Deep Learning (BEV033DLE)
Lecture 12 Variational Autoencoders

Czech Technical University in Prague

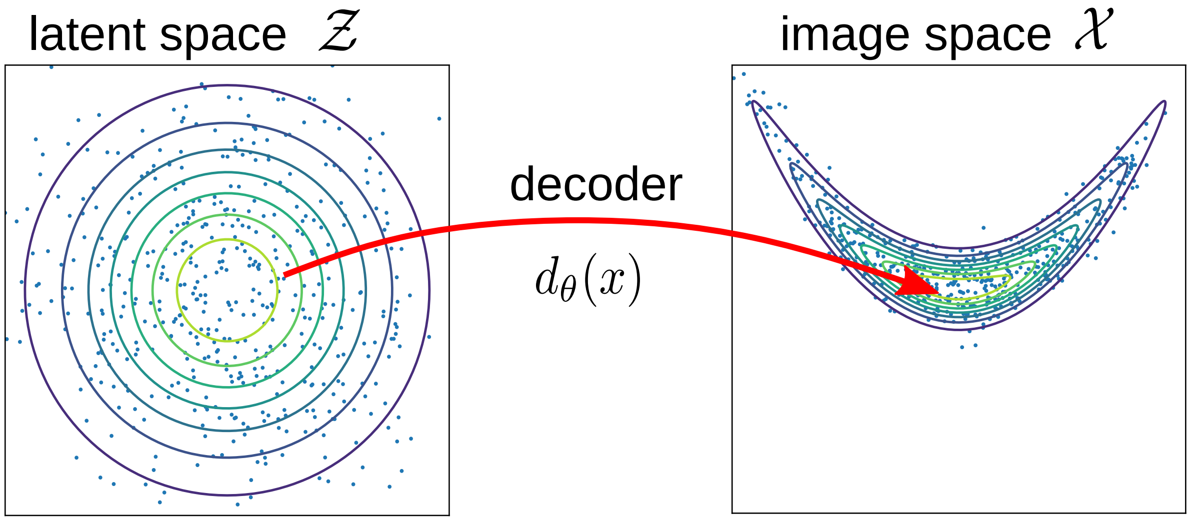
- Generative models in machine learning
- Variational autoencoders (VAE)
- Hierarchical VAE & diffusion models

Generative models

Generative models: Given training data $\mathcal{T} = \{x_j \mid j = 1, \ldots, \ell\}$ drawn i.i.d. from an unknown distribution $p_d(x)$, the goal is to learn a DNN model that allows to generate random instances of x similar to $x \sim p_d(x)$.

Approach this task by using *latent variable models:*

- fix a latent noise space $\mathcal{Z}$ and a distribution $p(z)$ on it,
- design a neural network d_θ that maps $\mathcal{Z}$ to the feature space $\mathcal{X}$,
- learn its parameters θ so that the resulting distribution $p_\theta(x)$ "reproduces" the data distribution.



(Gaussian) Variational Autoencoders

- latent space $\mathcal{Z} = \mathbb{R}^m$, prior distribution $p(z)$: $\mathcal{N}(0, \mathbb{I})$
- image space $\mathcal{X} = \mathbb{R}^n$, conditional distribution $p_\theta(x \,|\, z)$: $\mathcal{N}(\mu_\theta(z), \sigma^2 \mathbb{I})$
  The mapping $\mathcal{Z} \ni z \mapsto \mu_\theta \in \mathcal{X}$ is modelled in terms of a (deep, convolutional) *decoder network* $d_\theta \colon \mathcal{Z} \to \mathcal{X}$.
- Learning goal: maximise data log-likelihood

$$L(\theta; \mathcal{T}) = \mathbb{E}_{\mathcal{T}} \log p_\theta(x) = \mathbb{E}_{\mathcal{T}} \log \int_{\mathcal{Z}} dz\, p_\theta(x \,|\, z) p(z)$$

Computing $L(\theta)$ or $\nabla_\theta L(\theta)$ is not tractable! It would require to integrate the decoder mapping $d_\theta(z)$ over the latent space $\mathcal{Z}$.

Proposal: Use ELBO, i.e. a lower bound of the data log-likelihood

$$L(\theta) \geqslant L_B(\theta, q) = \mathbb{E}_{\mathcal{T}} \mathbb{E}_{q(z \,|\, x)} \Big[\log p_\theta(x \,|\, z) - \log \frac{q(z \,|\, x)}{p(z)} \Big]$$

(Gaussian) Variational Autoencoders

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May be we can apply the *EM algorithm* directly?

