Information Bottleneck Analysis of Deep Neural Networks

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May 18, 2024

Introduction/Background

Consider random vectors, denoted as $X : \Omega \to \mathbb{R}^n$ and $Y : \Omega \to \mathbb{R}^m$, where Ω represents the sample space. Let's assume that these random vectors have absolutely continuous probability density functions (PDF) denoted as $\rho(x)$, $\rho(y)$, and $\rho(x, y)$, respectively.

Entropy definitions

- differential entropy of X: $h(X) = -\mathbb{E} \log \rho(x)$.
- conditional entropy: $h(X \mid Y) = -\mathbb{E} \log \rho\left(X|Y\right) = -\mathbb{E}_Y \left(\mathbb{E}_{X|Y=y} \log \rho(X \mid Y = y)\right)$
- joint differential entropy: $h(X, Y) = -\mathbb{E} \log \rho(x, y)$

Mutual Information definition

Mutual Information between variables X and Y is defined as

$$I(X, Y) = h(X) + h(Y) - h(X, Y)$$

Besides, the following equations holds: $I(X; Y) = h(X) - h(X \mid Y) = h(Y) - h(Y \mid X)$

Information Bottleneck principle

Information Bottleneck

This concept was applied to DNNs in Shwartz-Ziv, Tishby (2017). The major idea of the IB approach is to track the dynamics of two MI values:

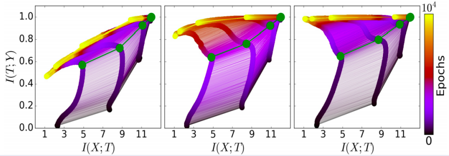
- $I(X; T)$ between the hidden layer output (T) and the DNN input (X)
- $I(Y; T)$ between the hidden layer output (T) and the target of the model (Y)

Authors formulated the fitting-compression hypothesis: training process consists of two phases:

- feature-extraction “fitting“ phase: both MI values grow
- representation “compression“ phase: $I(Y; T)$ grows while $I(X; T)$ decreases

Information Bottleneck Hypothesis

Firstly, classifier's construction based on the most significant features, next the internal representation is being compressed



Aim and Objectives

Problem Statement

Due to the challenging nature of estimating MI between high-dimensional random vectors, this hypothesis has only been verified for NNs of tiny sizes or specific types, such as quantized NNs

Research goals

- create the approach for the MI estimation that outperform previous methods in case of MI measurements between high-dimensional random variables
- provide the Information Bottleneck analysis for real neural networks via the proposed method

Method: proposed ideas

Key idea: Lossy compression

Our main goal is to precisely estimate MI between high-dimensional random vectors. To overcome the curse of dimensionality, we suggest to COMPRESS THE DATA:

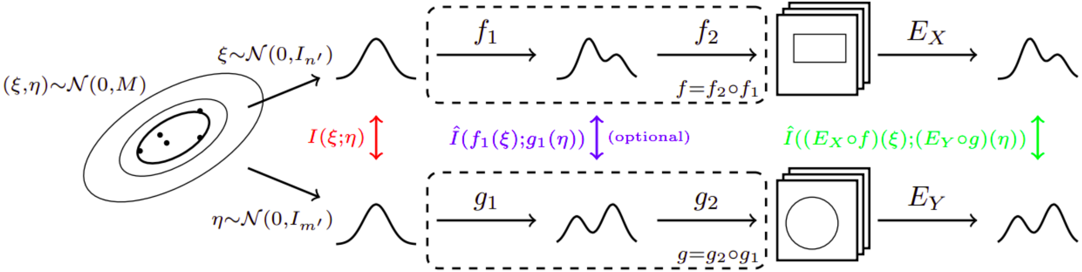
- learning the manifold with autoencoders
- applying conventional estimators (KDE, KL, WKL, ...) to the compressed representations

