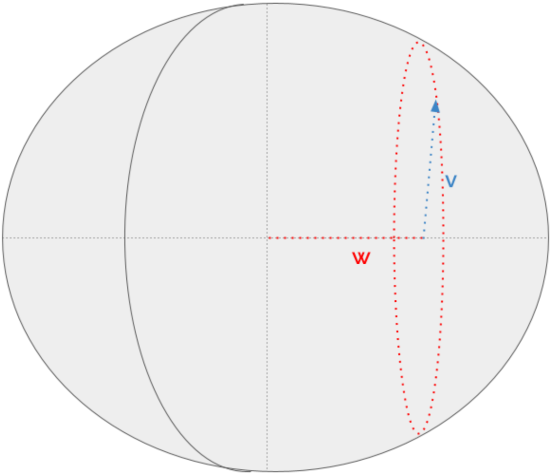
Sampling w from $g(w|\kappa, \theta)$



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

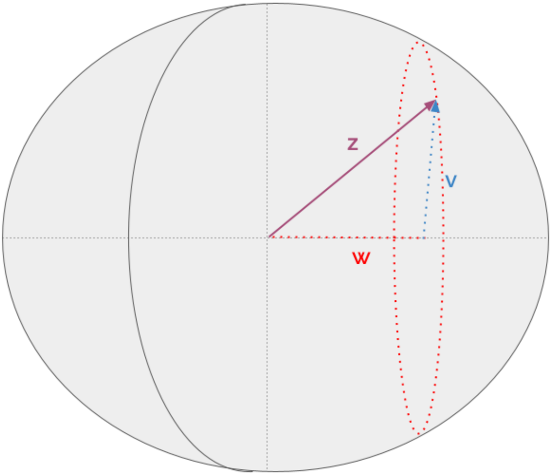
Sampling w from $g(w|\kappa)$

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



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

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



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

Transform z

Algorithm 3 Overview of the sampling method from $\mathcal{S}(\mu, \kappa)$

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: $u \leftarrow Normalize(e_1 - \mu)$
4: $U \leftarrow I - 2uu^T$
5: **return** $z' = U(\mu)z$

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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 4 Reparameterized Rejection Sampling (from [NRLB20])

$i \leftarrow 0$
repeat
    $i \leftarrow i + 1$
    Propose $\varepsilon_i \sim s(\varepsilon)$
    Simulate $u_i \sim \mathcal{U}[0, 1]$
until $u_i < \frac{g(h(\varepsilon_i,\theta);\theta)}{r(h(\varepsilon_i,\theta);\theta)}$
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

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
- 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

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