Computational Statistics

Hyperspherical Variational Auto-Encoders

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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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Sampling z' from vMF

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

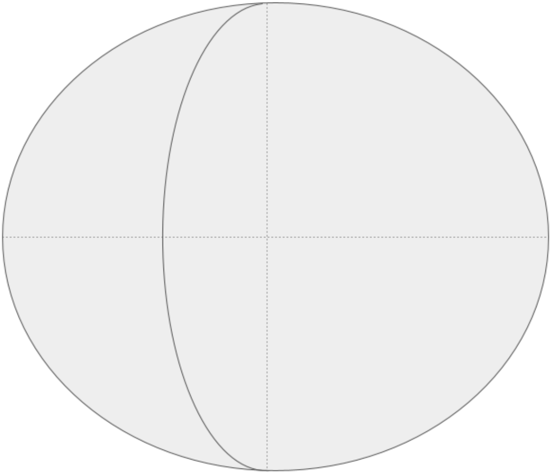
1: Sample $z \sim q(z|e_1, \kappa)$ where $e_1 = (1, 0, \ldots, 0)$
2: Compute Householder reflection $U(\mu)$ so that $U(\mu)e_1 = \mu$
3: **return** $z' = U(\mu)z$

Sampling z from vMF

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

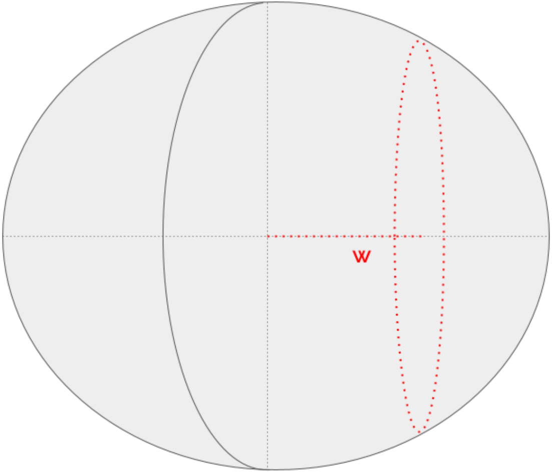
1: Sample $z \sim q(z|e_1, \kappa)$ where $e_1 = (1, 0, \dots, 0)$
2: Sample $w \in \mathbb{R} \sim g(w|\kappa)$ by acceptance rejection sampling
3: Sample $v \in \mathbb{R}^{d-1} \sim \mathcal{U}(S^{d-2})$ (uniform on the hypersphere S^{d-2} independent of w)
4: $z \leftarrow (w, \sqrt{1-w^2}v^T)^T$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

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

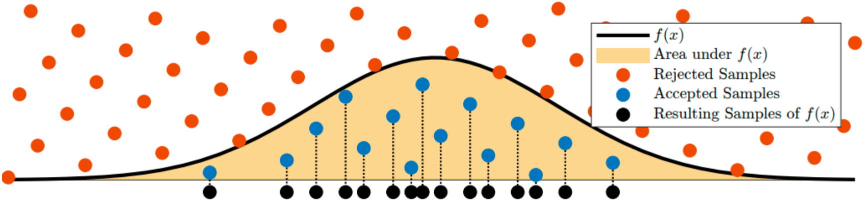


Illustration from [FH]

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

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

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

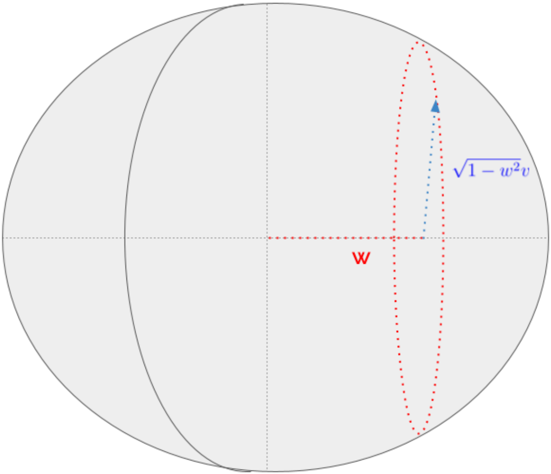
  - We compute its cumulative distribution function $F_W(w)$ and its inverse

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

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

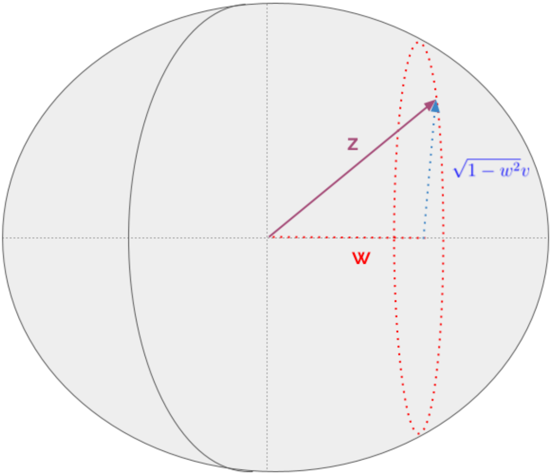
Sampling v from $\mathcal{U}(S^{d-2})$

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

Algorithm 3 Sampling 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** $(Y_i)_{i=1,\dots,d-1} \sim \mathcal{U}(S^{d-2})$

