Estimating Information Flow in Deep Neural Networks

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MIT, IBM Research, MIT-IBM Watson AI Lab

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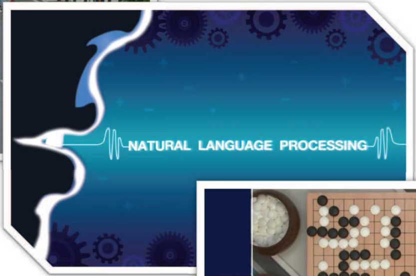
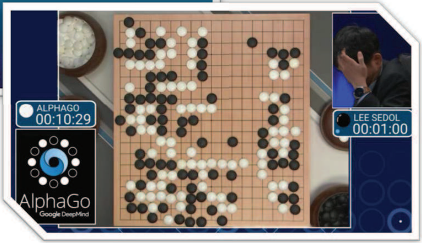
Deep Learning - What's Under the Hood?





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  - Structure of loss landscape
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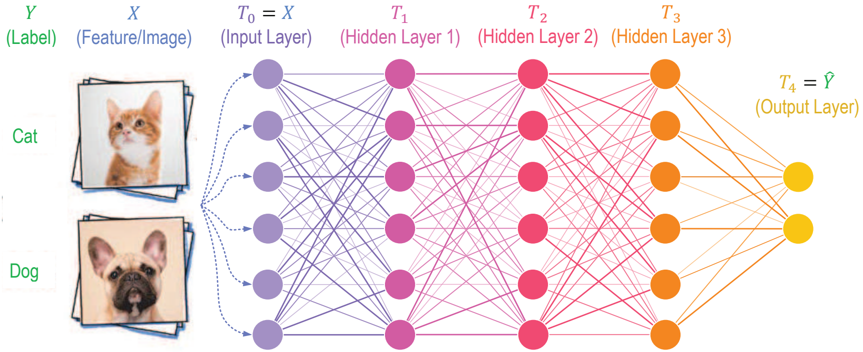
★ **Goal:** Mathematically analyze IB theory & test 'Compression'

(Deterministic) Feedforward DNN: Each layer $T_\ell = f_\ell(T_{\ell-1})$



Setup and Preliminaries

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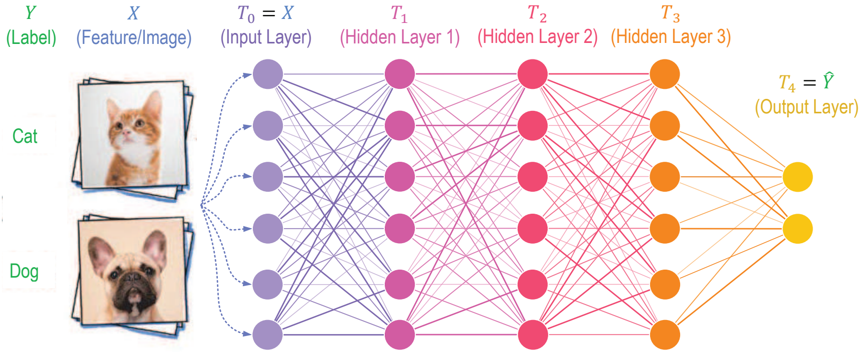

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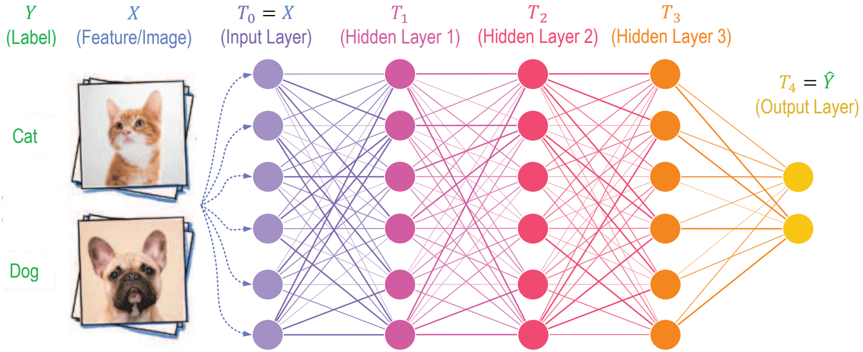