Main statement: MI can be measured between compressed representations

Let $\xi \colon \Omega \to \mathbb{R}^{n'}$ be an absolutely continuous random vector, and let $f \colon \mathbb{R}^{n'} \to \mathbb{R}^{n}$ be an injective piecewise-smooth mapping with Jacobian J_f,satisfying $n \geq n'$ and $\det\left(J_f^T J_f\right) \neq 0$ almost everywhere. Let either η be a discrete random variable, or (ξ, η) be an absolutely continuous random vector. Then

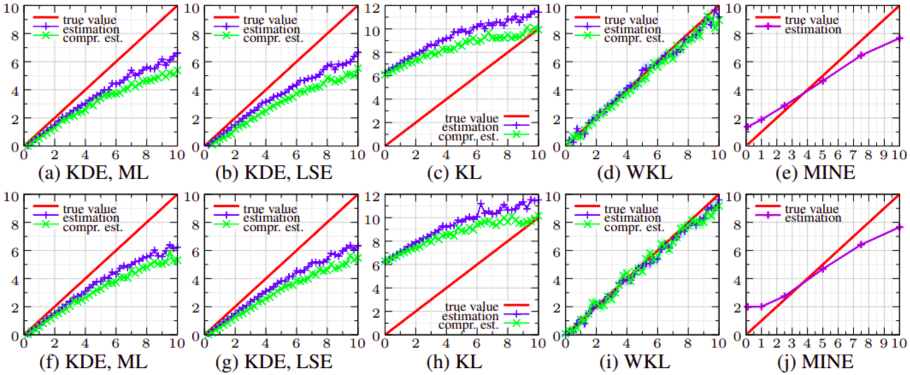
$$I(\xi; \eta) = I\left(f(\xi); \eta\right)$$

Experiments: Measure mutual information estimation quality on high-dimensional synthetic datasets



In order to observe and quantify the loss of information caused by the compression step, we split $f\colon \mathbb{R}^{n'} \to \mathbb{R}^n$ into two functions: $f_1\colon \mathbb{R}^{n'} \to \mathbb{R}^{n'}$ maps ξ to a structured latent representation of X (e.g., parameters of geometric shapes), and $f_2\colon \mathbb{R}^{n'} \to \mathbb{R}^n$ maps latent representations to corresponding high-dimensional vectors (e.g., rasterized images of geometric shapes). The same goes for $g = g_2 \circ g_1$

Results: comparison of different estimators on synthetic image datasets



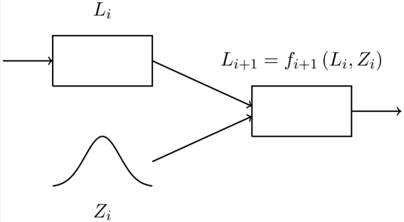
Maximum-likelihood and Least Squares Error KDE, Non-weighted and Weighted Kozachenko-Leonenko, MINE for 16×16 (first row) and 32×32 (second row) images of rectangles ($n = m = 4$), $5 \cdot 10^3$ samples. Along x axes is $I(X;Y)$, along y axes is $\hat{I}(X;Y)$.

MI estimation between neural network layers

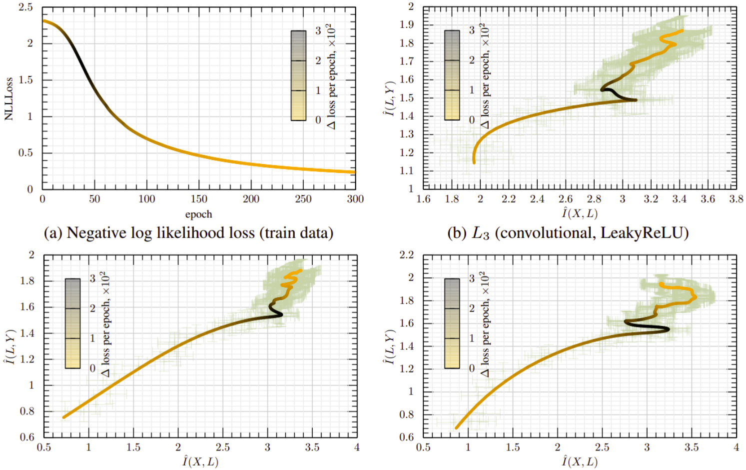
The architecture of the MNIST convolution-DNN classifier