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



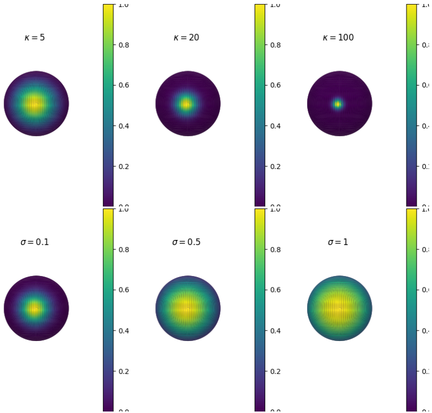
$$z = (w, \sqrt{1-w^2}v^T)^T$$

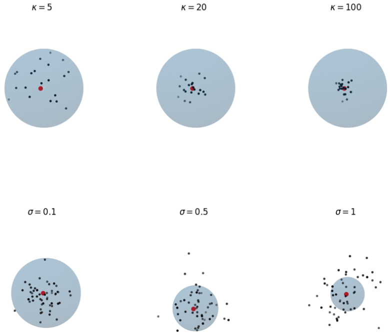
Algorithm 4 Overview of the sampling method from $vMF(\mu, \kappa)$

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 (gradient of the expected log-likelihood)

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

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:

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

- 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

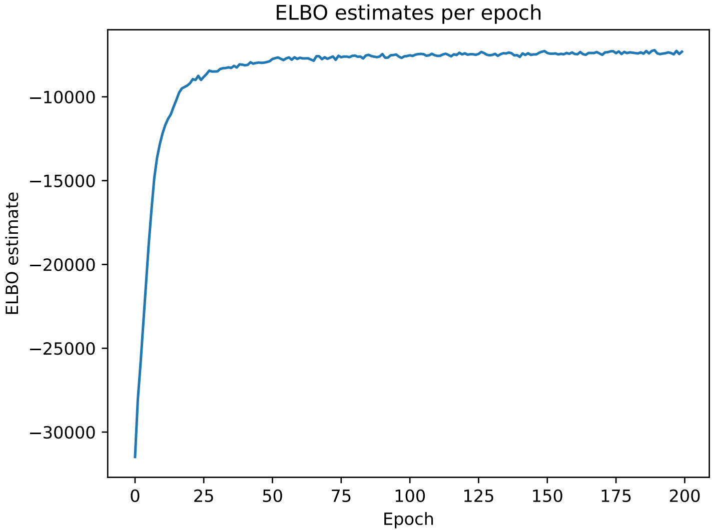
Loss computation

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

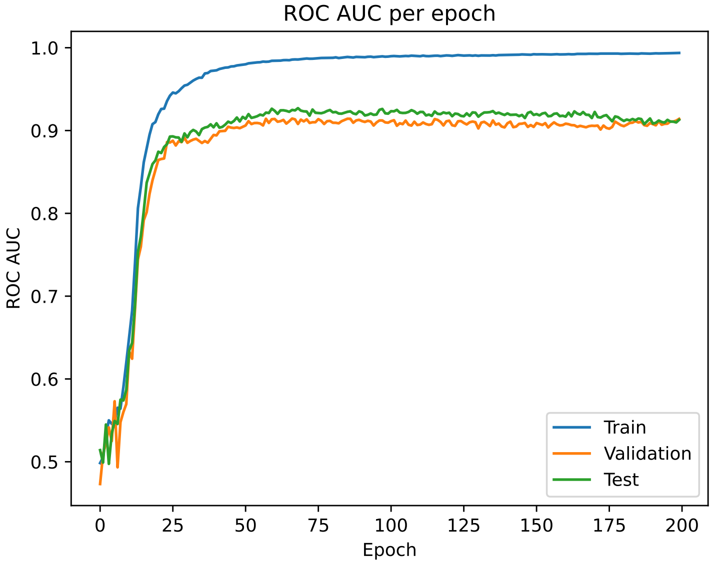
The formulas were explicity computed in the article.

