Why Does Deep Learning Work?

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Overview

1. Recap of IB principle
2. Information Geometry
3. Future Work

Information Bottleneck Principle

The central idea of IB-Theory is[1]

"Regularization by optimal intermediate representations"

[1] N. Tishby and N. Zaslavsky, "Deep learning and the information bottleneck principle," *CoRR*, vol. abs/1503.02406, 2015. arXiv: 1503.02406. [Online]. Available: http://arxiv.org/abs/1503.02406.

Mathematical Recapitulation

Given $p_{XY}(x, y)$ for the dataset, IB objective is as follows

$$L(p(\hat{X}|X)) = I(\hat{X}, X) - \beta I(\hat{X}, Y)$$

and probability distribution of minimum sufficient statistics (optimal) is

$$p^*(\hat{X}|X) = \underset{p(\hat{X}|X)}{\arg\min}\, L(p(\hat{X}|X))$$

So intermediate representation $\hat{X}$ is a stochastic compressed representation of X

True optimal and Empirical optimal

The optimal curve for different β with true distribution $p_{XY}(x, y)$ (in black) and with empirical distribution $\hat{p}_{XY}(x, y)$ estimated with finite samples in the dataset is as follows [2]

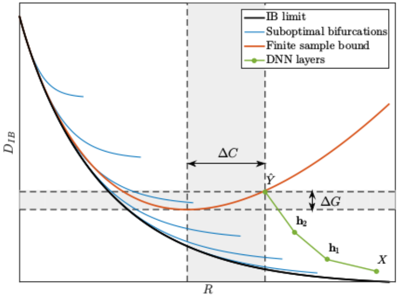

Figure: A qualitative information plane, with a hypothesized path of the layers in a typical DNN (green line) on the training data. The black line is the optimal achievable IB limit, and the blue lines are sub-optimal IB bifurcations.

[2] Figure taken from [1]

Two phase training dynamics - Generalization and Compression phase

First observed in [2]

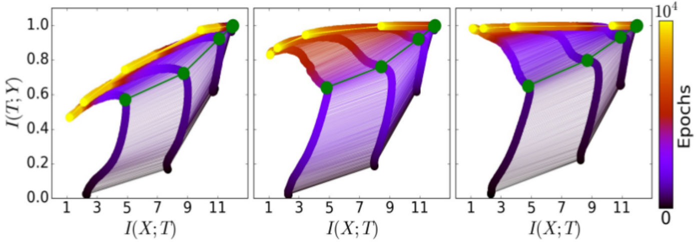

Figure: The evolution of the layers with the training epochs in the information plane. On the left - 5%, middle - 45%, and right - 85% of the data.

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[3] Figure taken from R. Shwartz-Ziv and N. Tishby, "Opening the black box of deep neural networks via information," *CoRR*, vol. abs/1703.00810, 2017. arXiv: 1703.00810. [Online]. Available: `http://arxiv.org/abs/1703.00810`

The Controversy

Paper [3] attacked the original paper claiming[4]

- IB-Theory is not fundamental theory
- Depends on specific activation used
- Showed two phase dynamics do not hold for RELU activation

But later more accurate MI estimators published and observed the two phases !

Even then , IB-Theory have issues in case of deterministic networks

[4] A. M. Saxe, Y. Bansal, J. Dapello, *et al.*, "On the information bottleneck theory of deep learning," in *International Conference on Learning Representations*, 2018. [Online]. Available: `https://openreview.net/forum?id=ry_WPG-A-`.

Resolution - Accurate Mutual Information estimation methods

Improvement in estimation methods

- Use more accurate MI estimation methods like EDGE, MINE [5]etc.
- Use tight bounded MI representations
- Research for which estimation method to use when

[5]MINE - I. Belghazi, S. Rajeswar, A. Baratin, *et al.*, "MINE: mutual information neural estimation," *CoRR*, vol. abs/1801.04062, 2018. arXiv: 1801.04062. [Online]. Available: http://arxiv.org/abs/1801.04062
EDGE - M. Noshad and A. O. H. III, "Scalable mutual information estimation using dependence graphs," *CoRR*, vol. abs/1801.09125, 2018. arXiv: 1801.09125. [Online]. Available: http://arxiv.org/abs/1801.09125

Problems with Mutual Information

Problem with mutual information is as follows:

- Difficult to estimate in practice fewer samples available.
- Suffers discontinuity in case of non-stochastic deterministic networks[6].
- No measure for robustness to noise.

