Variational Autoencoders

Machine Learning and Data Mining, 2021

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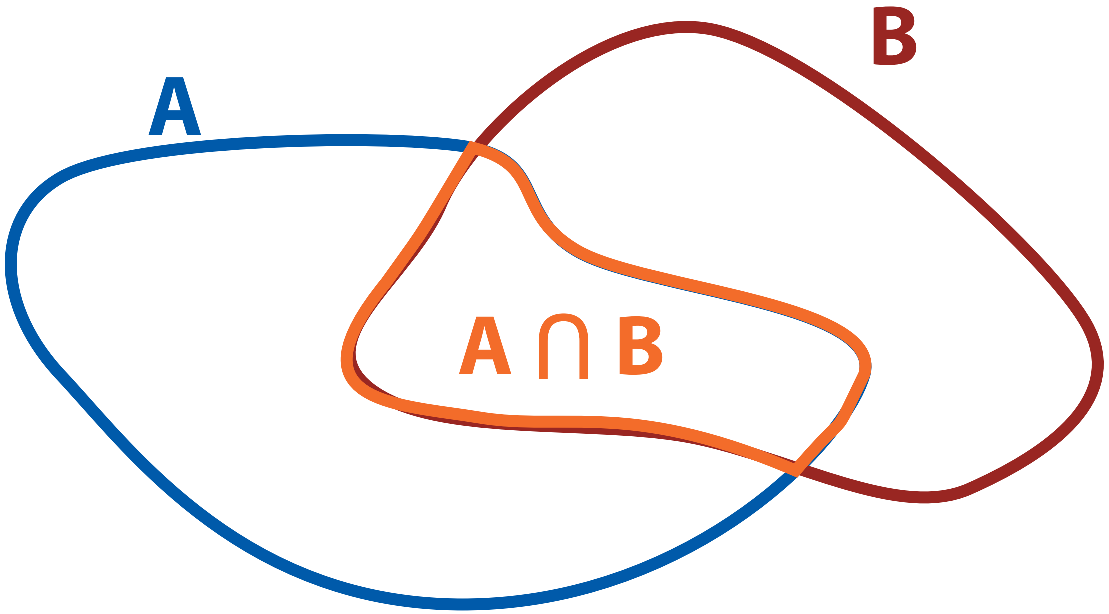
A few definitions

Conditional probability (recap)

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$



For PDF: $$p(x|y) = \frac{p(x,y)}{p(y)}$$

– i.e. we're renormalizing $p(x,y)$ as a distribution of only x for some fixed y

Entropy

- Entropy of a distribution:

$$\mathcal{H}(p) = -\mathbb{E}_{x\sim p(x)} \log p(x)$$

  - measure uncertainty of the random variable x
  - e.g., for the normal distribution it is proportional to $\log \sigma^2$ (the wider the distribution, the more uncertainty there is)

- Note that it equals to the expected negative log likelihood **of the correct hypothesis** (i.e., when the data is actually distributed as p)

Cross-entropy

- Cross-entropy between two distributions:

$$\mathcal{H}(p, q) = -\mathbb{E}_{x \sim p(x)} \log q(x)$$

- May be thought of as the expected negative log likelihood of q when the data is actually distributed as p

Kullback–Leibler divergence

$$D_{\mathrm{KL}}(p\,||\,q) \equiv \mathcal{H}(p,q) - \mathcal{H}(p)$$

$$= \mathbb{E}_{x\sim p(x)} \log \frac{p(x)}{q(x)}$$

- Interpretation: expected logarithm of the **likelihood ratio** between the true data distribution and distribution q when the data is actually distributed as p