Training curves for $\mathcal{N}$-VGAE

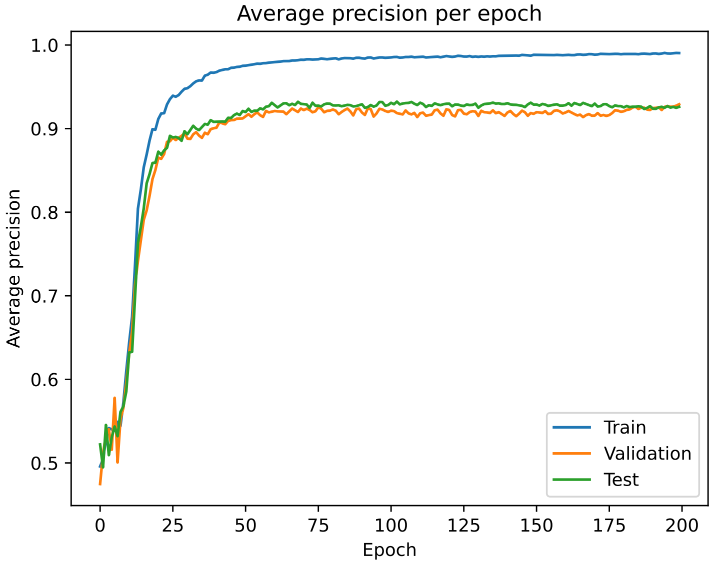
Latent dimension 16, learning rate 0.01. No KL divergence in loss.



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

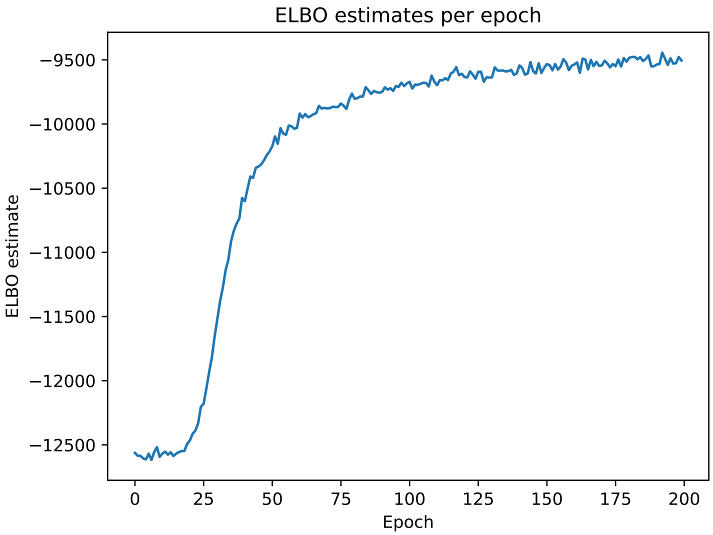


Average precision for $\mathcal{N}$-VGAE

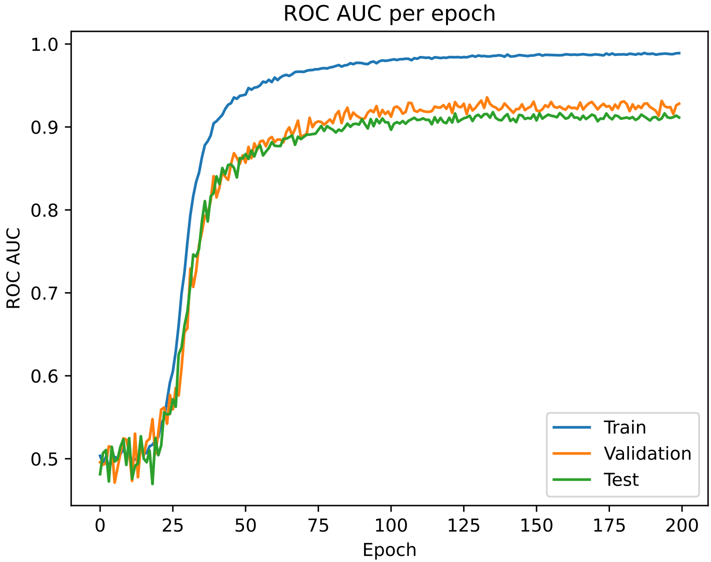


Training curves for $\mathcal{S}$-VGAE

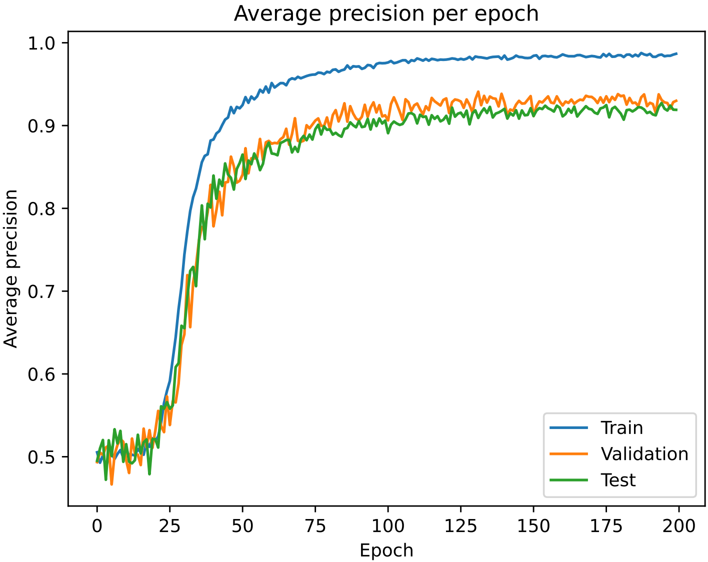
Latent dimension 16, learning rate 0.01. No KL divergence in loss.



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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