Information Bottleneck View of Deep Learning

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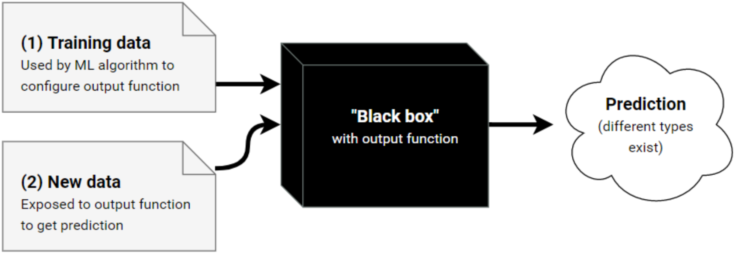
Overview

Outline

What does Deep Learning Do?

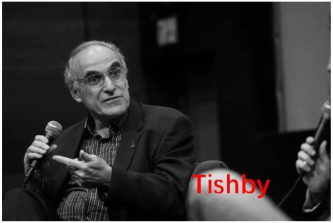
- Deep learning achieves lots of successes in diverse fields.



- How to open the black-box on its success?
- Some basic problems have not been solved:
  - Why stochastic gradient descent (SGD) works?
  - What's happening over training with SGD?
  - How sample size affects the training and generalization?
  - What's the optimal solutions of DNNs when they converge?

How to Open the Black-box?

- Tishby *et al.* [8]: open the black-box via information theory by
  - quantify the information flow along layers of DNNs.
  - characterize the phases over training.



Hinton: “It’s extremely interesting. I have to listen to it another 10,000 times to really understand it”.

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Sufficient Statistic

What captures the relevant properties in a sample about a parameter?

- Given i.i.d. samples $x^{(n)} \sim p(x|\theta)$

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Definition (Sufficient Statistics)

A *sufficient statistic*: $T(x^n)$ is a function of the sample such that

$$p\left(x^{(n)} \mid T\left(x^{(n)}\right) = t, \theta\right) = p\left(x^{(n)} \mid T\left(x^{(n)}\right) = t\right) \tag{1}$$

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- Sufficient statistics contain everything about θ from samples $x^{(n)}$.

There are always trivial sufficient statistics - e.g., the sample itself.

Definition (Minimal Sufficient Statistics)

One sufficient statistic $S(x^n)$ is called a *minimal sufficient statistic (MSS)* for θ in $p(x|\theta)$ if it is a function of any other sufficient statistics $T(x^n)$.

- $S(x^{(n)})$ gives the coarser sufficient description of the samples.
- S is unique (up to 1-1 map).

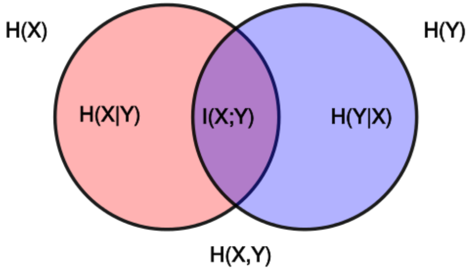
Sufficiency and Information

Definition (Mutual Information) [4]

For any two random variables X and Y with joint pdf $P(X = x, Y = y) = p(x, y)$, Shannon's mutual information $I(X; Y)$ is defined as

$$I(X; Y) = \mathbb{E}_{p(x,y)} \log \frac{p(x, y)}{p(x)p(y)} \quad (2)$$

- $I(X; Y) = H(X) - H(X \mid Y) = H(Y) - H(Y \mid X) \geqslant 0$



Properties of Mutual Information

Key properties of mutual information:

Theorem (Data-processing inequality)

When $X \to Y \to Z$ form a Markov chain, then

$$I(X;Z) \leqslant I(X;Y)$$

— data processing cannot increase (mutual) information

Sufficiency and Information

We can characterize sufficiency and minimality using mutual information:

Theorem (Sufficiency and Information)

