Learning Hierarchical Priors in VAEs

Alexej Klushyn, Nutan Chen, Richard Kurle, Botond Cseke, Patrick van der Smagt

Machine Learning Research Lab, Volkswagen Group, Munich, Germany

Abstract

We address the problem of learning informative latent representations in the context of variational autoencoders. To do this, we

- use a hierarchical prior to avoid the over-regularisation resulting from a standard normal prior distribution.
- formulate the learning problem as a constrained optimisation problem.
- introduce a graph-based interpolation method to evaluate the learned latent representation.

Variational Autoencoders as a Constrained Optimisation Problem

Rezende and Viola (2018) reformulate the VAE objective as the Lagrangian

$$\mathcal{L}(\theta, \phi; \lambda) \equiv \mathbb{E}_{p_\mathcal{D}(\mathbf{x})} \Big[\underbrace{\mathrm{KL}\big(q_\phi(\mathbf{z}|\mathbf{x}) \| p_0(\mathbf{z})\big)}_{\text{optimisation objective}} + \lambda \big(\underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \big[\mathcal{C}_\theta(\mathbf{x}, \mathbf{z}) \big] - \kappa^2}_{\text{inequality constraint}} \big) \Big]$$

of a constrained optimisation problem

$$\overbrace{\min_\theta}^{\text{M-step}} \underbrace{\max_\lambda \min_\phi}_{\text{E-step}} \mathcal{L}(\theta, \phi; \lambda) \quad \text{s.t.} \quad \lambda \geq 0.$$

Here, $\mathcal{C}_\theta(\mathbf{x}, \mathbf{z})$ is defined as the reconstruction-error-related term in $-\log p_\theta(\mathbf{x}|\mathbf{z})$. Thus, $\min_\theta \mathcal{L}$ and $\max_\lambda \min_\phi \mathcal{L}$ can be interpreted as M- and E-step, respectively, of the original EM-algorithm for training VAEs. Optimisation is performed by a quasi-gradient ascent/descent algorithm (GECO):

$$\lambda_t = \lambda_{t-1} \cdot \exp\big(\nu \cdot (\mathcal{C}_t - \kappa^2)\big) \quad \text{and} \quad (\theta_t, \phi_t) = (\theta_{t-1}, \phi_{t-1}) - \eta_t \, \partial_{(\theta,\phi)} \mathcal{L},$$

where $\Delta\lambda_t \cdot \partial_\lambda \mathcal{L} \geq 0$ and ν is the update's learning rate. We obtain the ELBO iff $\lambda = 1$; or if $0 \leq \lambda < 1$, a lower bound on the ELBO (see β-VAE formulation (Higgins et al., 2017)).

Hierarchical Priors for Learning Informative Latent Representations

The optimal empirical Bayes prior is the aggregated posterior distribution $p^*(\mathbf{z}) = \mathbb{E}_{p_\mathcal{D}(\mathbf{x})}\big[q_\phi(\mathbf{z}|\mathbf{x})\big]$. In order to express it, we use a hierarchical prior/two-layer stochastic model

$$p_0(\mathbf{z}) \equiv p_\Theta(\mathbf{z}) = \int p_\Theta(\mathbf{z}|\zeta) \, p(\zeta) \, \mathrm{d}\zeta$$

and learn the parameters by applying an importance-weighted lower bound on $\mathbb{E}_{p^*(\mathbf{z})}\big[\log p_\Theta(\mathbf{z})\big] \geq \mathbb{E}_{p_\mathcal{D}(\mathbf{x})} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \big[\mathcal{L}_{\mathrm{IW}}(\Theta, \Phi; \mathbf{z}) \big]$ (Burda et al., 2016):

$$\mathbb{E}_{p_\mathcal{D}(\mathbf{x})} \big[\mathrm{KL}\big(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\Theta(\mathbf{z})\big) \big] \leq \mathbb{E}_{p_\mathcal{D}(\mathbf{x})} \big[\mathcal{F}(\phi, \Theta, \Phi; \mathbf{x}) \big]$$

$$\equiv \mathbb{E}_{p_\mathcal{D}(\mathbf{x})} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \Big[\log q_\phi(\mathbf{z}|\mathbf{x}) - \underbrace{\mathbb{E}_{\zeta_{1:K} \sim q_\Phi(\zeta|\mathbf{z})} \Big[\log \frac{1}{K} \sum_{k=1}^K \frac{p_\Theta(\mathbf{z}, \zeta_k)}{q_\Phi(\zeta_k|\mathbf{z})} \Big]}_{\mathcal{L}_{\mathrm{IW}}(\Theta, \Phi; \mathbf{z})} \Big].$$

