The emergence of an

Information Bottleneck Theory *of* Deep Learning

Presentation for the conclusion of the Master Degree in Computer Science

By

Frederico Guth
Departamento de Ciência da Computação
Universidade de Brasília

Committee:

Téofilo de Campos (supervisor)
Universidade de Brasília

John Shawe-Taylor
University College London

Moacir Ponti
Universidade de São Paulo

Brasília, 20/01/2022

Universidade de Brasília

Agenda

1. Introduction
   - Problem and Research Objective
   - Research Questions and Methodology
2. Background
   - Machine Learning Theory (MLT)
   - Information Theoretic Learning (ITML)
   - MLT vs. ITML: “genealogy” and comparison
3. Information Bottleneck Theory new narrative
   - IB Principle and Relevance
   - IBT Main thesis and criticism
   - IB and Representation Learning: filling the gaps
   - Deep Learning phenomena in the IBT narrative
4. Conclusions

Problem

Practice-theory gap in Deep Learning Generalisation [Zha+16, Rah18].

IBT presents new perspective that may help fill this gap.

No comprehensive digest of IBT or comparison to MLT.

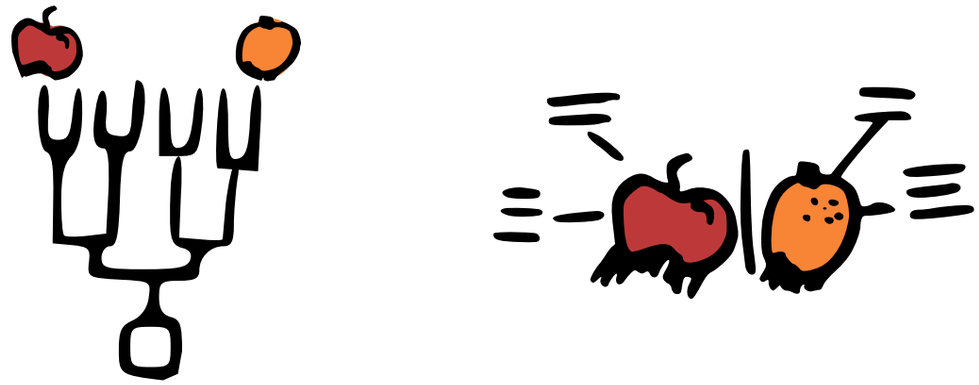
Objective

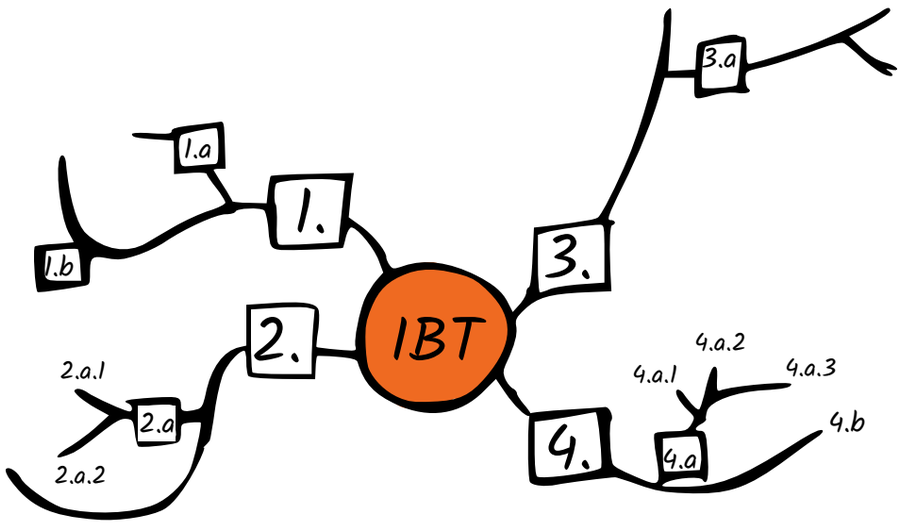
To investigate *to what extent* can IBT help us understand Deep Learning generalisation, presenting its strengths, weaknesses and research opportunities in a digest.

Research Questions

1. What are IBT fundamentals?
2. IBT and MLT differences and similarities?
3. Does IBT explain what MLT does?
4. Does IBT invalidate MLT results?
5. Can IBT explain phenomena currently not well understood?
6. IBT strengths?
7. IBT weaknesses?
8. What has been already developed in IBT?
9. IBT Research opportunities?