- T is sufficient statistics for θ in $p(x \mid \theta) \Longleftrightarrow$

$$I\left(T\left(x^{(n)}\right);\theta\right) = I\left(x^{(n)};\theta\right)$$

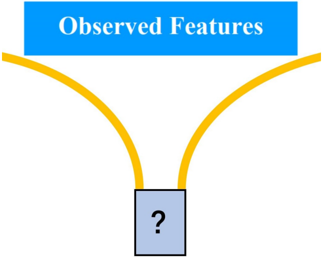
- If S is minimal sufficient statistics for θ in $p(x \mid \theta)$, then:

$$I\left(S\left(x^{(n)}\right);x^{(n)}\right) \leqslant I\left(T\left(x^{(n)}\right);x^{(n)}\right)$$

That is, among all sufficient statistics, minimality maintains the least mutual information on the samples $x^{(n)}$.

Relation to Learning Theory

- In a supervised manner, only samples $\{x^n, y^n\}_{n=1}^N \sim p(x, y)$ are given.
- Take the samples as random variables (X, Y)
- How to extract an efficient representation of the relevant information contained in a large set of features (X)?
- What information is relevant?
- The Information Bottleneck method [9, 10] answers this.



Information Bottleneck: Approximate MSS

- Given $(X, Y) \sim p(x, y)$, it suggests that the learning objective is to find the relevant part X with respect to Y, i.e., the MSS,

$$\begin{aligned} &\min_{T} I(X; T) \\ &\text{s.t. } I(T; Y) = I(X; Y) \end{aligned} \tag{3}$$

- However, $p(x, y)$ is not known and only samples are provided.
- $I(X; Y)$ is intractable.

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- $I(X; Y)$ is intractable.
- Minimal Sufficient Statistics (MSS) can be approximated:

$$\begin{aligned} &\min_{T} I(X; T) \\ &\text{s.t. } I(T; Y) = \alpha \end{aligned} \tag{4}$$

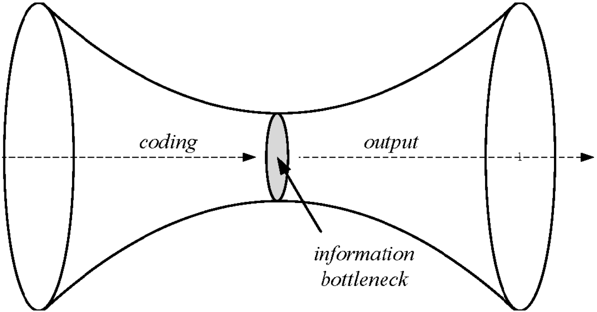
- T is called the Information Bottleneck between X and Y.

Why Information Bottleneck?

Definition

Compression: reduction in $I(X;T)$ over the course of training.

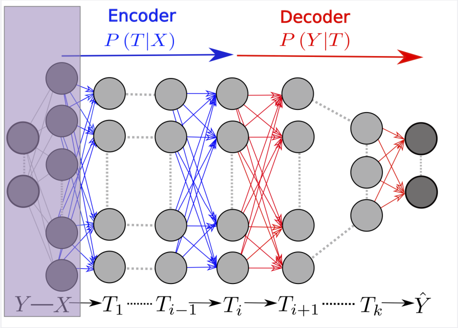
The codding is compressed smaller than α, as like the data through the bottleneck.



Outline

Information Flow along DNNs

Consider a feed-forward neural network

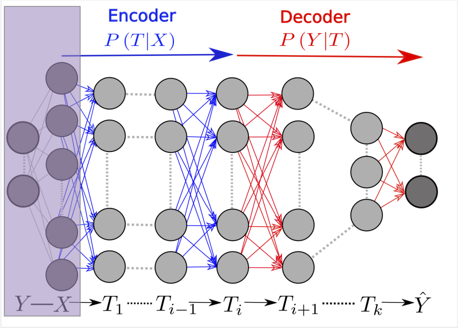


- Take the whole layer as a single random variable, in which the i-th hidden layer representation is processed from X:

$$T_i = \sigma_i \left(\boldsymbol{W}_i \sigma_{i-1} \left(\boldsymbol{W}_{i-1} \cdots \sigma_1 \left(\boldsymbol{W}_1 \boldsymbol{x} \right) \cdots \right) \right) \tag{5}$$

- Network layers form a Markov chain.