As a result, we arrive at the Lagrangian objective

$$\mathcal{L}_{\mathrm{VHP}}(\theta, \phi, \Theta, \Phi; \lambda) \equiv \mathbb{E}_{p_\mathcal{D}(\mathbf{x})} \Big[\mathcal{F}(\phi, \Theta, \Phi; \mathbf{x}) + \lambda \big(\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \big[\mathcal{C}_\theta(\mathbf{x}, \mathbf{z}) \big] - \kappa^2 \big) \Big],$$

where the constrained optimisation problem is formulated as

$$\overbrace{\min_{\Theta, \Phi}}^{\text{M-step}} \underbrace{\min_\theta}_{\text{empirical Bayes}} \underbrace{\max_\lambda \min_\phi}_{\text{E-step}} \mathcal{L}_{\mathrm{VHP}}(\theta, \phi, \Theta, \Phi; \lambda) \quad \text{s.t.} \quad \lambda \geq 0.$$

This leads to the following double-loop method: (i) update the upper bound (empirical Bayes) via (Θ, Ψ); (ii) solve the constrained optimisation problem w.r.t. (θ, λ, ψ).

Optimisation: to be in line with previous literature and to facilitate the comparison with the original VAE framework, we use the β-parametrisation: $\beta = \frac{1}{\lambda}$.

Our goal is to obtain a tight lower bound on the log-likelihood. This holds when $\beta = 1$ (ELBO). To guarantee that the optimisation process finishes at $\beta = 1$—provided the constraint is fulfilled—we propose the following update:

$$\beta_t = \beta_{t-1} \cdot \exp\big[\nu \cdot f_\beta(\beta_{t-1}, \mathcal{C}_t - \kappa^2; \tau) \cdot (\mathcal{C}_t - \kappa^2)\big],$$

where $f_\beta(\beta, \delta; \tau) \equiv \big(1 - H(\delta)\big) \cdot \tanh\big(\tau \cdot (\beta - 1)\big) - H(\delta)$; H is the Heaviside function; and τ is a slope parameter.
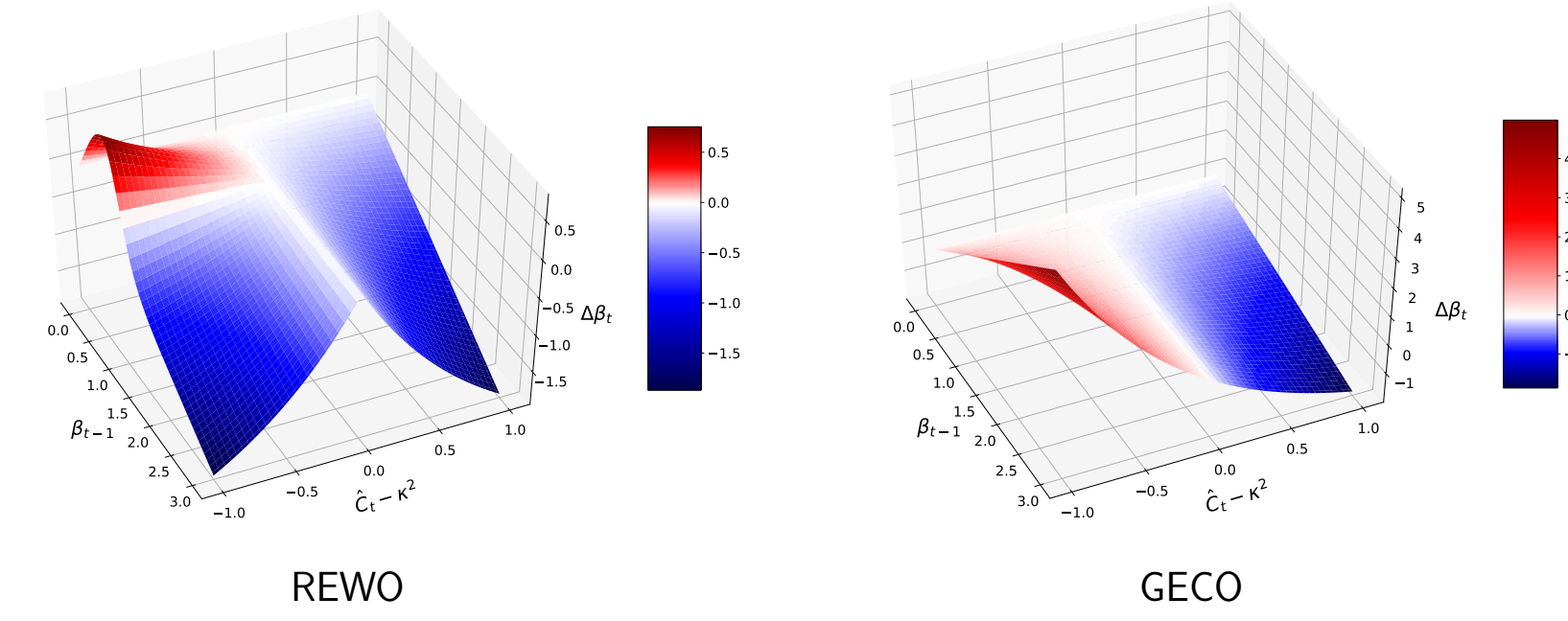
Comparison of β-update schemes: $\Delta\beta_t = \beta_t - \beta_{t-1}$ as a function of β_{t-1} and $\mathcal{C}_t - \kappa^2$ for $\nu = 1$ and $\tau = 3$.

