Deep Generative Models (Latent Variable Models)

Aapo Hyvärinen for the NNDL course, 25 April 2025

- Definition of deep latent variable models (DLVM)
- ▶ How to estimate an DLVM? Why maximum likelihood is difficult.
- Approximations of likelihood: Variational Autoencoders (VAE)
- Estimation of DLVM by classification: Generative Adversarial Networks (GAN)
- Problem of identifiability
- (Nonlinear) Independent Component Analysis

Literature: Prince's book Chapters 15, 17 (only part of the material)



Deep Latent Variable Models (DLVM): general definition

- Express observed data x as a function of latent vector z
 - latent = hidden, i.e. unobserved
- Model (hypothetical) data generation in two stages
 - ightharpoonup z is sampled from a "prior" p(z)
 - Given the sampled z, sample x from the "likelihood" p(x|z)
 - ► Terminological note: not quite the same "likelihood" as earlier
 - Formal definition:

$$p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x}|\mathbf{z})p(\mathbf{z})$$

where heta is a vector of parameters, e.g. in a neural network

- Typically, prior $p(\mathbf{z})$ is something very simple, e.g. independent z_i , and not dependent on any parameters
- Likelihood $p(\mathbf{x}|\mathbf{z})$ models some kind of "mixing", e.g.
 - ▶ Mixing of real-life "sources" in a measurement system
 - Mixing of image features when composing pixels
- Generative model is a term with many meanings; we use it in the same sense as a (deep) latent-variable model.



Background: covariance matrix and whiteness

▶ We define the covariance matrix as

$$[cov(\mathbf{z})]_{ij} = cov(z_i, z_j) = E\{z_i z_j\} - E\{z_i\} E\{z_j\}$$
 (1)

or simply for zero-mean data:

$$cov(\mathbf{z}) = E\{\mathbf{z}\mathbf{z}^T\} \tag{2}$$

We have for any linear transformation:

$$cov(Mz) = Mcov(z)M^{T}$$
 (3)

We often define the z_i to be uncorrelated, and to have unit variance

$$cov(\mathbf{z}) = \mathbf{I} \tag{4}$$

This is properly called whiteness.

▶ It is easy to linearly transform data to be white ("whitening")



Deep Latent Variable Models: Very basic instance

- Simplest thing is to use white Gaussian latent variables
 - ▶ Define prior $p(\mathbf{z})$ so that \mathbf{z} zero-mean white Gaussian $\mathcal{N}(\mathbf{0}, \mathbf{I})$, implying the entries z_i are mutually independent
- A mixing $p_{\theta}(\mathbf{x}|\mathbf{z})$ widely used in DL: nonlinear transformation with additive Gaussian noise

$$\mathbf{x} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) + \mathbf{n},\tag{5}$$

with \mathbf{n} white Gaussian noise, \mathbf{f}_{θ} is some nonlinear function (NN)

dim(x) can be larger than dim(z): leads to dimension reduction like autoencoders



Degenerate case

Could we omit any noise, just invertible transformation?

$$\mathbf{x} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) \tag{6}$$

- In the case without noise, it is important that dim(x) ≤ dim(z), otherwise the distribution of x is degenerate
 - i.e., totally concentrated in a lower-dimensional manifold
 - This leads to all kinds of problems: even pdf does not exist!
- An interesting approach is to assume the dimensions equal, which leads to (normalizing) flows (not treated here)
- For the time being, we assume dimension reduction dim(x) >> dim(z),and therefore noise has to be there so that the pdf exists and there is no degeneracy

Estimation of generative models by maximum likelihood

- Let's first consider maximum likelihood estimation
- ▶ But to compute the likelihood requires we *integrate out* the **z**:

$$p_{\theta}(\mathbf{x}) = \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z} \tag{7}$$

If we could compute this, we could compute the log-likelihood:

$$\log L(\theta; \mathbf{x}_1, \dots, \mathbf{x}_N) = \sum_{i=1}^N \log p_{\theta}(\mathbf{x}_i)$$
 (8)

▶ But there is a multidimensional integral — perhaps even worse than in EBM!

