1 Generative modelling

Learn $p_{\text{model}} \approx p_{\text{data}}$, sample from p_{model}.

- Explicit density:
  - Approximate:
    - Variational: VAE, Diffusion
    - Markov Chain: Boltzmann machine
  - Tractable:
    - Autoregressive: FVSBN/NADE/MADE, Pixel(C/R)NN, WaveNet/TCN, Autor. Transf.,
    - Normalizing Flows
- Implicit density:
  - Direct: Generative Adversarial Networks
  - MC: Generative Stochastic Networks

Autoencoder: $X \rightarrow Z \rightarrow X$, $g \circ f \approx \text{id}$, f and g are NNs. Optimal linear autoencoder is PCA.
Undercomplete: $|Z| < |X|$, else overcomplete.
Overcomp. is for denoising, inpainting.
Latent space should be continuious and interpolable. Autoencoder spaces are neither, so they are only good for reconstruction.

2 Variational AutoEncoder (VAE)

Sample z from prior $p_\theta(z)$, to decode use conditional $p_\theta(x \mid z)$ defined by a NN.
$D_{\text{KL}}(P\|Q) \coloneqq \int_x p(x) \log \frac{p(x)}{q(x)} \mathrm{d}x$: KL divergence, measure similarity of prob. distr.
$D_{\text{KL}}(P\|Q) \neq D_{\text{KL}}(Q\|P)$, $D_{\text{KL}}(P\|Q) \geq 0$
Likelihood $p_\theta(x) = \int_z p_\theta(x \mid z) p_\theta(z) \mathrm{d}z$ is hard to max., let enc. NN be $q_\phi(z \mid x)$, $\log p_\theta(x^i) = \mathbb{E}_z \left[\log p_\theta(x^i \mid z)\right] - D_{\text{KL}}(q_\phi(z \mid x^i) \| p_\theta(z)) + D_{\text{KL}}(q_\phi(z \mid x^i) \| p_\theta(z \mid x^i))$. Red is intractable, use ≥ 0 to ignore it; Orange is reconstruction loss, clusters similar samples; Purple makes posterior close to prior, adds cont. and interp. Orange − Purple is **ELBO**, maximize it.

$x \xrightarrow{\text{enc}} \mu_{z|x}, \Sigma_{z|x} \xrightarrow{\text{sample}} z \xrightarrow{\text{dec}} \mu_{x|z}, \Sigma_{x|z} \xrightarrow{\text{sample}} \hat{x}$
Backprop through sample by reparametr.: $z = \mu + \sigma\epsilon$. For inference, use μ directly.
Disentanglement: features should correspond to distinct factors of variation. Can be done with semi-supervised learning by making z conditionally independent of given features y.

2.1 β-VAE

Disentangle by $\max_{\theta,\phi} \mathbb{E}_x \left[\mathbb{E}_{z \sim q_\phi} \log p_\theta(x \mid z)\right]$ s.t. $D_{\text{KL}}(q_\phi(z \mid x) \| p_\theta(z)) < \delta$, with KKT: max Orange − βPurple.

