Auto-Encoding Variational Bayes

Diederik P (Durk) Kingma, Max Welling
University of Amsterdam
Ph.D. Candidate, advised by Max

Durk Kingma

Max Welling

UNIVERSITEIT VAN AMSTERDAM

Problem class

- Directed graphical model:

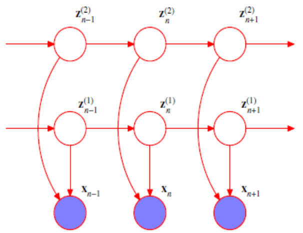
  x : observed variable

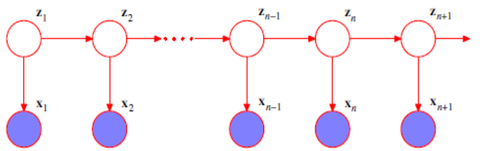
  z : latent variables (continuous)

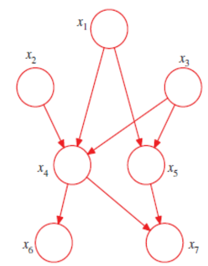
  θ : model parameters

  $p_\theta(\mathbf{x},\mathbf{z})$: joint PDF

  - Factorized, differentiable







- Hard case: intractable posterior distribution $p_\theta(\mathbf{z}|\mathbf{x})$

  e.g. neural nets as components

- We want fast approximate posterior inference per datapoint
  - After inference, learning params is easy

Approximate Inference/Learning methods

- MCMC / Monte Carlo EM
  - often too slow / scaling issues
- Wake-Sleep
  - Improper
- Why not pure MAP / Maximization?
  - Heavlily overfits with high dimensional $\mathbf{z}$'

Auto-Encoding Variational Bayes

Idea:

- Learn neural net to approximate the posterior
  - $q_{\varphi}(z|x)$ with 'variational parameters' φ
  - one-shot approximate inference
  - akin to the recognition model in Wake-Sleep

- Construct estimator of the variational lower bound
  which we can optimize jointly w.r.t. **φ** jointly with **θ**

  -> Stochastic gradient ascent

Variational Lower Bound of the marg. lik.

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = KL(q_{\mathbf{z}|\mathbf{x}}||p_{\mathbf{z}|\mathbf{x}}) + \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x})$$

$$\text{where} \quad \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \left[\log p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) - \log q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\right)$$

Monte Carlo estimator of the variational bound

Shorthand:

$$f_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{z}) = \log p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) - \log q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$$

$$\mathcal{L}(\boldsymbol{\theta},\boldsymbol{\phi};\mathbf{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\left[f_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{z})\right] \simeq \frac{1}{L}\sum_{l=1}^{L} f_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{z}^{(l)})$$

$$\text{where} \quad \mathbf{z}^{(l)} \sim q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \quad \text{(samples)}$$

Can we differentiate through the sampling process w.r.t. φ ?

Key reparameterization trick

Construct samples $z \sim q_\varphi(z|x)$ in two steps:

1. $\varepsilon \sim p(\varepsilon)$ *(random seed independent of φ)*
2. $z = g(\varphi, \varepsilon, x)$ (differentiable perturbation)

such that $z \sim q_\varphi(z|x)$ (the correct distribution)

Examples:

- if $q(z|x) \sim N(\mu(x), \sigma(x)^2)$
  $\varepsilon \sim N(0,I)$
  $z = \mu(x) + \sigma(x) * \varepsilon$
- (approximate) Inverse CDF
- Much more possibilities (see paper)

SGVB estimator

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}) = \int q_{\boldsymbol{\phi}}(\mathbf{z}) \left[\log p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) - \log q_{\boldsymbol{\phi}}(\mathbf{z})\right] d\mathbf{z}$$

$$\simeq \frac{1}{L} \sum_{l=1}^{L} \left(\log p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}^{(l)}) - \log q_{\boldsymbol{\phi}}(\mathbf{z}^{(l)})\right)$$

$$\text{where} \quad \boldsymbol{\epsilon}^{(l)} \sim p(\boldsymbol{\epsilon}) \quad \text{(samples from noise variable)}$$

$$\mathbf{z}^{(l)} = g(\boldsymbol{\epsilon}^{(l)}, \boldsymbol{\phi})$$

$$\text{(such that} \quad \mathbf{z}^{(l)} \sim q_{\boldsymbol{\phi}}(\mathbf{z}))$$

Really simple and appropriate for differentiation w.r.t. **φ** and **θ**!

