

Computational Statistics

Hyperspherical Variational Auto-Encoders

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2. Sampling method
3. Reparameterization Trick
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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 $e_1 = (1, 0, \dots, 0)$
 - 2: Compute Householder reflection $U(\mu)$ so that $U(\mu)e_1 = \mu$
 - 3: **return** $z' = U(\mu)z$
-

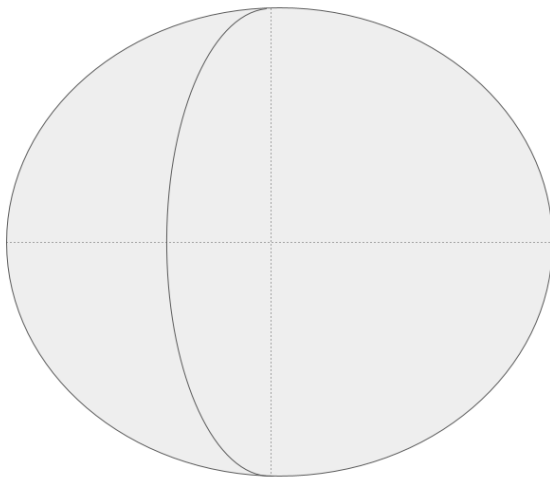


Algorithm 2 Overview of the sampling method from $\text{vMF}(\mu, \kappa)$

- 1: Sample $z \sim q(z|\mathbf{e}_1, \kappa)$ where $\mathbf{e}_1 = (1, 0, \dots, 0)$
 - 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 $U(\mu)\mathbf{e}_1 = \mu$
 - 6: **return** $z' = U(\mu)z \sim q(z'|\mu, \kappa)$
-



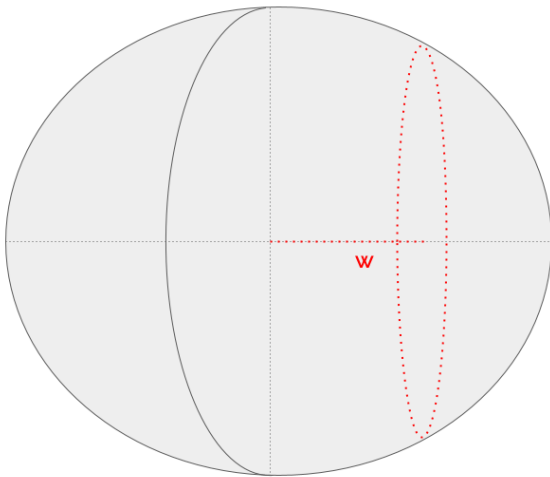
Sampling w from $g(w|\kappa, \theta)$



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

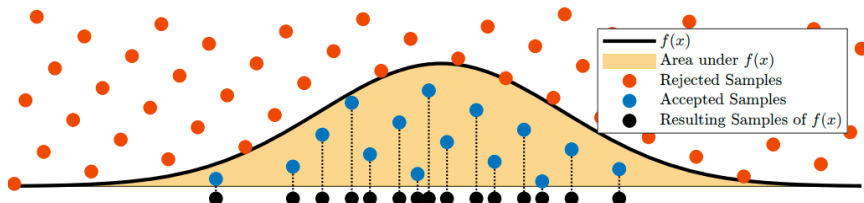


Illustration from [FH]



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

■ Case $d = 3$: faster to use inverse transformation method

- The vMF distribution explicitly writes :

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

- $(w, \sqrt{1 - w^2} v^T)^T \sim \text{vMF}(e_1, \kappa)$ 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

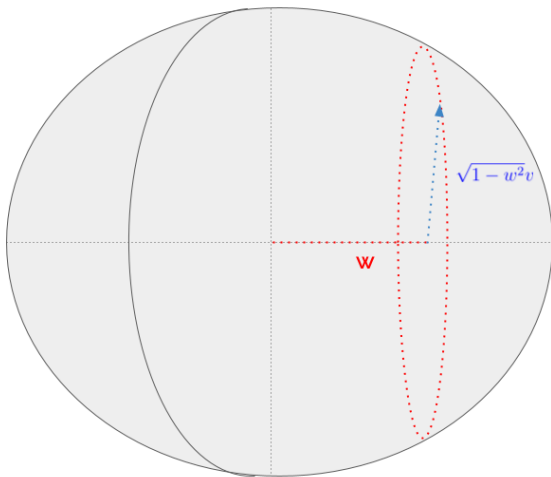
$$F_W^{-1}(u) = \frac{1}{\kappa} \ln(\exp(-\kappa) + 2 \sinh(\kappa) u)$$