Likelihood computation in very basic model

Considering very "simple" model considered above:

$$\mathbf{x} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) + \mathbf{n} \tag{9}$$

with Gaussian white **z**, and **n** Gaussian of variance σ^2

▶ We have (assuming random vectors are all of dim d)

$$p_{\theta}(\mathbf{x}|\mathbf{z}) = \frac{1}{(2\pi)^{d/2}\sigma^d} \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{x} - \mathbf{f}_{\theta}(\mathbf{z})\|^2\right) d\mathbf{z} \qquad (10)$$

$$\rho_{\mathbf{z}}(\mathbf{z}) = \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2} \|\mathbf{z}\|^2\right)$$
 (11)

Since $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z})$, the integration we need to do is:

$$p_{\theta}(\mathbf{x}) = \int \frac{1}{(2\pi\sigma)^d} \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{x} - \mathbf{f}_{\theta}(\mathbf{z})\|^2 - \frac{1}{2} \|\mathbf{z}\|^2\right) d\mathbf{z}$$
(12)

- Nobody knows an analytical solution
 - ... unless **f** is linear
- Numerical integration extremely difficult, as always



Estimation by MAP approximation of likelihood

- ➤ Since exact likelihood in a DLVM (=generative model) is very difficult to compute, resort to approximations
- ► The simplest approximation is *Maximum A Posteriori (MAP)*
 - ► Treat the latent variables like parameters, maximize likelihood with respect to them as well

$$\max_{\boldsymbol{\theta}, \mathbf{z}_1, \dots, \mathbf{z}_N} \sum_{i=1}^N \log p_{\boldsymbol{\theta}}(\mathbf{x}_i | \mathbf{z}_i) + \log p(\mathbf{z}_i)$$
 (13)

Often works well, but computation may be hard since so many quantities to optimize: proportional to N which can be millions.

Estimation by Variational Autoencoders (VAE)

- Approximation of likelihood based on variational inference
- "variational" \approx uses an approximative function that is also optimized as part of the approximation
 - ▶ Here approximation of conditional pdf $p(\mathbf{z}|\mathbf{x})$ by $q_{\alpha}(\mathbf{z}|\mathbf{x})$
 - If approximation by q_{α} is exact for some α , method finds that and approximation of likelihood becomes exact too
- Approximator q_{α} should be easy to evaluate and easy to sample from (cf. noise in NCE)
- The objective is called ELBO, "evidence lower bound":

$$J(\theta) = \max_{\alpha} \sum_{i=1}^{N} \int q_{\alpha}(\mathbf{z}|\mathbf{x}(i)) \log \frac{p_{\theta}(\mathbf{x}(i), \mathbf{z})}{q_{\alpha}(\mathbf{z}|\mathbf{x}(i))} d\mathbf{z}$$

which "internally" maximizea lpha to make approximation good

- ightharpoonup Integration in ELBO is relatively easy by sampling from q!
- A lot of details omitted here...



Model usually used with Variational Autoencoders (VAE)

- Although VAE is a general estimation method, it is usually associated with a particular model (almost defined above)
 - 1. Latent vector $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_m)$, i.e. white / independent, as above
 - 2. Observed data:

$$\mathbf{x} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) + \mathbf{n} \tag{14}$$

with $\mathbf{f}: \mathbb{R}^m \to \mathbb{R}^d$, where m usually much less than d

- Main point is to reduce dimension: manifold learning
- "Training a VAE" typically means estimating this model using the ELBO
- ► A lot of confusion in the literature because of this double meaning of "VAE"



VAE as autoencoder

- ▶ The estimation crucially includes posterior $p(\mathbf{z}|\mathbf{x})$, approximated by q
- Intuitively plausible: to estimate the model, you have to infer the latents
- ▶ The **z** are then used to generate the data as

$$\hat{\mathbf{x}} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) \tag{15}$$

and due to Gaussian noise **n**, the least-squares error $\|\mathbf{x} - \hat{\mathbf{x}}\|^2$ appears in the objective

- This turns out to be very similar to a dimension-reducing autoencoder:
 - ightharpoonup (Probabilistic) encoding by $q_{\alpha}(\mathbf{z}|\mathbf{x})$
 - \triangleright Decoding by \mathbf{f}_{θ}
 - ... but more complicated than earlier autoencoders
- It is fashionable to use a VAE for simple dimension reduction, but an ordinary AE would often be a better idea!
 - IMHO: only use VAE if you have a good reason
- ► (For more on VAEs, see Wikipedia entry, or Prince's book)

Another estimation approach, based on classification

- Consider fundamental problem:
 - We are given two data sets,

$$\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$$
 and $\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_N)$

- How to measure the similarity of the underlying distributions, p_x and p_y , based on those data sets? (no pdf's given)
- Related to problem of defining a divergence (see EBM1 slides)
 - but here we have no pdf's, only data: methods considered in earlier lectures cannot be used
- In general, a very difficult problem
- Approach here:
 - 1. Train a classifier to discriminate between X and Y
 - 2. If classification works well (high accuracy)
 - ightarrow the datasets are very different from each other
 - 3. If classification fails (close to chance level)
 - \rightarrow the datasets are similar to each other
- lacktriangle Distance between distributions \sim Classification accuracy



