Deep Generative Models

Lecture 2

Roman Isachenko

Moscow Institute of Physics and Technology

Autumn, 2021

Recap of previous lecture

We are given i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^n \in X$ (e.g. $X = \mathbb{R}^m$) from unknown distribution $\pi(\mathbf{x})$.

Goal

We would like to learn a distribution $\pi(\mathbf{x})$ for

- evaluating $\pi(\mathbf{x})$ for new samples (how likely to get object $\mathbf{x}$?);
- sampling from $\pi(\mathbf{x})$ (to get new objects $\mathbf{x} \sim \pi(\mathbf{x})$).

Instead of searching true $\pi(\mathbf{x})$ over all probability distributions, learn function approximation $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

Divergence

- $D(\pi||p) \geq 0$ for all $\pi, p \in \mathcal{S}$;
- $D(\pi||p) = 0$ if and only if $\pi \equiv p$.

General divergence minimization task

$$\min_{\boldsymbol{\theta}} D(\pi||p).$$

Recap of previous lecture

Forward KL

$$KL(\pi || p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\boldsymbol{\theta})} d\mathbf{x} \rightarrow \min_{\boldsymbol{\theta}}$$

Reverse KL

$$KL(p || \pi) = \int p(\mathbf{x}|\boldsymbol{\theta}) \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x})} d\mathbf{x} \rightarrow \min_{\boldsymbol{\theta}}$$

Maximum likelihood estimation (MLE)

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

Maximum likelihood estimation is equivalent to minimization of the Monte-Carlo estimate of forward KL.

Recap of previous lecture

Likelihood as product of conditionals

Let $\mathbf{x} = (x_1, \dots, x_m)$, $\mathbf{x}_{1:j} = (x_1, \dots, x_j)$. Then

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}); \quad \log p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{j=1}^{m} \log p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}).$$

MLE problem for autoregressive model

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \sum_{j=1}^{m} \log p(x_{ij}|\mathbf{x}_{i,1:j-1}\boldsymbol{\theta}).$$

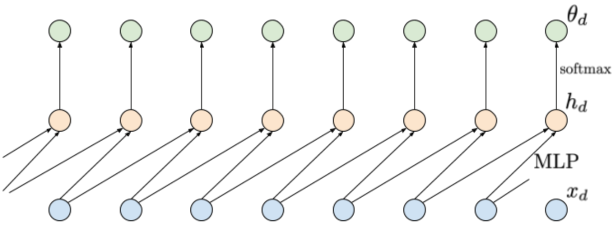
Sampling

$$\hat{x}_1 \sim p(x_1|\boldsymbol{\theta}), \quad \hat{x}_2 \sim p(x_2|\hat{x}_1, \boldsymbol{\theta}), \dots, \quad \hat{x}_m \sim p(x_m|\hat{\mathbf{x}}_{1:m-1}, \boldsymbol{\theta})$$

New generated object is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m)$.

Recap of previous lecture

Autoregressive MLP



Autoregressive RNN

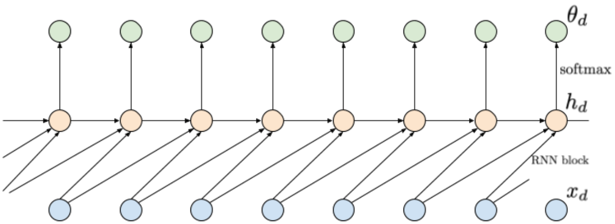
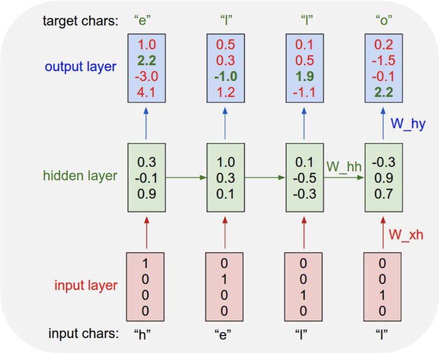


image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

Char RNN

Model tries to predict the next token (single letter) from previous context.