Information Flow along DNNs



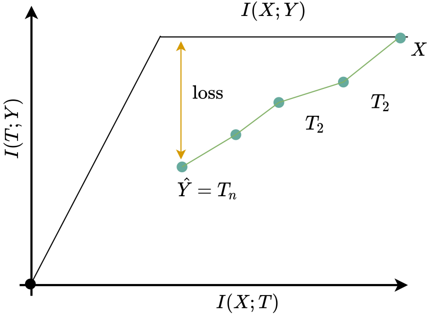
- From data processing inequality, the information is lost along layers.

$$I(Y;X) \geqslant I(Y;T_1) \geqslant I(Y;T_i) \geqslant \ldots \geqslant I(Y;\tilde{Y})$$
$$H(X) \geqslant I(X;T_1) \geqslant I(X;T_i) \geqslant \ldots \geqslant I(X;\tilde{Y})$$

Learning by Forgetting?

Looking at networks in the information plane:

- Stacking multiple layers makes the representation increasingly minimal.
- Minimizing usual Cross-Entropy loss $H(T, Y)$ maximizes the mutual information $I(T; Y)$.
- Layer-processing and regularization of DNNs: maximizing $I(T; Y)$ while minimizing $I(X; T)$ to some extent.



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Question 1: Compression helps?

- Compression promotes better generalization [3]

$$P\left[\left|\mathrm{err}_{\text{test}} - \text{err}_{\text{train}}\right| > \epsilon\right] < O\left(\frac{I(X;T)}{n\epsilon^2}\right) \tag{6}$$

Conjecture: SGD Has Two Phases

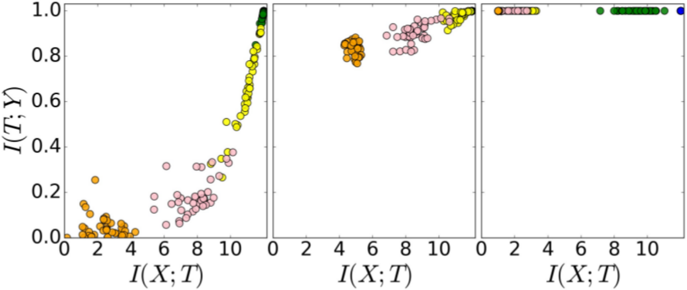


Figure: The dynamics of mutual information between hidden layers (red points represent deep layers) and the inputs X or labels Y (Traning Start, Middle, End).

- SGD training present two phases:
  - fitting (left $\to$ middle): increase of $I(X;T)$ and $I(T;Y)$.
  - compression (middle $\to$ right): increase of $I(T;Y)$ and decrease of $I(X;T)$.

Different Sample Sizes

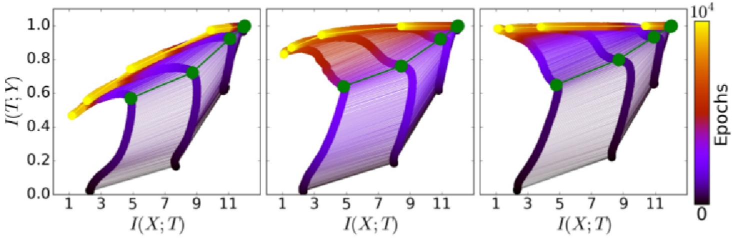


Figure: Training with 5%, 45%, 85% of the data, respectively.

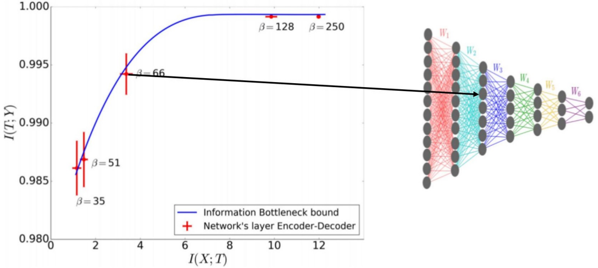
- Small sample size loses label information (the compression phase).
- Causes over-fitting, which can be prevented by early stopping.