$$D_{\mathrm{KL}}(p\,||\,q) \geq 0$$

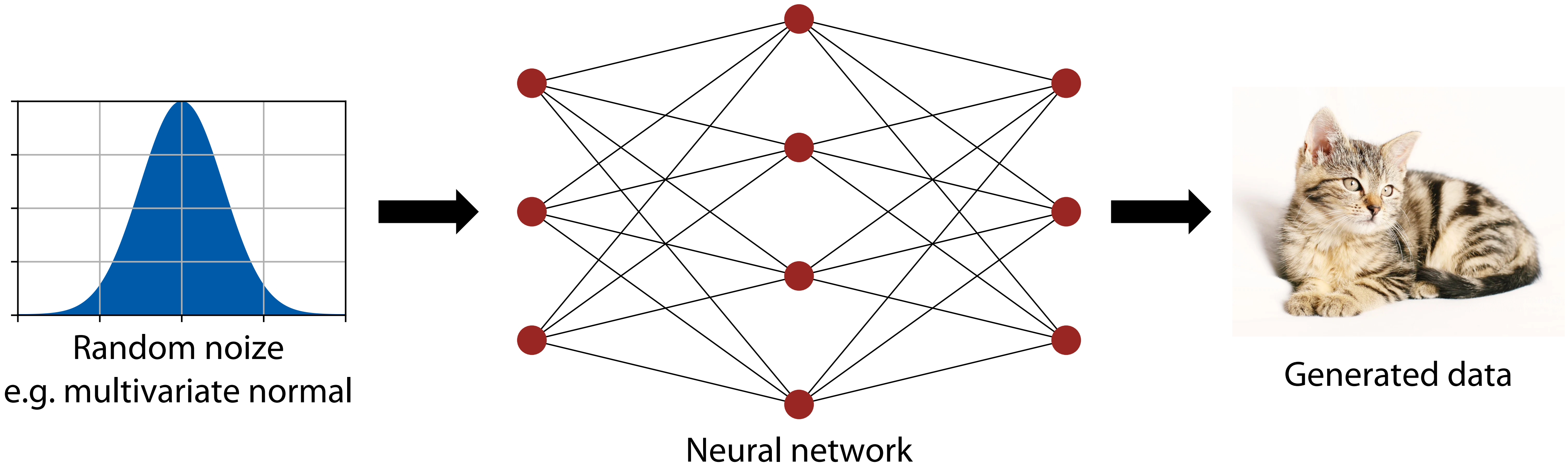
$$D_{\mathrm{KL}}(p\,||\,q) = 0 \quad \Leftrightarrow \quad p = q \text{ (almost everywhere)}$$

Generative modelling

Problem setup (recap)

- Given a set of training objects $\{x_i\}$
- We want to approximate their population distribution $p_{\text{data}}(x)$
- E.g., with some distribution $p_\theta(x)$ parametrized with θ
- To be able to sample new objects $x' \sim p_\theta$, that are similar to $\{x_i\}$

How can a neural network generate data? (recap)



- This makes the generated object being a **differentiable function** of the network parameters

Cat image attribution: https://pixabay.com/users/chiemsee2016-1892688/

Modelling the probability density

- Generated object: $x' = G_\theta(z)$,
- Latent code: $z \sim p_z$ (sampled from some fixed distribution)

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$$p_\theta(x \mid z) = \mathcal{N}(x \mid \underbrace{\mu = G_\theta(z)}, \Sigma = \mathbb{I}\underbrace{\sigma^2})$$

I.e. the network generates not just a single object,
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$$p_\theta(x) = \int p_\theta(x, z) dz = \int p_\theta(x \mid z) \underbrace{p_z}(z) dz = \mathbb{E}_{z \sim \underbrace{p_z}} p_\theta(x \mid z)$$

prior on z

How can we train it?

- To train the model, we'd want to maximize the expected log likelihood:

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  - we only have closed forms for $p_\theta(x \mid z)$ and $p_z(z)$

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  - we only have closed forms for $p_\theta(x \mid z)$ and $p_z(z)$
- Sampling $z \sim p_z$, $x \sim p_{\text{data}}$ and then maximizing the likelihood is typically not very productive
  - Like this, z contains no information about x, and the network will likely learn just to ignore it and always predict the same object

The posterior

- Assume we're able to calculate (and sample from) the posterior $p_\theta(z|x)$
- Note that:

$$\log p_\theta(x) = \mathbb{E}_{z\sim p_\theta(z|x)} \log\left[p_\theta(x)\frac{p_\theta(z|x)}{p_\theta(z|x)}\right]$$

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So, for the log-likelihood we're sampling not all z values, but only those corresponding to this particular x

Maximizing this encourages placing high probability mass on many z values that could've generated x