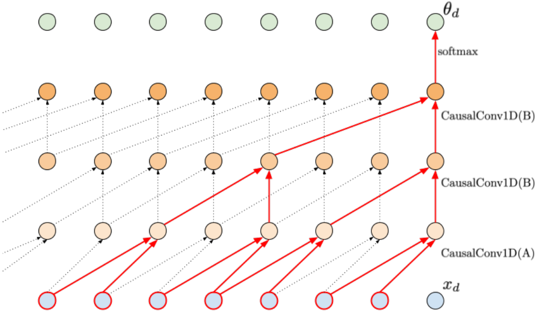



```
PANDARUS:
Alas, I think he shall be come approached and the day
When little srain would be attain'd into being never fed,
And who is but a chain and subjects of his death,
I should not sleep.

Second Senator:
They are away this miseries, produced upon my soul,
Breaking and strongly should be buried, when I perish
The earth and thoughts of many states.

DUKE VINCENTIO:
Well, your wit is in the care of side and that.

Second Lord:
They would be ruled after this chamber, and
my fair nues begun out of the fact, to be conveyed,
Whose noble souls I'll have the heart of the wars.

Clown:
Come, sir, I will make did behold your worship.

VIOLA:
I'll drink it.
```

image credit: http://karpathy.github.io/2015/05/21/rnn-effectiveness

Autoregressive models

- Convolutions could be used for autoregressive models, but they have to be **causal**.
- Try to find and understand the difference between Conv A/B.

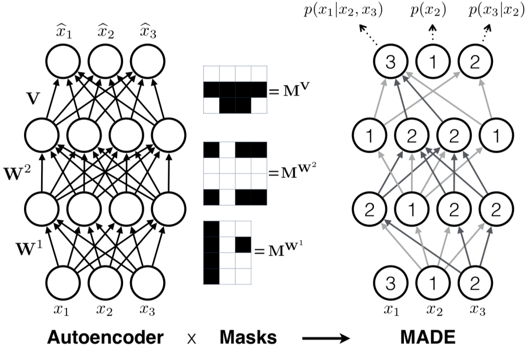


- Could learn long-range dependecies.
- Do not suffer from gradient issues.
- Easy to estimate probability for given input, but hard generation of new samples (the sequential process).

image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

MADE

- Vanila autoencoder is not a generative model.
- Let mask the weight matrices to make the model generative: $\mathbf{W}_M = \mathbf{W} \cdot \mathbf{M}$.



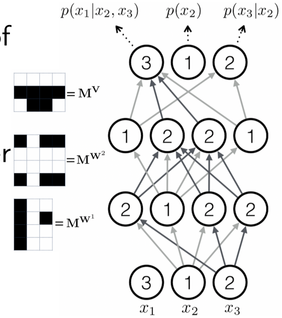
- The question is how to create matrices **M** which produce the autoregressive property?

Germain M. et al. Made: Masked autoencoder for distribution estimation, 2015

MADE

Masks generation

- Define the ordering of input elements from 1 to m.
- Assign the random number k from 1 to $m-1$ to each hidden unit. The number gives the maximum number of input units to which the unit can be connected.
- Connect each hidden unit with number k with the previous layer units which has the number is **less or equal** than k.
- Connect each output unit with number k with the previous layer units which has the number is **less** than k.

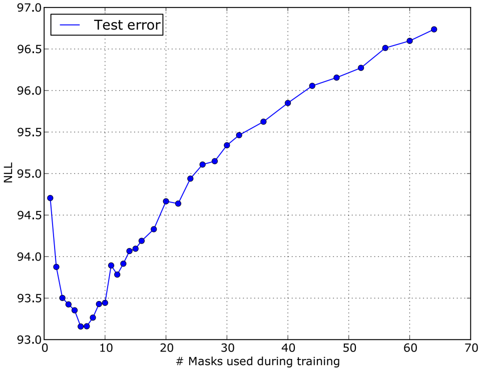


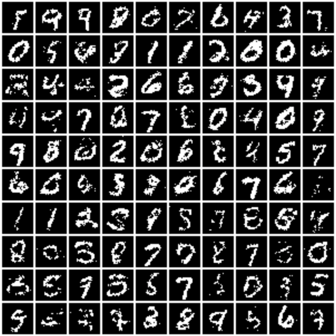
Germain M. et al. Made: Masked autoencoder for distribution estimation, 2015

MADE

Possible variations

- Order agnostic training (missing values in partially observed input vectors can be imputed efficiently);
- Connectivity-agnostic training (cheap ensembling).





Germain M. et al. Made: Masked autoencoder for distribution estimation, 2015

WaveNet

Goal

Efficient generation of raw audio waveforms with natural sounds.

