Mutual Information in Deep Learning

程昊
Emal: haocheng_louis@163.com
腾讯-优图实验室

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   - What is mutual information?
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What is mutual information?

First, we define the **information** of a random variable X as $H(X)$:

$$H(X) = -\sum_{p_i} p_i \log p_i$$

$H(X)$ measures the uncertainty of a random variable.
$H(X)$ achieves maximum when X follows uniform distribution.

A mathematical theory of communication   link

What is mutual information?

The **mutual information (MI** between two **discrete** random variable X and Y is defined as :

$$I(X;Y) = \sum_{x,y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} = H(X) - H(X|Y)$$

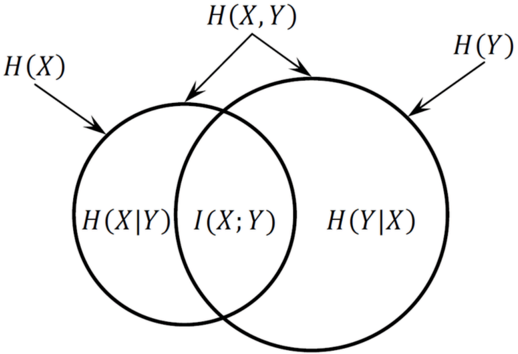
Similarly, the **MI** between two **continous** random variable X and Y is defined as:

$$I(X;Y) = \iint_{x,y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} = H(X) - H(X|Y)$$

MI measures the amount of information obtained about one random variable through observing the other random variable.

Relationship between Entropy and Mutual Information

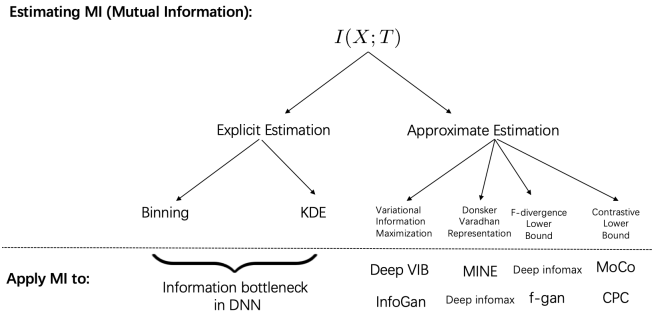
$$I(X;Y) = \sum_{x,y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} = H(X) - H(X|Y) = H(Y) - H(Y|X)$$



MI can represent higher order relationship among variables.

How to estimate mutual information?

There are two ways to estimate mutual information in practice:



Usually, explicit estimation is **non-parametric** method while approximate estimation is **parametric** method.

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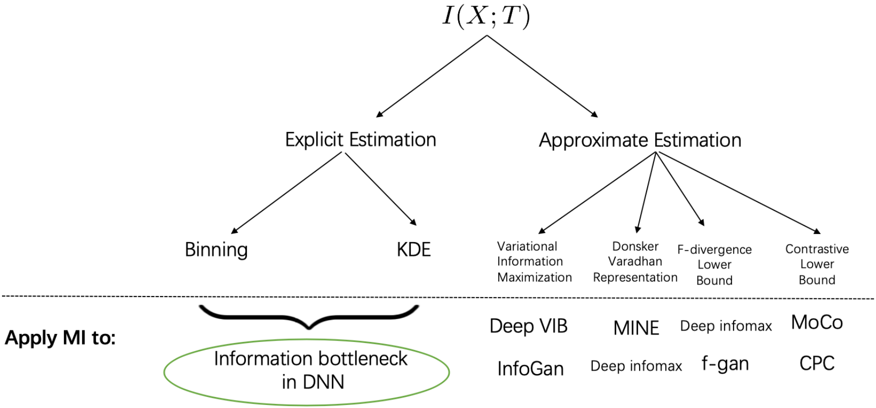
MI in Deep Learning

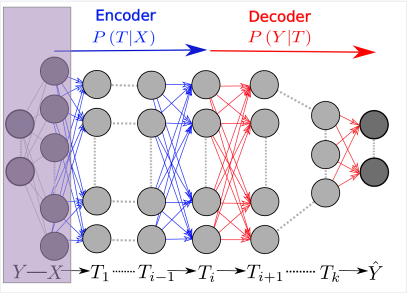
Estimating MI (Mutual Information):



Information Bottleneck (MI as visualization tool)