[6] R. A. Amjad and B. C. Geiger, "How (not) to train your neural network using the information bottleneck principle," *CoRR*, vol. abs/1802.09766, 2018. arXiv: 1802.09766. [Online]. Available: http://arxiv.org/abs/1802.09766.

Dependence Criterion

Instead of MI as dependence criterion use more robust criterion which captures

- **inform about** Y - $\hat{X}$ should be sufficient statistics
- **be maximally compressed** - representation $\hat{X}$ should not tell about X
- **admit a simple decision function** - Y can be estimated from $\hat{X}$ using simple functions
- **be robust** - small noise should not change $\hat{X}$ with big differences

First two are captured by mutual information criterion but there is a need for criterion which captures last two too !

Hilbert Schmidt Independence Criteria

An alternate criterion HSIC was first introduced in paper[7] which gave one of the most interesting application of IB principle

"Deep Learning without Back-Propagation"

[7] W.-D. K. Ma, J. P. Lewis, and W. B. Kleijn, *The hsic bottleneck: Deep learning without back-propagation*, 2019. arXiv: 1908.01580 [cs.LG].

PyGlow: Python Package for Information Theory of Deep Learning

PyGlow

Information Theory of Deep Learning

[8]

[8] GitHub repo on: https://github.com/spino17/PyGlow
PyGlow Docs: https://pyglow.github.io/

Need for Geometric Reformulation

Need for a geometric framework of information theory:

- Models should not be specified with particular value of parameter[9].
- Learning dynamics should be independent of parameters.
- Distance measure in information theory is non-euclidean.
- Coordinate-free formulation to make deep connections of information theory with DL visible.

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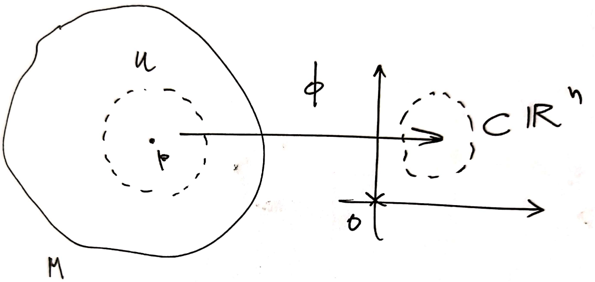
[9] G. Desjardins, K. Simonyan, R. Pascanu, *et al.*, *Natural neural networks*, 2015. arXiv: 1507.00210 [stat.ML].

Manifolds - Topological spaces which locally looks like $\mathbb{R}^n$.

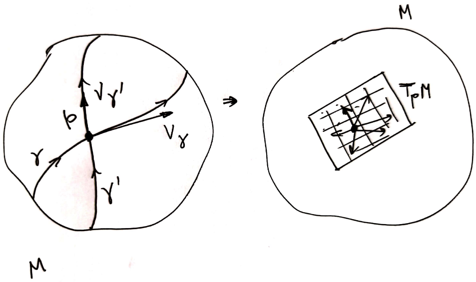


For any point $p \in M$, there exists an open set U such that we have a homeomorphism from U to $\mathbb{R}^n$.

Ingredients - Vectors

Vectors - Objects that captures the rate with which a function $f\colon M \to \mathbb{R}$ on manifold changes along a curve $\gamma\colon [0,1] \to M$. They live in tangent space T_pM.

$$V_\gamma[f] = \frac{\mathrm{d} f \circ \gamma(\lambda)}{\mathrm{d}\lambda}\Big|_{\lambda=0}$$



Basis of T_PM - $\{\partial_\alpha = \frac{\partial}{\partial x^\alpha}\Big|_p\}_{\alpha=1\ldots n}$

Ingredients - One-forms

One-forms - Objects that take vectors from abstract objects to a point in $\mathbb{R}^n$ (components of vectors in common treatments). They live in cotangent dual space T_p^*M.

$$df(V) := V[f] \in \mathbb{R}$$

This object is called as gradient of a function f. We now define dual basis ω_α of T_p^*M, which are dual to the coordinate basis of T_pM as

$$\omega_\alpha\left(\frac{\partial}{\partial x^\beta}\bigg|_p\right) := \delta^\alpha_\beta$$