Solution

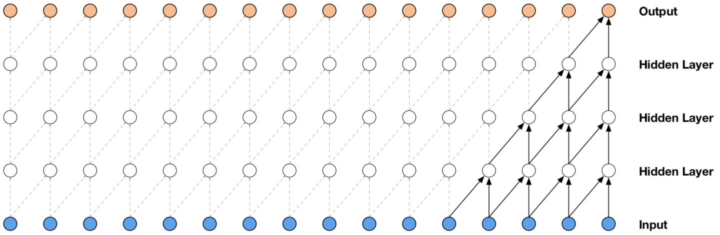
Autoregressive model

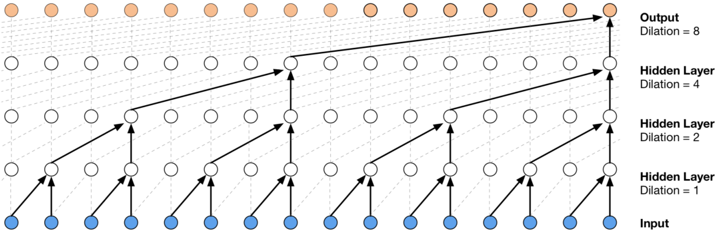
$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{t=1}^{T} p(x_t|\mathbf{x}_{1:t-1}, \boldsymbol{\theta}).$$

- Each conditional $p(x_t|\mathbf{x}_{1:t-1}, \boldsymbol{\theta})$ models the distribution for the timestamp t.
- The model uses **causal** dilated convolutions.

Oord A. et al. Wavenet: A generative model for raw audio, 2016

WaveNet





Oord A. et al. Wavenet: A generative model for raw audio, 2016

PixelCNN

Goal

Model a distribution $\pi(\mathbf{x})$ of natural images.

Solution

Autoregressive model on 2D pixels

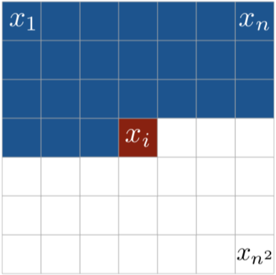
$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{\text{width}\times\text{height}} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}).$$

- We need to introduce the ordering of image pixels.
- The convolution should be **masked** to make them causal.
- The image has RGB channels, these dependencies could be addressed.

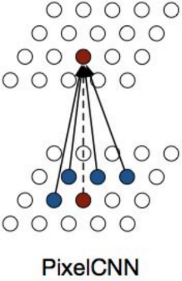
Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

PixelCNN

Raster ordering

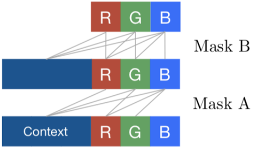


Dependencies between pixels



Masked convolution kernel

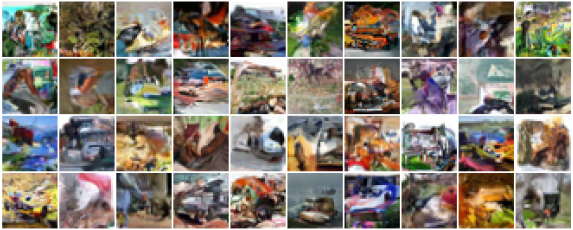
1	1	1
1	0	0
0	0	0



Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

PixelCNN

CIFAR-10 generated samples



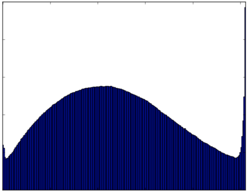
CIFAR-10 perfomance

Model	NLL Test (Train)
Uniform Distribution:	8.00
Multivariate Gaussian:	4.70
NICE [1]:	4.48
Deep Diffusion [2]:	4.20
Deep GMMs [3]:	4.00
RIDE [4]:	3.47
PixelCNN:	3.14 (3.08)
Row LSTM:	3.07 (3.00)
Diagonal BiLSTM:	**3.00** (2.93)

Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

PixelCNN++

CIFAR-10 pixel values distribution



- Standard PixelCNN outputs softmax probabilities for values $\{0, 255\}$ (256 outputs feature maps).
- Categorical distribution do not know anything about numerical relationships (220 is close to 221 and far from 15).
- If pixel value is not presented in the training dataset, it won't be predicted.
- (Look at the edges of the distributions: they have higher probability mass).