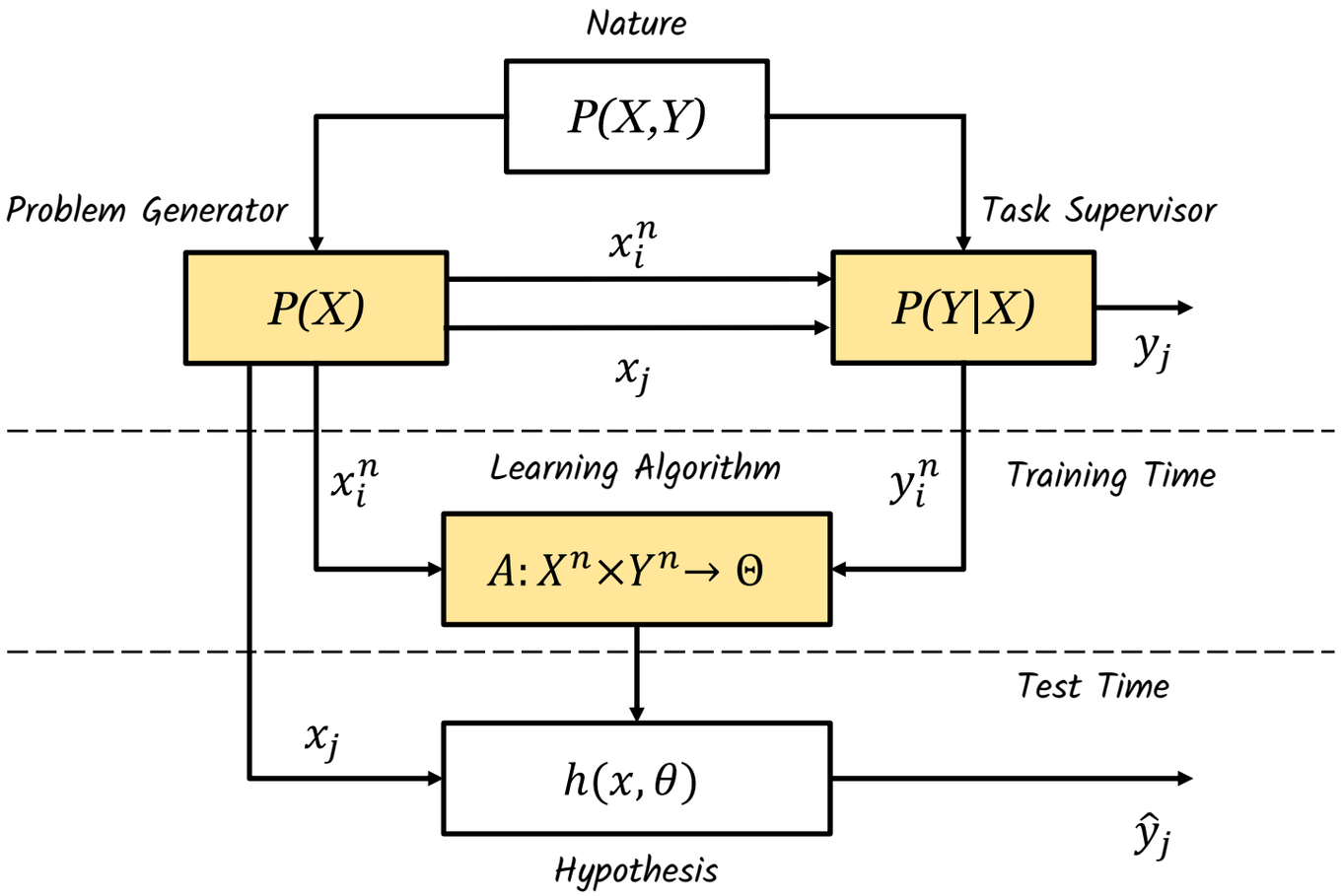
Methodology

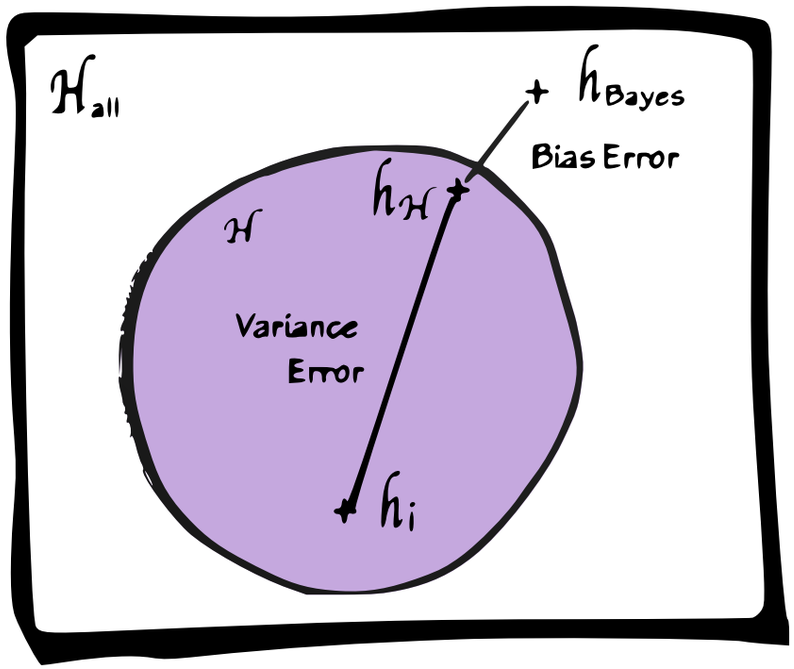




Machine Learning Theory

Learning as search in the hypothesis space

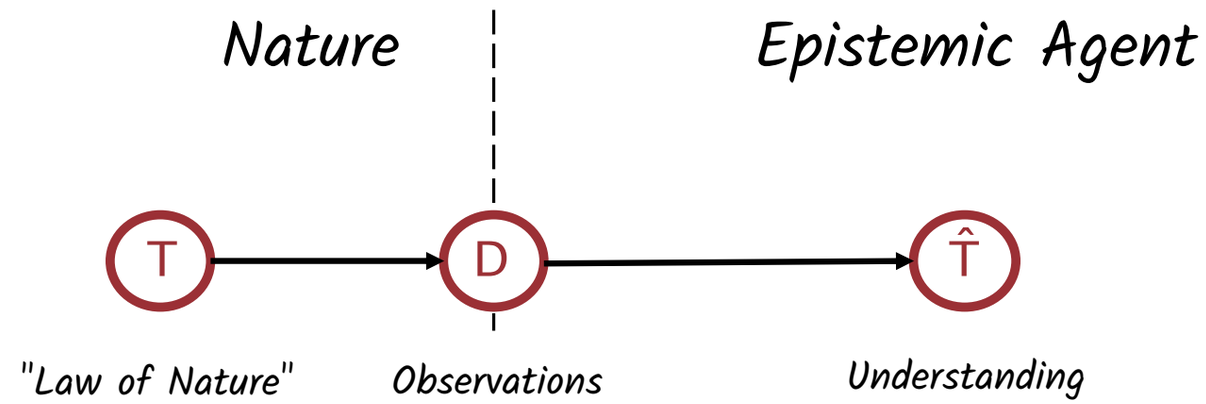




$$h_{\mathcal{H}} = \arg\min_{h \in \mathcal{H}} \hat{\mathrm{R}}_S(h)$$

Information Theoretical Learning

Learning as a communication problem



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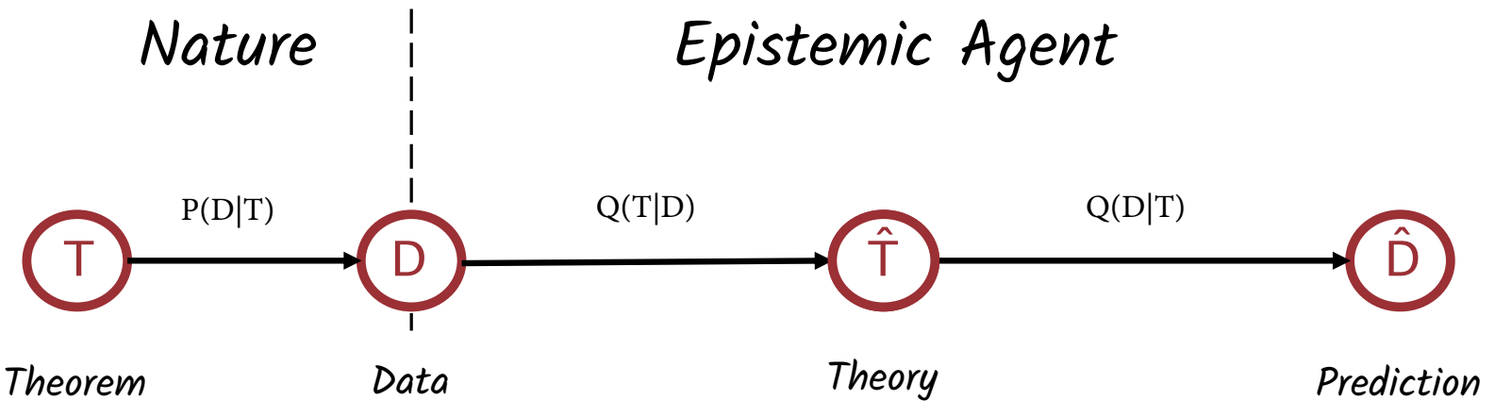

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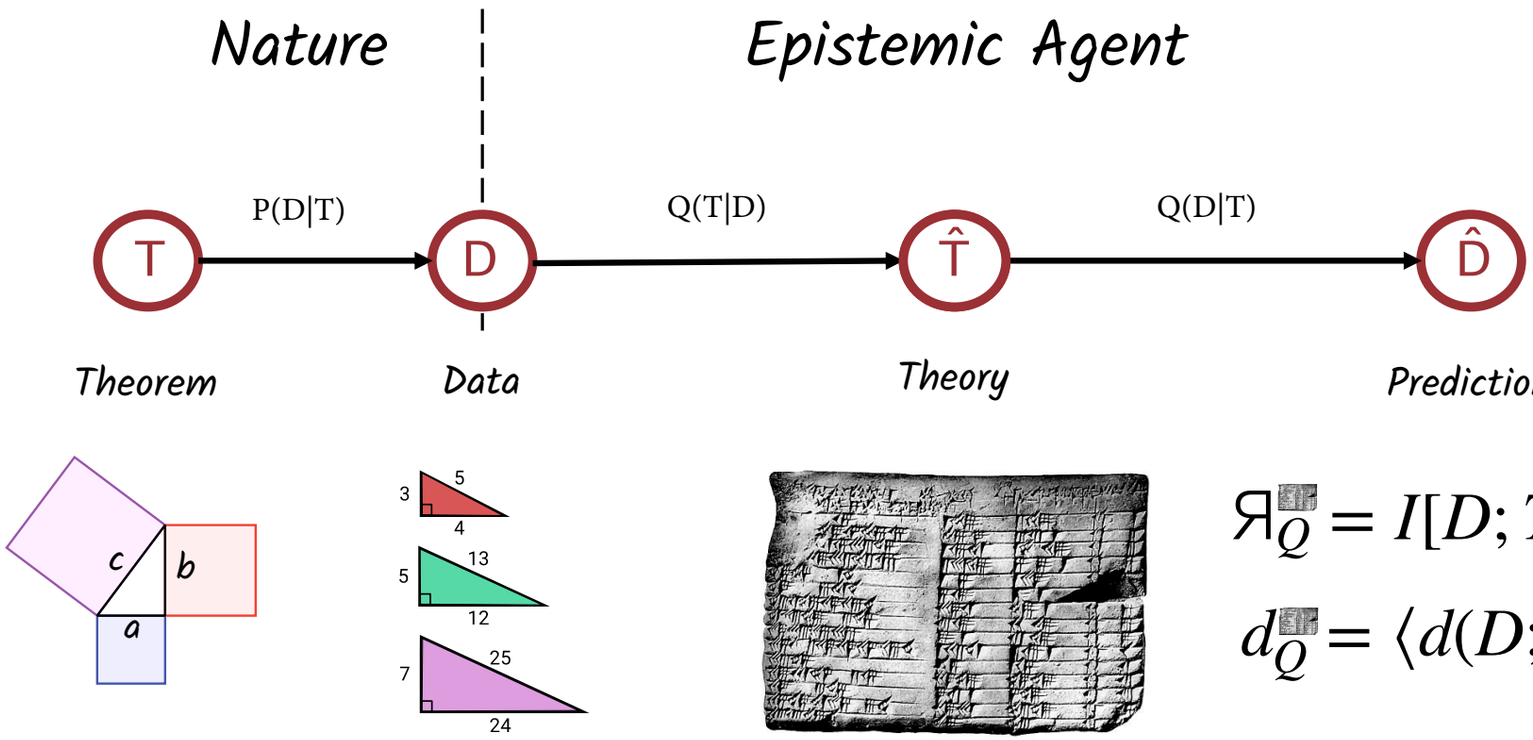

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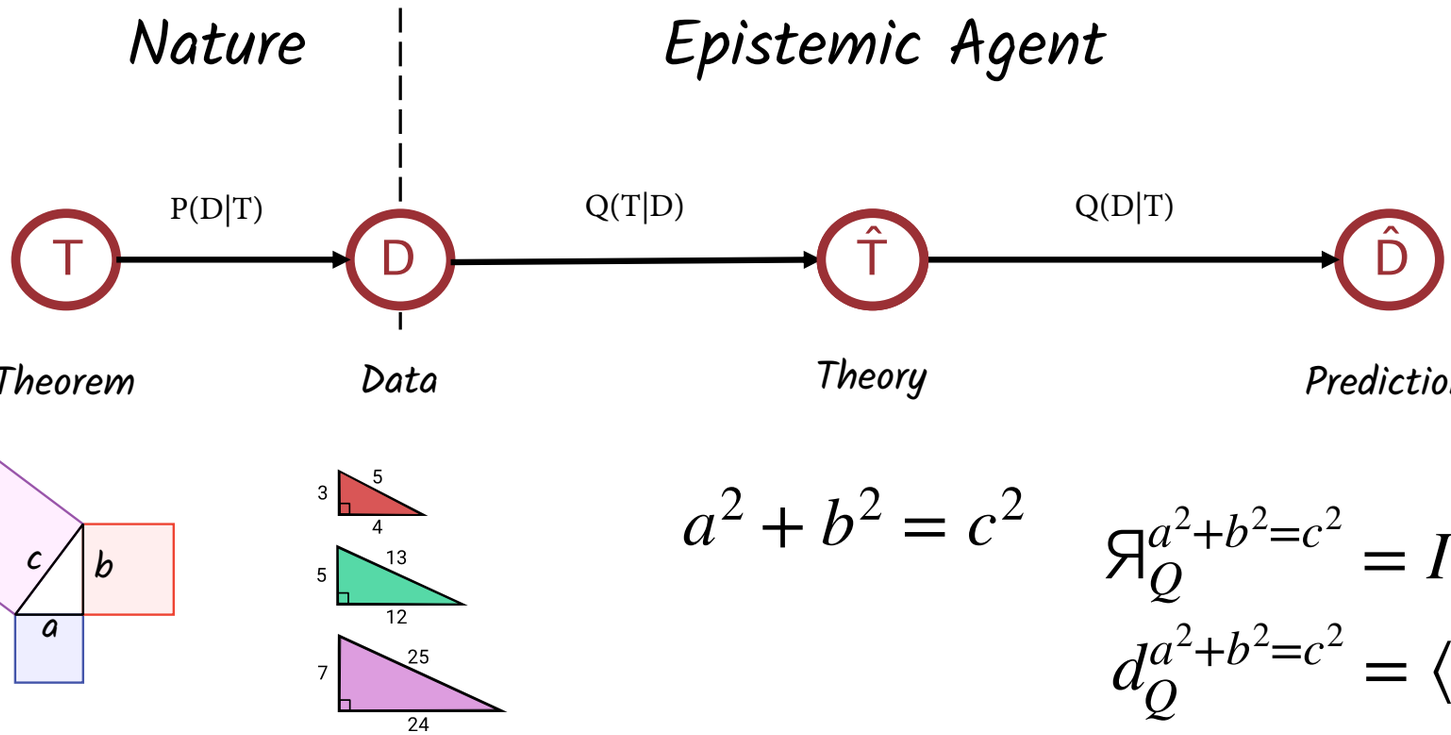

