[CoLike]
Complete Likelihood Objective
for Latent Variable Models

Mikhail Arkhipov
Mary Vikhreva

Generative Modelling Supervised Setting

Given a model

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

and a sample of data

$$\{(x_1, z_1), ..., (x_N, z_N)\}$$

Parameters θ can be obtained by maximization of complete log-likelihood of the data

$$\theta^* = \arg\max_\theta \mathscr{L}_c(\theta) = \arg\max_\theta \sum_i \log p_\theta(x_i, z_i)$$

Generative Modelling **Latent Variable** Setting

Given a model

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

and an incomplete sample of data

$$\{x_1, ..., x_N\}$$

Parameters θ can be obtained by maximization of **marginal** log-likelihood of the data

$$\theta^* = \arg\max_\theta \sum_i \log p_\theta(x_i) = \arg\max_\theta \sum_i \log \int_z p_\theta(x_i, z) dz$$

Additional Assumptions to Latent Variable Setting

Given a model

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

and an incomplete sample of data

$$\{x_1, ..., x_N\}$$

We add

a sample $\{z_1, ..., z_N\}$ from prior $p(z)$

and say that

$\{z_1, ..., z_N\}$ are pairs for $\{x_1, ..., x_N\}$ with unknown order

Generative Modelling with **Complete Likelihood** Objective

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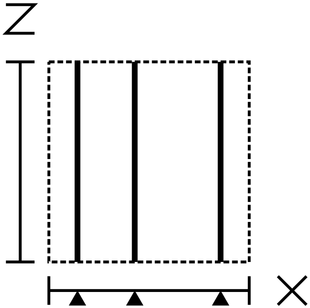
Under these assumptions Complete Likelihood is known up to a permutation

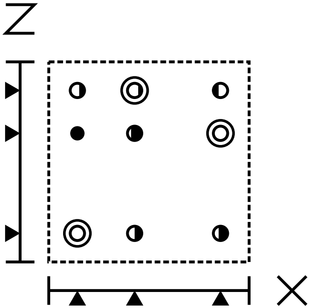
$$\mathcal{L}_c(\theta,\pi) = \sum_i \log p_\theta(x_i, z_{\pi(i)})$$

This allows us to perform Maximum Likelihood estimation over both permutation and parameters

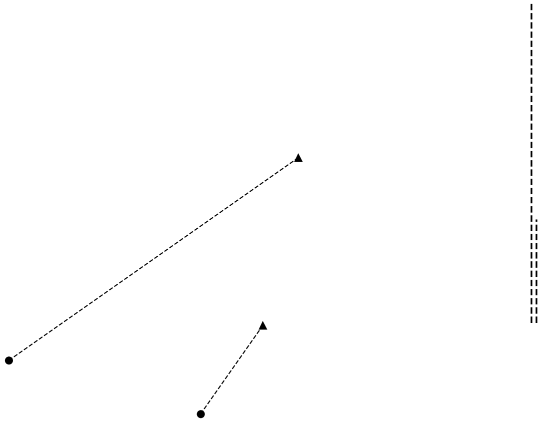
$$\theta^*,\pi^* = \arg\max_{\theta,\pi} \mathcal{L}_c(\theta,\pi)$$

Marginal Likelihood vs. Complete Likelihood





How strong is the assumption?



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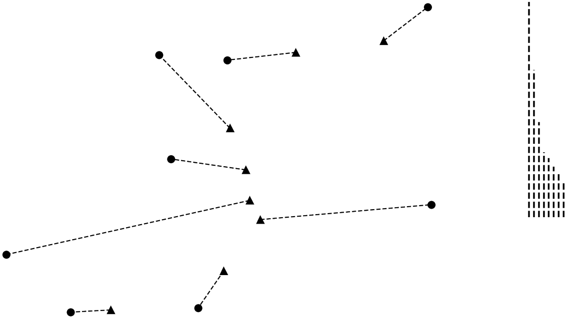

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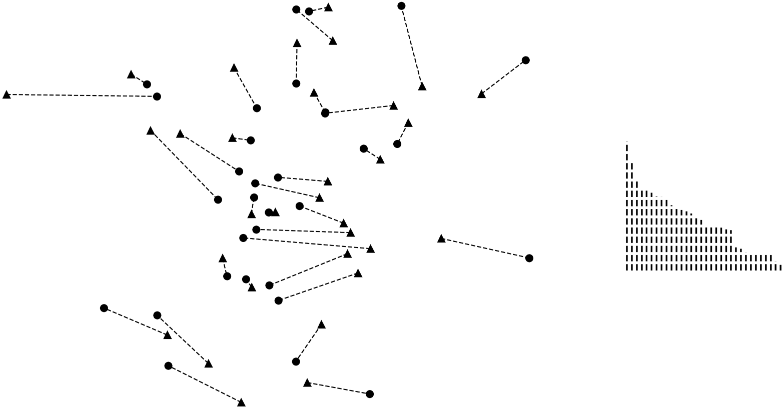