Basis of T_p^*M - $\{dx^\alpha\}_{\alpha=1\ldots n}$

Ingredients - Metric Tensor

Metric Tensor - Gives a notion of length (via infinitesimal lengths) on the manifold. $g_p \colon T_pM \times T_pM \to \mathbb{R}$ as

$$g_p(U, V) = \langle U, V \rangle$$

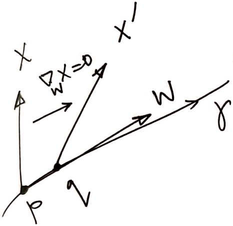
for any $U, V \in T_pM$. In coordinate basis,

$$g = g_{\alpha\beta}(p) dx^\alpha \otimes dx^\beta$$

for example: $ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2$ is infinitesimal length on sphere in spherical coordinates basis.

Ingredients - Affine Connections

Affine Connection - Provides us with a definition of parallel transport and directional derivative.



For a vector $X \in T_pM$, the parallel transport vector $X' \in T_qM$ along the curve γ with tangent vector W is

$$X'^{\alpha}(q) = X^{\alpha}(p) - \Gamma^{\alpha}_{\beta\gamma}(p) W^{\gamma} X^{\beta} \Delta\lambda$$

where $\Gamma^{\alpha}_{\beta\gamma}$ are christoffel symbols which captures curvi-linearity of coordinate systems.

Affine Connections

The covariant derivative $\nabla_W X$ w.r.t to connection ∇ is given by

$$\nabla_W X = \frac{\mathrm{d}X^\alpha}{\mathrm{d}\lambda} + \Gamma^\alpha_{\beta\gamma} W^\gamma X^\beta$$

Metric Induced Connection:

- Metric compatibility - X[g(Y, Z)] = 0 for Y, Z being parallel transported along X.
- Torsion Free - $\Gamma^\alpha_{\beta\gamma} = \Gamma^\alpha_{\gamma\beta}$.

These restriction are enough to obtain closed form expression for christoffel symbols

$${}^{LC}\Gamma^\alpha_{\beta\gamma} = \frac{1}{2} g^{\alpha\lambda}(\partial_\gamma g_{\lambda\beta} + \partial_\beta g_{\gamma\lambda} - \partial_\lambda g_{\beta\gamma})$$

where ${}^{LC}\Gamma^\alpha_{\beta\gamma}$ is Levi-Civita christoffel symbols.

Fundamental Theorem of Riemannian Geometry - The above Levi-Civita connections are unique.

Information Manifolds - (M, g, ∇, ∇^*)

Conjugate-Connection Manifolds - Spaces of allowed parameters for a statistical decision making problem. The CCM's have a dual structure of connections (∇, ∇^*) with ∇^* defined by:

$$X[g(Y, Z)] = g(\nabla_X Y, Z) + g(Y, \nabla^\star_X Z)$$

for any arbitrary vector fields X, Y and Z.

Note: $(\nabla^\star)^\star = \nabla$. Equivalent definition -

$$\langle U, V \rangle = \langle \prod_{\gamma(t)}^{\nabla} U, \prod_{\gamma(t)}^{\nabla^\star} V \rangle$$

which is statement that dual connections are metric-preserving. Note from this definition Levi-Civita Connection is self-dual $({}^{LC}\nabla, {}^{LC}\nabla^* = {}^{LC}\nabla)$

Statistical Manifolds

A statistical manifold (M, g, C) is a manifold equipped with a metric tensor g and a totally symmetric 3-tensor C Amari-Chentsov tensor where

$$C(X, Y, Z) := \langle \nabla_X Y - \nabla^{\star}_X Y, Z \rangle$$

or in component form

$$C^k_{ij} = \Gamma^k_{ij} - \tilde{\Gamma}^k_{ij}$$

Also for given pair $(\Gamma^{\alpha}_{\beta\gamma}, \tilde{\Gamma}^{\alpha}_{\beta\gamma})$, we have a self-dual connection

$$^{LC}\nabla = \frac{1}{2}(\nabla + \nabla^{\star})$$

which from fundamental theorem of Riemannian Geometry is Levi-Civita connections.

One-parameter family of Conjugate Connections

For a given $(\Gamma^{\alpha}_{\beta\gamma}, \tilde{\Gamma}^{\alpha}_{\beta\gamma})$ with Amari-Chentsov tensor $C^{\alpha}_{\beta\gamma}$.