Converged Layers are Close to the IB Bound

- Given data $\{x^n, y^n\}_{n=1}^{N} \sim p(x, y)$, Information Bottleneck (IB) Lagrangian can be defined as

$$\min_{T} I(X; T) - \beta I(T; Y) \tag{7}$$

- Given different βs, the IB Lagrangian can be solved.
- The solutions form the IB bound curve (blue).
- Claim: The solutions of DNNs converge to the IB bound: DNNs are minimizing the IB Lagrangian objective.



Black Box is Opened? Problem Solved?

However, the findings in [7] shows that these claims may not hold true in the general case ...

- Compression dynamics may be a general feature of DNNs.
  - or may not, but influenced by the non-linearities employed by DNN.
- Generalization performance may not relate to the information plane behaviour
  - compression may occur to a subset of features if the task demands it.

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How to improve the compression.

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Question 2: How to further compress the representation?

- Solve IB objective with smaller α.

$$\begin{aligned} &\min_T I(X;T) \\ &\text{s.t. } I(T;Y) = \alpha \end{aligned} \tag{9}$$

Information Bottleneck Lagrangian

- The constrained IB objective is equivalent to the following IB Lagrangian,

$$\min_{p(t|x)} I(X;T) - \beta I(T;Y) \tag{10}$$

- $p(t|x)$ is the conditional probability given x (encoder function)
- β is the trade-off hyper-parameter balancing fitting and compression.
- Solvable when $p(x, y)$ are known [9].

IB Solution

Theorem (Tishby, 1998)

The optimal assignment, that minimizes IB Lagrangian, satisfies the equation

$$p(t \mid x) = \frac{p(t)}{Z(x, \beta)} \exp \left[-\beta \sum_{y} p(y \mid x) \log \frac{p(y \mid x)}{p(y \mid t)} \right]$$

where the distribution $p(y \mid t)$ in the exponent is given via Bayes' rule, as,

$$p(y \mid t) = \frac{1}{p(t)} \sum_{x} p(y \mid x) p(t \mid x) p(x)$$

Proof Sketch (pt.1)

Introducing Lagrangian multipliers, $\lambda(x)$ for the normalization of the conditional distributions $p(t \mid x)$ at each x, IB Lagrangian becomes

$$\begin{aligned}\mathcal{L} &= I(X,T) - \beta I(T,Y) - \sum_{x,t} \lambda(x) p(t \mid x) \\ &= \sum_{x,t} p(t \mid x) p(x) \log \left[\frac{p(t \mid x)}{p(t)} \right] - \beta \sum_{t,y} p(t,y) \log \left[\frac{p(t \mid y)}{p(t)} \right] \\ &\quad - \sum_{x,t} \lambda(x) p(t \mid x)\end{aligned} \tag{11}$$

Taking derivatives with respect to $p(t \mid x)$ for given x and t, one obtains

$$\begin{aligned}\frac{\delta \mathcal{L}}{\delta p(t \mid x)} &= p(x)[1 + \log p(t \mid x)] - \frac{\delta p(t)}{\delta p(t \mid x)}[1 + \log p(t)] \\ &\quad - \beta \sum_y \frac{\delta p(t \mid y)}{\delta p(t \mid x)} p(y)[1 + \log p(t \mid y)] \\ &\quad - \beta \frac{\delta p(t)}{\delta p(t \mid x)}[1 + \log p(t)] - \lambda(x)\end{aligned}$$

Proof Sketch (pt. 2)