We experienced that the double-loop method behaves as a layer-wise pre-training. Thus, we propose an algorithm (REWO) that separates training into two phases:

- Initial phase: to enforce a reconstruction optimisation, we start with $\beta \ll 1$ and optimise $\mathcal{L}_{\mathrm{VHP}}$ w.r.t. (θ, ϕ), until $\mathcal{C}_t < \kappa^2$.
- Main phase: after $\mathcal{C}_t < \kappa^2$ is fulfilled, we optimise $\mathcal{L}_{\mathrm{VHP}}$ w.r.t. $(\Theta, \Phi, \theta, \phi)$ and update β.
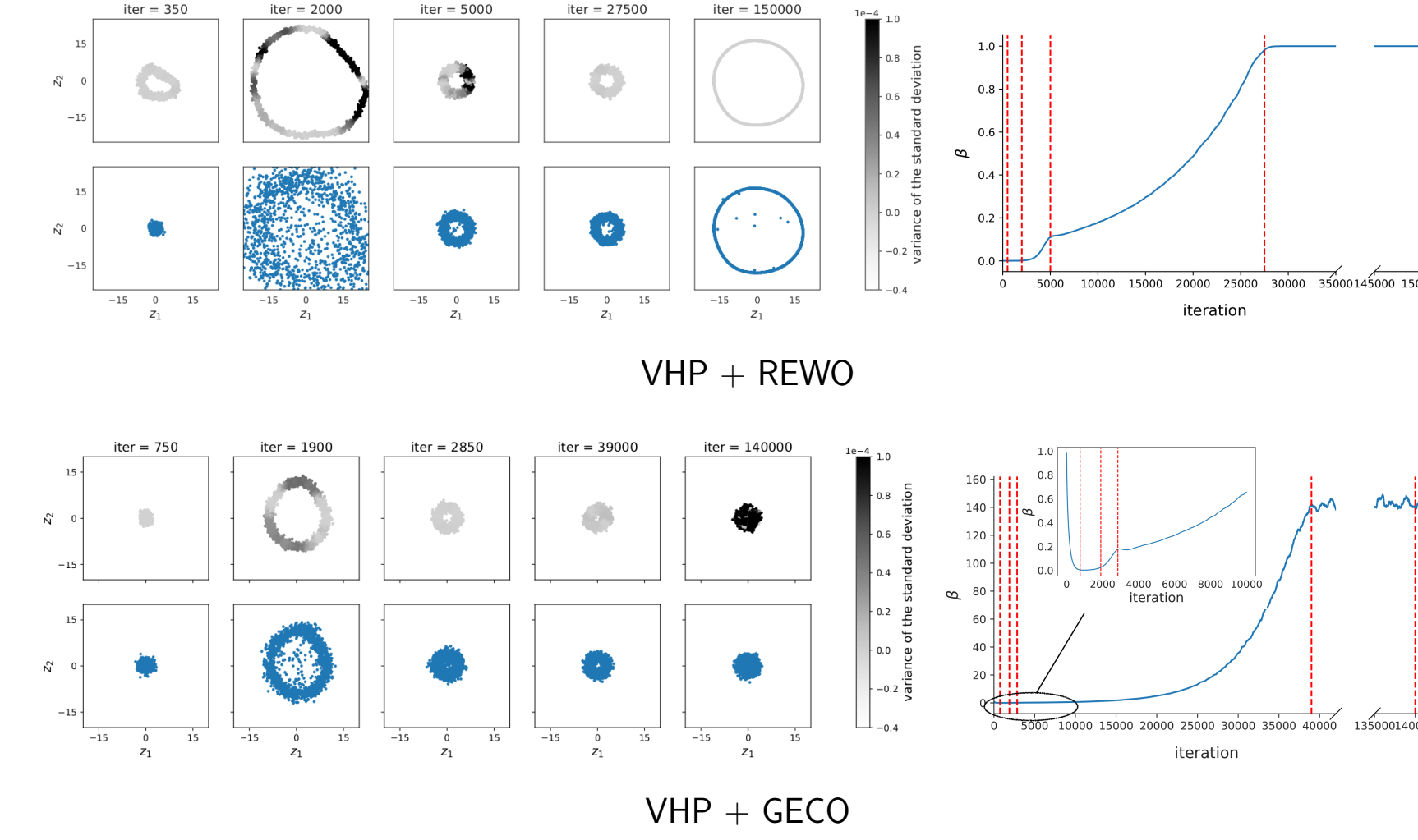
Graph-Based Interpolation