Auto-Encoding Variational Bayes
Online algorithm

repeat

$$\mathbf{x} \leftarrow \text{random datapoint or minibatch}$$
$$\boldsymbol{\epsilon} \leftarrow \text{sample from } p(\boldsymbol{\epsilon})$$
$$g_{\boldsymbol{\theta}}, g_{\boldsymbol{\phi}} \leftarrow \nabla_{\boldsymbol{\theta},\boldsymbol{\phi}} \widetilde{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}, g(\boldsymbol{\epsilon}, \boldsymbol{\phi}))$$
$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \cdot g_{\boldsymbol{\theta}}$$
$$\boldsymbol{\phi} \leftarrow \boldsymbol{\phi} + \alpha \cdot g_{\boldsymbol{\phi}}$$

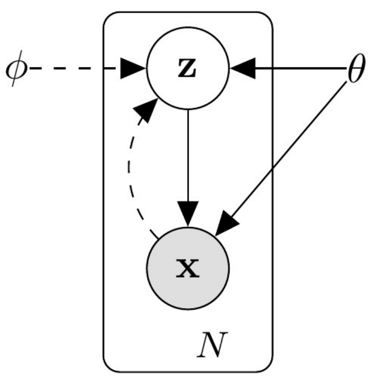
until convergence

Backprop
(Torch7 / Theano)

e.g. Adagrad

Scales to very large datasets!

Model used in experiments



$$p_{\boldsymbol{\theta}}(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$$

$$p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}(\mathbf{z}), \sigma(\mathbf{z})\mathbf{I})$$

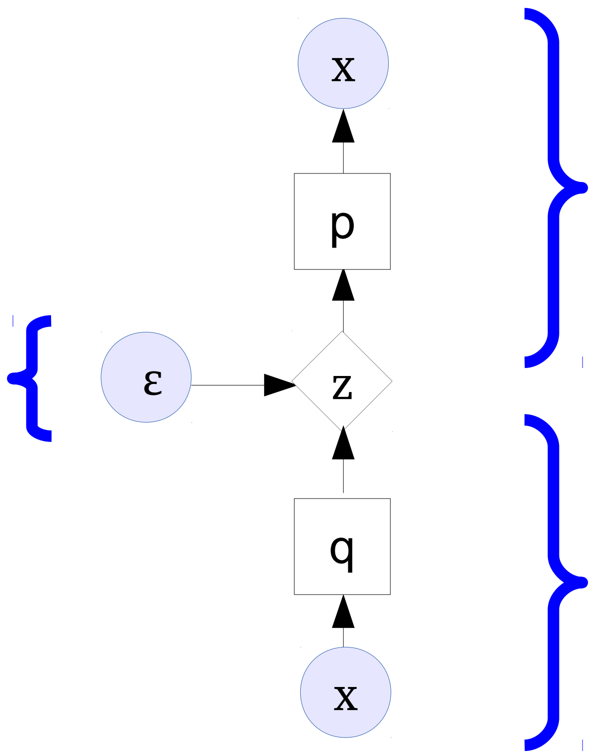
$$q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}(\mathbf{x}), \sigma(\mathbf{x})\mathbf{I})$$

$$\widetilde{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}) = \underbrace{\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}^{(l)})}_{\text{(noisy) negative reconstruction error}} + \underbrace{\log p_{\boldsymbol{\theta}}(\mathbf{z}^{(l)}) - \log q_{\boldsymbol{\phi}}(\mathbf{z}^{(l)}|\mathbf{x})}_{\text{regularization terms}}$$

$$\text{where} \quad \mathbf{z}^{(l)} \sim q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$$