3 Autoregressive generative models

Autoregression: use data from the same input variable at previous time steps
Discriminative: $P(Y \mid X)$, generative: $P(X, Y)$, maybe with Y missing. Sequence models are generative: from $x_i \ldots x_{i+k}$ predict x_{i+k+1}.
Tabular approach: $p(\mathbf{x}) = \prod_i p(x_i \mid \mathbf{x}_{<i})$, needs 2^{i-1} params. Independence assumption is too strong. Let $p_{\theta_i}(x_i \mid \mathbf{x}_{<i}) = \text{Bern}(f_i(\mathbf{x}_{<i}))$, where f_i is a NN. **Fully Visible Sigmoid Belief Networks**: $f_i = \sigma(\alpha_0^{(i)} + \boldsymbol{\alpha}^{(i)} \mathbf{x}_{<i}^\mathsf{T})$, complexity n^2, but model is linear.
Neural Autoregressive Density Estimator: add hidden layer. $\mathbf{h}_i = \sigma(\mathbf{b} + \mathbf{W}_{\cdot,<i}\mathbf{x}_{<i})$, $\hat{x}_i = \sigma(c_i + \mathbf{V}_{i,\cdot}\mathbf{h}_i)$. Order of $\mathbf{x}$ can be arbitrary but fixed. Train by max log-likelihood in $O(TD)$, can use 2nd order optimizers, can use **teacher forcing**: feed GT as previous output.
Extensions: Convolutional; Real-valued: conditionals by mixture of gaussians; Order-less and deep: one DNN predicts $p(x_k \mid x_{i_1} \ldots x_{i_j})$.
Masked Autoencoder Distribution Estimator: mask out weights s.t. no information flows from $x_d \ldots$ to $\hat{x}_d$. Large hidden layers needed. Trains as fast as autoencoders, but sampling needs D forward passes.
PixelRNN: generate pixels from corner, dependency on previous pixels is by RNN (LSTM).
PixelCNN: also from corner, but condition by CNN over context region (perceptive field) $\Rightarrow$ parallelize. For conditionals use masked convolutions. Channels: model R from context, G from R + cont., B from G + R + cont. Training is parallel, but inference is sequential $\Rightarrow$ slow. Use conv. stacks to mask correctly.
NLL is a natural metric for autoreg. models, hard to evaluate others.
WaveNet: audio is high-dimensional. Use dilated convolutions to increase perceptive field with multiple layers.
AR does not work for high res images/video, convert the images into a series of tokens with an AE: Vector-quantized VAE. The codebook is a set of vectors. $x \xrightarrow{\text{enc}} z \xrightarrow{\text{codebook}} z_q \xrightarrow{\text{dec}} \hat{x}$.
We can run an AR model in the latent space.

3.1 Attention

$\mathbf{x}_t$ is a convex combination of the past steps, with access to all past steps. For $X \in \mathbb{R}^{T \times D}$: $K = XW_K, V = XW_V, Q = XW_Q$. Check pairwise similarity between query and keys via dot product: let attention weights be $\boldsymbol{\alpha} = \text{Softmax}(QK^\mathsf{T}/\sqrt{D})$, $\boldsymbol{\alpha} \in \mathbb{R}^{1 \times T}$. Adding mask M to avoid looking into the future:

$$X = \text{Softmax}\left(\frac{(XW_Q)(XW_K)^\mathsf{T}}{\sqrt{D}} + M\right)(XW_V)$$

Multi-head attn. splits W into h heads, then concatenates them. Positional encoding injects information about the position of the token. Attn. is $O(T^2 D)$.

4 Normalizing Flows

VAs dont have a tractable likelihood, AR models have no latent space. Want both. Change of variable for $x = f(z)$: $p_x(x) = p_z(f^{-1}(x)) \left|\det \frac{\partial f^{-1}(x)}{\partial x}\right| = p_z(f^{-1}(x)) \left|\det \frac{\partial f(z)}{\partial z}\right|^{-1}$. Map $Z \rightarrow X$ with a deterministic invertible f_θ. This can be a NN, but computing the determinant is $O(n^3)$. If the Jacobian is triangular, the determinant is $O(n)$. To do this, add a coupling layer:

$$\begin{pmatrix} y^A \\ y^B \end{pmatrix} = \begin{pmatrix} h(x^A, \beta(x^B)) \\ x^B \end{pmatrix}$$

, where β is any model, and h is elementwise.

$$\begin{pmatrix} x^A \\ x^B \end{pmatrix} = \begin{pmatrix} h^{-1}(y^A, \beta(y^B)) \\ y^B \end{pmatrix}, J = \begin{pmatrix} h' & h'\beta' \\ 0 & 1 \end{pmatrix}$$

Stack these for expressivity, $f = f_k \circ \ldots f_1$
$p_x(x) = p_z(f^{-1}(x)) \prod_k \left|\det \frac{\partial f_k^{-1}(x)}{\partial x}\right|$.
Sample $z \sim p_z$ and get $x = f(z)$. To get the prob. of x, use the formula above.