The nodes of the graph $\mathbf{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$ are obtained by randomly sampling N samples from the prior distribution:

$$\mathbf{z}_n, \zeta_n \sim p_\Theta(\mathbf{z}|\zeta) \, p(\zeta), \quad n = 1, \ldots, N.$$

The graph is constructed by connecting each node by undirected edges to its k-nearest neighbours. The edge weights are the Euclidean distances (latent space) between the node pairs.

Artificial Pendulum

Latent representation of the pendulum data at different iteration steps when optimising $\mathcal{L}_{\mathrm{VHP}}(\theta, \phi, \Theta, \Phi; \beta)$ with REWO and GECO, respectively. The top row shows the approximate posterior; the greyscale encodes the variance of its standard deviation. The bottom row shows the hierarchical prior.
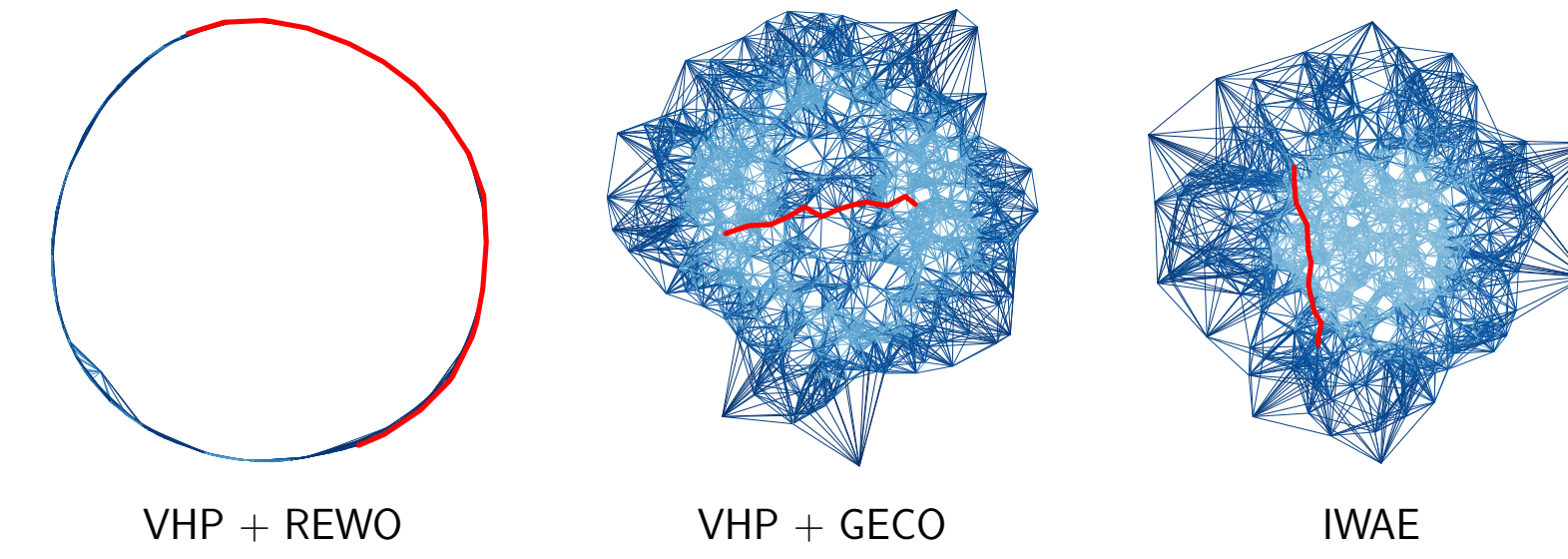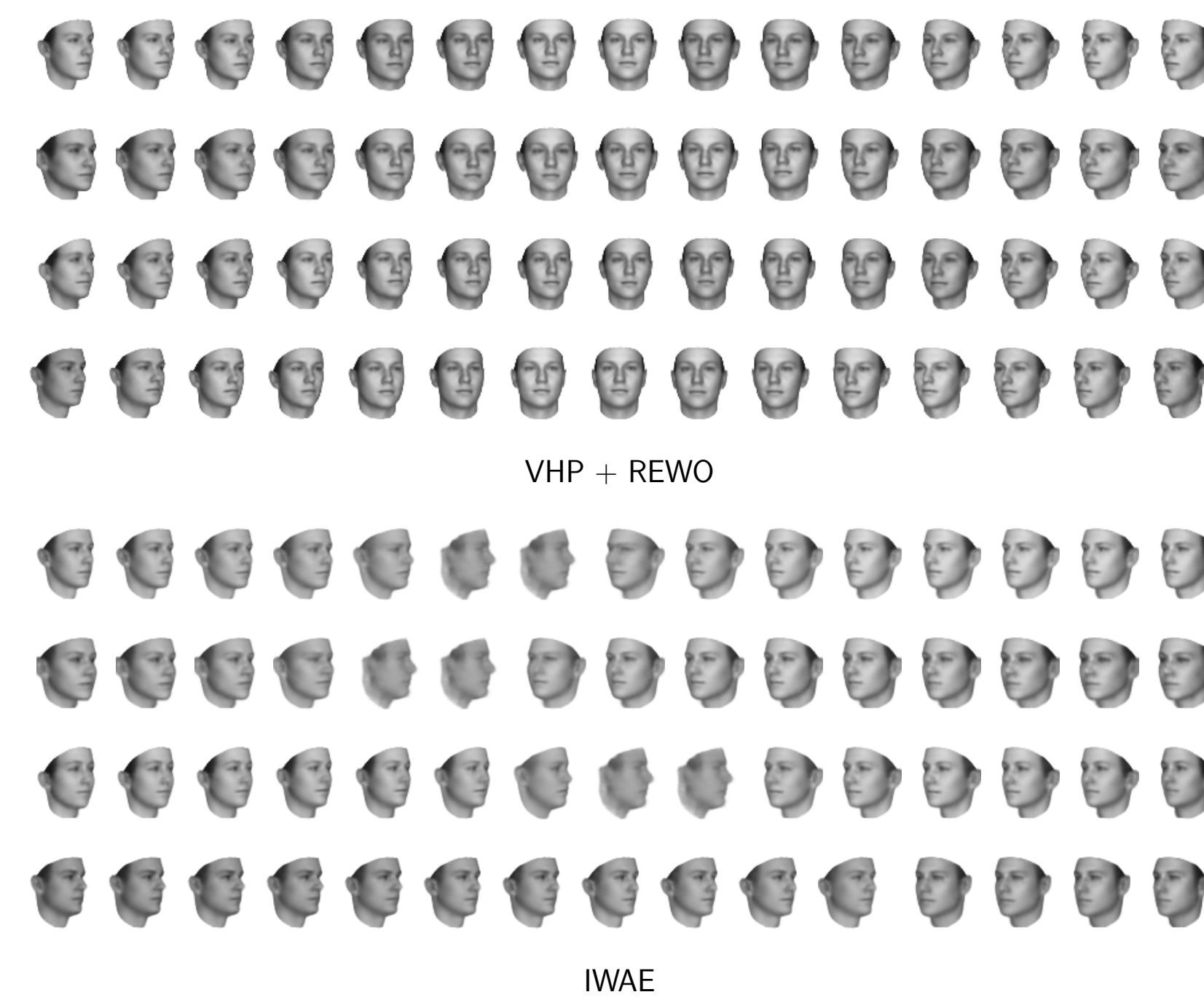