Tishby et al. believes that the DNN training is actually optimizing the following objective:

$$\min I(X;T) - \beta I(T;Y)$$

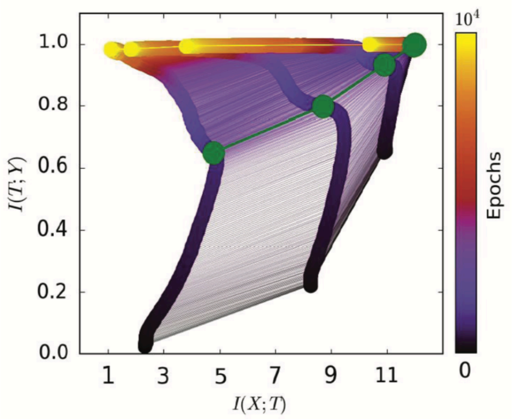


where T is the feature of each layer, X is the input and Y is the label.

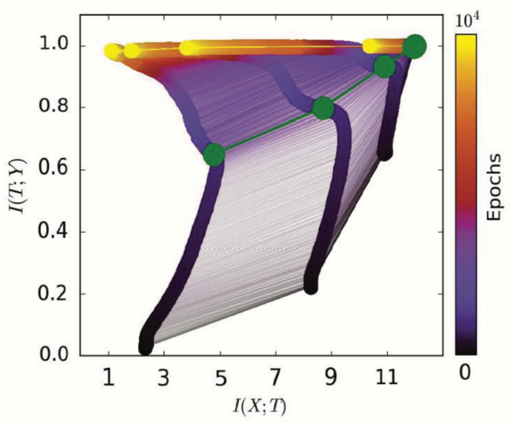
Opening the Black Box of Deep Neural Networks via Information. Arxiv:1703.00810

Tishby et al. use **binning** to estimate MI. In this case:

$$I(X;T) = \iint_{x,t} p(x,t) \log \frac{p(x,t)}{p(x)p(t)} \approx \sum_{x,t} p(x,t) \log \frac{p(x,t)}{p(x)p(t)}$$



Information Bottleneck (MI as visualization tool)



- Phase 1: $I(X;T)$ and $I(T;Y)$ both increases, which indicates the network memorizes the information about the input.
- Phase 2: $I(X;T)$ decreases while $I(T:Y)$ increases, which indicates that the network drops unimportant information to generalize.

Information Bottleneck (MI as visualization tool)

Andrew Michael Saxe et al. find that two phase phenomenon disappears in RELU case.

They use KDE (Kernel Density Estimation) to estimate mutual information, which is more practical than binning. In KDE (gaussian kernel), each sample forms a gaussian distribution. The overall distribution is the sum of all the gaussian distribution.

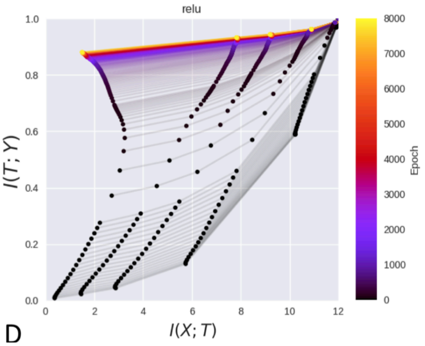
$$p(X) = \frac{1}{N}\sum_{i=1}^{N} p(X_i)$$

where $p(X_i)$ is a gaussian distribuiton centered at X_i.

On the Information Bottleneck Theory of Deep Learning. ICLR 2018

Information Bottleneck (MI as visualization tool)

Here the picture shows IB in RELU case (KDE estimation).



It seems that except for the last layer, all the other layers do not have the second compression phase.

Information Bottleneck (MI as visualization tool)

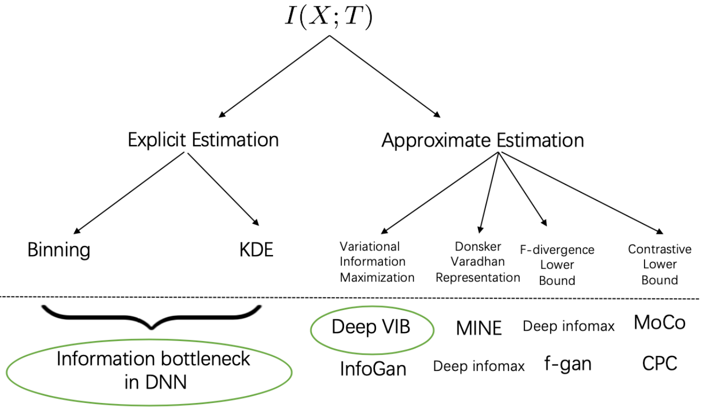
Which is right (Dose second phase really exist in RELU case)?