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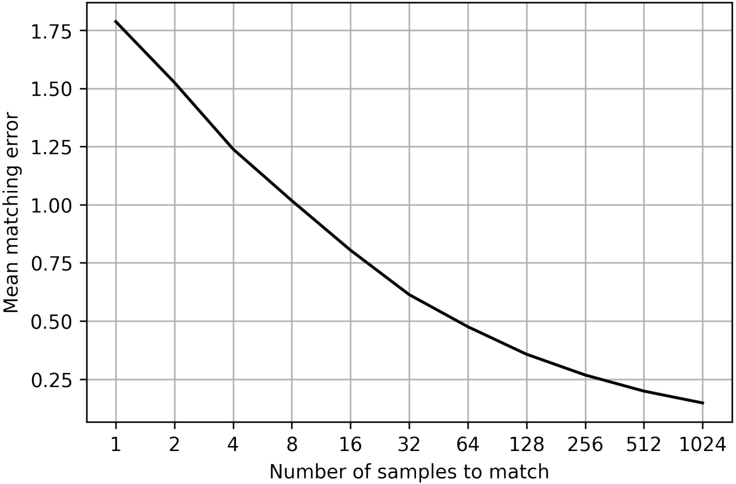


Links to Supervised Settings

Threre is a known supervised problem Broken Sample[1] or Linear Regression With Shuffled Labels[2]:

$$y_i = \mathbf{w}^T \mathbf{x}_{\pi(i)} + \varepsilon_i$$

This problem is common e.g. in tracking[3] and signal processing[4].

[1] [DeGroot et al. 1976] The Matching Problem for Multivariate Normal Data
[2] [Hsu et. al 2017] Linear Regression Without Correspondence
[3] [Bewley et al. 2016] Simple Online and Realtime Tracking
[4] [Haghighatshoar and Caire 2017] Signal Recovery from Unlabeled Samples

Link to Unsupervised Learning by Predicting Noise[5]

Setting:

data sample $\{x_1, ..., x_N\}$

sample from spherical prior $\{y_1, ..., y_N\}$

model f_θ that maps x to y domain

Objective:

$$\max_{\theta} \max_{\pi} \sum_{i} \mathbf{y_i}^T f_\theta(\mathbf{x}_{\pi(i)})$$

[5] [Bojanowski and Joulin 2017] Unsupervised Learning by Predicting Noise

Links to Optimal Transport

The Optimal Transport task for matching distributions P_X and P_Y is stated as

$$W_c(P_X, P_Y) = \inf_{\Gamma(P_X, P_Y)} \mathbb{E}_{X,Y \sim \Gamma}[c(X, Y)]$$

where $\Gamma(P_X, P_Y)$ is a family of joint distributions with marginals P_X and P_Y.
This problem is equivalent to[6]

$$W_c(P_X, P_Y) = \inf_{\substack{Q(Z|X): \\ Q_Z = P_Z}} \mathbb{E}_{X \sim P_X} \mathbb{E}_{Z \sim Q(Z|X)}[c(X, G(Z))]$$

where Q_Z is the marginal of $Q(Z|X)$, while G and $Q(Z|X)$ are a deterministic functions

[6][Tolstikhin et al. 2017] Wasserstein auto-encoders

Links to Optimal Transport

The objective is hard to optimize due to $Q_Z = P_Z$ constraint

$$W_c(P_X, P_Y) = \inf_{\substack{Q(Z|X): \\ \mathbf{Q_Z = P_Z}}} \mathbb{E}_{X \sim P_X} \mathbb{E}_{Z \sim Q(Z|X)} [c(X, G(Z))]$$

Wasserstein AutoEncoder suggests relaxation of original objective

$$\min_{G} \min_{Q(Z|X)} \mathbb{E}_{X \sim P_X} \mathbb{E}_{Z \sim Q(Z|X)} [c(X, G(Z)] + \beta D(Q_Z, P_Z)$$

where D is arbitrary discrepancy measure

Links to Optimal Transport

Consider encoderless case

$$W_c = \sup_{\Gamma \in \Pi(P_X, P_Y)} \mathbb{E}_{X,Y \sim \Gamma}\left[c(X,Y)\right] = \sup_{\Gamma \in \Pi(P_X, P_Z)} \mathbb{E}_{X,Z \sim \Gamma}\left[c(X,G(Z))\right]$$