Graph-based interpolation of the pendulum movement. The graph is based on the respective prior. The red curves depict the interpolations, the bluescale indicates the edge weight.
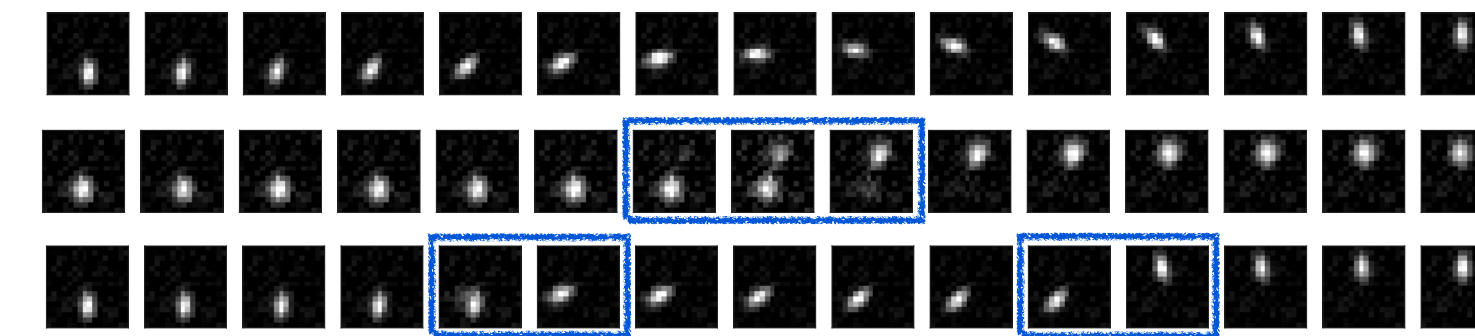
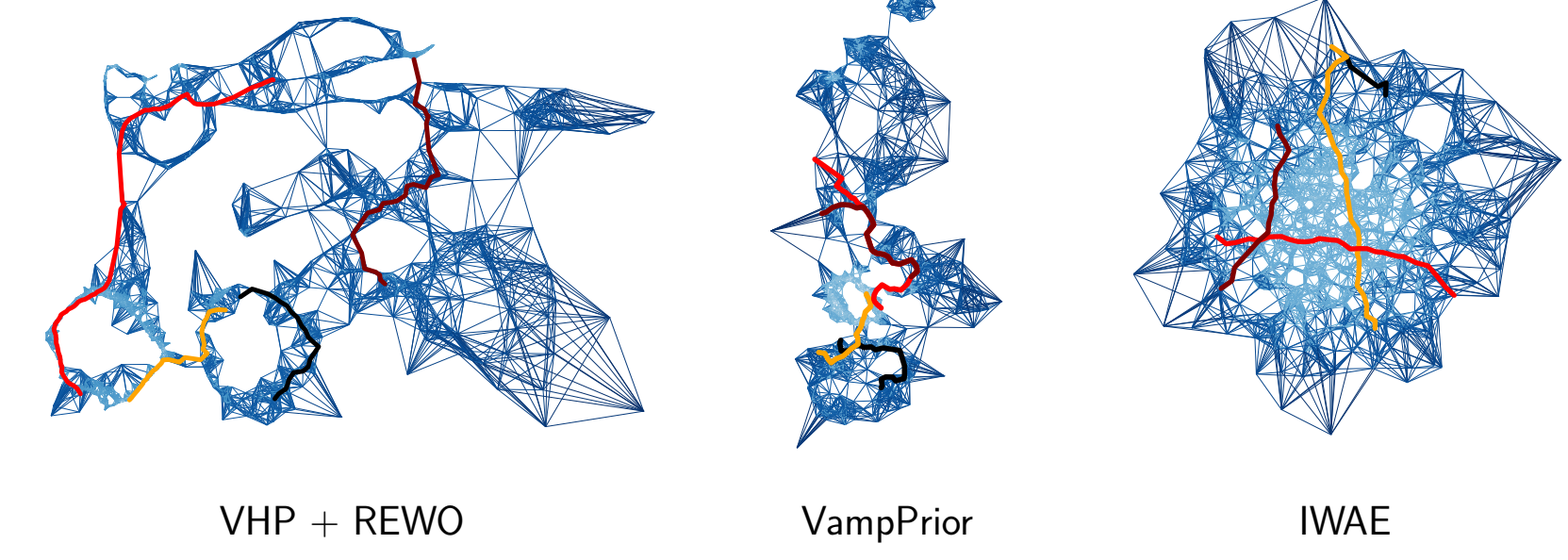top: VHP + REWO, middle: VHP + GECO, bottom: IWAE