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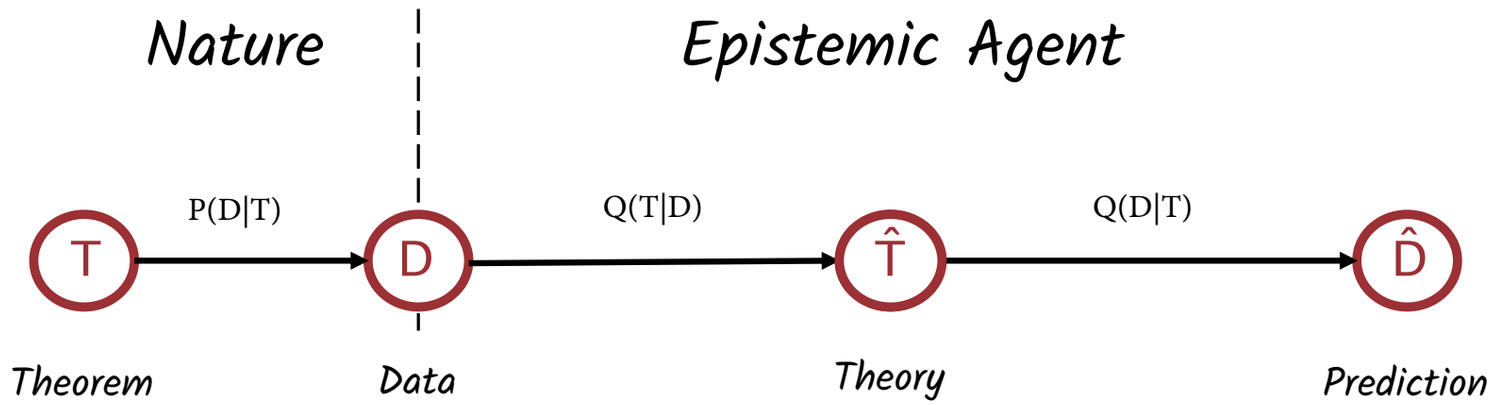
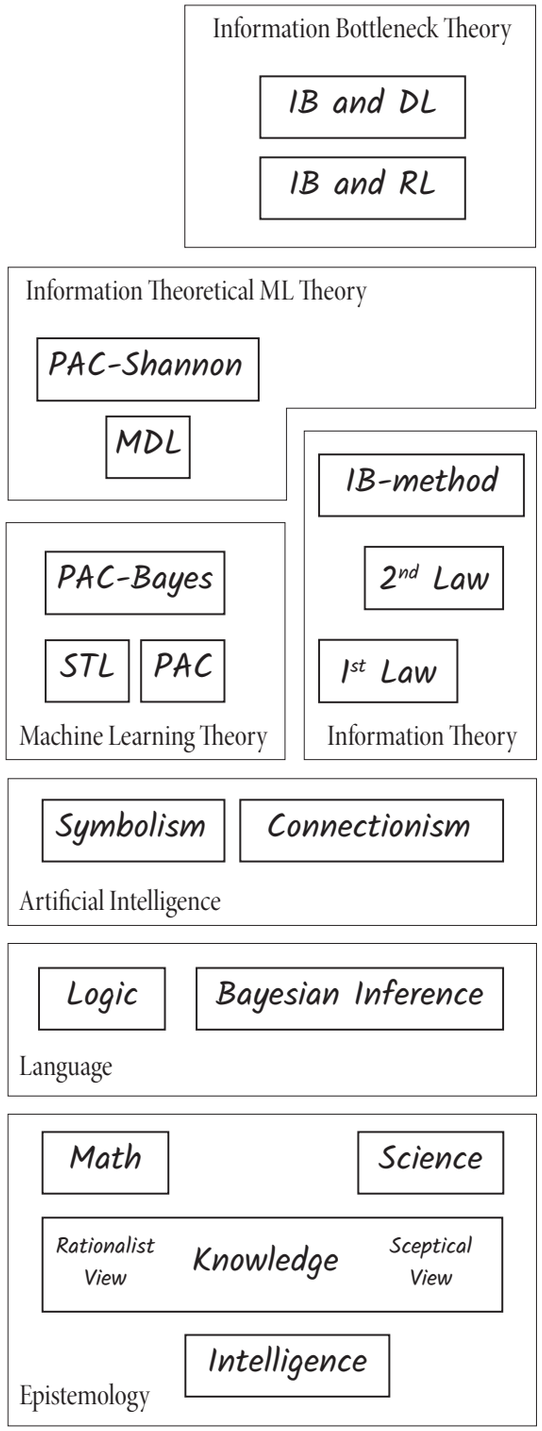
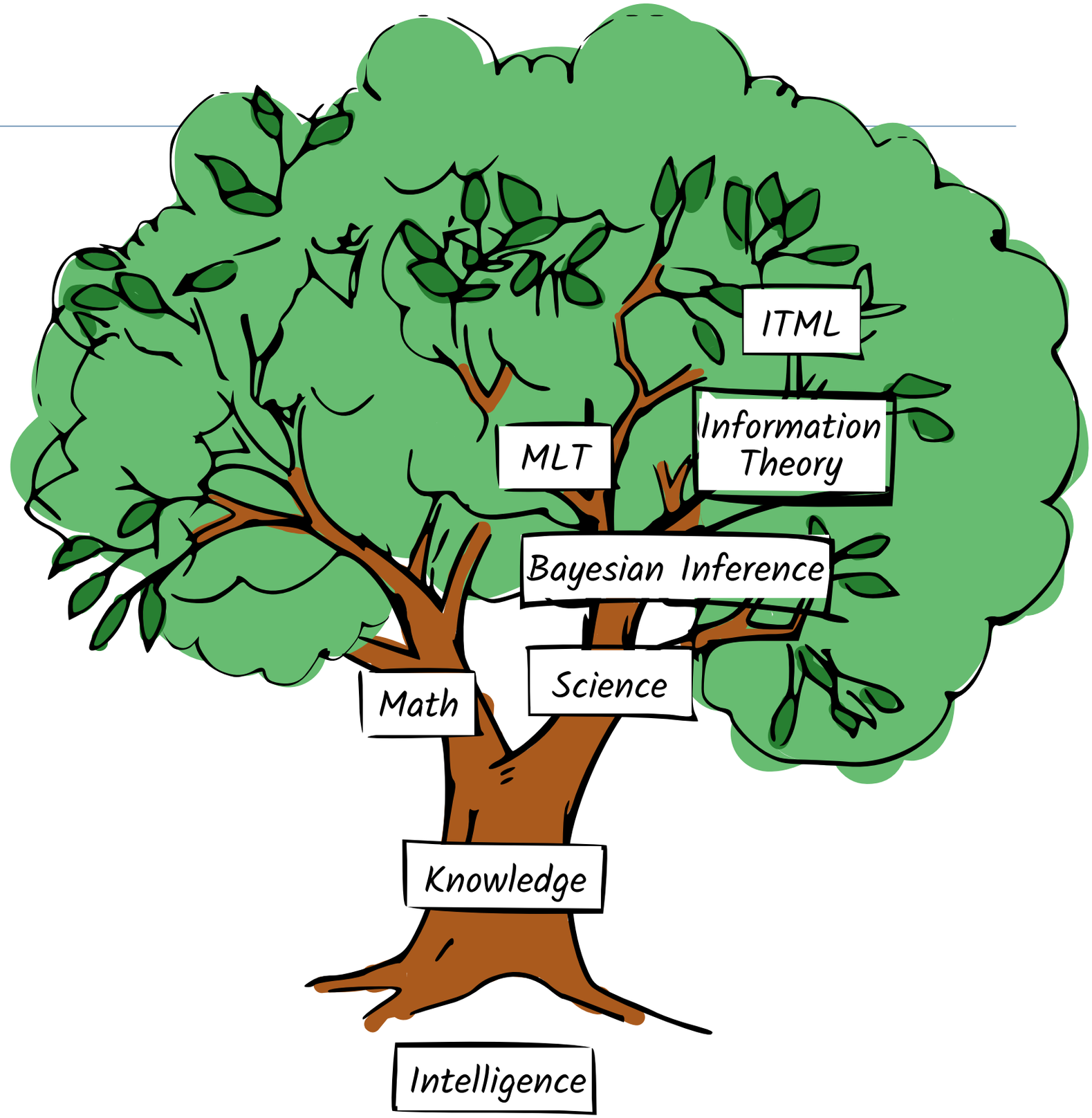


$$\text{Я}(\epsilon) \equiv \min_{Q:\ \langle d(x;z)\rangle \leq \epsilon} I[D;\hat{T}]$$

MLT vs. ITML

From the ground up





MLT

- P(X,Y) is fixed, no “time” parameter;
- Optimisation problem: search;
- Loss-metric agnostic (Risk function);

ITML

- P(X,Y) is fixed, no “time” parameter;
- Optimisation problem: compression;
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- Hypothesis-space dependent;
- Task independent;
- Continuous random variables;
- Possibly infinite input and target spaces;
- Unknown P(Y|X) can be deterministic;
- Independent sampling;