When both P_X and P_Z are empirical distributions[7]

$$W_c = \sup_{\pi} \sum_i c\left(x_i, y_{\pi(i)}\right)$$

and for quadratic cost function

$$W_c = \sum_i ||x_i - y_{\pi(i)}||_2^2 = \sum_i ||x_i - G(z_{\pi(i)})||_2^2$$

[7] [Patrini et al. 2018] Sinkhorn AutoEncoders

Links to Optimal Transport

The function

$$W_c = \sum_i ||x_i - y_{\pi(i)}||_2^2 = \sum_i ||x_i - G(z_{\pi(i)})||_2^2$$

is identical to CoLike objective for Gaussian $p_\theta(x|z)$ and uniform prior $p(z)$

$$\begin{aligned}
\mathcal{L}_c &= \sup_\pi \sum_i \log p_\theta\left(x_i \middle| z_{\pi(i)}\right) p\left(z_{\pi(i)}\right) \\
&= \log c_z + \sup_\pi \sum_i \left(-\frac{d}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}\left\|x_i - G\left(z_{\pi(i)}\right)\right\|_2^2\right) \\
&= C + \sum_i \left\|x_i - G\left(z_{\pi(i)}\right)\right\|_2^2
\end{aligned} \tag{1}$$

Algorithm

Direct evaluation of CoLike objective

$$\mathcal{L}_c(\theta,\pi) = \sum_i \log p_\theta(x_i, z_{\pi(i)})$$

requires evaluations of $p_\theta(x_i, z_k)$ for every pair x_i and z_k for $i \in \{1,\ldots,N\}$ and $k \in \{1,\ldots,N\}$.
This amounts to N^2 evaluations of $p_\theta(x|z)$.
However, for non-autoregressive models, the neural network can be evaluated only N times, since decoder $p_\theta(x|z)$ takes only z as an input, while autoregressive models require x as an input.

Algorithm

Furthermore, finding optimal permutation requires solving combinatorial optimization problem.
The solution can be found with **Hungarian** algorithm with complexity $O(N^3)$.

Algorithm

Problem:

For large datasets, N^2 evaluations might be infeasible.

Solution:

Minibatch approximation for optimal permutation.

0. Sample z_i for each x_i
1. Sample minibatch of pairs (x_i, z_i)
2. Find optimal permutatin π^* for minibatch
3. Permute z_i in the training set according to π^*
4. Compute loss and perform gradient step for θ according to π^*
5. Go to step 1.

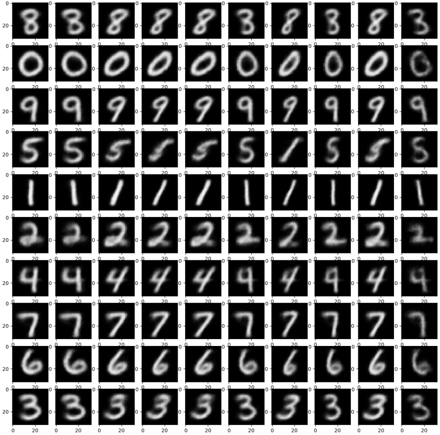
Discrete Latents out of the box

Setting:

- MNIST dataset
- Convolutional $p_\theta(x|z)$ from DCGAN
- 1 categorical latent with 10 classes
- 2 uniform continuous latents

Rows - distinct categorical latents.

Columns - random samples of continuos variables.



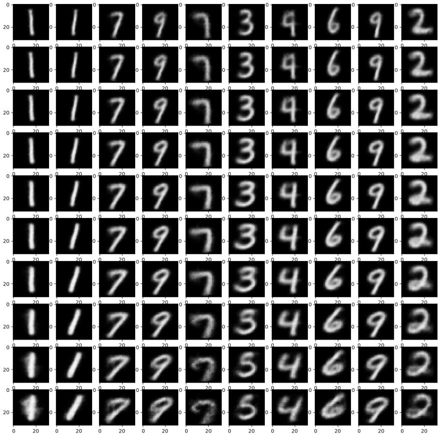
Discrete Latents out of the box

Setting:

- MNIST dataset
- Convolutional $p_\theta(x|z)$ from DCGAN
- 1 categorical latent with 10 classes
- 2 uniform continuous latents

Rows - traverse of one continuos latent.

Columns - samples of categorical and one continuous latents.



Likelihood on binarized MNIST

Setting:

- Statically binarized MNIST dataset
- 2 hidden layer MLP $p_\theta(x|z)$ with hidden dimensionality 500
- Gaussian latents
- RealNVP to approximate posterior after training
- Evidince is estimated using 1000 importnace weigthed samples from RealNVP posterior

Mehod	$dim(z)$	$p(x)$	Dataset size
VAE	2	-205.07	32
CoLike	2	-200.65	32
VAE	2	-171.43	256
CoLike	2	-170.04	256
VAE	2	-176.80	1024
CoLike	2	-151.18	1024
VAE	2	-152.61	50000
CoLike	2	-157.92	50000