Pendulum reconstructions of the graph-based interpolations (red curve). Discontinuities are marked by blue boxes.

3D Faces

Graph-based interpolations along the learned 32-dimensional latent manifold. The graph is based on samples from the respective prior distribution.
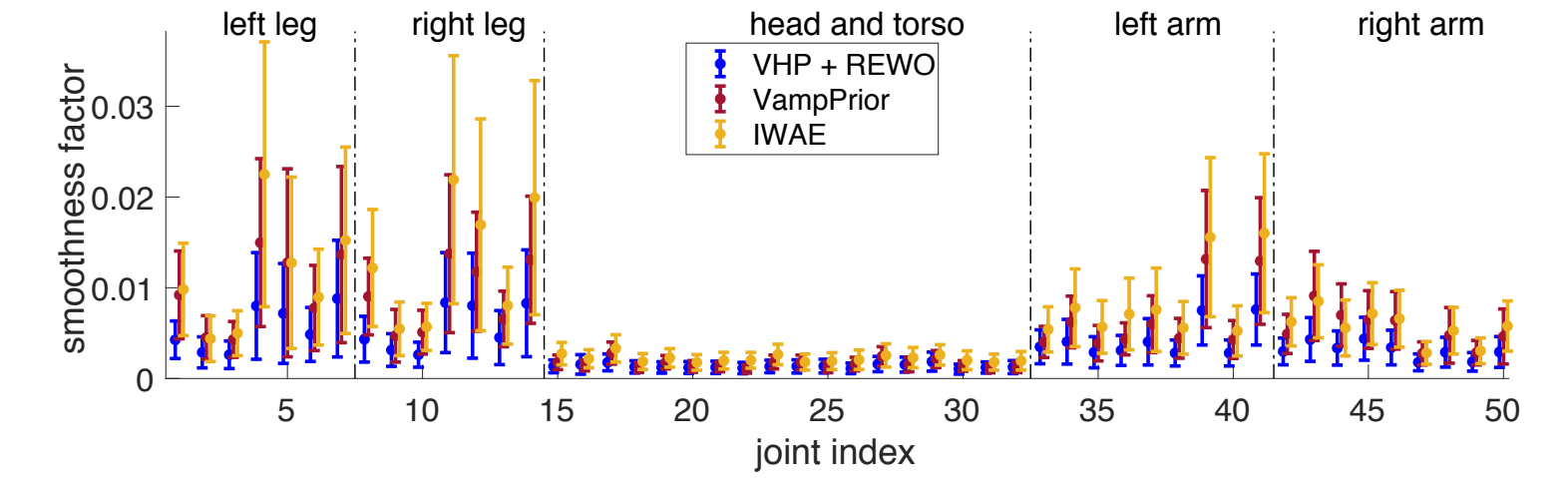
Human Motion

