LU-Net: Invertible Neural Networks Based on Matrix Factorization

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Abstract

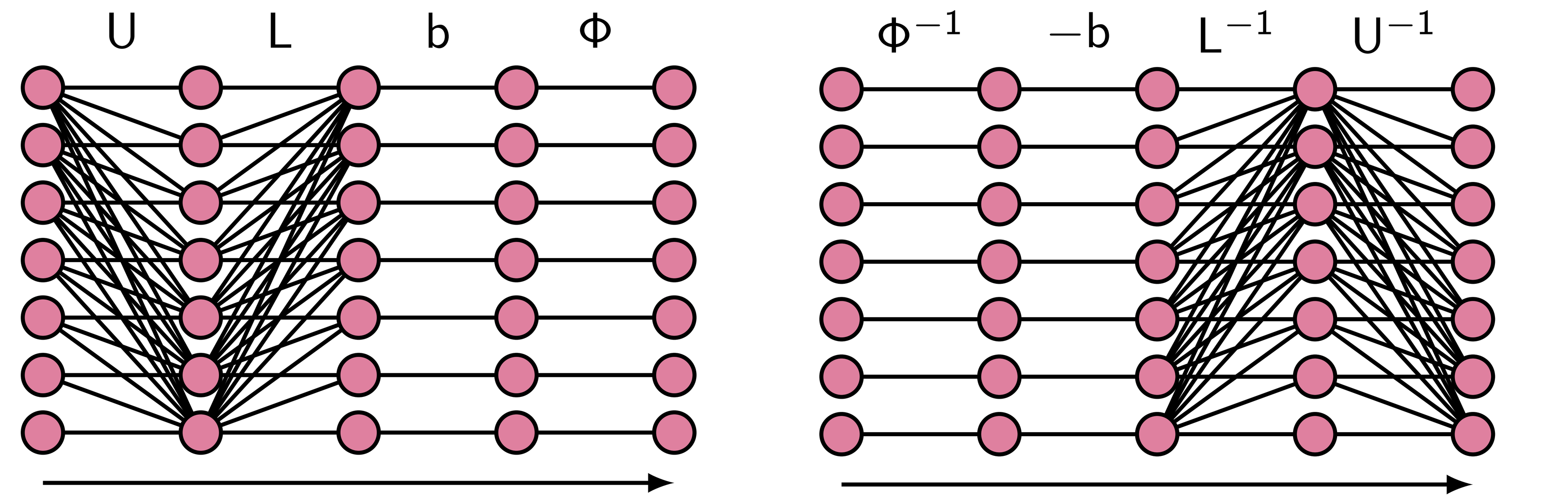
LU-Net is a simple and fast architecture for invertible neural networks (INNs) that is based on the factorization of quadratic weight matrices $A = LU$, where L is a lower triangular matrix with ones on the diagonal and U an upper triangular matrix. Instead of learning a fully occupied matrix A, we learn L and U separately. If combined with an invertible activation function, such a layer can easily be inverted whenever the diagonal entries of U are different from zero. Also, the computation of the determinant of the Jacobian matrix is cheap. Consequently, the LU-Net architecture allows for cheap likelihood computation via the change of variables formula and can be trained according to the maximum likelihood principle.

Training via Maximum Likelihood

Let $x \in \mathbb{R}^D$ denote some D-dimensional input and let $M \geq 2$ specify the number of LU layers, where each layer of LU-Net is a map $\mathbb{R}^D \to \mathbb{R}^D$. Hence, $f : \mathbb{R}^D \to \mathbb{R}^D$ denotes the output of LU-Net. Given a dataset $\mathcal{D} = \{x^{(n)}\}_{n=1}^N$ and the set of model parameters $\theta = \{U^{(m)}, L^{(m)}, b^{(m)}\}_{m=1}^M$, our training objective is to maximize the likelihood on $\mathcal{D}$. By using the change of variables formula, the chain rule of calculus and given the fact that the determinant of a triangular matrix is the product of its diagonal entries, we obtain the following expression for the negative log likelihood as training loss function:

