Finding geodesics on uncertain manifolds

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Background. We consider the geometry of *variational autoencoders (VAEs)* (Rezende et al., 2014; Kingma & Welling, 2014). The VAE generative process of $\mathbf{x} \in \mathbb{R}^D$ is

$$\mathbf{x}|\mathbf{z} \sim \mathcal{N}\left(\boldsymbol{\mu}(\mathbf{z}), \mathrm{diag}\left(\boldsymbol{\sigma}^2(\mathbf{z})\right)\right), \tag{1}$$

where $\mathbf{z} \in \mathbb{R}^d$ is a latent variable, and $\boldsymbol{\mu} : \mathbb{R}^d \to \mathbb{R}^D$ and $\boldsymbol{\sigma} : \mathbb{R}^d \to \mathbb{R}^D$ are neural networks representing mean and standard deviation of the generator.

This generator can be viewed as a stochastic mapping,

$$\mathbf{x} = f(\mathbf{z}) = \boldsymbol{\mu}(\mathbf{z}) + \boldsymbol{\sigma}(\mathbf{z}) \odot \epsilon, \qquad \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \tag{2}$$

such that a stochastic manifold is spanned. Arvanitidis et al. (2018) have shown that the expected metric of this stochastic manifold is a Riemannian metric, such that standard differential geometry can be applied to interpret the latent space. Here we consider the computation of geodesics under the expected Riemannian metric.

Computing geodesics. Shortest paths under the expected metric are known to minimize (Hauberg, 2018)

$$\mathcal{E}(\mathbf{c}) = \frac{1}{2}\int_a^b \|\dot{\mathbf{c}}_t\|^2_{\mathbf{M}_{\mathbf{c}_t}} \mathrm{d}t, \tag{3}$$

where $\mathbf{c} : [a, b] \to \mathbb{R}^d$ is a curve with derivative $\dot{c}$ and $\mathbf{M}$ is the expected metric. Using that the noise ϵ is normally distributed we can discretize this expression as

$$\mathcal{E} \approx \frac{1}{2}\sum_{n=1}^{N-1} \mathbb{E}\Big[\Big\|\mathcal{N}(\boldsymbol{\mu}(\mathbf{c}_n), \quad \mathrm{diag}(\boldsymbol{\sigma}^2(\mathbf{c}_n))) - \mathcal{N}(\boldsymbol{\mu}(\mathbf{c}_{n+1}), \mathrm{diag}(\boldsymbol{\sigma}^2(\mathbf{c}_{n+1})))\Big\|^2\Big]. \tag{4}$$

This expression can easily be evaluated in closed-form, and it is what we will optimize with respect to the unknown curve $\mathbf{c}$ connecting two points.

Parametrizing geodesics. In an effort to build efficient algorithms, we here propose to approximate the curve $\mathbf{c}$ with a quadratic curve per dimension,

$$c_i(t) = a_i t^2 + b_i t + c_i, \qquad i = 1, \ldots, d. \tag{5}$$

By fixing the end-points of $\mathbf{c}$ we then have d unknown parameters, which we find with gradient-based optimization.

Warm-starting. Following Arvanitidis et al. (2018) we model $\boldsymbol{\sigma}^2$ with an RBF network (Que & Belkin, 2016)

$$1/\boldsymbol{\sigma}^2(\mathbf{z}) = g(\mathbf{z}) = \mathbf{W}\exp(-\gamma\|\mathbf{z} - \bar{\mathbf{z}}\|^2). \tag{6}$$

Here $\mathbf{W}$ is the trainable weight matrix while γ and $\bar{z}$ are the bandwidth and center for the basis function. Arvanitidis et al. (2018) find that shortest paths tend to follow the "ridges" of $g(\mathbf{z})$, so we propose to first maximize the curve with respect to g and use this to initialize the optimization of $\mathcal{E}$. This is beneficial as the RBF network is significantly faster to evaluate than the deep neural network $\boldsymbol{\mu}$.

Two-moons illustration. We illustrate our algorithm on the synthetic two-moons data, and find that the proposed method works well. Figure 1 shows example results.

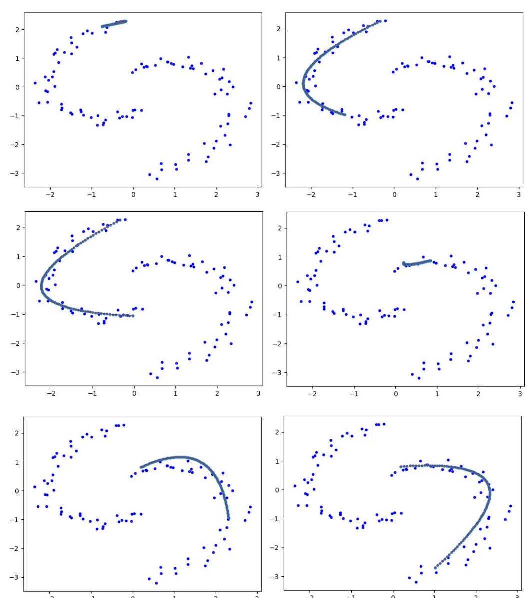

Figure 1. Geodesics obtained in latent space

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Acknowledgments. SH was supported by a research grant (15334) from VILLUM FONDEN. This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement n^{o} 757360).