EM-algorithm corresponds to block-coordinate ascent of $L_B(\theta, q)$ w.r.t. θ and q

E-step fix θ_t, set $q_t(z \,|\, x) = \arg\max_q L(\theta_t, q) \Rightarrow q_t(z \,|\, x) = p_{\theta_t}(z \,|\, x)$

M-step fix $q_t(z \,|\, x)$, maximise $\theta_{t+1} = \arg\max_\theta \mathbb{E}_{\mathcal{T}} \mathbb{E}_{q_t(z \,|\, x)} \log p_\theta(x \,|\, z)$

No, it is not feasible because computing

$$p_{\theta_t}(z \,|\, x) = \frac{p_{\theta_t}(x \,|\, z) p(z)}{\int dz' \, p_{\theta_t}(x \,|\, z') p(z')}$$

would require to integrate the decoder mapping.

(Gaussian) Variational Autoencoders

Way out: choose a class of *amortised inference* models $q_\varphi(z \,|\, x)$

$$z \,|\, x \sim \mathcal{N}\big(\mu_\varphi(x), \operatorname{diag}(\sigma_\varphi^2(x))\big)$$

The mapping $x \mapsto \big(\mu_\varphi(x), \sigma_\varphi(x)\big)$ is modelled in terms of a (deep, convolutional) *encoder network* $e_\varphi(x) = \big(\mu_\varphi(x), \sigma_\varphi(x)\big)$.

The ELBO criterion reads now

$$L_B(\theta, \varphi) = \mathbb{E}_{\mathcal{T}}\Big[\mathbb{E}_{q_\varphi(z \,|\, x)} \log p_\theta(x \,|\, z) - D_{KL}(q_\varphi(z \,|\, x) \,\|\, p(z))\Big]$$

Can we maximise it by gradient ascent w.r.t. θ and φ?

- $\mathbb{E}_{\mathcal{T}}$: SGD with mini-batches ✓
- $D_{KL}(q_\varphi(z \,|\, x) \,\|\, p(z))$: both Gaussians factorise and the KL-divergence decomposes into a sum over components $\sum_{i=1}^{m} D_{KL}(q_\varphi(z_i \,|\, x) \,\|\, p(z_i))$. The KL-divergence of univariate Gaussian distributions can be computed in closed form! ✓

(Gaussian) Variational Autoencoders

$$L_B(\theta,\varphi) = \mathbb{E}_{\mathcal{T}}\Big[\mathbb{E}_{q_\varphi(z\,|\,x)} \log p_\theta(x\,|\,z) - D_{KL}(q_\varphi(z\,|\,x) \,\|\, p(z))\Big]$$

- $\nabla_\theta \mathbb{E}_{q_\varphi(z\,|\,x)} \log p_\theta(x\,|\,z)$: use SGD by sampling $z \sim q_\varphi(z\,|\,x)$. ✓
- $\nabla_\varphi \mathbb{E}_{q_\varphi(z\,|\,x)} \log p_\theta(x\,|\,z)$: this gradient is *critical*.
  We can not replace $\mathbb{E}_{q_\varphi(z\,|\,x)}$ by a sample $z \sim q_\varphi(z\,|\,x)$, because it will depend on φ!

Re-parametrisation trick: Simple solution for Gaussians:

$$z \sim \mathcal{N}(\mu,\sigma^2) \iff \epsilon \sim \mathcal{N}(0,1) \text{ and } z = \sigma\epsilon + \mu$$

Now, if μ and σ depend on φ:

$$\nabla_\varphi \mathbb{E}_{z\sim\mathcal{N}(\mu_\varphi,\sigma_\varphi^2)}[f(z)] = \mathbb{E}_{\epsilon\sim\mathcal{N}(0,1)}\big[\nabla_\varphi f(\sigma_\varphi\epsilon + \mu_\varphi)\big]$$

(Gaussian) Variational Autoencoders

Overall, the learning step for a (Gaussian) VAE is pretty simple:

Fetch a mini-batch x from training data

1. apply the encoder network $e_\varphi(x) \mapsto \big(\mu_\varphi(x), \sigma_\varphi(x)\big)$ and compute $q_\varphi(z \,|\, x)$
2. compute the KL-divergence $D_{KL}(q_\varphi(z \,|\, x) \,\|\, p(z))$
3. sample a batch $z \sim q_\varphi(z \,|\, x)$ with reparametrisation
4. apply the decoder network $d_\theta(z) \mapsto \mu_\theta(z)$ and compute $\log p_\theta(x \,|\, z)$
5. combine the ELBO terms and let PyTorch compute the derivatives and make an SGD step.