- Tishby shows the with RELU, the network still have the compression phase with more advanced estimator (code is not released).
- Some researchers prove the second phase exists with a specific estimator (EDGE).
- It is still an open problem. However, the ideology of IB is valuable in understanding neural networks and has inspired other great works.

MI in Deep Learning

Estimating MI (Mutual Information):

Apply MI to:



Variational Information Maximization

$$\begin{aligned}
I(x;z) &= H(z) - H(z|x) \\
&= H(z) + \mathbb{E}_{p(x,z)}\left[\log \frac{p(x,z)}{p(x)}\right] \\
&= H(z) + \mathbb{E}_{p(x)}\left[\mathbb{E}_{p(z|x)}\left[\log p(z|x)\right]\right] \\
&= H(z) + \mathbb{E}_{p(x)}\left[\mathbb{E}_{p(z|x)}\left[\log \frac{p(z|x)}{q_\theta(z|x)}\right] + \mathbb{E}_{p(z|x)}\left[\log q_\theta(z|x)\right]\right] \\
&= H(z) + \mathbb{E}_{p(x)}\left[\underbrace{D_{\mathrm{KL}}\left(p(z|x)||q_\theta(z|x)\right)}_{\geq 0} + \mathbb{E}_{p(z|x)}\left[\log q_\theta(z|x)\right]\right] \\
&\geq H(z) + \mathbb{E}_{p(x)}\left[\mathbb{E}_{p(z|x)}\left[\log q_\theta(z|x)\right]\right],
\end{aligned}$$

Main idea: Let q_θ is parameterized by a neural network.

Deep Variational Information BottleNeck. ICLR 2017

Deep VIB (MI as regularizer)

Suppose $Y \leftrightarrow X \leftrightarrow Z$ forms a Markov chain. We want to learn an efficient model $p(z|x)$ from IB perspective. Then our goal is to minimize:

$$\min I(X;Z) - \beta I(Z;Y)$$

In the above formulation, $p(y|z)$ in $I(Z;Y)$ and $p(z)$ in $I(X;Z)$ are hard to compute (intratable).

$$p(y|z) = \int \frac{p(y|x)p(z|x)p(x)}{p(z)}dx \qquad p(z) = \int p(z|x)p(x)dx$$

Thus we use $q(y|z)$ and $r(z)$ to approximate them, where $q(y|z)$ is parameterized by a neural network and we assume $r(z)$ follows a standard gaussian distribution. The loss becomes:

$$-\frac{1}{N}\sum_{n=1}^{N}\int dz\, p(z|x_n)\log q(y_n|z) - \beta \mathsf{KL}[p(z|x_n), r(z)] \quad \textit{similar to VAE !}$$

Deep Variational Information BottleNeck. ICLR 2017

Deep VIB (MI as regularizer)

By applying reparameterization trick:

$$p(z|x)dz = p(\epsilon)d\epsilon$$

, where $z = f(x, \epsilon)$ is a deterministic function of x and Gaussian random variable ϵ. The final loss is

$$L = -\frac{1}{N}\sum_{n=1}^{N} \mathbb{E}_{]\epsilon\sim p(\epsilon)}[-\log q(y_n|f(x_n,\epsilon))] + \beta \mathsf{KL}[p(z|x_n), r(z)]$$