Variational auto-encoder

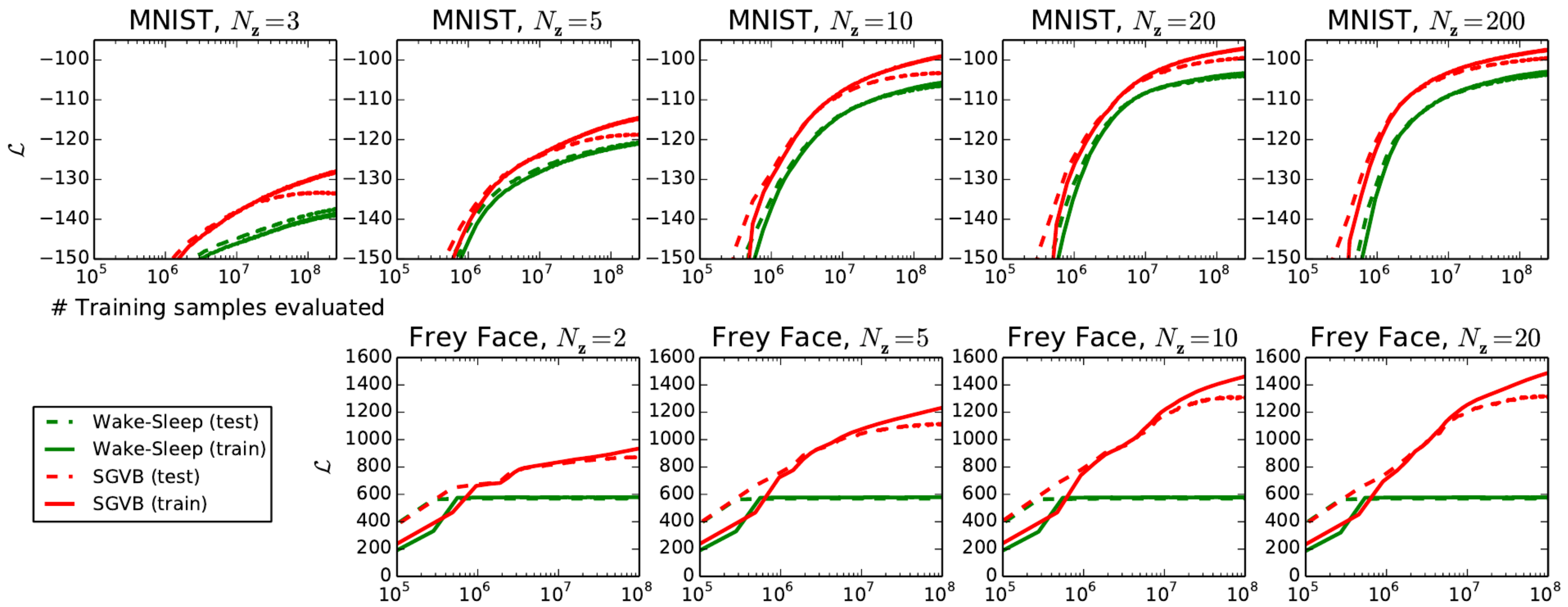
injected noise



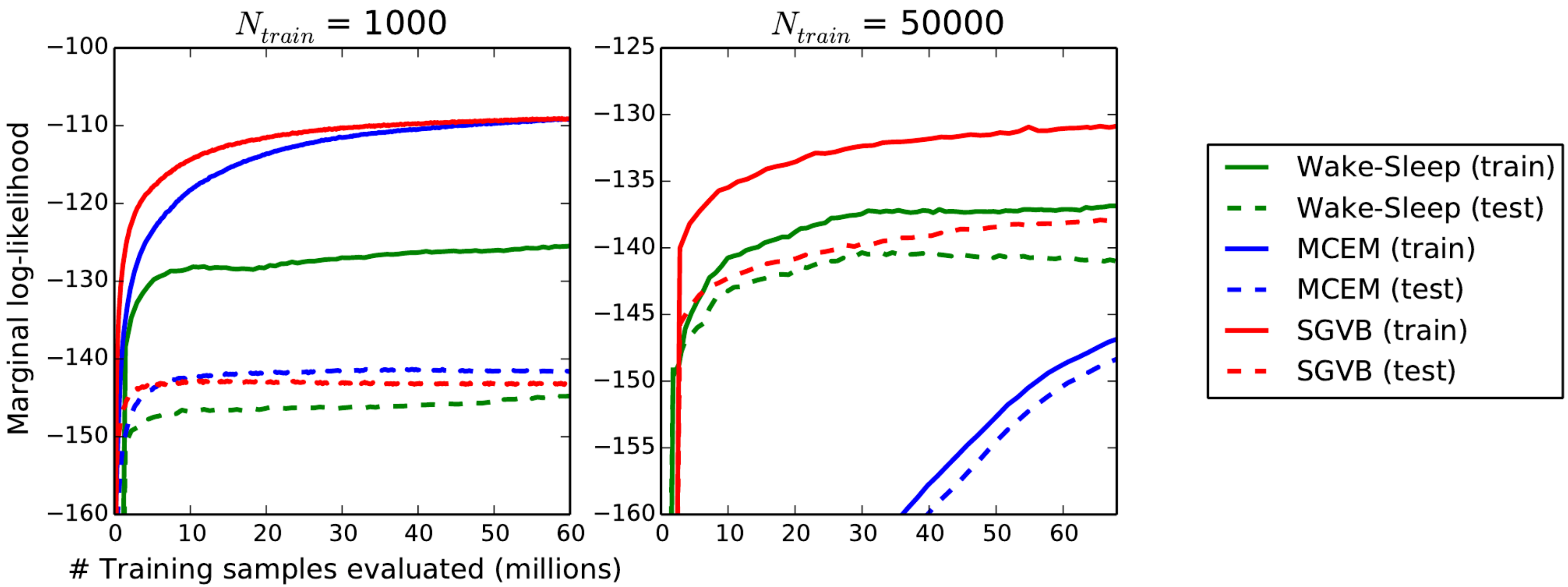
p(z) and p(x|z)
(decoder)

q(z|x) = N(μ,σ)
(encoder)