- 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 ν from $\mathcal{U}(S^{d-2})$

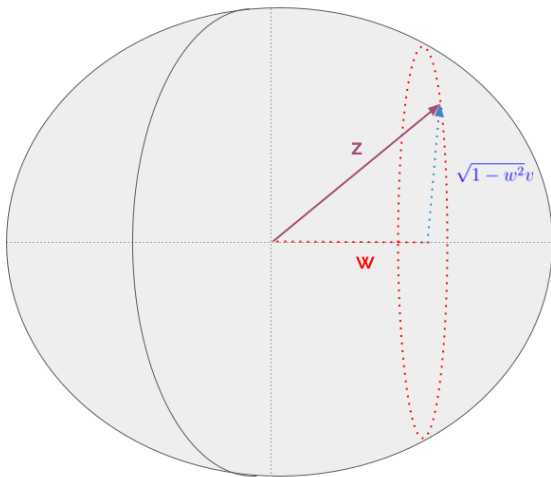
- $\mathcal{N}(0, I_{d-1})$ is rotationally symmetric around the origin
- $f_{Y_1, \dots, Y_{d-1}} = \frac{1}{\sqrt{2\pi}^{d-1}} \exp(-(Y_1^2 + \dots + Y_{d-1}^2)/2) = \frac{1}{\sqrt{2\pi}^{d-1}} \exp(-1^2/2)$
which is constant in all of the angular variables.

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

- 1: Generate $d - 1$ iid variables (X_i) from $\mathcal{N}(0, 1)$
 - 2: $Y_i \leftarrow \frac{X_i}{\sqrt{X_1^2 + \dots + X_{d-1}^2}}$
 - 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 $e_1 = (1, 0, \dots, 0)$
 - 2: Compute Householder reflection $U(\mu)$ so that $U(\mu)e_1 = \mu$
 - 3: $u \leftarrow \text{Normalize}(e_1 - \mu)$
 - 4: $U \leftarrow I - 2uu^T$
 - 5: **return** $z' = U(\mu)z$
-