$$
\begin{aligned}
-\ln \mathscr{L}(\theta|\mathcal{D}) = \; & \frac{1}{2} \cdot N \cdot D \cdot \ln(2\pi) + \frac{1}{2} \sum_{n=1}^{N} \sum_{d=1}^{D} f_d(x^{(n)}|\theta)^2 \\
& - \sum_{n=1}^{N} \sum_{m=1}^{M} \sum_{d=1}^{D} \ln \phi'^{(m)} \left((L^{(m)} U^{(m)} x^{(n)})_d + b_d^{(m)} \right) \\
& - N \cdot \sum_{m=1}^{M} \sum_{d=1}^{D} \ln \left| u_{d,d}^{(m)} \right| \longrightarrow \min
\end{aligned}
$$

Illustration of one LU layer



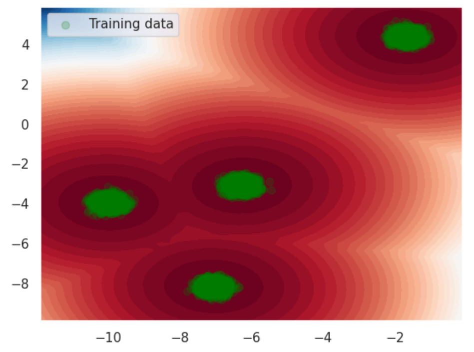
normalizing sequence:

$$
\begin{aligned}
x &\mapsto Ux \\
&\mapsto LUx \\
&\mapsto LUx + b \\
&\mapsto \Phi(LUx + b) \\
&= f(x) =: z
\end{aligned}
$$

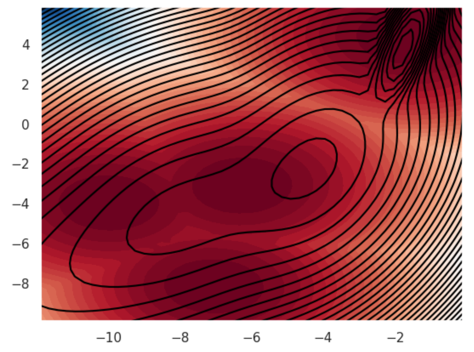
generating sequence:

$$
\begin{aligned}
z &\mapsto \Phi^{-1}(z) \\
&\mapsto \Phi^{-1}(z) - b \\
&\mapsto L^{-1}(\Phi^{-1}(z) - b) \\
&\mapsto U^{-1}L^{-1}(\Phi^{-1}(z) - b) \\
&= f^{-1}(z) = x
\end{aligned}
$$