Generative adversarial networks: basic idea

- ► A principle of training deep generative networks (DLVM)
- Adjust parameters of the latent variable model so that the distribution of generated data is as close as possible to the distribution of the observed data
- In more detail, repeat the following:
 - 1. Generate data from the model with current parameters $oldsymbol{ heta}$
 - Train another NN to discriminate between this generated data and the real data
 - Consider the negative of the objective minimized by the classifier (as a simple proxy for classification error) as a measure of distance between distributions
 - 4. Reduce that distance by gradient descent on heta
- Converges, in theory, when the data generated from model has same distribution as real data
 - That means we fit the model to the data perfectly!
 - lacktriangle We must have found the optimal $oldsymbol{ heta}$
- This is kind of SSL?



Generative adversarial networks: some typical choices

- While GAN is a general principle for estimating DLVM, usually it is used with a particular model:
 - 1. Latent vector $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_m)$, i.e. white / independent, as above
 - 2. Observed data:

$$\mathbf{x} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) \tag{16}$$

with $\mathbf{f}: \mathbb{R}^m o \mathbb{R}^d$

(here, m can be just about anything, more relaxed than VAE)

- ▶ When people say they "train a GAN" it usually means fitting this model with the GAN principle
 - ambiguous, just like "training a VAE" we saw above
- Classifier is pretty much always logistic
- Typically: size of generated dataset = size of real data set
- Optimization by stochastic gradient, but there are some special problems...



Generative adversarial networks: definition

- ▶ Denote by **X** the whole observed dataset $\mathbf{x}_1, \dots, \mathbf{x}_N$
- ► Assume *generative NN*

$$\mathbf{x} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) \tag{17}$$

where **z** is sampled from $\mathcal{N}(\mathbf{0}, \mathbf{I})$, and $\boldsymbol{\theta}$ are NN parameters

- ▶ Denote by $\mathbf{Y}(\theta)$ a sample of "artificial" data generated using the above Eq. (17) with parameter θ .
- ▶ Denote by $J_{lr}(\mathbf{X}, \mathbf{Y}; \alpha)$ the loss (=negative likelihood) of logistic regression, α being parameters of a discriminating NN
 - Likelihood (negative loss) is *maximized* to learn classification:

$$\max_{\alpha} -J_{lr}(\mathbf{X}, \mathbf{Y}(\boldsymbol{\theta}); \boldsymbol{\alpha}) \tag{18}$$

- (Signs may be confusing: trying to follow literature here)
- ► The GAN learning principle is then

$$\min_{\boldsymbol{\theta}} \max_{\alpha} -J_{lr}(\mathbf{X}, \mathbf{Y}(\boldsymbol{\theta}); \alpha) \tag{19}$$



Generative adversarial networks as minimax problem

Consider the GAN optimization problem we just derived:

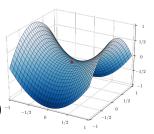
$$\min_{\boldsymbol{\theta}} \max_{\alpha} -J_{\mathsf{lr}}(\mathbf{X}, \mathbf{Y}(\boldsymbol{\theta}); \alpha) \tag{20}$$

where J_{lr} is negative likelihood of logistic regression.

- This is *adversarial*: The generating network is trying to choose θ so that the discriminator NN fails
- Minimax problem: interleaved minimization and maximization
- → Tries to find a saddle point
- ► Note: No way you could transform it to "min-min" by changing signs

$$\min_{\boldsymbol{\theta}} \max_{\boldsymbol{\alpha}} -J(\boldsymbol{\theta}, \boldsymbol{\alpha}) = \min_{\boldsymbol{\theta}} - \min_{\boldsymbol{\alpha}} J(\boldsymbol{\theta}, \boldsymbol{\alpha})^{-1}$$

since now negative sign appears in the middle; it is not $\min_{\theta,\alpha} J(\theta,\alpha)$



saddle point

Generative adversarial networks: optimization

How to actually solve the optimization of:

$$\min_{\boldsymbol{\theta}} \max_{\alpha} -J_{\mathsf{lr}}(\mathbf{X}, \mathbf{Y}(\boldsymbol{\theta}); \alpha) \tag{21}$$