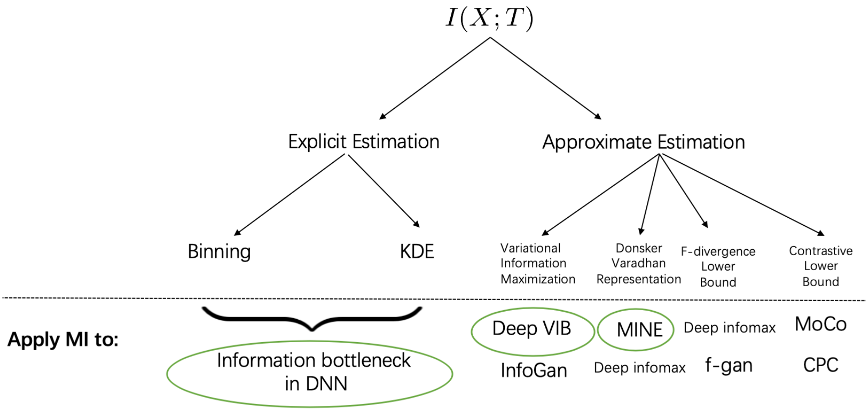
The first term equals to the traditional loss of supervised learning, while the second term pushes $p(z|x)$ follows a standard gaussian distribution. Thus Deep VIB introduces a regularizer to traditional supervised learning.

Result of Deep VIB on MNIST:

Model	error
Baseline	1.38%
Dropout	1.34%
Dropout (Pereyra et al., 2017)	1.40%
Confidence Penalty	1.36%
Confidence Penalty (Pereyra et al., 2017)	1.17%
Label Smoothing	1.40%
Label Smoothing (Pereyra et al., 2017)	1.23%
VIB ($\beta = 10^{-3}$)	**1.13%**

MI in Deep Learning

Estimating MI (Mutual Information):



MINE: MI as regularizer

Donsker-Varadhan Representation:

$$I(x,z) = \sup_{\theta} \mathbb{E}_{p(x,z)}[T_\theta(x,z)] - \log \mathbb{E}_{p(x)p(z)}[e^{T_\theta(x,z)}]$$

$$\begin{aligned}
I(x;z) &= D_{\mathrm{KL}}\left(p(x,z)||p(x)p(z)\right) \\
&= \mathbb{E}_{p(x,z)}\left[\log \frac{p(x,z)}{p(x)p(z)}\right] \\
&= \mathbb{E}_{p(x,z)}\left[\log\left(\frac{q(x,z)}{p(x)p(z)}\frac{p(x,z)}{q(x,z)}\right)\right] \\
&= \mathbb{E}_{p(x,z)}\left[\log \frac{q(x,z)}{p(x)p(z)}\right] + \underbrace{D_{\mathrm{KL}}\left(p(x,z)||q(x,z)\right)}_{\geq 0} \\
&\geq \mathbb{E}_{p(x,z)}\left[\log \frac{q(x,z)}{p(x)p(z)}\right]
\end{aligned}$$

let $q(x,z) = \frac{1}{K}p(x)p(z)e^{T_\theta(x,z)} = \frac{p(x)p(z)e^{T(x,z)}}{\int\int p(x')p(z')e^{T_\theta(x',z')}dz'dx'}$

Then
$$\begin{aligned}
D_{\mathrm{KL}}\left(p(x,z)||p(x)p(z)\right) &\geq \sup_{\theta} \mathbb{E}_{p(x,z)}\left[\log \frac{p(x)p(z)e^{T_\theta(x,z)}}{Kp(x)p(z)}\right] \\
&= \sup_{\theta} \mathbb{E}_{p(x,z)}\left[\log \frac{e^{T_\theta(x,z)}}{\mathbb{E}_{p(x)p(z)}\left[e^{T_\theta(x,z)}\right]}\right] \\
&= \sup_{\theta} \mathbb{E}_{p(x,z)}\left[T_\theta(x,z)\right] - \log \mathbb{E}_{p(x)p(z)}\left[e^{T_\theta(x,z)}\right]
\end{aligned}$$

Main idea: Let T_θ is parameterized by a neural network.

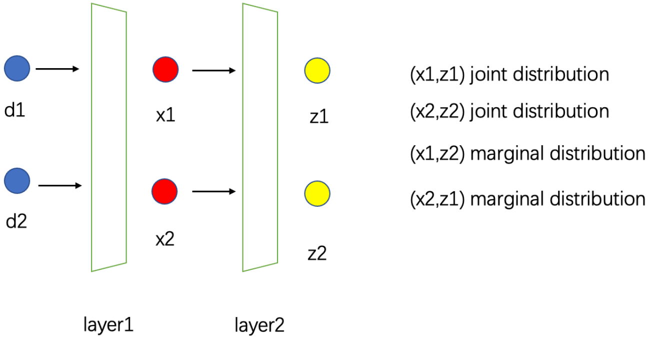
MINE: Mutual Information Neural Estimation. ICML 2018

MINE: MI as regularizer

How can we sample x and z ?

$$I(x,z) = \sup_{\theta} \mathbb{E}_{p(x,z)}[T_\theta(x,z)] - \log \mathbb{E}_{p(x)p(z)}[e^{T_\theta(x,z)}]$$

Suppose x and z are features of data from the first layer and second layer respectively.