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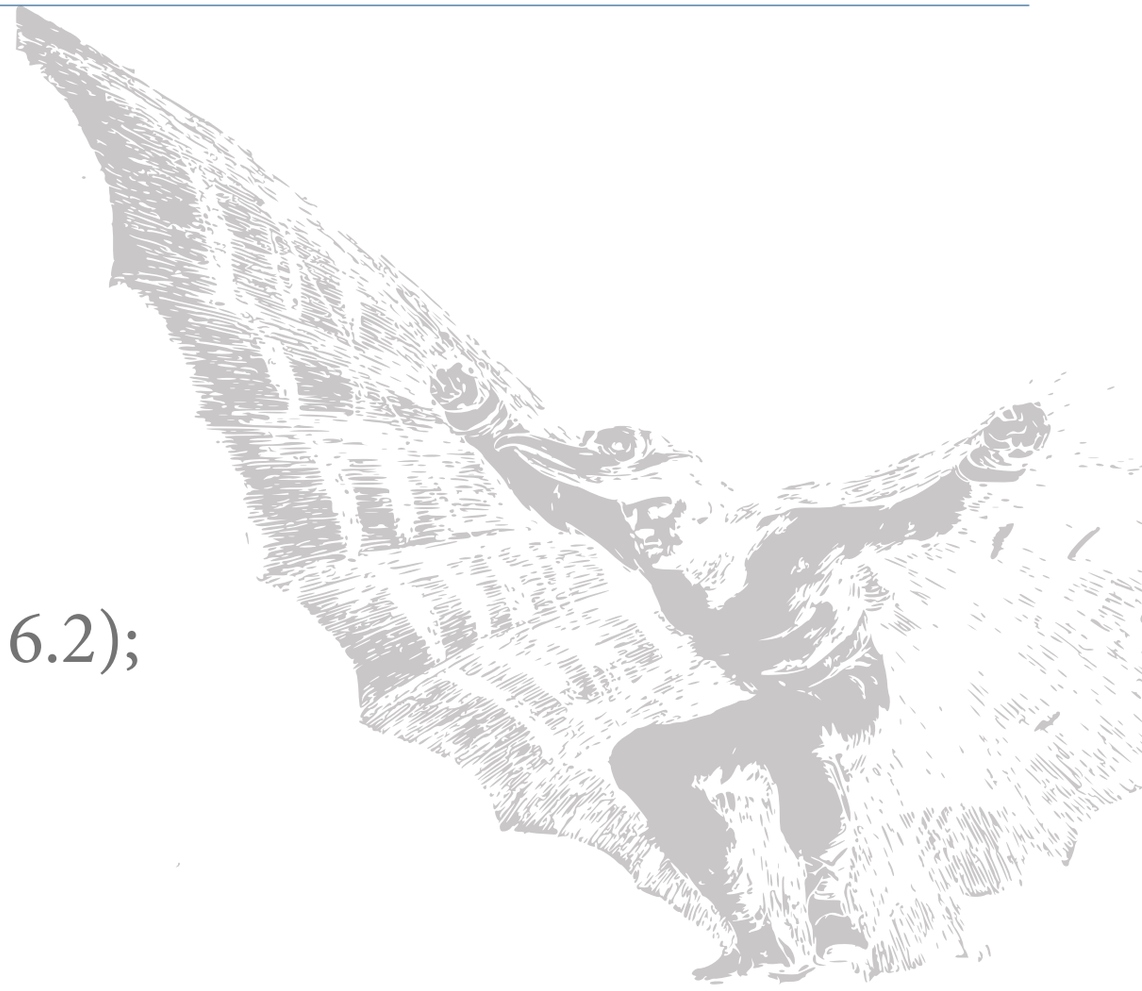
Answering Research Questions 1 to 4

If MLT ≡ ITML, what is the point ?



MLT vs ITML (IBT included):

Share most assumptions;

Differences are conciliable choices:
e.g. MDL[HVC93] and PAC-Shannon (sec. 6.2);

What is the point? A new narrative.

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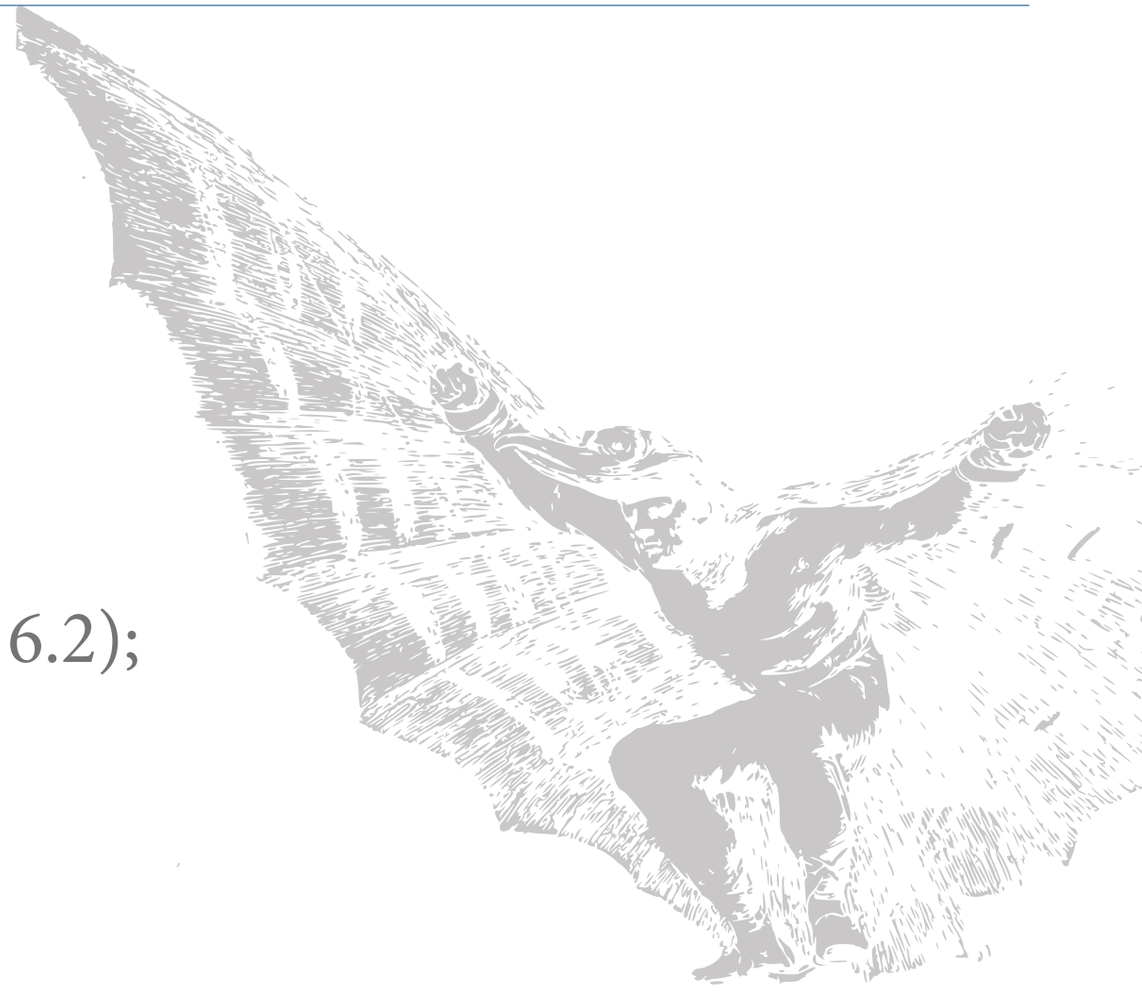

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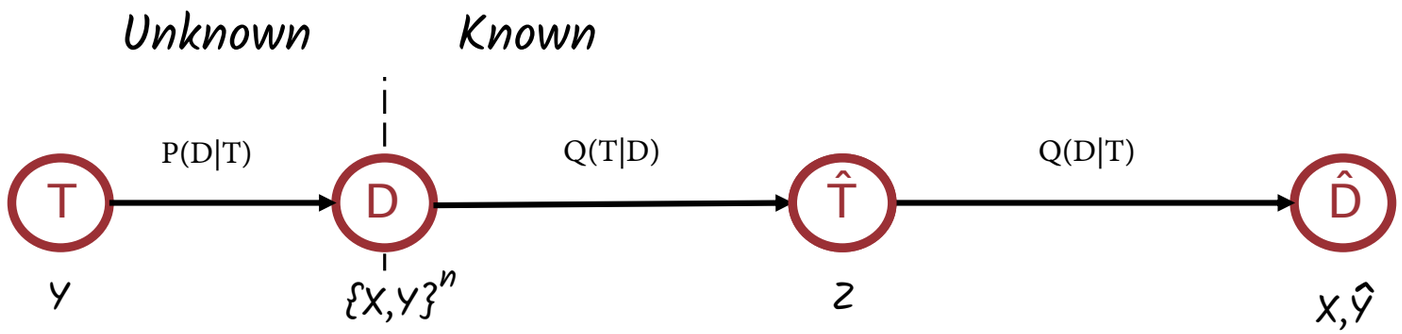
IB Principle

Relevance through a target variable

An arbitrary distortion function is an arbitrary feature selection [TPB99].



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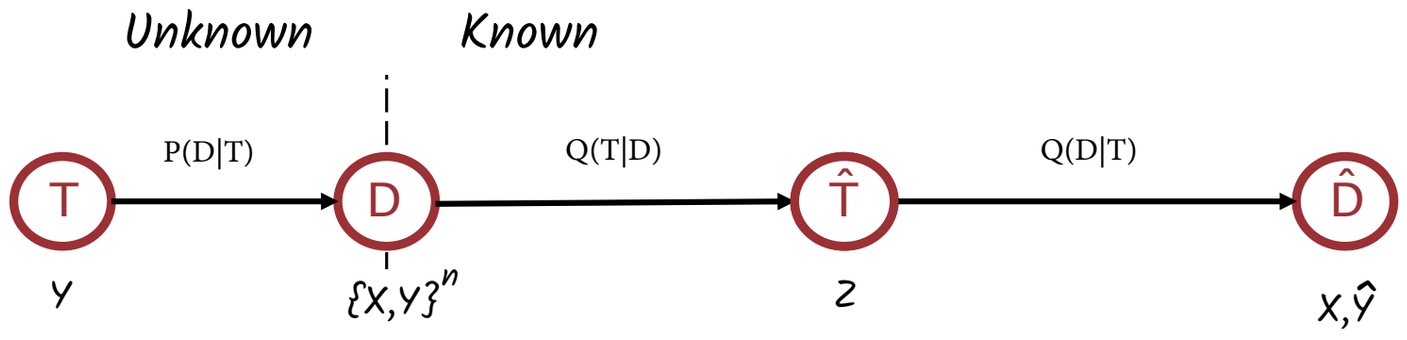