Approximate inference

Approximate inference

- In practice, $p_\theta(z|x)$ is typically intractable
- Let's try to approximate it with another parametric distribution $q_\phi(z|x)$
  - E.g., $q_\phi(z|x) = \mathcal{N}\left(z \middle| \mu_\phi(x), \mathbb{I}\sigma_\phi^2(x)\right)$, where μ_ϕ and σ_ϕ^2 are outputs of a neural network
- And use it for the likelihood calculation, i.e.:

$$[\log p_\theta(x)]_{\mathrm{approx.},\phi} = \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x,z) + \mathcal{H}\left(q_\phi(z|x)\right)$$

Approximate inference

- Let's check how bad this approximation is:

$$\log p_\theta(x) - [\log p_\theta(x)]_{\text{approx.},\phi} =$$

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$$= \mathbb{E}_{z\sim q_\phi(z|x)}\left[-\log p_\theta(z|x) + \log q_\phi(z|x)\right]$$

$$= D_{\mathrm{KL}}\left(q_\phi(z|x) \| p_\theta(z|x)\right) \geq 0$$

Approximate inference

- We've shown that:

$$\log p_\theta(x) - [\log p_\theta(x)]_{\text{approx.},\phi} = D_{\text{KL}}\big(q_\phi(z|x) \big\| p_\theta(z|x)\big) \geq 0$$

- I.e., our approximate log-likelihood is the **lower bound** for the true log-likelihood
  - Also called evidence lower bound (ELBO) or variational lower bound

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- I.e., our approximate log-likelihood is the **lower bound** for the true log-likelihood
  – Also called evidence lower bound (ELBO) or variational lower bound
- The better q approximates the posterior – the closer the bound is to the actual log-likelihood
- Also, if we maximize the lower bound, we'll maximize the likelihood as well!

Alternative form

$$\mathrm{ELBO} = [\log p_\theta(x)]_{\text{approx.},\phi} = \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x,z) + \mathcal{H}\left(q_\phi(z|x)\right)$$

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Variational autoencoder (VAE)

Variational autoencoder

- Let's make use our choices for $p_\theta(x \mid z)$, $p_z(z)$ and $q_\phi(z \mid x)$:

$$p_z(z) = \mathcal{N}(z \mid 0, \mathbb{I})$$

$$p_\theta(x \mid z) = \mathcal{N}(x \mid \mu = G_\theta(z), \Sigma = \mathbb{I}\sigma^2)$$

$$q_\phi(z|x) = \mathcal{N}\left(z \middle| \mu_\phi(x), \mathbb{I}\sigma_\phi^2(x)\right)$$

- And see how we can optimize the two ELBO terms:

$$\mathrm{ELBO} = \underbrace{\mathbb{E}_{z \sim q_\phi(z|x)} \log p_\theta(x|z)}_{\text{Data term}} - \underbrace{D_{KL}\left(q_\phi(z|x) \| p(z)\right)}_{\text{Regularizer}} \to \max_{\theta,\phi}$$

The data term

$$\mathbb{E}_{z \sim q_\phi(z|x)} \log p_\theta(x|z)$$

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$$q_\phi(z|x) = \mathcal{N}\left(z\middle|\ \mu_\phi(x), \mathbb{I}\sigma_\phi^2(x)\right)$$

- Take object x from the dataset
- Calculate the posterior $q_\phi(z|x)$
- Sample latent code z_ϕ from the posterior
- Calculate the log-likelihood for this pair (x, z_ϕ):

$$\log p_\theta(x|z) = -\frac{1}{2\sigma^2}\sum_i \left(x_i - G_\theta(z_\phi)_i\right)^2 + const$$

Sum over the components of the data vector

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“decoder”

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How do we backpropagate through z (to optimize wrt ϕ)?