We can sample the data by disrupting the order.

Estimation acuracy:

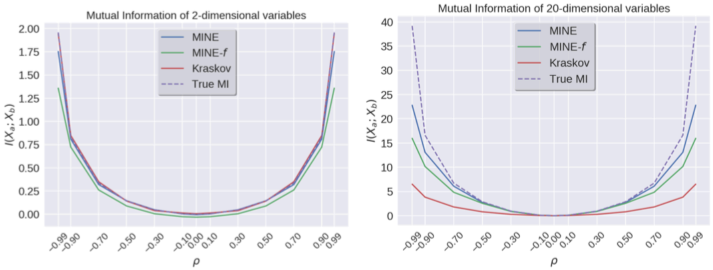


Figure 1. Mutual information between two multivariate Gaussians with component-wise correlation $\rho \in (-1, 1)$.

MINE (MI as regularizer)

MINE in GAN:

Vanilla Gan objective is :

$$\min_G \max_D V(D, G) = \mathbb{E}_{P_X}[\log D(X)] + \mathbb{E}_{P_Z}[log(1 - D(G(Z)))]$$

Write Z as $Z = [\epsilon, c]$, then the generator objective becomes:

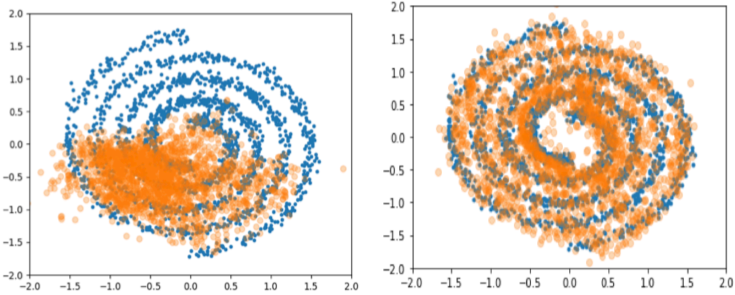
$$\max_G \mathbb{E}[\log(D(G([\epsilon, c])))]$$

In MINE, the generator objective has a regularization term:

$$\max_G \mathbb{E}[\log(D(G([\epsilon, c])))] + \beta I(G([\epsilon, c]); c)$$

The calculation of $\beta I(G([\epsilon, c]); c)$ needs T_θ parameterized by a neural network.

Comparison with GAN and GAN+MINE:



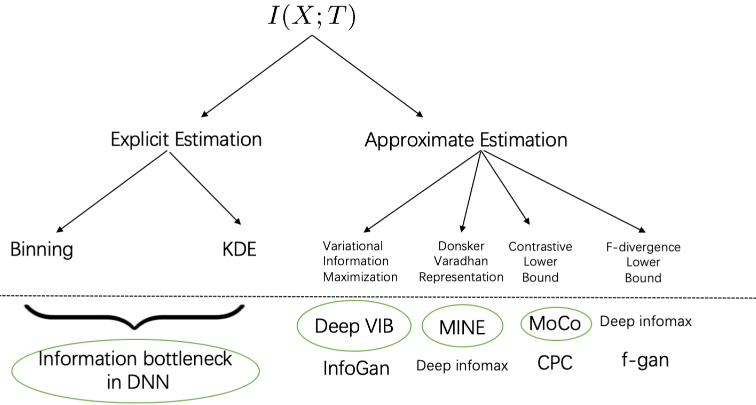
(a) GAN

(b) GAN+MINE

MI in Deep Learning

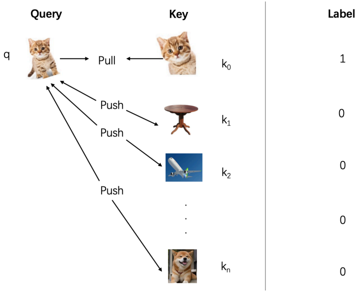
Estimating MI (Mutual Information):

Apply MI to:



MoCo (MI as objective function)

Goal: Learn a good representation by instance discrimination.