Results:
Marginal likelihood lower bound

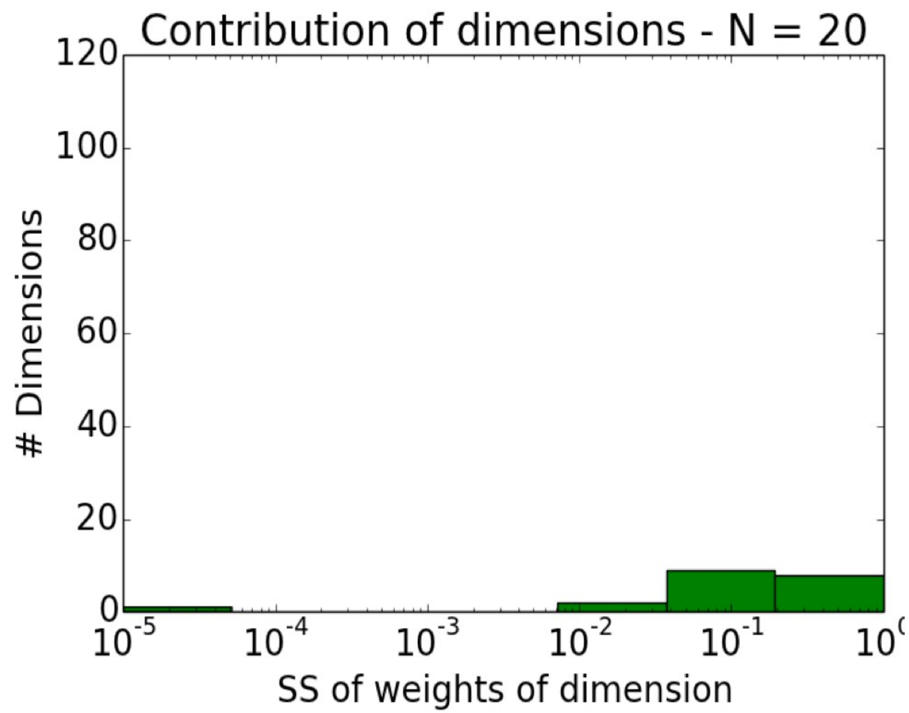


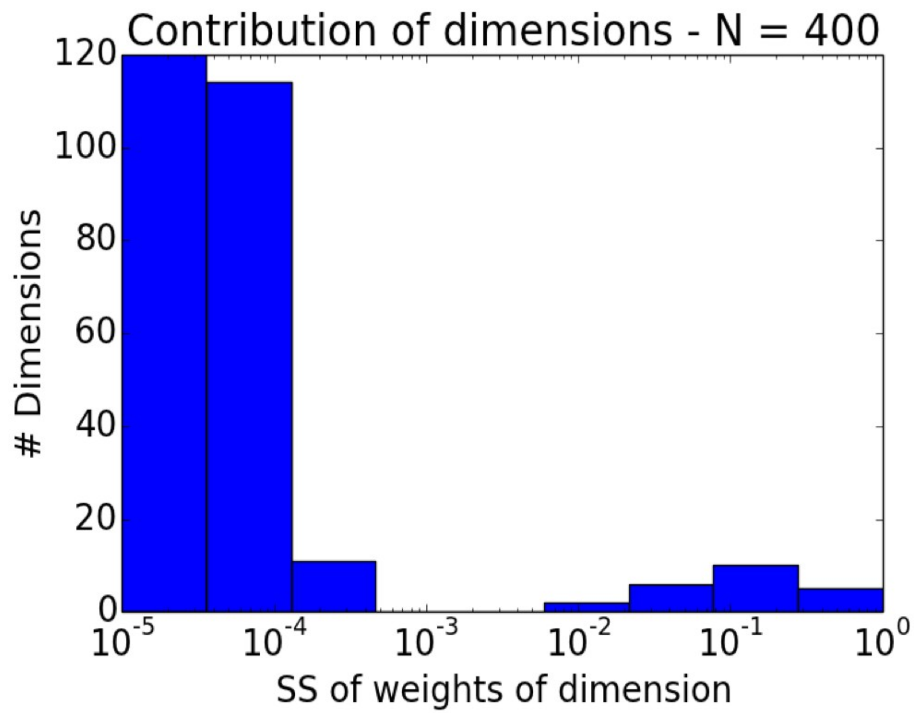
Results: Marginal log-likelihood



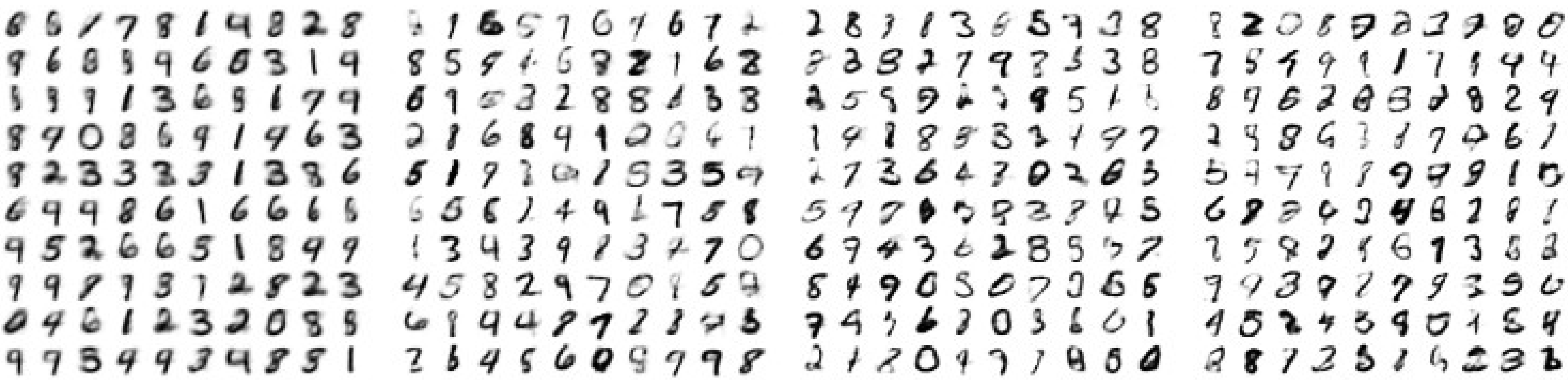
Monte Carlo EM does not scale well to large datasets