Likelihood on binarized MNIST

Mehod	$dim(z)$	$p(x)$	Dataset size	Active Units
VAE	2	-152.61	50000	2
CoLike	2	-157.92	50000	2
VAE	8	-100.94	50000	8
CoLike	8	-108.36	50000	8
VAE	32	-93.80	50000	18
CoLike	32	-110.09	50000	32

A latent unit (a single dimension of z) is active when the variance of its expectation with respect to x is larger than 0.01[8]: $A_u > 0.01$ where $A_u = Cov_x(\mathbb{E}_{u \sim q_\phi(u|x)}[u])$

[8] [Burda et al. 2015] Importance weighted autoencoders

Language Modelling with Latent Variables

Setting:

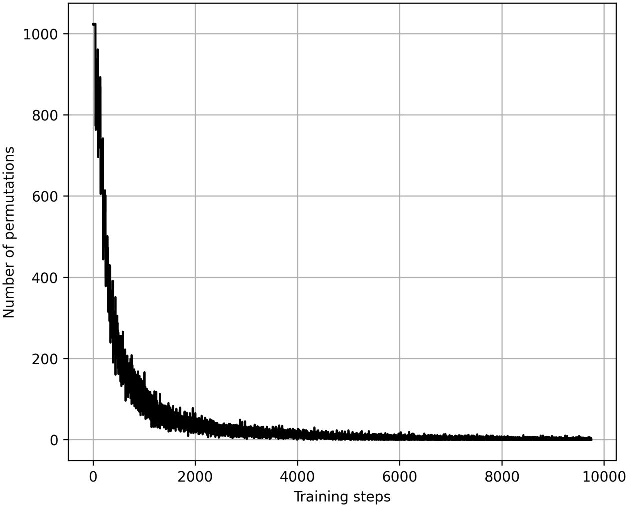
- SNLI dataset
- Single layer autoregressive unidirectional LSTM $p_\theta(x|z)$
- z is concatenated to each input
- LSTM hidden size - 512
- Gaussian latents
- $dim(z) = 32$

Mehod	$dim(z)$	PPL	Active Units
VAE	32	21.67	1
VAE FB[9]	32	22.00	32
CoLike	8	25.81	32

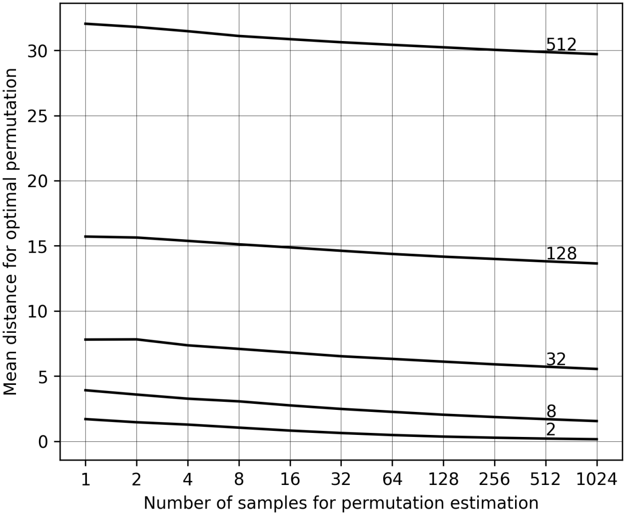
[9] VAE FB - VAE with free bits objective with KL constraint to be grater that 7.0

[Kingma et al. 2017] Improved Variational Inferencewith Inverse Autoregressive Flow

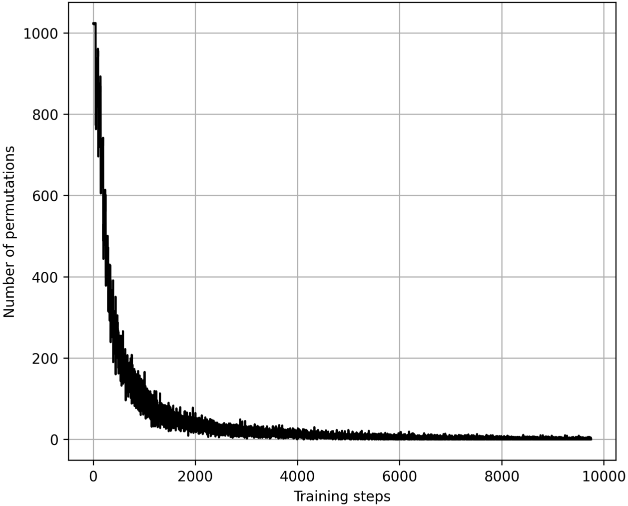
Challenges. Permutation saturation



Challenges. Dimensionality



Challenges. Permutation saturation



Conclusion

- New probabilistic objective for training latent variables models
- Approximate solution with partial permutation is proposed
- Promising results for discrete latentents and low-dimensional latents
- Robustness to posterior collapse for autoregressive models

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