The loss (which is also called InfoNCE) is:

$$L_q = -\log \frac{\exp(q \cdot k_0)}{\sum_{i=0}^{n} \exp(q \cdot k_i)}$$

It can be shown that this loss is actually maximizing the mutual information of the two views of the image.

Momentum Contrast for Unsupervised Visual Representation Learning. CVPR 2020

MoCo (MI as objective function)

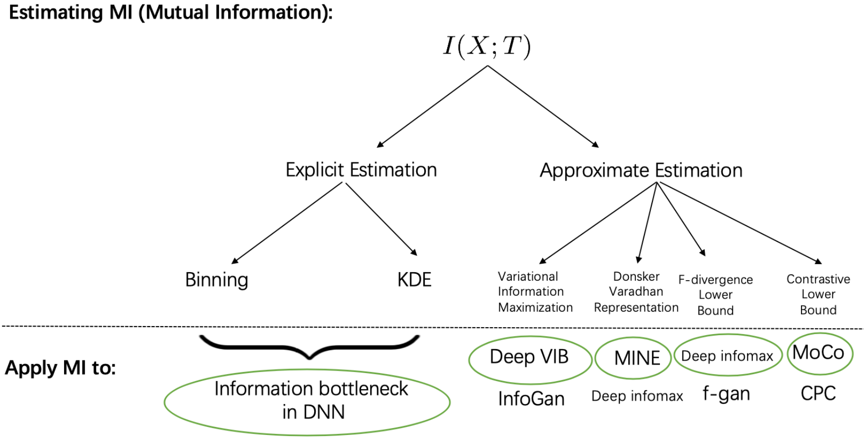
Contrastive lower bound:

$$
\begin{aligned}
I(x;z) - \log N &= \mathbb{E}_S\left[\log \frac{p(x^*|z^*)}{p(x^*)}\right] - \log N \\
&= \mathbb{E}_S\left[\log\left(\frac{p(x^*|z^*)}{p(x^*)}\frac{1}{N}\right)\right] \\
&= \mathbb{E}_S\left[\log\left(\frac{1}{\frac{p(x^*)}{p(x^*|z^*)}}\frac{1}{N}\right)\right] \\
&\geq \mathbb{E}_S\left[\log \frac{1}{1+\frac{p(x^*)}{p(x^*|z^*)}(N-1)}\right] \\
&= \mathbb{E}_S\left[-\log\left(1+\frac{p(x^*)}{p(x^*|z^*)}(N-1)\right)\right] \\
&= \mathbb{E}_S\left[-\log\left(1+\frac{p(x^*)}{p(x^*|z^*)}(N-1)\mathbb{E}_{S-\{x^*\}}\left[\frac{p(x|z^*)}{p(x)}\right]\right)\right] \\
&= \mathbb{E}_S\left[-\log\left(1+\frac{p(x^*)}{p(x^*|z^*)}\sum_{j=1}^{N-1}\frac{p(x_j|z^*)}{p(x_j)}\right)\right] \\
&= \mathbb{E}_S\left[-\log\left(1+\frac{\sum_{j=1}^{N-1}\frac{p(x_j|z^*)}{p(x_j)}}{\frac{p(x^*)}{p(x^*|z^*)}}\right)\right] \\
&= \mathbb{E}_S\left[\log \frac{\frac{p(x^*|z^*)}{p(x^*)}}{\frac{p(x^*|z^*)}{p(x^*)}+\sum_{j=1}^{N-1}\frac{p(x_j|z^*)}{p(x_j)}}\right] \\
&\approx \mathbb{E}_S\left[\log \frac{h_\theta(x^*,z^*)}{h_\theta(x^*,z^*)+\sum_{j=1}^{N-1}h_\theta(x_j,z^*)}\right] \\
&= \mathbb{E}_S\left[\log \frac{h_\theta(x^*,z^*)}{\sum_{x\in S}h_\theta(x,z^*)}\right],
\end{aligned}
$$

Comparison with MoCo and other self-supervised methods.