- ▶ In principle, optimize $\max_{\alpha} -J_{lr}(\mathbf{X}, \mathbf{Y}(\theta); \alpha)$ until convergence, and then take gradient step with respect to θ .
- This leads to another interpretation: $\max_{\alpha} -J_{lr}(\mathbf{X}, \mathbf{Y}(\theta); \alpha)$ is objective being minimized, but it is *changing* (learned?)
- In practice, could just do stochastic gradient method with respect to θ and α in alternation

$$\alpha \leftarrow \alpha - \mu_{\theta} \nabla_{\alpha} J_{\mathsf{lr}}(\mathbf{X}, \mathbf{Y}(\theta); \alpha) \tag{22}$$

$$\theta \leftarrow \theta + \mu_{\alpha} \nabla_{\theta} J_{lr}(\mathbf{X}, \mathbf{Y}(\theta); \alpha)$$
 (23)

for minibatches $\tilde{\mathbf{X}}, \tilde{\mathbf{Y}}(\boldsymbol{\theta})$, and two step sizes $\mu_{\boldsymbol{\theta}}, \mu_{\boldsymbol{\alpha}}$.

Very challenging in practice! Beware of instability!



Generative adversarial networks: applications

Overwhelmingly, in data generation (image, video)



(Karras et al, 2018)

- ► GAN's were the beginning of the Generative AI boom
- Now, partly superseded by generative diffusion models
 - In diffusion models, standard optimization problem: not adversarial

- 1) Accurate model of data distribution?
 - ► E.g. Energy-based models (Done!)

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 - Contrastive learning, autoencoders, many kinds of SSL
- 4) Reveal identifiable structure in data, "disentangle" latent quantities?
 - ► Independent Component Analysis (next)

Problem of identifiability

- Do we actually estimate the model properly?
- Do we actually get the "correct" **f** in the model

$$\mathbf{x} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}) \tag{24}$$

- Definition: a model is *identifiable* if for two different values of θ , the distributions of the data p_x are different
- Identifiability means it is *possible* to find the underlying θ from the data x, assuming x is generated from the model
 - ▶ In practice, it means there is some *hope* of a unique solution
 - ... but a DL algorithm can give different solutions even for an identifiable model
 - Local minima, random initial points
- ► For data generation, we may not care about identifiability (?)
- But for understanding data, identifiability is paramount



Unidentifiability of Gaussian latent variables

- Consider the original Gaussian, white latent vector z
- ▶ We have for any *orthogonal* transformation $\mathbf{z}' = \mathbf{U}\mathbf{z}$:

$$cov(\mathbf{z}') = \mathbf{U}cov(\mathbf{z})\mathbf{U}^T = \mathbf{U}\mathbf{I}\mathbf{U}^T = \mathbf{I}$$
 (25)

- ► The covariance stays the same! (for white **z**)
- But a zero-mean gaussian pdf depends only on the covariance
- \Rightarrow **z** and **z**' have same distribution
- ightharpoonup Define heta' that gives a neural network such that

$$\mathbf{f}_{\theta'}(\zeta) = \mathbf{f}_{\theta}(\mathbf{U}^{T}\zeta) \tag{26}$$

Then we have:

$$\mathbf{x}' = \mathbf{f}_{\boldsymbol{\theta}'}(\mathbf{z}') \tag{27}$$

- ▶ Data is same **x** in both cases, but $\theta \neq \theta'$ (and **z** and **z**' follow the same prior)
- $\Rightarrow \theta$ is not identifiable (and neither is z)



Practical implication of unidentifiability

- Suppose you train a VAE (in the usual sense) on, say, some scientific data
- Crucially: it makes no sense to interpret the individual components as corresponding to some scientific phenomena
 - We already saw this with dimension-reducing autoencoders
- However, this is very often done in the literature, due to general ignorance of this problem
- Same thing applies to a GAN (but such interpretation is rare with GAN)

ICA as an identifiable linear generative model

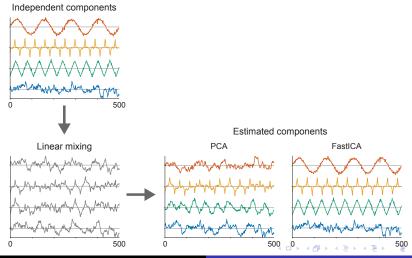
Linear independent component analysis (ICA)

$$\mathbf{x} = \mathbf{A}\mathbf{s} \tag{28}$$

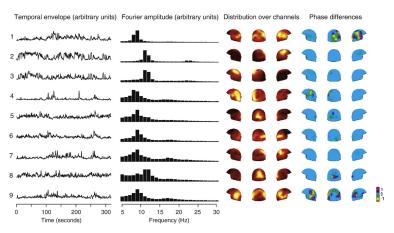
- $\mathbf{x} \in \mathbb{R}^d$ is the observed data
- ► A matrix of constant parameters describing "mixing"
- Assuming independent, non-Gaussian latent variables s_j , $j=1,\ldots,d$ (in basic case, dimensions are equal for ${\bf s}$ and ${\bf x}$)
- ICA is identifiable:
 - Observing only x we can recover both A and s
- Fundamental point: non-Gaussianity of the latents enables identifiability
 - together with independence
 - But this works only in linear case...