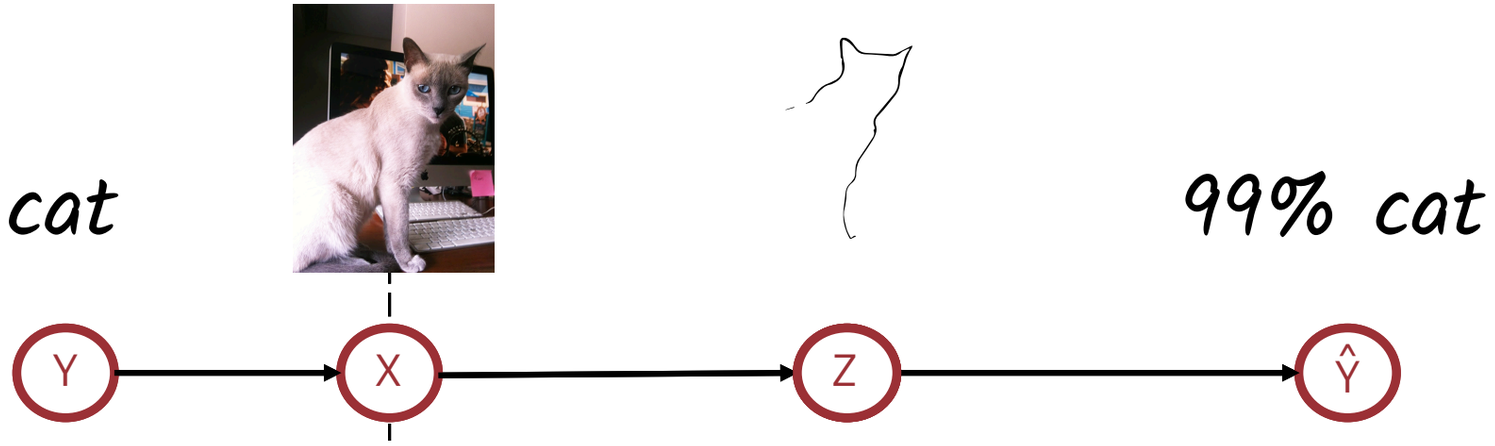

Relevance is task-dependent.

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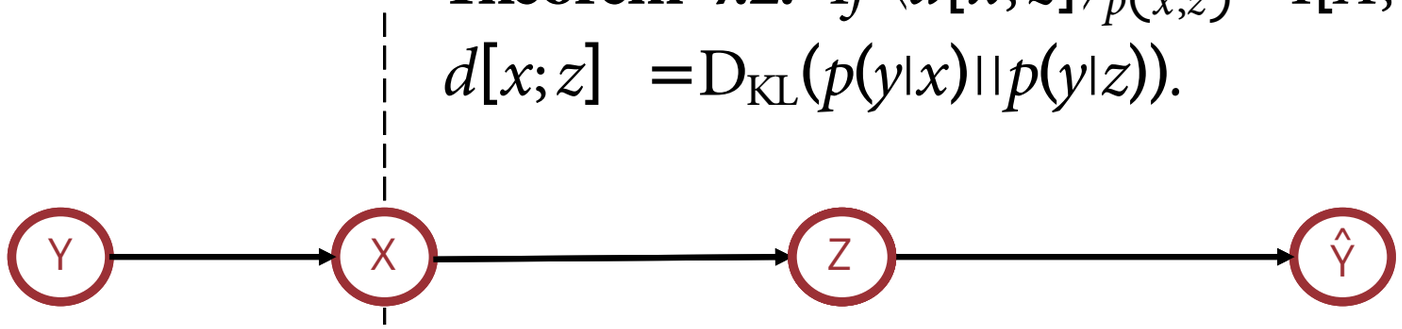
Theorem 7.2. *If* $\langle d[x;z]\rangle_{p(x,z)} = \mathrm{I}[X;Y] - \mathrm{I}[Z;Y]$, *then* $d[x;z] = \mathrm{D}_{\mathrm{KL}}(p(y|x)||p(y|z))$.

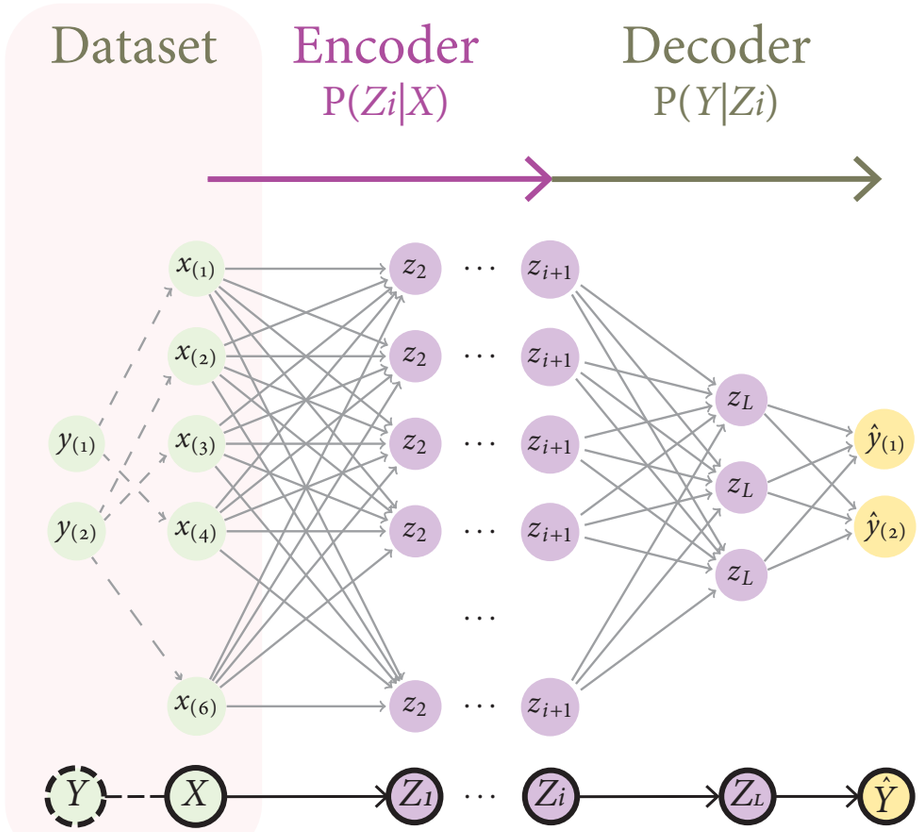


$$\text{Я}^{\text{IB}}(\epsilon) = \min_{Q:\ I[X;Y]-I[Z;Y]\leq\epsilon} I[Z;X]$$

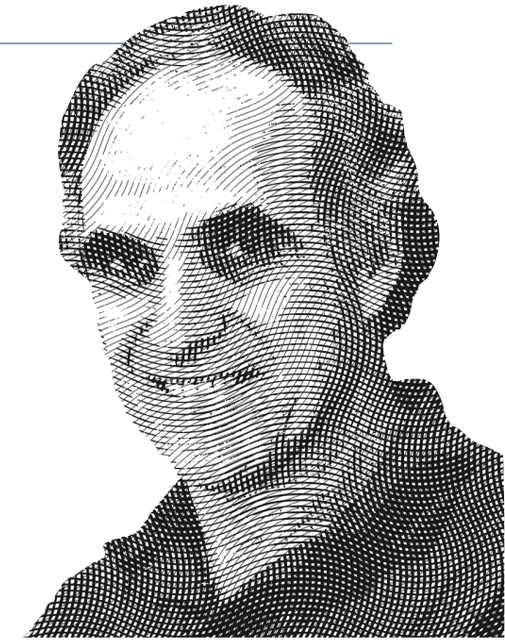
Relevance is task-dependent. $\mathscr{L}(Z) = I[Z;X] + \beta I[Z;Y]$

Information Bottleneck Theory

Information Bottleneck principle applied to Deep Learning



[TZ15a, ST17]



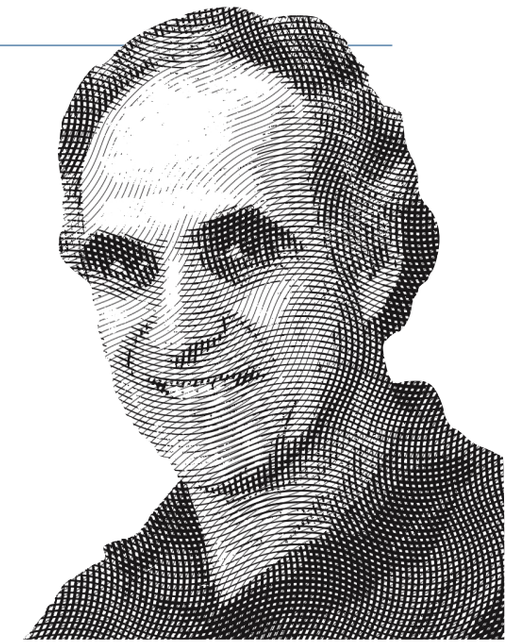
Naftali Tishby

What for?

Analysis, opening the "black-box" [ST17].