method	architecture	#params (M)	accuracy (%)
Exemplar [17]	R50w3×	211	46.0 [38]
RelativePosition [13]	R50w2×	94	51.4 [38]
Jigsaw [45]	R50w2×	94	44.6 [38]
Rotation [19]	Rv50w4×	86	55.4 [38]
Colorization [64]	R101*	28	39.6 [14]
DeepCluster [3]	VGG [53]	15	48.4 [4]
BigBiGAN [16]	R50	24	56.6
	Rv50w4×	86	61.3
methods based on contrastive learning follow:			
InstDisc [61]	R50	24	54.0
LocalAgg [66]	R50	24	58.8
CPC v1 [46]	R101*	28	48.7
CPC v2 [35]	$\text{R170}^{*}_{\text{wider}}$	303	65.9
CMC [56]	$\text{R50}_{\text{L+ab}}$	47	$64.1^{\dagger}$
	$\text{R50w2}\times_{\text{L+ab}}$	188	$68.4^{\dagger}$
AMDIM [2]	$\text{AMDIM}_{\text{small}}$	194	$63.5^{\dagger}$
	$\text{AMDIM}_{\text{large}}$	626	$68.1^{\dagger}$
MoCo	R50	24	60.6
	RX50	46	63.9
	R50w2×	94	65.4
	R50w4×	375	**68.6**

MI in Deep Learning



Deep Infomax: MI as objective function

Goal: Learn a good representation by maximize the mutual information between input and output.

Global MI:

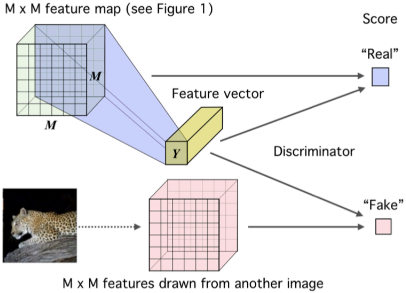


Figure 2: **Deep InfoMax (DIM) with a global MI$(X;Y)$ objective.** Here, we pass both the high-level feature vector, Y, and the lower-level $M \times M$ feature map (see Figure 1) through a discriminator to get the score. Fake samples are drawn by combining the same feature vector with a $M \times M$ feature map from another image.

Learning deep representations by mutual information estimation and maximization. ICLR 2019

Deep Infomax (MI as objective function)

Local MI:

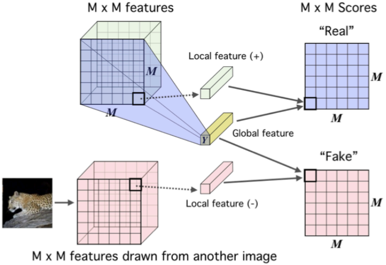


Figure 3: **Maximizing mutual information between local features and global features.** First we encode the image to a feature map that reflects some structural aspect of the data, e.g. spatial locality, and we further summarize this feature map into a global feature vector (see Figure 1). We then concatenate this feature vector with the lower-level feature map *at every location*. A score is produced for each local-global pair through an additional function (see the Appendix A.2 for details).

Deep Infomax (MI as objective function)

Estimate MI in Deep InfoMax:

The authors propose three MI estimators (DV, JSD, InfoNCE) in the paper and show the estimator based on Jensen-Shannon Divergence (JSD) is the most practical. The estimotor is presented as:

$$I_{w,\phi}^{\text{JSD}} = \mathbb{E}_P[-sp(-T_w(x, E_\phi(x)))] - \mathbb{E}_{P\times\tilde{P}}[sp(T_w(x^{'}, E_\phi(x)))]$$

where x is the input. E_ϕ is the encoder to map the input to output. T_w is a parameterized neural network. $\mathbb{E}_P$ represents the joint distribution bewteen input and output. $\mathbb{E}_{P\times\tilde{P}}$ represents the marginal distribution between input and output. $sp(z) = \log(1 + e^z)$ is the softplus function.

Derivation can be found here. Recommend to see f-gan first.

Deep Infomax (MI as objective function)

Comparison with Deep InfoMax and other methods:

Table 1: Classification accuracy (top 1) results on CIFAR10 and CIFAR100. DIM(L) (i.e., with the local-only objective) outperforms all other unsupervised methods presented by a wide margin. In addition, DIM(L) approaches or even surpasses a fully-supervised classifier with similar architecture. DIM with the global-only objective is competitive with some models across tasks, but falls short when compared to generative models and DIM(L) on CIFAR100. Fully-supervised classification results are provided for comparison.