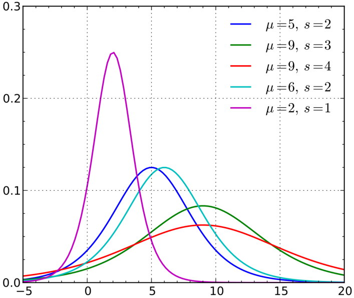
Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

PixelCNN++

Mixture of logistic distributions

$$p(x|\mu, s) = \frac{\exp^{-(x-\mu)/s}}{s(1+\exp^{-(x-\mu)/s})^2};$$

$$p(x|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi}) = \sum_{k=1}^{K} \pi_k p(x|\mu_k, s_k);$$



To adopt probability calculation to discrete values:

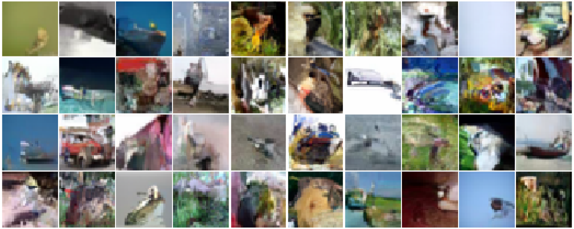
$$P_d(x|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi}) = P(x+0.5|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi}) - P(x-0.5|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi})$$

For the edge case of 0, replace $x - 0.5$ by $-\infty$, and for 255 replace $x + 0.5$ by $+\infty$.

Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

PixelCNN++

CIFAR-10 generated samples

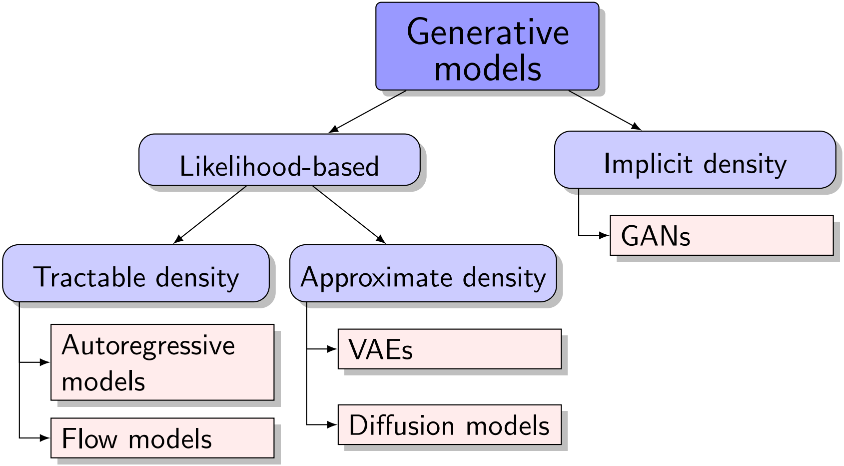


CIFAR-10 perfomance

Model	Bits per sub-pixel
Deep Diffusion (Sohl-Dickstein et al., 2015)	5.40
NICE (Dinh et al., 2014)	4.48
DRAW (Gregor et al., 2015)	4.13
Deep GMMs (van den Oord & Dambre, 2015)	4.00
Conv DRAW (Gregor et al., 2016)	3.58
Real NVP (Dinh et al., 2016)	3.49
PixelCNN (van den Oord et al., 2016b)	3.14
VAE with IAF (Kingma et al., 2016)	3.11
Gated PixelCNN (van den Oord et al., 2016c)	3.03
PixelRNN (van den Oord et al., 2016b)	3.00
PixelCNN++	**2.92**

Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

Generative models zoo



Bayesian framework

Bayes theorem

$$p(\mathbf{t}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{\int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}}$$

- $\mathbf{x}$ – observed variables, $\mathbf{t}$ – unobserved variables (latent variables/parameters);
- $p(\mathbf{x}|\mathbf{t})$ – likelihood;
- $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}$ – evidence;
- $p(\mathbf{t})$ – prior distribution, $p(\mathbf{t}|\mathbf{x})$ – posterior distribution.

Meaning

We have unobserved variables $\mathbf{t}$ and some prior knowledge about them $p(\mathbf{t})$. Then, the data $\mathbf{x}$ has been observed. Posterior distribution $p(\mathbf{t}|\mathbf{x})$ summarizes the knowledge after the observations.