Linear ICA can separate "sources" from mixtures



Real example of ICA: Brain source separation



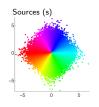
(Hyvärinen, Ramkumar, Parkkonen, Hari, 2010)

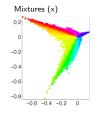
How to formulate ICA in the nonlinear case?

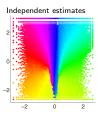
- Can we extend ICA to nonlinear case, get identifiable DLVM?
- A simple extension of nonlinear ICA is not identifiable
- ▶ If we define nonlinear ICA model for random variables x_i as

$$\mathbf{x} = \mathbf{f}(\mathbf{z}) \tag{29}$$

we cannot recover original sources, even if z_i are non-Gaussian.







Darmois construction to prove non-identifiability

For any x_1, x_2 , can always construct $y = g(x_1, x_2)$ independent of x_1 as

$$g(\xi_1, \xi_2) = P(x_2 < \xi_2 | x_1 = \xi_1)$$
(30)

- After obtaining such independent variables we can find a scalar function $h(x_1)$, $h(x_2)$ that transform to any distribution we want
- With nonlinear transformations, non-Gaussianity is meaningless since it can be changed arbitrarily
- Using this construction, we could even take x₁ as independent component which is absurd



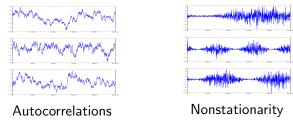






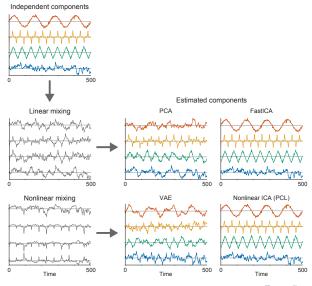
Temporal structure helps in nonlinear ICA

- ► Theory above considered i.i.d. sampled random variables
- What if we have time series? with specific temporal structure?



▶ Identifiability of nonlinear ICA can be proven Can find original sources!

Nonlinear ICA can separate "sources" from mixtures



One identifiable source model: Temporal dependencies

- Assume mixing model $x_t = f(s_t)$ where
 - \mathbf{x}_t observed *n*-dimensional time series
 - ightharpoonup s_t latent *n*-dimensional independent time series
 - ▶ **f** invertible (bijective) mixing
- Assume s_t^i temporally dependent and non-Gaussian (and some technical constraints)
- ► E.g., non-Gaussian AR model with non-quadratic G:

$$\log p(s_t^i | s_{t-1}^i) = G(s_t^i - \rho s_{t-1}^i)$$

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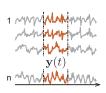
- This is Identifiable!
- Why would this work? Impose independence over time lags → more constraints → unique solution
- Estimation by VAE, GAN, even MLE possible; also more heuristic SSL methods (next)



► SSL on temporal dependencies

- SSL on temporal dependencies
- Take short time windows as new data

$$\mathbf{y}(t) = \big(\mathbf{x}(t),\mathbf{x}(t-1)\big)$$



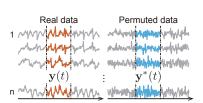
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Create randomly time-permuted data

$$\mathbf{y}^*(t) = \big(\mathbf{x}(t), \mathbf{x}(t^*)\big)$$

with t^* a random time point.



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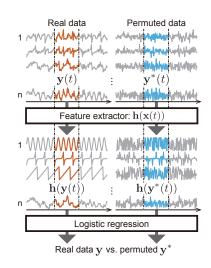
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- ▶ Train NN to discriminate y from y*
- Performs Nonlinear ICA for temporally dependent components!
 Quite surprising...



Conclusion on generative models

- Deep Latent Variable Models: one approach to unsupervised modelling of data
- Alternative to energy-based models
- Estimation of DLVM is challenging
 - EBMs may be better from that viewpoint
- Strength: DLVM automatically generates new data points
 - GANs were original success in GenAl
- ▶ DL often uses trivial models for latents: Gaussian and white
- ⇒ Serious problems of identifiability
- Nonlinear ICA solves identifiability
 - ▶ More difficult than linear ICA where non-Gaussianity is enough
 - We need e.g. nonstationarity or temporal dependencies