Then for a continous parameter λ, $\lambda C^{\alpha}_{\beta\gamma}$ is also totally symmetric tensor and can be Amari-Chentsov tensor of some other pair of dual connections $(\nabla^{-\lambda}, (\nabla^{-\lambda})^* = \nabla^{\lambda})$ with christoffel symbols as:

$$\Gamma^{\lambda}_{ijk} = \Gamma^{0}_{ijk} - \frac{\lambda}{2} C_{ijk}$$
$$\Gamma^{-\lambda}_{ijk} = \Gamma^{0}_{ijk} + \frac{\lambda}{2} C_{ijk}$$

where Γ^{0}_{ijk} is Levi-Civita connections.

Fundamental Theorem of Information Geometry - A manifold $(M, g, \nabla^{-\lambda}, \nabla^{\lambda})$ is ∇^{λ}-flat if and only if it is $\nabla^{-\lambda}$-flat.

Big Question - How can we obtain above structures ?

Two ways to obtain CCM structure (g, ∇, ∇^*) canonically from the problem is:

- From divergence considered in the problem to capture dissimilarity between probability distributions.
- From probability distribution itself by using max-log likelihood principle.

Conjugate Connection Structure from Divergences

Divergence:
$D\colon M \times M \to [0, \infty)$ on a manifold M with a local chart $\theta \subset \mathbb{R}^D$ with following properties

- $D(\theta : \theta') \geq 0 \;\forall\; \theta, \theta' \in \Theta$ where equality holds if and only if $\theta = \theta'$.
- $\partial_{i,.} D(\theta, \theta')\Big|_{\theta=\theta'} = \partial_{.,j} D(\theta, \theta'\Big|_{\theta=\theta'} = 0 \;\forall i, j$
- $-\partial_{.,i}\partial_{.,j} D(\theta, \theta')\Big|_{\theta=\theta'}$ is positive-definite.

We can also define a dual-divergence by swapping the arguments

$$D^\star(\theta, \theta') = D(\theta, \theta')$$

Intuition:

$$\begin{aligned}
D(\theta, \theta + \delta\theta) &= D(\theta, \theta) + \frac{\partial}{\partial\theta^i} D\Big|_\theta \delta\theta + \frac{\partial^2}{\partial\theta^i \partial\theta^j} D\Big|_\theta \delta\theta^i \delta\theta^j \\
&= \frac{\partial^2}{\partial\theta^i \partial\theta^j} D\Big|_\theta \delta\theta^i \delta\theta^j \\
&= \partial_{i,j} D(\theta, \theta')\Big|_\theta \delta\theta^i \delta\theta^j
\end{aligned}$$

Conjugate Connection Structure from Divergences

we define the conjugate connection structure naturally induced by divergence $D(\theta, \theta')$ as follows:

- $g := -\partial_{i,j} D(\theta, \theta')\Big|_{\theta=\theta'}$
- $\Gamma_{ijk} := -\partial_{ij,k} D(\theta, \theta')\Big|_{\theta=\theta'}$
- $\tilde{\Gamma}_{ijk} := -\partial_{k,ij} D(\theta, \theta')\Big|_{\theta=\theta'}$

Conjugate Connection Structure from Probability Distribution

Let $\mathfrak{P}$ be a parametric family of probability distribution

$$\mathfrak{P} = \{p_\theta(X)\}_{\theta \in \Theta}$$

where Θ is parameter space. Order of parameter space is dimension of parameter space. We use the familiar log-likelihood function

$$l(\theta; x) = \log p_\theta(x)$$

We now define metric as

$$I(\theta) = g_{ij} = \mathbb{E}_\theta[\partial_i l \partial_j l]$$

This relates with the Cramer-Rao lower bound on variance of estimator

$$Var_\theta[\hat{\theta}_n(x)] \geq \frac{1}{n} I^{-1}(\theta)$$

Conjugate Connection Structure from Probability Distribution

Now we define two types of connections which is naturally defined in terms of the above probability distribution

- Exponential connection - ${}^{e}\Gamma_{ijk} := \mathbb{E}_\theta[(\partial_i\partial_j l)\partial_k l]$
- Mixing connection - ${}^{m}\Gamma_{ijk} := \mathbb{E}_\theta[(\partial_i\partial_j l + \partial_i l \partial_j l)\partial_k l]$

For a complete treatment on the subject refer the paper[10].