Bayesian framework

Let consider the case, where the unobserved variables $\mathbf{t}$ is our model parameters $\boldsymbol{\theta}$.

- $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$ – observed samples;
- $p(\boldsymbol{\theta})$ – prior parameters distribution (we treat model parameters $\boldsymbol{\theta}$ as random variables).

Posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

Bayesian inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta}$$

Note the difference from

$$p(\mathbf{x}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}.$$

Bayesian framework

Posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

Bayesian inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta}$$

If evidence $p(\mathbf{X})$ is intractable (due to multidimensional integration), we can't get posterior distribution and perform the precise inference.

Maximum a posteriori (MAP) estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \big(\log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\big)$$

Bayesian framework

MAP estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \big(\log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\big)$$

Estimated $\boldsymbol{\theta}^*$ is a deterministic variable, but we could treat it as a random variable with density $p(\boldsymbol{\theta}|\mathbf{X}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$.

Dirac delta function

$$\delta(x) = \begin{cases} +\infty, & x = 0; \\ 0, & x \neq 0; \end{cases} \quad \int \delta(x)dx = 1; \; \int f(x)\delta(x-y)dx = f(y).$$

MAP inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta} \approx p(\mathbf{x}|\boldsymbol{\theta}^*).$$

Latent variable models (LVM)

MLE problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

Challenge

$p(\mathbf{x}|\boldsymbol{\theta})$ could be intractable.

Extend probabilistic model

Introduce latent variable $\mathbf{z}$ for each sample $\mathbf{x}$

$$p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}); \quad \log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}).$$

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}) d\mathbf{z}.$$

Motivation

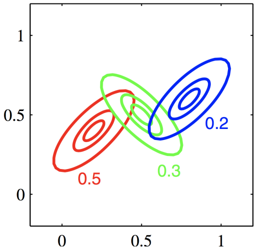
The distributions $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ and $p(\mathbf{z})$ could be quite simple.

Latent variable models (LVM)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z})d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

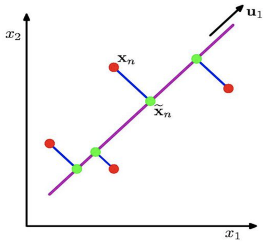
Examples

Mixture of gaussians



- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\mathbf{z}}, \boldsymbol{\Sigma}_{\mathbf{z}})$
- $p(\mathbf{z}) = \text{Categorical}(\mathbf{z}|\pi)$

PCA model



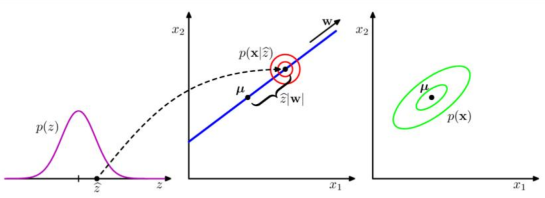
- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \boldsymbol{\Sigma}_{\mathbf{z}})$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$

Bishop C. Pattern Recognition and Machine Learning, 2006

Latent variable models (LVM)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

PCA goal: Project original data $\mathbf{X}$ onto a low dimensional latent space while maximizing the variance of the projected data.



$\boldsymbol{x} = W\boldsymbol{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$

- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \boldsymbol{\Sigma}_{\mathbf{z}})$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$

Bishop C. Pattern Recognition and Machine Learning, 2006

Incomplete likelihood

MLE

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}).$$

Since $\mathbf{Z}$ is unknown, maximize **incomplete likelihood**.

MILE problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \log p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log \int p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}) d\mathbf{z}_i =$$

$$= \arg\max_{\boldsymbol{\theta}} \log \sum_{i=1}^{n} \int p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta}) p(\mathbf{z}_i) d\mathbf{z}_i.$$

Summary

- MADE model is an autoregressive autoencoder with masked dense layers.
- WaveNet and PixelCNN models use masked causal convolutions (1D or 2D) to get autoregressize model.
- PixelCNN++ proposes to use discretized mixture of logistics for output distribution.
- Bayesian inference is a generalization of most common machine learning tasks. It allows to construct MLE, MAP and bayesian inference, to compare models complexity and many-many more cool stuff.
- LVM introduce latent representation of observed samples to make model more interpretable.