Sampling results

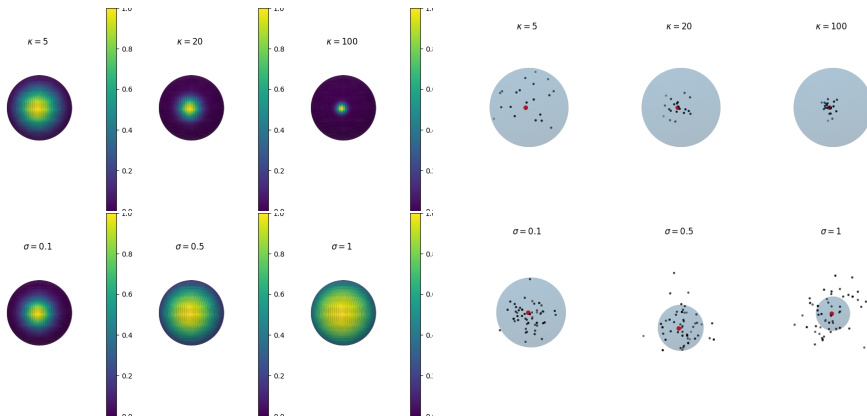


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Reparameterization Trick

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  $\varepsilon_i$ 
```



By noting $\pi(\varepsilon|\theta)$ the distribution of the resulting ε , we have (gradient of the expected log-likelihood)

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

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:

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

- 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

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$$\mathcal{L}_{\mathcal{KL}} = \mathcal{KL}(q(z|\mu, \kappa) || p(z))$$

-

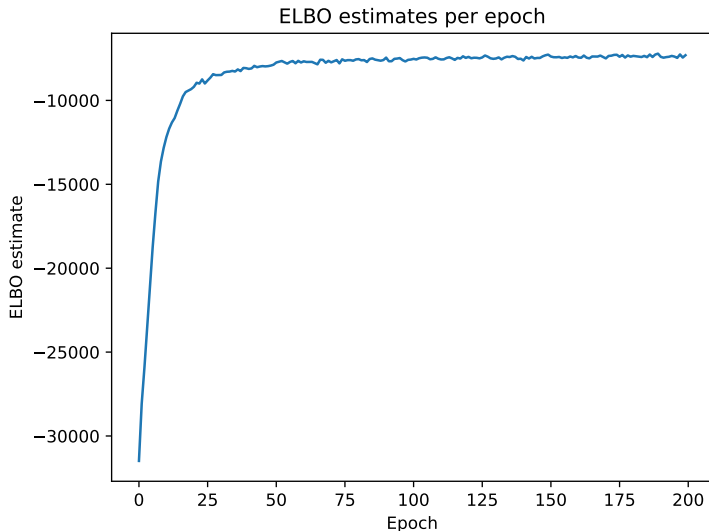
$$\nabla_{\kappa} \mathcal{L}_{\mathcal{KL}}$$

The formulas were explicitly computed in the article.

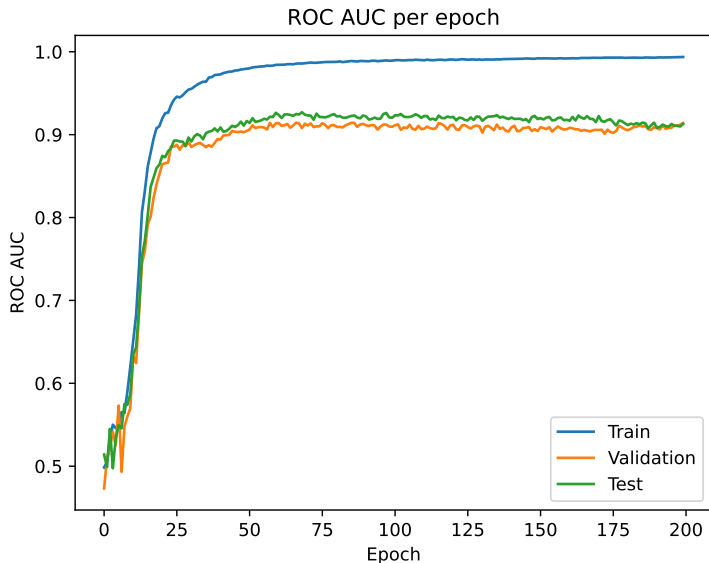


Training curves for \mathcal{N} -VGAE

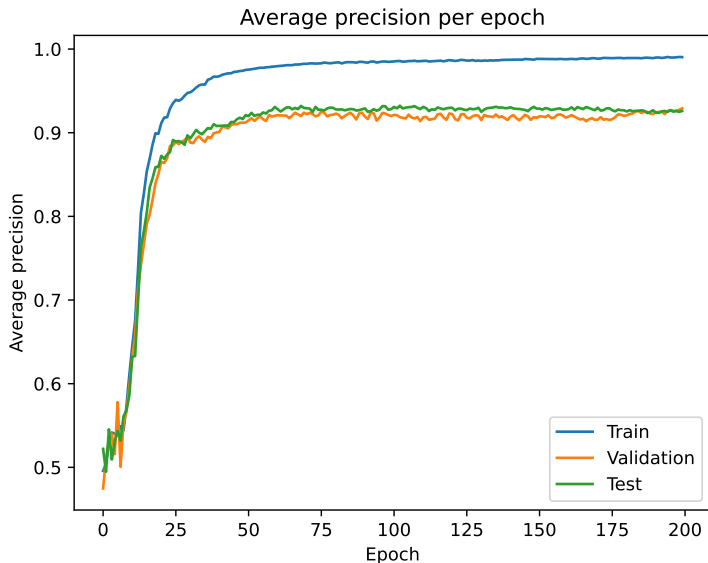
Latent dimension 16, learning rate 0.01. No KL divergence in loss.