[10] F. Nielsen, *An elementary introduction to information geometry*, 2018. arXiv: 1808.08271 [cs.LG].

Why this is relevant in Deep Learning?

Natural Gradient Descent - If the problem has non-euclidean information manifold (which is the case most of the time) then the update rule in gradient descent algorithm is given by

$$\theta_{t+1} = \theta_t - \eta_t \tilde{\nabla} l(\theta)$$

Here $\tilde{\nabla}$ is natural gradient defined as[11]

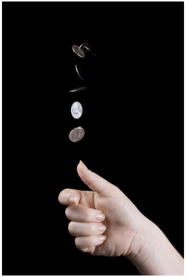
$$\tilde{\nabla} l(\theta) = G^{-1} \nabla l(\theta)$$

where $\nabla = (\frac{\partial}{\partial x^1}, \ldots, \frac{\partial}{\partial x^n})$ is usual gradient and $G = g_{\alpha\beta}$.

[11] S.-i. Amari, "Natural gradient works efficiently in learning," *Neural Computation*, vol. 10, no. 2, pp. 251–276, 1998. DOI: 10.1162/089976698300017746. eprint: https://doi.org/10.1162/089976698300017746. [Online]. Available: https://doi.org/10.1162/089976698300017746.

Scope of Future Work - Classical VS Non-Classical Models

Classical Probability - Source of stochastic outcome comes from the missing of intractable hidden variables from the dynamics. For example: tossing of coin[12]



Non-classical Probability - Stochastic outcomes are intrinsic even if the dynamics is complete (no local hidden variables missing). For example: quantum probability

[12] Image Source - https://www.bellevuerarecoins.com/history-coin-flip/

Scope of Future Work - Bell's Inequality

How to distinguish between classical and non-classical probabilities?

"Bell's Inequality"

Classical Probability - Obeys Bell's Inequality.

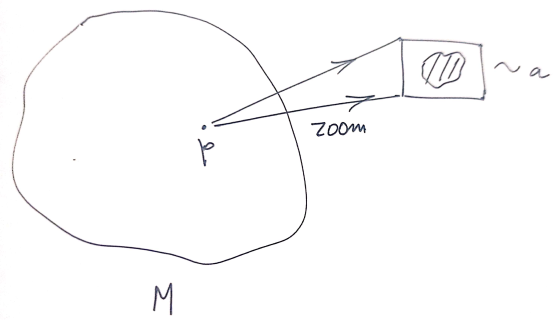
Non-Classical Probability - Does not obey Bell's inequality.[13]

[13] J. S. Bell, "On the einstein podolsky rosen paradox," in *Speakable and Unspeakable in Quantum Mechanics*, Cambridge University Press, 2004 [1964], pp. 14–21.

Scope of Future Work - Classical VS Non-Classical Models

Two main features of dynamical theories which obey Bell's Inequality:

- Counter-factual definiteness.
- Local hidden variables.



In this diagram above, a is the order of intrinsic uncertainty. For quantum mechanics a is $\hbar$.

Scope of Future Work - Classical VS Non-Classical Models

Classical information manifolds are non-classical information manifolds in the limit $a \longrightarrow 0$.
For reverse, from classical information manifolds to non-classical information manifolds, the process is called

"Quantization"

Quantization: real chart coordinates $\theta_\alpha \in \mathbb{R} \longrightarrow$ matrix-valued operators Θ_α (finite or infinite dimensional)

$$[\Theta_\alpha, \Theta_\beta] \sim a\Delta_{\alpha\beta}\mathbb{I}$$

where $\Delta_{\alpha\beta}$ quantifies uncertainty coefficient between different pairs (α, β).

Scope of Future Work - Are Deep Neural Networks non-classical?

Do hidden layers have non-classical stochastic nature ?

"Analyse Classical Information Manifolds for DNN"

Thank You

References I

[1] N. Tishby and N. Zaslavsky, "Deep learning and the information bottleneck principle," *CoRR*, vol. abs/1503.02406, 2015. arXiv: 1503.02406. [Online]. Available: http://arxiv.org/abs/1503.02406.

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References III

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