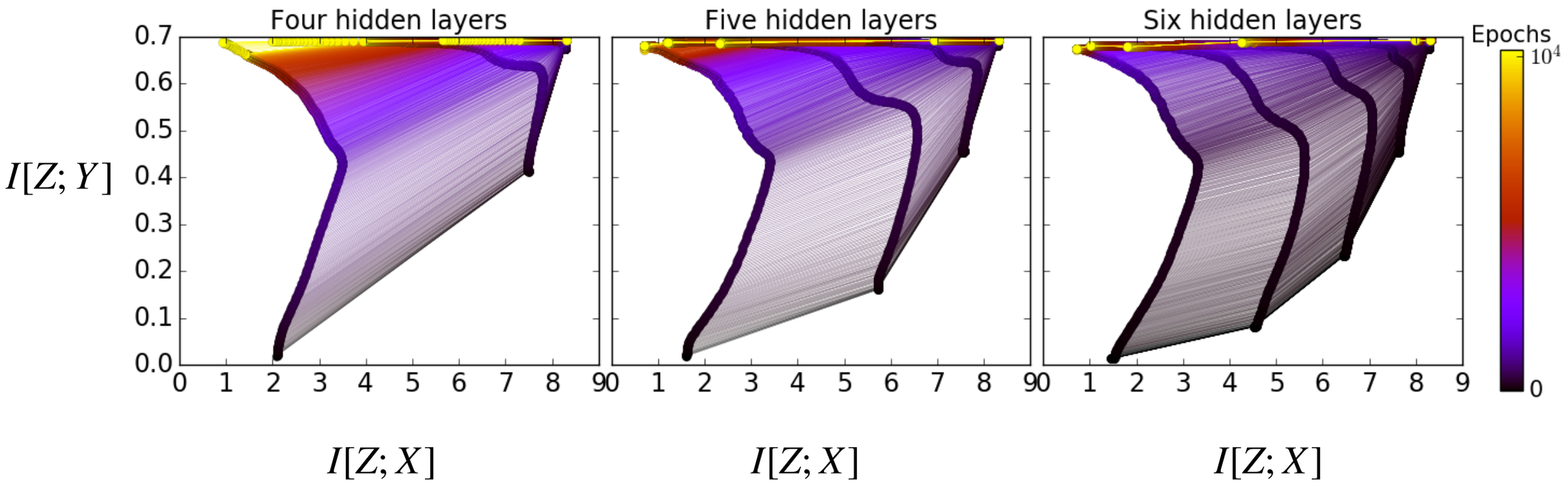
IBT Main thesis

Learning is forgetting



Naftali Tishby

Phase transition during training:
Fitting phase vs. Compression phase.



IBT Criticism

"Throwing the baby with the bathwater"?

Several papers challenged IBT initial efforts [Sax+18, Gol+19, CHO19] for different reasons:

- Discrete versus continuous random variables;
- IB is ill-posed for deterministic or invertible functions;
- Information in the activations: Stochastic mapping? Why? How?
- Information measurement did not convince;
- "Just an analysis tool" versus "a new Deep Learning Theory";
- Analysis overlooked for lack of confidence in the theory.

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> *'I would not call [IBT] a proven rigorous theory' — Tishby*[Tis20].

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IB and Representation Learning

Filling the gaps

Prof. Soatto's team extensive body of work [Ach19, Ach+19, ARS17, AS18b, AS19, CS18, Cha+19a]:

- Addresses the problem of bounding the information in the activations;
- Explains the emergence of generalisation and disentanglement;
- Shows the crucial role of noise in generalisation;
- Proposes a variational method for estimating mutual information;
- Relates IBT with MLT (PAC-Bayes).

Stefano Soatto

Alessandro Achille

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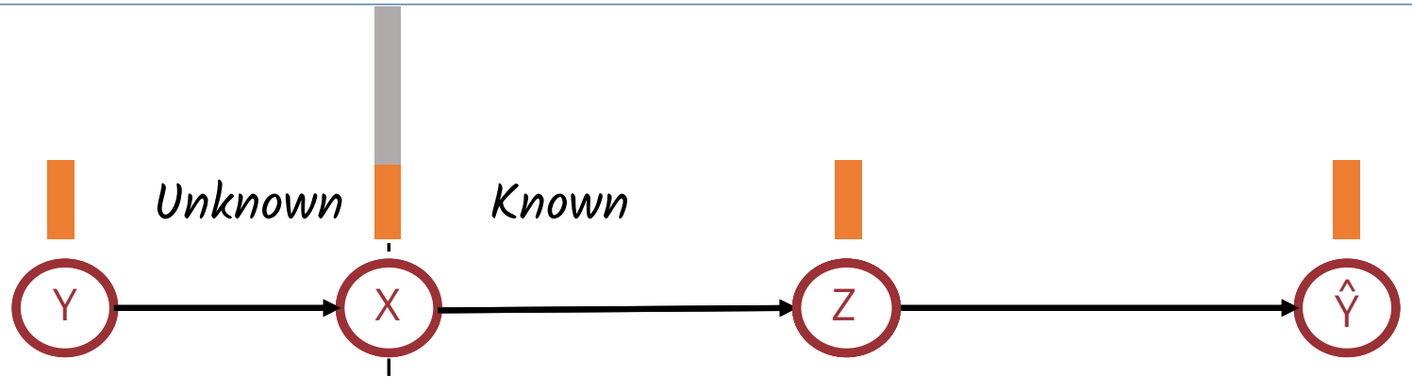
Alessandro Achille

Desiderata for Representations → Activations IB → Activations IB x Weights IB → IB Learning X Deep Learning

Desiderata for Representations

What is a good representation?



The best representation $Z := P(Z|X)$ of data X for task $Y := P(Y|X)$ is [AS18a]:

sufficient: $I[Z;Y] = I[X;Y]$ → accuracy

invariant: $\eta \perp Y \rightarrow I[\eta;Y] = 0 \rightarrow I[\eta;Z] = 0$

minimal: $I[Z;X] = I[Z;Y]$ → generalisation

disentangled: $TC(Z) = D_{KL}(P(Z) \| \prod_{i=1}^{n} P(Z_i)) = 0$ → explainability

sufficient    minimal

Desiderata for Representations

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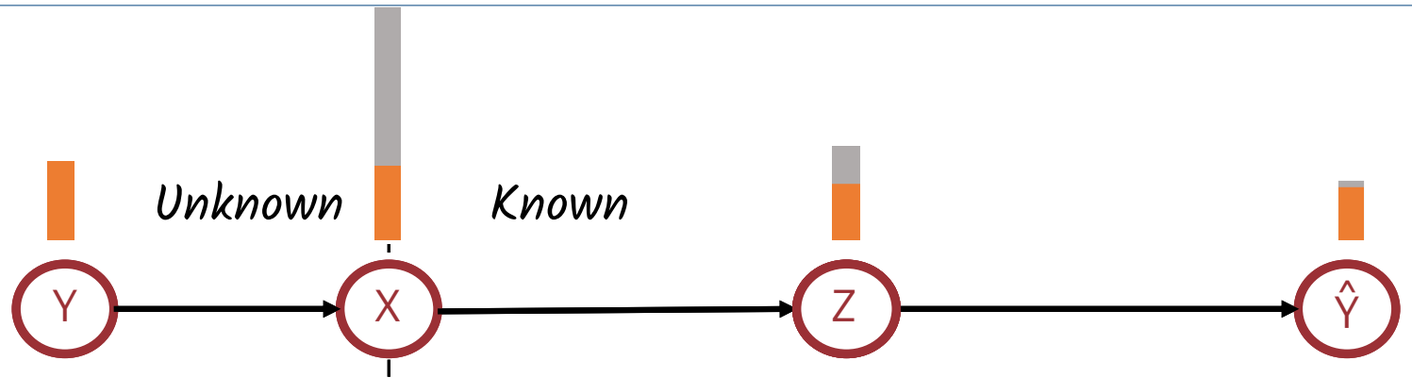

A good representation can be formulated as:

$$Z := \arg\min I[Z;X] \qquad \text{minimal/invariant}$$

s.t.

$$0 \leq I[X;Y] - I[Z;Y] \qquad \text{sufficient}$$

$$0 \leq TC(Z)\,. \qquad \text{disentangled}$$

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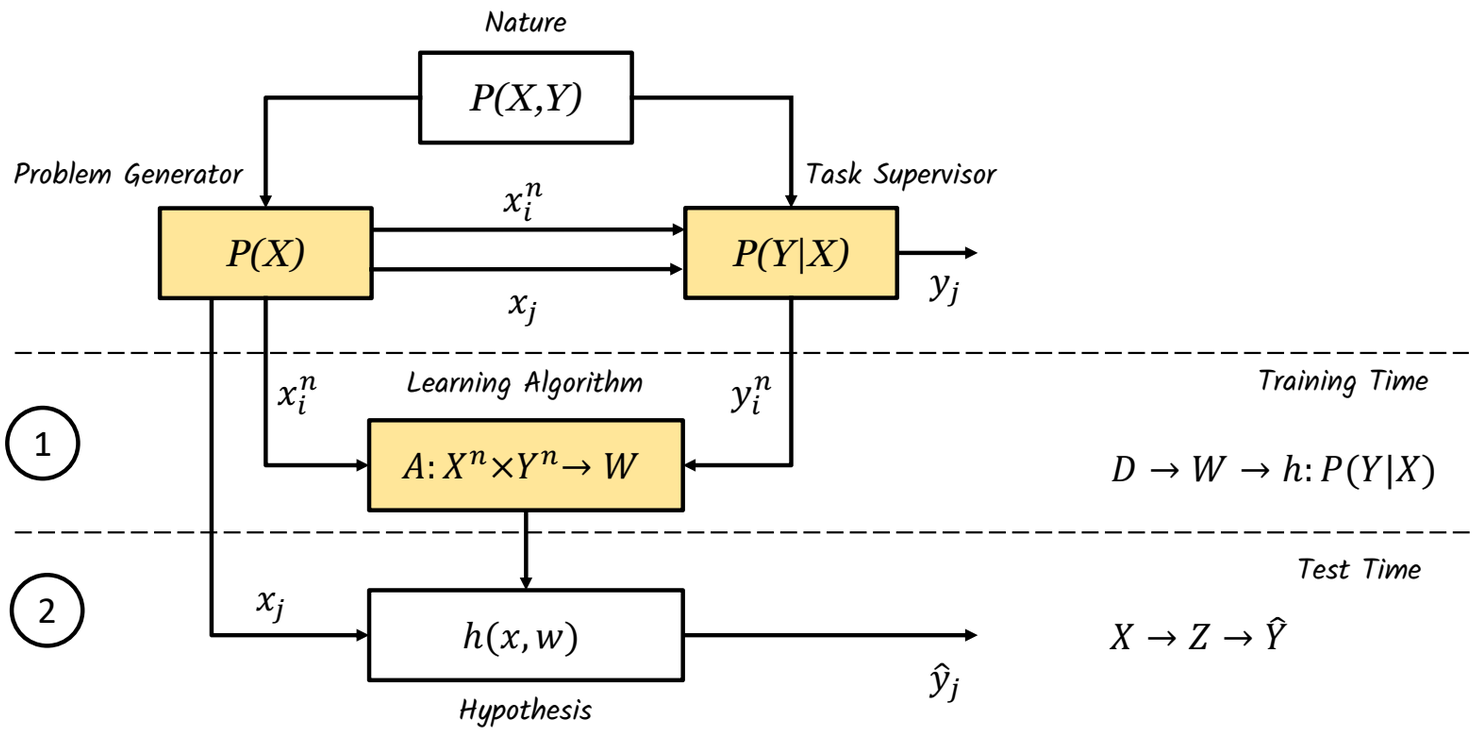
Using the Lagrangian relaxation:

$$L(Z) = \underbrace{H_{p,q}[Y|Z] + \beta^{-1}\{I[Z;X] + TC(Z)\}}_{\text{[TPB99, ST17]}} \qquad \text{Activations IB [AS18a]}$$

The IB "Achille's heel"

Two levels of representations



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Activations IB
[TPB99, ST17]

Activations IB is incomputable:

Z is a representation of yet not observed future data.