Backpropagating through randomness

Reparametrization trick:

- To sample $z_\phi \sim \mathcal{N}\left(\mu_\phi(x), \sigma_\phi^2(x)\right)$,
- we first sample $\xi \sim \mathcal{N}(0,1)$,
- then set $z_\phi = \xi \cdot \sigma_\phi(x) + \mu_\phi(x)$

Regularizer term

$$\text{ELBO} = \underbrace{\mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z)}_{\textbf{Data term}} - \underbrace{D_{KL}\big(q_\phi(z|x) \| p(z)\big) \to}_{\textbf{Regularizer}} \max_{\theta,\phi}$$

- p_z is $\mathcal{N}(0, \mathbb{I})$
- $q_\phi(z|x)$ is a normal with $\mu = \mu_\phi(x), \Sigma = \mathbb{I}\sigma_\phi^2(x)$
- KL divergence between them can be calculated analytically
- Proove that:
  - KL is additive for factorizing distributions $D_{KL}(p_x p_y \| q_x q_y) = D_{KL}(p_x \| q_x) + D_{KL}(p_y \| q_y)$,
  - KL between two univariate normal distributions is:

$$D_{KL}\left(\mathcal{N}(\mu_1, \sigma_1^2) \| \mathcal{N}(\mu_2, \sigma_2^2)\right) = \log\frac{\sigma_2}{\sigma_1} + \frac{\sigma_1^2 + (\mu_2 - \mu_1)^2}{2\sigma_2^2} - \frac{1}{2}$$

Discussion

VAE vs GANs

- In the tasks of image generation GANs are typically better
  - VAEs tend to produce blurry results due to the nature of the MSE loss
  - Note that MSE loss between images does not reflect our perception of image quality or similarity:

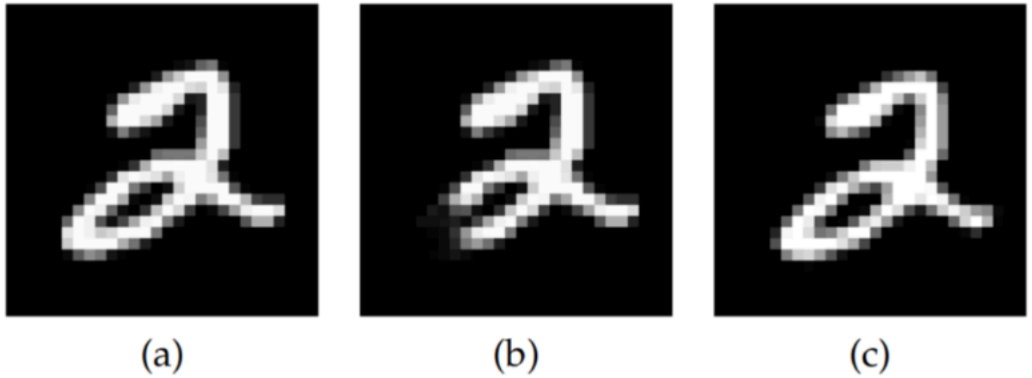

Image (b) — slightly altered image (a), image (c) — image (a) shifted by several pixels.
Under MSE metric, image (b) is much closer to (a), than (c) to (a).

  - There are some further advancements in VAEs that perform better (e.g., adversarial VAE)

VAEs vs GANs

- VAE is easier to train – no min-max game, just a single optimization objective
- The encoder gives you the mapping from objects to the latent representation
  - This lets you do things like interpolation between objects, anaylyzing latent space, etc.
- VAEs give you explicit access to the estimated data PDF

Bayesian neural networks in a nutshell

- Variational inference and ELBO optimization are very powerful techniques
- Also applied in bayessian neural networks
- The main idea is to treat the weights as random variables, with some prior distribution on them, i.e., the model is $p(y|x) = \mathbb{E}_{w \sim p(w)}[p(y|x,w)]$
- Approximate posterior $p(w|X,Y)$ with a parametric distribution $q_\phi(w)$
  – Something easy to sample from - allowing for the reparametrisation trick, and allowing the analytic calculation of KL divergence wrt prior
- Optimize ELBO:

$$\mathrm{ELBO} = \mathbb{E}_{w \sim q_\phi} \log p(y|x,w) - D_{\mathrm{KL}}\left(q_\phi(w) \parallel p(w)\right)$$

Bayessian neural networks in a nutshell

- Having found the approximate posterior $q_\phi(w)$, use expected w for prediction
- May also sample different weights from $q_\phi(w)$ to estimate the uncertainty of the prediction
- Different priors favor different properties of the network
  - E.g., log-uniform prior helps removing noisy weights and thus finding sparse solutions (as was shown in https://arxiv.org/abs/1701.05369)

Thank you!

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