According the following derivatives $\frac{\delta p(t)}{\delta p(t|x)} = p(x)$ and $\frac{\delta p(t|y)}{\delta p(t|x)} = p(x \mid y)$, we have

$$\frac{\delta \mathcal{L}}{\delta p(t \mid x)} = p(x) \left\{ \log \left[\frac{p(t \mid x)}{p(t)} \right] - \beta \sum_y p(y \mid x) \log \left[\frac{p(y \mid t)}{p(y)} \right] - \frac{\lambda(x)}{p(x)} \right\}$$

Finally, obtain the variational condition:

$$\frac{\delta \mathcal{L}}{\delta p(t \mid x)} = p(x) \left[\log \frac{p(t \mid x)}{p(t)} + \beta \sum_y p(y \mid x) \log \frac{p(y \mid x)}{p(y \mid t)} - \tilde{\lambda}(x) \right] = 0$$

which is equivalent to equation (16) for $p(t \mid x)$,

$$p(t \mid x) = \frac{p(t)}{Z(x, \beta)} \exp\left(-\beta D_{KL}[p(y \mid x) \mid p(y \mid t)]\right)$$

with

$$Z(x, \beta) = \exp[\beta \tilde{\lambda}(x)] = \sum p(t) \exp\left(-\beta D_{KL}[p(y \mid x) \mid p(y \mid t)]\right)$$

Blahut-Arimoto Algorithm

- The above self consistent equations suggest a natural method for finding the unknown distributions, at every value of β.
- These equations can be turned into converging, alternating iterations

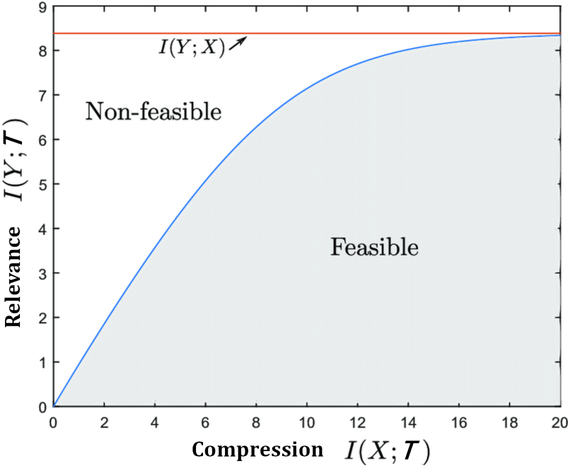
Blahut-Arimoto Algorithm

The minimization is performed by the converging alternating iterations. Denoting by k the iteration step,

$$\begin{cases} p_k(t \mid x) = \frac{p_k(t)}{Z_k(x,\beta)} \exp(-\beta d(x,t)) \\ p_{k+1}(t) = \sum_x p(x) p_k(t \mid x) \\ p_{k+1}(y \mid t) = \sum_y p(y \mid x) p_k(x \mid t) \end{cases} \tag{12}$$

Relevance-Compression Region

- The $I(X;T)$ and $I(T;Y)$ can be computed and plotted in the information plane given different β.



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How to Achieve It for Unknow Distribution?

Challenges:

- Only samples $\{x_i, y_i\}_{i=1}^{N}$ are available.
- $p(x, y)$ is not known.
- Mutual Information $I(X; T)$ is intractable.

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Solution:

- Parameterize the encoder function: $T = f_\phi(x)$ in DNNs.
- The minimization of IB Lagrangian reduces to

$$\min_{\phi} I(X; f_\phi(X)) - \beta I(f_\phi(X); Y) \tag{13}$$

- Therefore, minimize $I(X; f_\phi(X))$, maximize $I(f_\phi(X); Y)$

Maximize $I(T; Y)$

Using the fact that the KL-divergence is always positive, we have

$$\mathrm{KL}[p(Y \mid T), q(Y \mid T)] \geqslant 0 \Longrightarrow \int p(y \mid t) \log p(y \mid t) dy \geqslant \int p(y \mid t) \log q(y \mid t) dy$$

and hence,

$$\begin{aligned} I(T, Y) &\geqslant \int p(y, t) \log \frac{q(y \mid t)}{p(y)} dydt \\ &= \int p(y, t) \log q(y \mid t) dydt - \int p(y) \log p(y) dy \\ &= -\underbrace{(-\int p(y, t) \log q(y \mid t) dydt)}_{\text{cross-entropy}} + H(Y) \end{aligned}$$

where the entropy of labels $H(Y)$ is independent of the optimization procedure and so can be ignored.