The stochastic modification of a network serves as a proxy to determine the information-theoretic properties of the original model. The stochasticity enables proper MI estimation between layers of the network

L_1: Conv2d(1, 8, ks=3), LeakyReLU(0.01)
L_2: Conv2d(8, 16, ks=3), LeakyReLU(0.01)
L_3: Conv2d(16, 32, ks=3), LeakyReLU(0.01)
L_4: Dense(32, 32), LeakyReLU(0.01)
L_5: Dense(32, 10), LogSoftMax



Let's observe corresponding information plane plots for this network...



(a) Negative log likelihood loss (train data)

(b) L_3 (convolutional, LeakyReLU)

(c) L_4 (fully-connected, LeakyReLU)

(d) L_5 (fully-connected, LogSoftMax)

Dynamics of information-theoretic quantities during the training of DNNs are indeed non-trivial

Conclusion & Scientific novelty

Conclusion

- We have shown that it is possible to apply information analysis to compressed representations of datasets or models' outputs
- We have also developed a framework to test conventional mutual information estimators complemented with the proposed lossy compression step
- information plane experiment with the MNIST dataset classifier has been carried out

Scientific Novelty

- the idea of compression is the key novelty of this research
- proposed method outperforms existing approaches for the MI evaluation
- Information Bottleneck hypothesis was deeply explored and new MI dynamics dependencies were observed

Outcomes

Papers

- I. Butakov, *A. Tolmachev*, S. Malanchuk, A. Neopryatnaya, A. Frolov, K. Andreev **Information Bottleneck Analysis of Deep Neural Networks via Lossy Compression** (accepted to ICLR 2024, Poster)
- I.D. Butakov, S.V. Malanchuk, A.M. Neopryatnaya, *A. D. Tolmachev*, K. V. Andreev, S. A. Kruglik, E. A. Marshakov, A. A. Frolov **High-Dimensional Dataset Entropy Estimation via Lossy Compression** // Journal of Communications Technology and Electronics, 2021, № 66, pp. 764–768

Conferences

- 66th All-Russian Scientific Conference of MIPT, April 2024 (oral talk)
- All-Russian Summer School on Machine Learning SMILES-2023, Altai, August 20-31, 2023 (poster session, received *“Best poster“ prize*)
- 65th All-Russian Scientific Conference of MIPT, April 2023 (oral talk)

Outlook & Acknowledgements

Future plans

- edit and submit our paper about MI estimation via Normalizing Flows to NeurIPS 2024
- provide additional theoretical bounds for the MI estimation methods
- explore the Information Bottleneck hypothesis for a broader set of neural networks

Acknowledgements

I thank my colleagues and research advisor A.A. Frolov for the fruitful and exciting work!

Thank you for your attention!

Additional theory

Statement 3. *Let X, Y, and Z be random variables such that $I(X;Y)$ and $I((X,Z);Y)$ are defined. Let f be a function of two arguments such that $I(f(X,Z);Y)$ is defined. If there exists a function g such that $X = g(f(X,Z))$, then the following inequalities hold:*

$$I(X;Y) \leq I(f(X,Z);Y) \leq I((X,Z);Y)$$

In this context, $f(X,Z)$ can be interpreted as compressed noisy data, X as denoised data, and g as a perfect denoising dencoder. This statement justifies the proposed lossy compression method in cases where the data lost by compression can be considered as independent random noise.

Corollary 3. *Let X, Y, Z, f, and g satisfy the conditions of the Statement 3. Let also random variables (X,Y) and Z be independent. Then $I(X;Y) = I(f(X,Z);Y)$.*

We note that (a) the presented bounds cannot be further improved unless additional assumptions are made about the function f; (b) additional knowledge about the connection between X, Y, and Z is required to properly utilize the bounds. Other bounds can also be derived [16, 28, 44], but they do not take advantage of the compression aspect.