Robustness to high-dimensional latent space



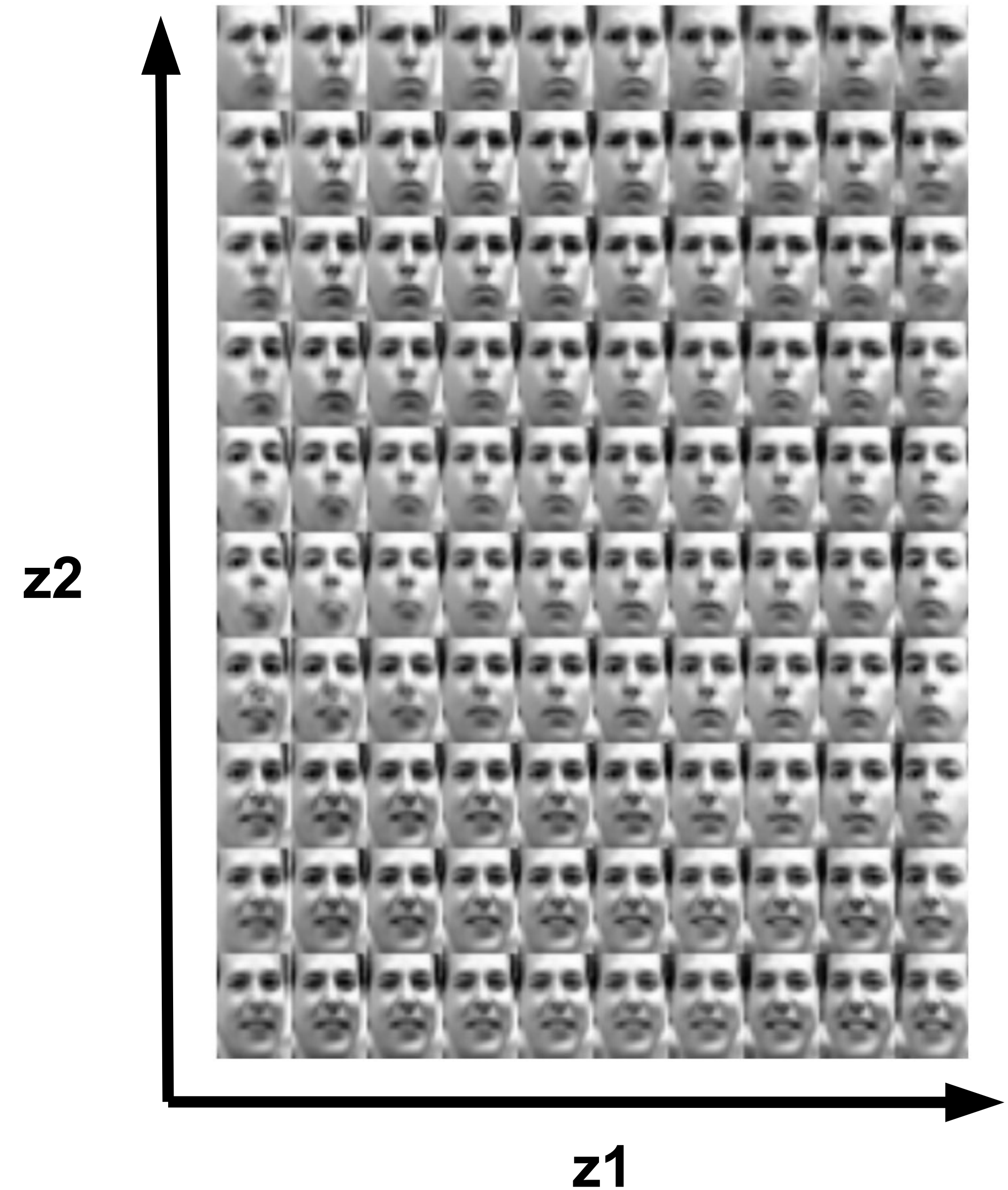


Samples from MNIST (simple ancestral sampling)