Valid min I[Z;X] during training → memorise indexes of each label.

Once the weights are fixed, not a stochastic mapping.

No access to true distribution P(X,Y).

Rethinking Generalisation

Cross-entropy decomposition and overfitting

Problem: Deep Learning pseudo-paradox [Zha+16].
→ can fit random labels, yet generalise;

Cross-entropy decomposition, assuming $D \sim P(D \mid \theta)$ [AS18a]:

$$\underbrace{H_{p,q}[D \mid W]}_{\text{intrinsic error}} = \underbrace{H_p[D \mid \theta]}_{\text{sufficiency}} + \underbrace{I[\theta; D \mid W]}_{\text{efficiency}} + D_{KL}(p \parallel q) - \underbrace{I[D; W \mid \theta]}_{\text{memorisation}}$$

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Naïve solution:

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Naïve solution:

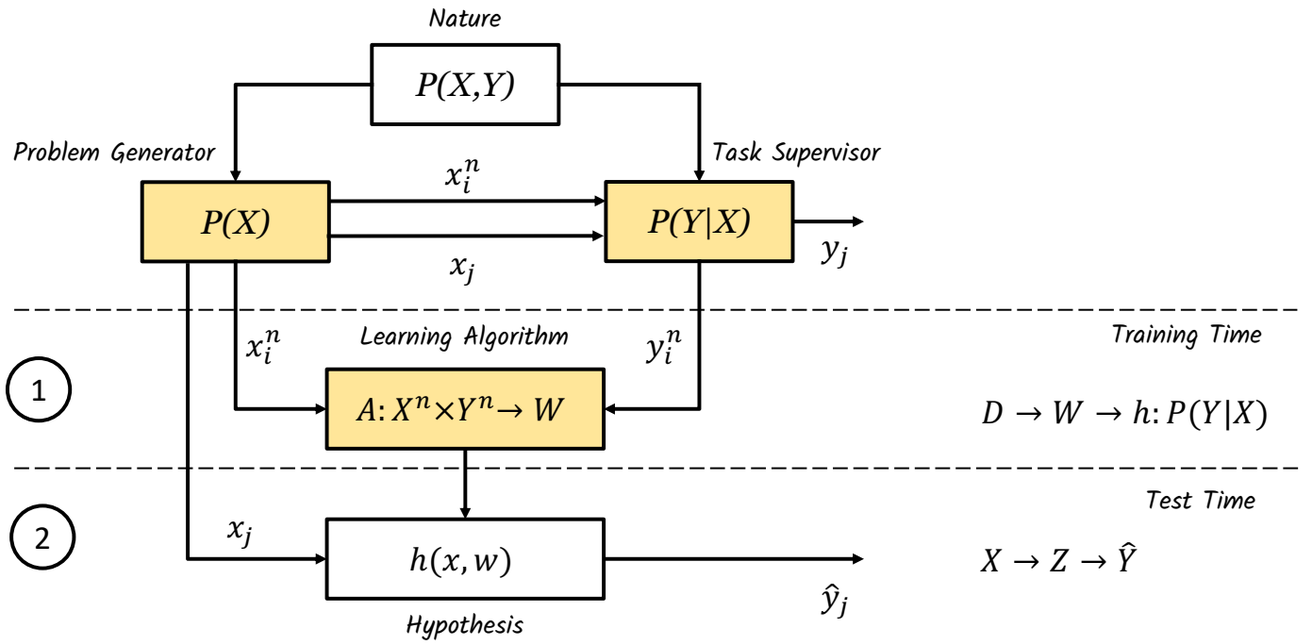
$$L(W) = H_{p,q}[D \mid W] + I[D; W \mid \theta]$$ intractable, θ is unknown.

But we can upper bound $I[D; W \mid \theta]$:

$$L(W) = H_{p,q}[D \mid W] + \beta^{-1} I[D; W]$$ Weights IB [AS18a, AS19]

Activations IB vs. Weights IB

Where is the information in Deep Neural Networks?



Weights IB
[AS18a, AS19]

$$\mathscr{L}(W) = H_{p,q}[D \mid W] + \beta^{-1} I[D; W]$$

$$\mathscr{L}(Z) = H_{p,q}[Y \mid Z] + \beta^{-1} I[Z; X]$$

Activations IB
[TPB99, ST17]

Activations IB vs. Weights IB

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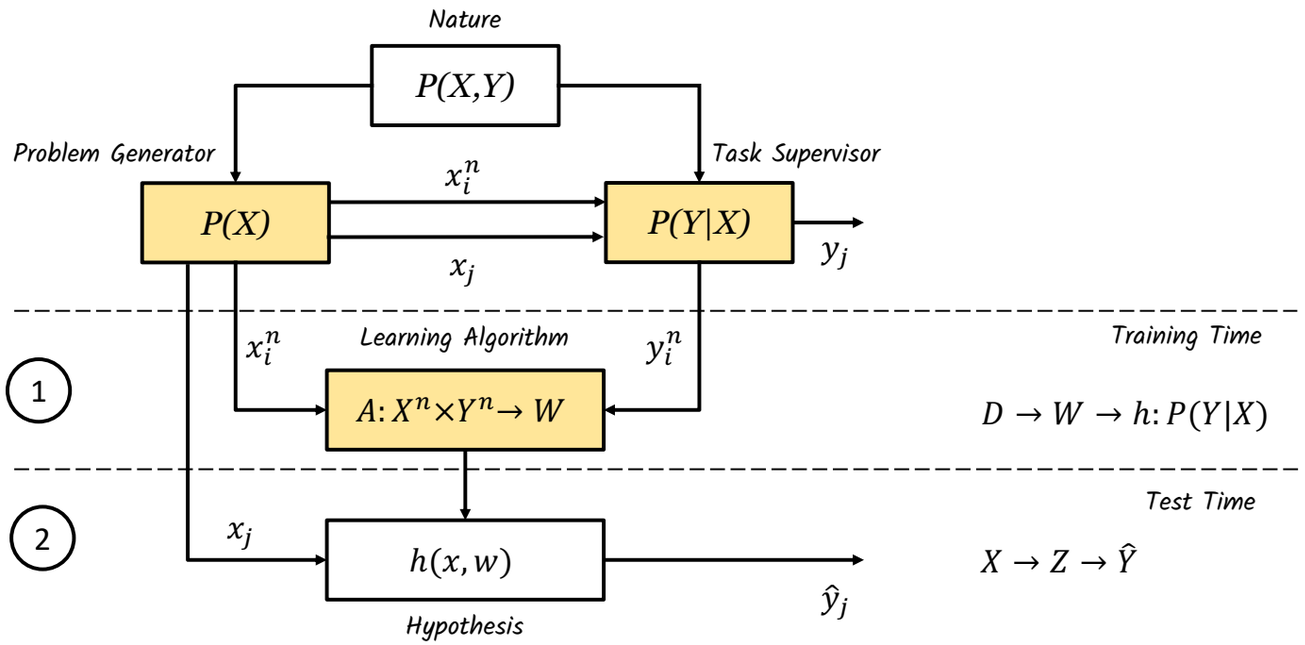

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$$\mathscr{L}(Z) = H_{p,q}[Y \mid Z] + \beta^{-1} I[Z; X]$$

Activations IB
[TPB99, ST17]

Bound [C.8 in AS18a]:

$$I[Z; X] \leq I[W; D] \leq \underbrace{\log |F(w^*)|}$$

Fisher Information

Deep Learning

Reality

Deep Learning components:

DNN Architecture: deep

SGD Optimiser

Large Dataset: P(X,Y) is noisy

Loss function: usually cross-entropy

$$\mathscr{L}(W) = H_{p,q}[D \mid W]$$

IBT Learning

Ideal

$$\mathscr{L}(W) = H_{p,q}[D \mid W] + \underbrace{\beta^{-1} I[D; W]}_{\text{regulariser}}$$

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IBT Learning

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Ways to reduce information:

Explicit regulariser in the loss function:
Information Dropout [As18b]

Implicit by architecture:
Reduce dimension (layers, max-pooling)
Add noise (dropout)

Problem [Zha+16]:
Generalisation without regularisers in the loss or architecture.

Can layers explain it all?