Model	CIFAR10			CIFAR100		
	conv	fc (1024)	$Y(64)$	conv	fc (1024)	$Y(64)$
Fully supervised	75.39			42.27		
VAE	60.71	60.54	54.61	37.21	34.05	24.22
AE	62.19	55.78	54.47	31.50	23.89	27.44
β-VAE	62.4	57.89	55.43	32.28	26.89	28.96
AAE	59.44	57.19	52.81	36.22	33.38	23.25
BiGAN	62.57	62.74	52.54	37.59	33.34	21.49
NAT	56.19	51.29	31.16	29.18	24.57	9.72
DIM(G)	52.2	52.84	43.17	27.68	24.35	19.98
DIM(L) (DV)	**72.66**	**70.60**	**64.71**	**48.52**	**44.44**	**39.27**
DIM(L) (JSD)	**73.25**	**73.62**	**66.96**	**48.13**	**45.92**	**39.60**
DIM(L) (infoNCE)	**75.21**	**75.57**	**69.13**	**49.74**	**47.72**	**41.61**

Deep Infomax (MI as objective function)

Comparison with Deep InfoMax and other methods:

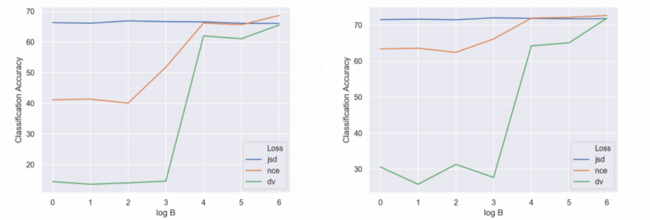
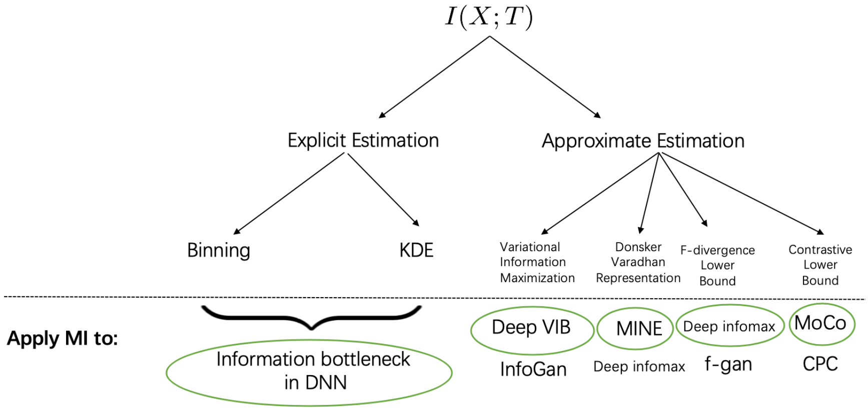


Figure 9: Classification accuracies (left: global representation, Y, right: convolutional layer) for CIFAR10, first training DIM, then training a classifier for 1000 epochs, keeping the encoder fixed. Accuracies shown averaged over the last 100 epochs, averaged over 3 runs, for the infoNCE, JSD, and DV DIM losses. x-axis is log base-2 of the number of negative samples (0 mean one negative sample per positive sample). JSD is insensitive to the number of negative samples, while infoNCE shows a decline as the number of negative samples decreases. DV also declines, but becomes unstable as the number of negative samples becomes too low.

MI in Deep Learning

Estimating MI (Mutual Information):



Content

Apply MI in Your Own Research

- When your research (problem) involves calculating the similarity (correlation) between two random variables, consider using MI as a criterion.
- Choosing a proper estimator is essential. You may try different estimators and select the best.

Other Reading Materials

- What Makes for Good Views for Contrastive Learning? NeurIPS2020
  Analyze what is good views for contrastive learning via information bottleneck
- L_DMI: A Novel Information-theoretic Loss Function for Training Deep Nets Robust to Label Noise. NeurIPS2019
  Apply a variant form of mutual information to learn with noisy labels

Reference

- Opening the Black Box of Deep Neural Networks via Information. Arxiv:1703.00810
- On the Information Bottleneck Theory of Deep Learning. ICLR 2018
- Learning deep representations by mutual information estimation and maximization. ICLR 2019
- MINE: Mutual Information Neural Estimation. ICML 2018
- Learning deep representations by mutual information estimation and maximization. ICLR 2019
- Momentum Contrast for Unsupervised Visual Representation Learning. CVPR 2020
- InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets. NIPS 2016
- f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization. NIPS 2016
- http://karangrewal.ca/blog/mutual-information-objectives/

Thanks!