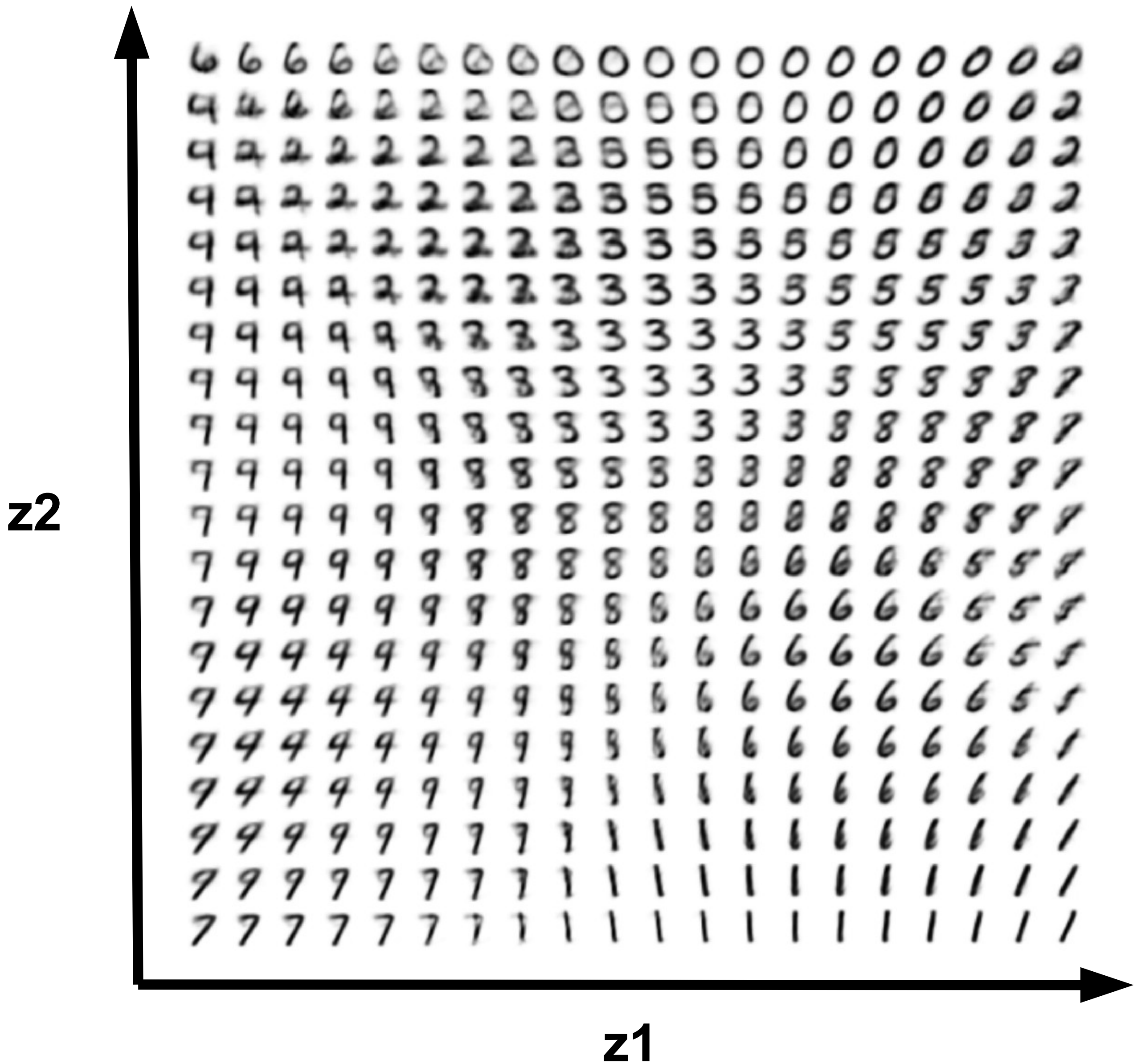


(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

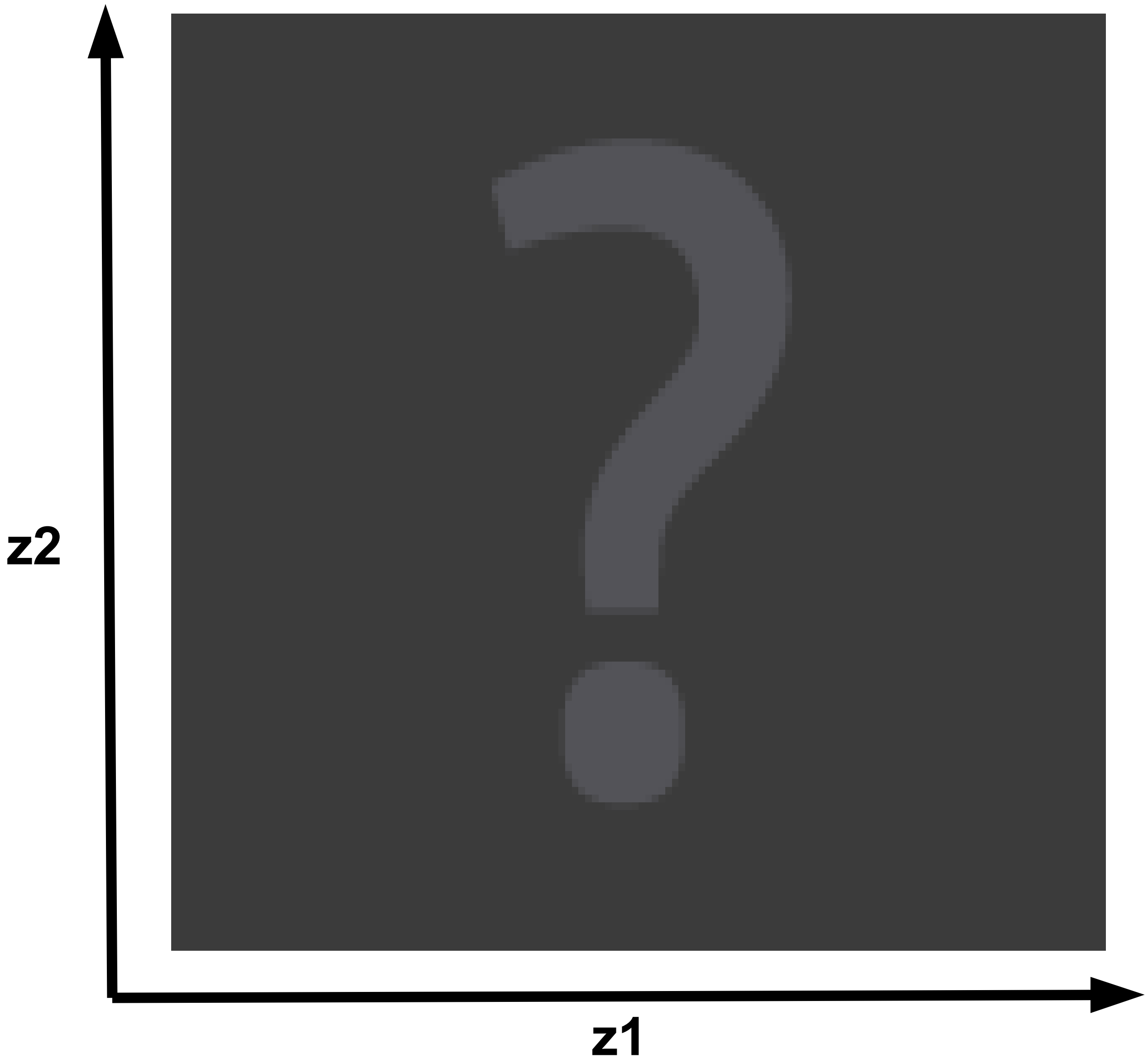
2D Latent space: Frey Face



2D Latent space: MNIST

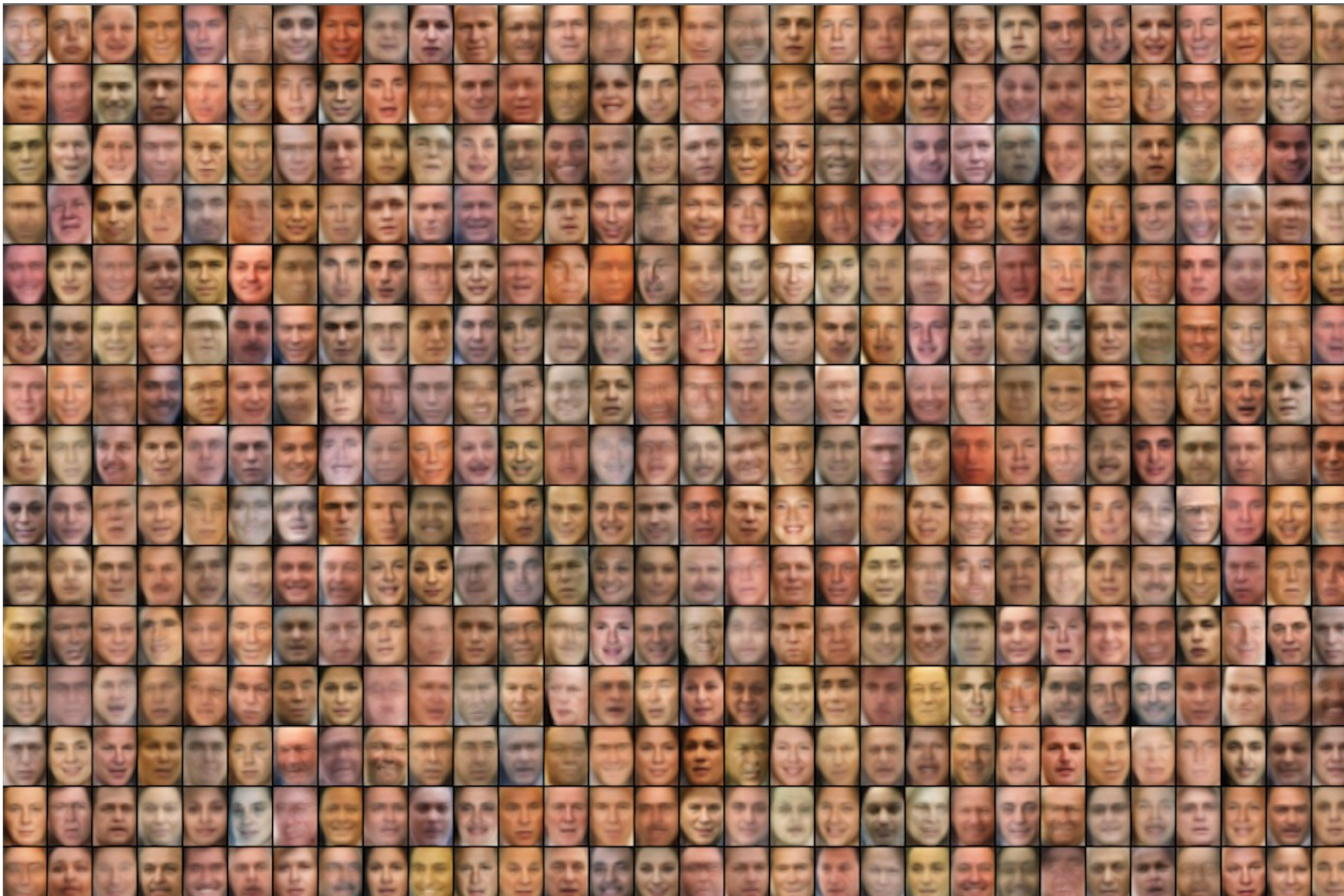


3D latent space: MNIST



Time: z3

Labeled Faces in the Wild (random samples from generative model)



Potential applications

- Representation learning
- Deep generative models of images, video, audio
- Optimal compression (bits-back coding)
- Broader applications of SGVB estimator:

  e.g. learning posterior of the global parameters

- Also see very recent paper:
  "Stochastic Back-propagation and Variational Inference in Deep Latent Gaussian Models"

  [*Danilo J. Rezende, Shakir Mohamed, Daan wierstra*, 2014]

Conclusion

- Auto-Encoding Variational Bayes
  - Applies to almost any directed model with continuous latent variables
  - Optimizes a lower bound of the marginal likelihood
  - Scales to very large datasets
  - Simple
  - Fast

Thanks!

https://github.com/y0ast/Variational-Autoencoder.git