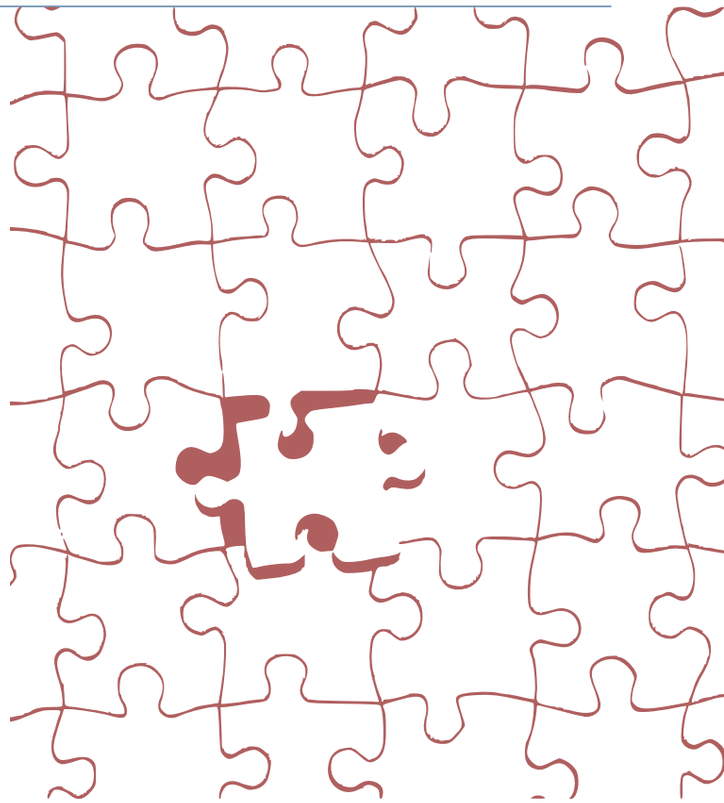
The role of noise in SGD

The last piece of the puzzle

Chaudhari and Soatto [CS18] prove with theory and empirical evidence that:

SGD performs variational inference with implicit loss;

SGD implicit loss has an information regulariser term.



$$\mathscr{L}(W) = H_{p,q}[D \mid W] + \underbrace{\beta^{-1} I[D; W]}_{\text{SGD implicit regulariser}}$$

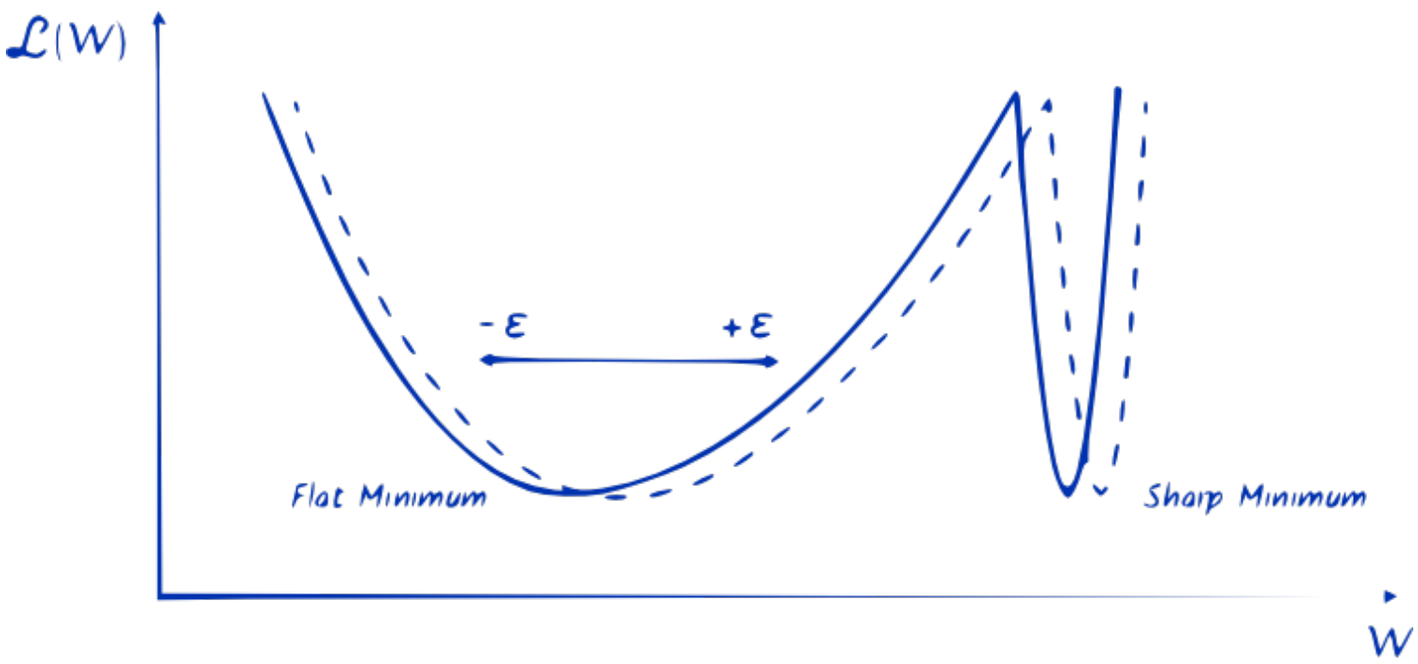
Deep Learning phenomena in the IBT narrative

Answering Research Question 5: Part I

Generalisation despite model capacity/expressiveness:
Information in the weights as the *effective* capacity measure.

Deep Learning bias towards disentangled representations:
SGD → I[W;D] implicit regulariser → upper-bound on I[Z;X]+TC

Scarcity of sharp minima in SGD optimisation:
SGD → low I[W;D] → low Fisher Information → curvature of loss



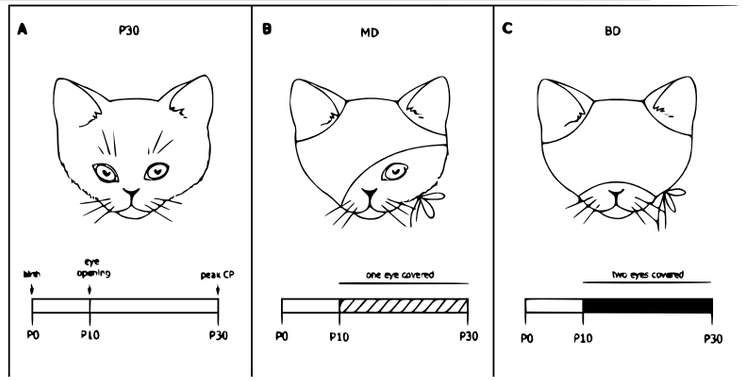
Deep Learning phenomena in the IBT narrative

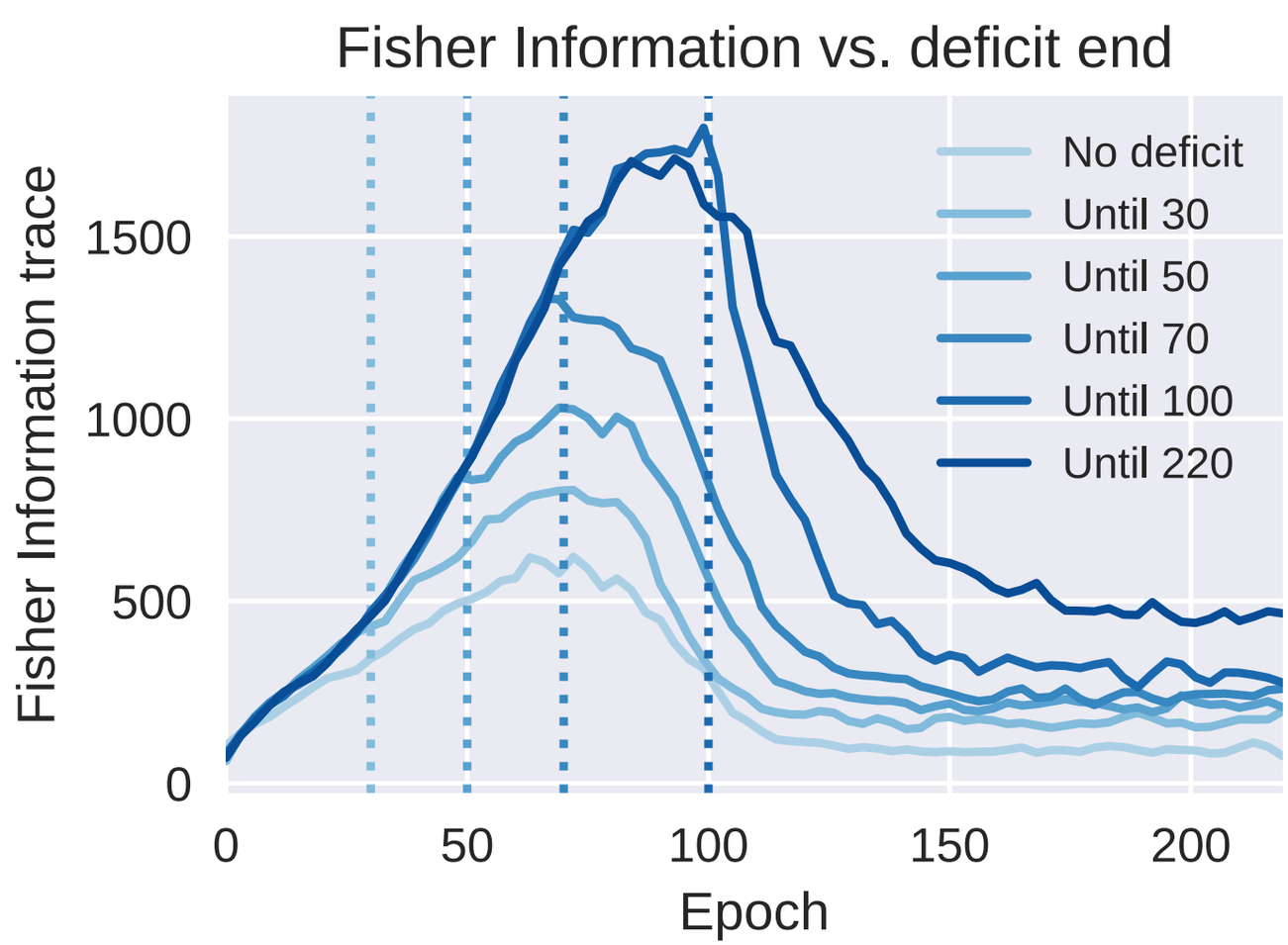
Answering Research Question 5: Part II

Critical Learning Periods:

Deficit → higher Fisher Information → memorisation

Phase transition → Fitting phase/high curvature





Conclusion

IBT strengths, weaknesses and research opportunities

Strengths

Narrative: connects seemly unrelated phenomena and practices;

Analysis: information in the weights "opens the black-box";

Task-dependent loss: not arbitrary ;

Weaknesses

Lack of rigour: overlooking important assumptions;

Discredit: critiques were hardly unjustified;

fragmentation: Literature is still very fragmented;

Conclusion

IBT strengths, weaknesses and research opportunities

Research Opportunities

PAC reformulation: β unifies (ϵ, δ);

New optimisation strategies: different approaches for the fitting and compression phases;

Transfer learning: Validate topologies of learning tasks built from IBT(e.g. Task2Vec [Ach+19]), with empirical ones (e.g. Taskonomy[Zam+18]);

IBT

far from being rigorous and complete

is an emerging theory with a compelling narrative and many open opportunities.

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