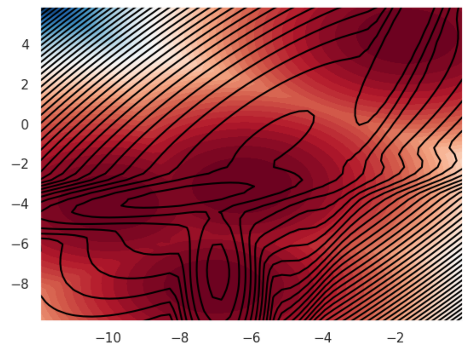
Gaussian Mixture



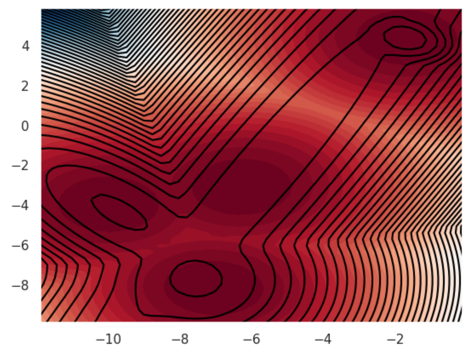
Training data



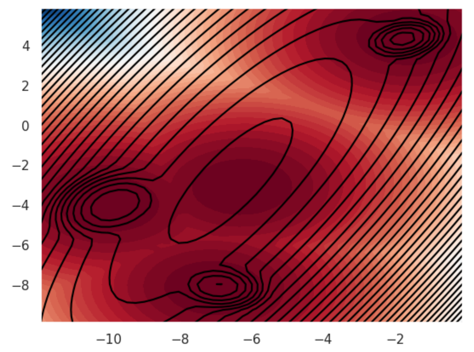
2 LU layers



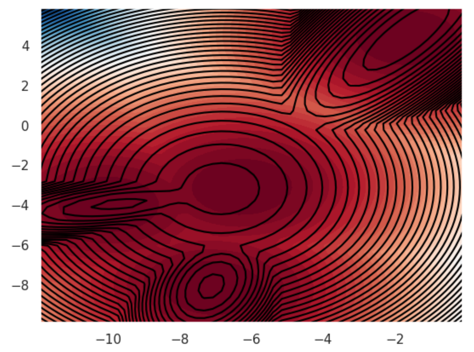
3 LU layers



5 LU layers

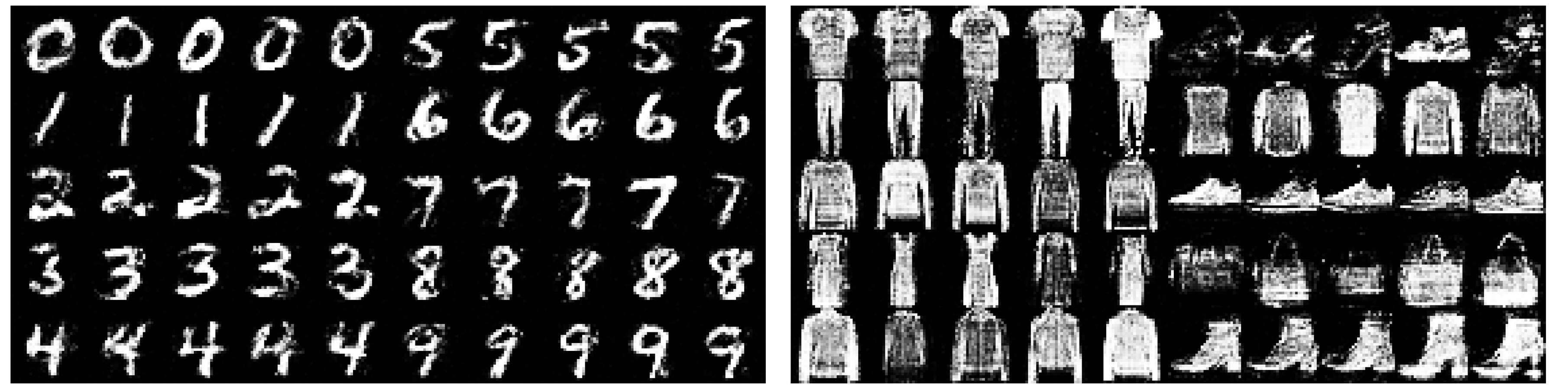


8 LU layers

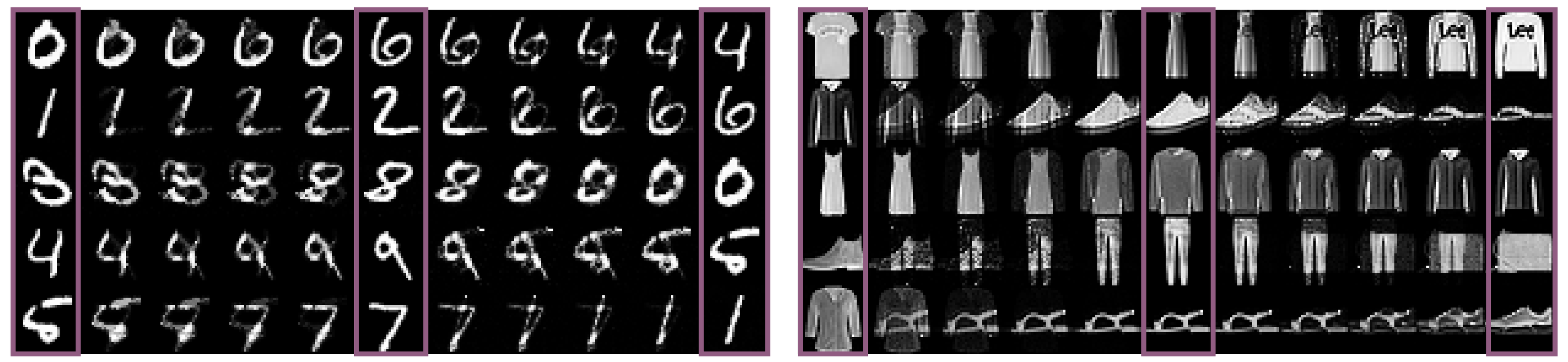


12 LU layers

MNIST and Fashion MNIST



LU-Net: Randomly generated samples of MNIST and Fashion MNIST

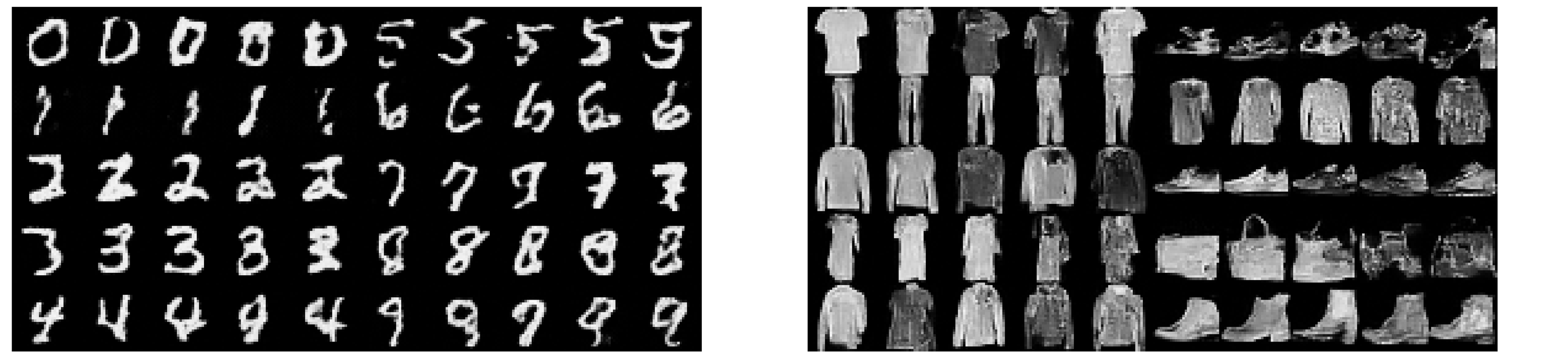


LU-Net: Samples of MNIST and Fashion MNIST generated by interpolating in latent space of LU-Net

Comparison with RealNVP

model	num weight parameters	GPU memory usage	num epochs training	test NLL
LU-Net	4.92 M	1,127 MiB	40	3.2424 bits/pixel
RealNVP	5.39 M	3,725 MiB	100	5.6819 bits/pixel

model	train epoch	optimization step	density per image	sampling per image
LU-Net	7.32 sec	1.2 ms	37.10 ms	45.15 ms
RealNVP	99.88 sec	56.0 ms	259.15 ms	1.03 ms



RealNVP: Randomly generated samples of MNIST and Fashion MNIST

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Code. `https://github.com/spenquitt/LU-Net-Invertible-Neural-Networks`

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