Tractable Upper Bound for $I(X; T)$

When the conditional distribution $p(t|x)$ is know, upper bounding $I(X; T)$ is possible [2],

$$
\begin{aligned}
I(X;T) &\equiv \mathbb{E}_{p(x,t)}\left[\log \frac{p(t \mid x)}{p(t)}\right] \\
&= \mathbb{E}_{p(x,t)}\left[\log \frac{p(t \mid x)q(t)}{q(t)p(t)}\right] \\
&= \mathbb{E}_{p(x,t)}\left[\log \frac{p(t \mid x)}{q(t)}\right] - \mathrm{KL}(p(t)\|q(t)) \\
&\leqslant \mathbb{E}_{p(x)}[\mathrm{KL}(p(t \mid x)\|q(t))]
\end{aligned}
\tag{14}
$$

Tractable Upper Bound for $I(X;T)$

- Since we have

$$I(X;T) \leqslant \mathbb{E}_{p(x)}[\mathrm{KL}(p(t \mid x) \| q(t))] \tag{15}$$

- This bound is tight when $q(t) = p(t)$.
- A Normal distribution is always utilized for $q(t)$ [2, 5], i.e.,

$$q(t) \sim \mathcal{N}(0, 1)$$

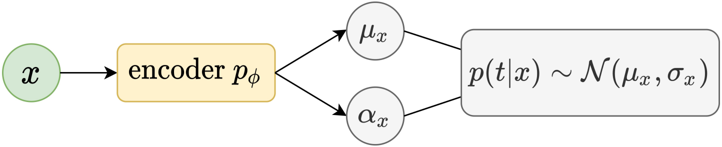
- Minimizing the upper bound can limit the capacity of a stochastic representation.

Implementation: Reparameterization Trick

Therefore, minimizing $I(X;T)$ reduces to the following,

$$\min I(X;T) \equiv \min_{\phi} \mathbb{E}_{p(x)}[KL(\underbrace{p_{\phi}(t \mid x)}_{\text{Encoder}} \,\|\, \underbrace{q(t)}_{\text{fixed}})]$$

- How to obtain the conditional distribution $p_{\phi}(t|x)$ in DNNs?
- Reparameterization: Sample t from the parameterized distribution:



- Finally, solve the following problem,

$$\min \mathrm{KL}\left[\mathcal{N}(\mu_x, \sigma_x) \| \mathcal{N}(0,1)\right] \tag{16}$$

Compression Promotes Clustering

The IB curve can be plotted by varying the hyper-parameter β [1, 6].

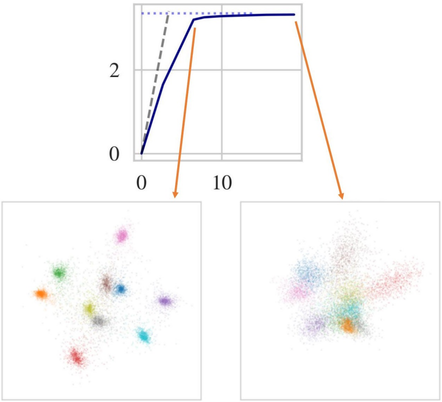


Figure: The IB curve plotted on MNIST dataset and clustering results.

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Summary

- In DNNs, relevant information in X is useful for predicting Y.
- Relevant information are refined and redundant information in X are compressed.

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- Relevant information are refined and redundant information in X are compressed.

- IB Lagrangian can be taken as objective for further compression.
- For known $p(x, y)$, which only exists for very special cases, the IB Lagrangian problem has a closed-form solution.
- For unknown $p(x, y)$, a tractable upper variational bound for $I(X; T)$ can be regarded as a substitute.
- Appropriate compression can improve the generalization.

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