Area under ROC curve for \mathcal{N} -VGAE

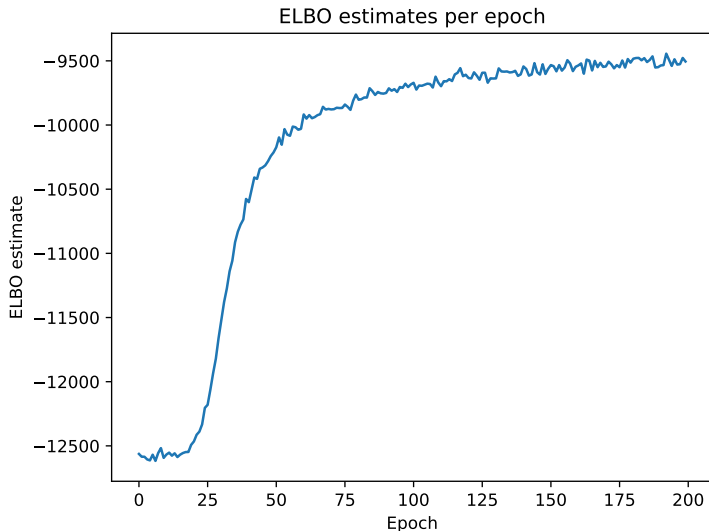


Average precision for \mathcal{N} -VGAE

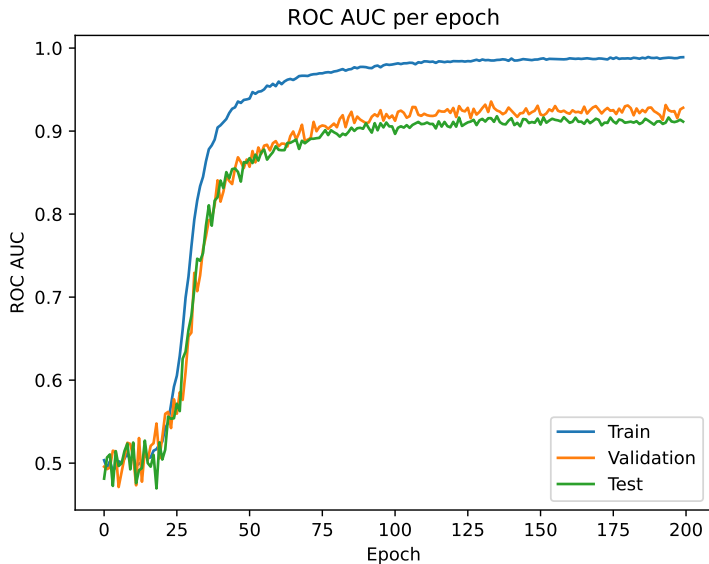


Training curves for \mathcal{S} -VGAE

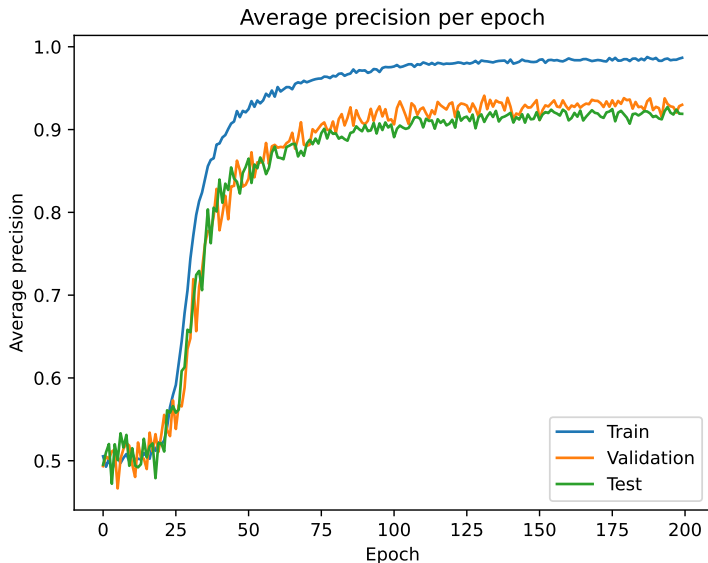
Latent dimension 16, learning rate 0.01. No KL divergence in loss.



Area under ROC curve for \mathcal{S} -VGAE



Average precision for \mathcal{S} -VGAE



Impact of dimension d on \mathcal{S} -VGAE

vmf d8 : mean auc : 0.90, 0.004638416275088545
vmd d8 : mean ap : 0.90, 0.006861910798200132
vmf d16 : mean auc : 0.91, 0.005106467210129149
vmd d16 : mean ap : 0.91, 0.002400819600884836
vmf d32 : mean auc : 0.92, 0.003988671804848861
vmd d32 : mean ap : 0.92, 0.006771540977322898
vmf d64 : mean auc : 0.92, 0.004086768956130232
vmd d64 : mean ap : 0.92, 0.006337561094050328



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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





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