Graph-based interpolation of human motions. The graphs are based on the (learned) prior distributions. The bluescale indicates the edge weight. The coloured lines represent four interpolated movements.

top: VHP + REWO, middle: VampPrior, bottom: IWAE
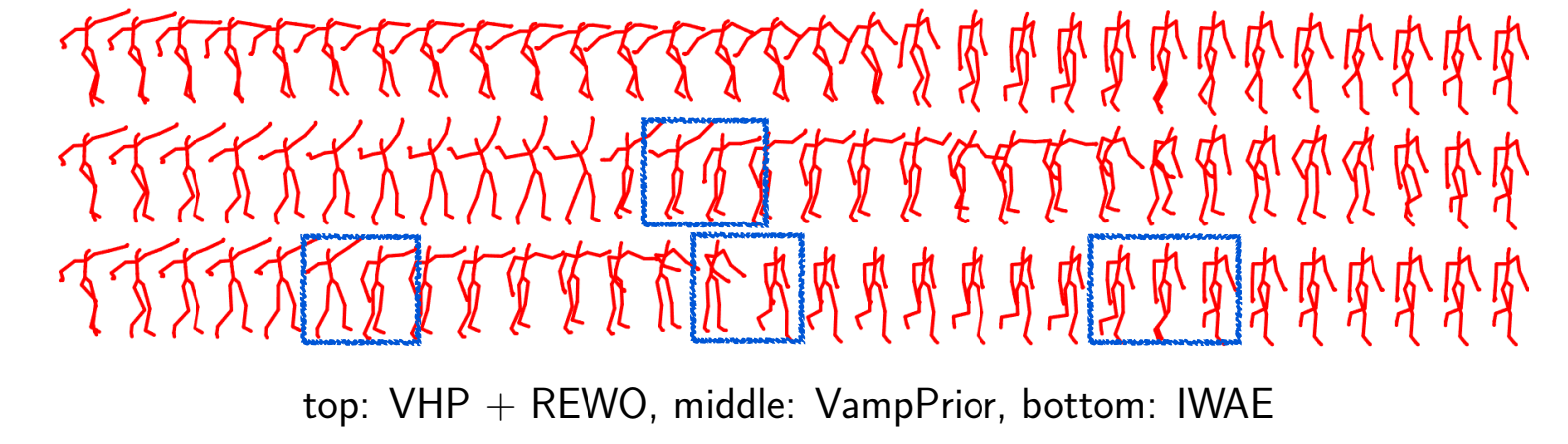
Human-movement reconstructions of the graph-based interpolations (red curve). Discontinuities are marked by blue boxes.

Smoothness measure of the human-movement interpolations. For each joint, the mean and standard deviation of the smoothness factor are displayed. Smaller values correspond to smoother movements.

MNIST, Fashion-MNIST, & OMNIGLOT

Negative test log-likelihood estimated with 5,000 importance samples

	DYNAMIC MNIST	STATIC MNIST	FASHION-MNIST	OMNIGLOT
VHP + REWO	78.88	82.74	225.37	101.78
VHP + GECO	95.01	96.32	234.73	108.97
VAMPPRIOR	80.42	84.02	232.78	101.97
IWAE (L=1)	81.36	84.46	226.83	101.57
IWAE (L=2)	80.66	82.83	225.39	101.83

References

Burda, Y. et al. (2016). Importance weighted autoencoders. *ICLR*.

Higgins, I. et al. (2017). Beta-VAE: Learning basic visual concepts with a constrained variational framework. *ICLR*.

Kingma, D. P. and Welling, M. (2014). Auto-encoding variational Bayes. *ICML*.

Rezende, D. J. and Viola, F. (2018). Taming VAEs. *CoRR*.

Tomczak, J. and Welling, M. (2018). VAE with a VampPrior. *AISTATS*.

Contact

alexej.klushyn@argmax.ai

botond.cseke@argmax.ai