Strengths and weaknesses of VAEs

- concise model, simple objective (ELBO), can be optimised by SGD ✓
- local optima, *posterior collapse*: some latent components collapse to $q_\varphi(z_i \,|\, x) = p(z_i)$, i.e. they carry no information. ✗
- amortised inference models $q_\varphi(z \,|\, x)$ have not enough expressive power to close the gap between $L(\theta)$ and $L_B(\theta, \varphi)$ for complex data distributions ✗

Hierarchical Variational Autoencoders

Closing the gap between $L(\theta)$ and $L_B(\theta, \varphi)$:

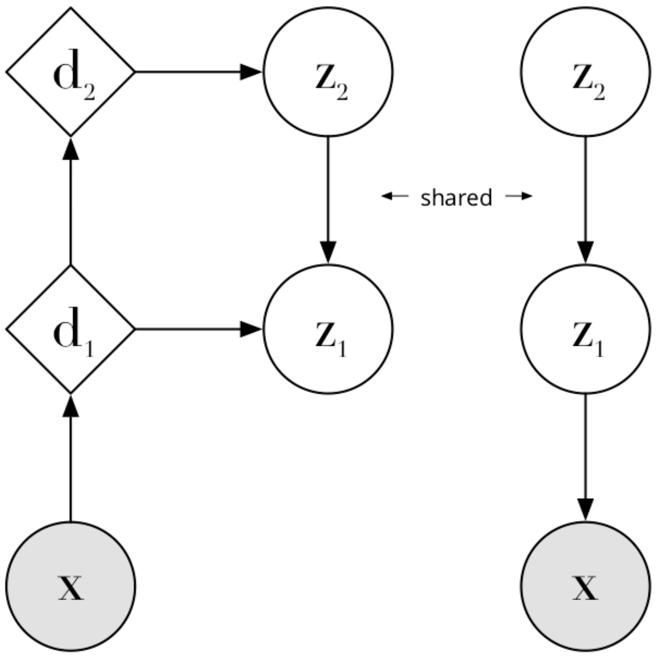
The latent state z consists of variable groups $z_1, \ldots, z_m$.

$$p_\theta(x, z) = p(z_m) \prod_{i=1}^{m-1} p_\theta(z_i \,|\, z_{>i})\, p_\theta(x \,|\, z); \quad q_\varphi(z \,|\, x) = q_\varphi(z_m \,|\, x) \prod_{i=1}^{m-1} q_\varphi(z_i \,|\, z_{>i}, x).$$

The encoder shares parameters with the decoder, by assuming

$$q_{\theta,\varphi}(z_i \,|\, z_{>i}, x) \propto p_\theta(z_i \,|\, z_{>i}) d_i(z_i, x, \varphi),$$

where the functions d_i are hidden layer outputs of a deterministic encoder network whose forward direction is reverse to the factorisation order of the model.



Hierarchical Variational Autoencoders

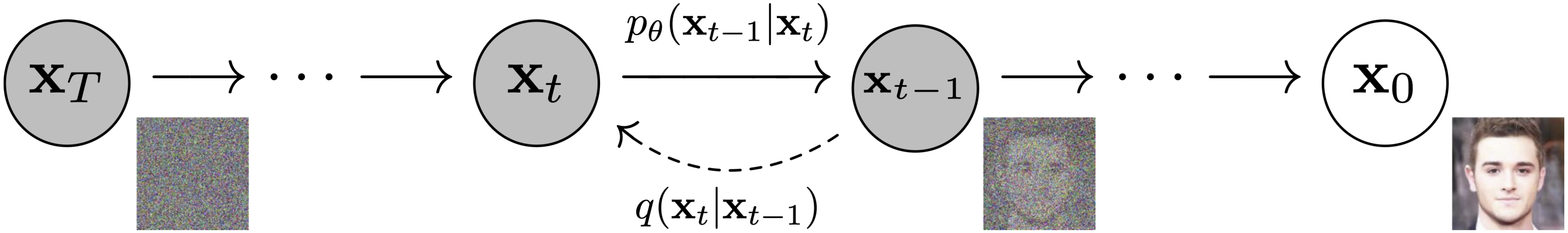
Hierarchical VAEs can be learned by maximising ELBO.

For instance

$$D_{KL}(q_\varphi(z\,|\,x)\,\|\,p(z)) = D_{KL}(q_\varphi(z_m\,|\,x)\,\|\,p(z_m)) + \int dz_m\, q_\varphi(z_m\,|\,x) D_{KL}(q_\varphi(z_{m-1}\,|\,z_m, x)\,\|\,p_\theta(z_{m-1}\,|\,z_m)) + \dots$$

A. Vahdat et al., NeurIPS 2020: A Deep Hierarchical VAE trained on CelebA data.

Diffusion Models



Diffusion models are homogeneous hierarchical VAEs defined on image sequences $x_0, x_1, \ldots, x_t, \ldots$.

- The decoder is given by $p_\theta(x_{t-1} \,|\, x_t)$ and is implemented by a deep network (typically a UNet). Its parameters θ are shared for all t.
- The encoder $q(x_t, \,|\, x_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t} x_{t-1}, \beta_t \mathbb{I})$ is fixed and gradually adds Gaussian noise to the data.

The limiting distribution of the encoder (for $t \to \infty$) is pixel-wise independent Gaussian noise.

The limiting distribution of the trained decoder matches the data distribution.

Diffusion Models

J. Ho et al., NeurIPS 2020, Denoising diffusion probabilistic models