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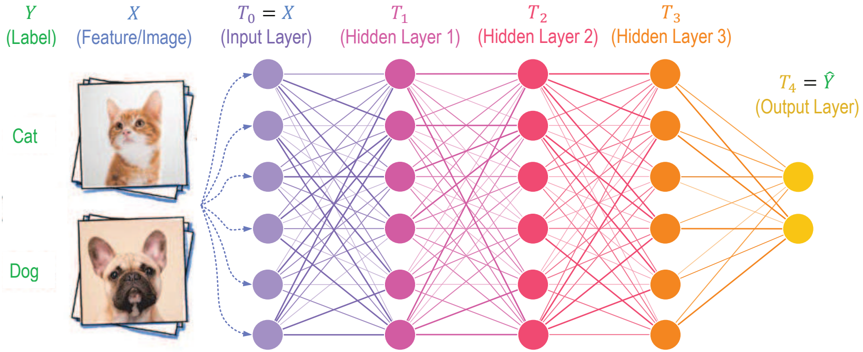

- **Joint Distribution:** $P_{X,Y} \quad \Longrightarrow \quad P_{X,Y} \cdot P_{T_1,\ldots,T_L|X}$
- **Information Plane:** Evolution of $\big(I(X;T_\ell), I(Y;T_\ell)\big)$ during training

$$\left[I(A;B) = \mathsf{D}_{\mathsf{KL}}(P_{A,B} \| P_A \otimes P_B) \overset{\text{Discrete}}{=} \sum_{a,b} P_{A,B}(a,b) \log \frac{P_{A,B}(a,b)}{P_A(a) P_B(b)} \right]$$

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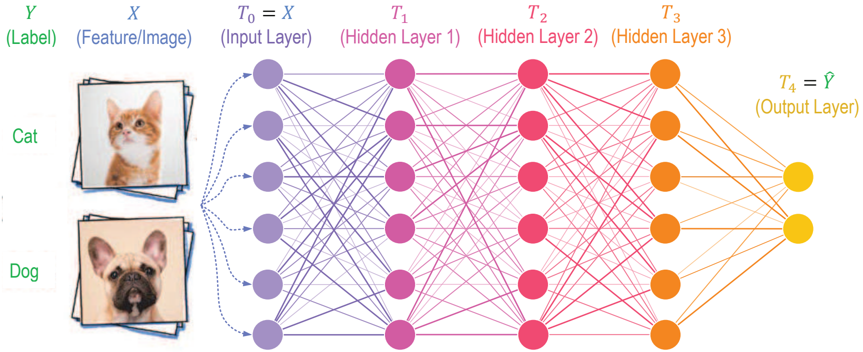

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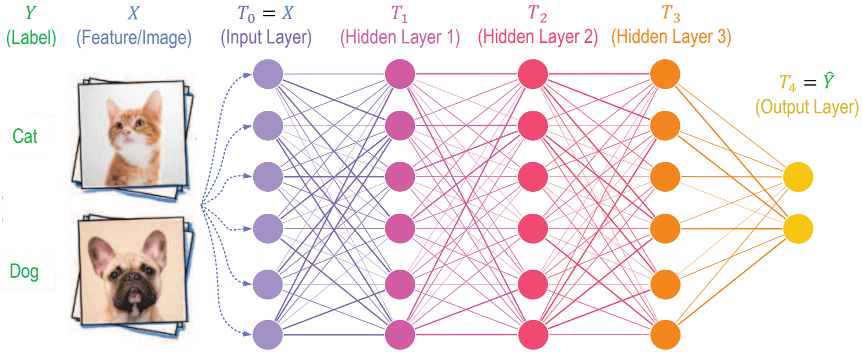

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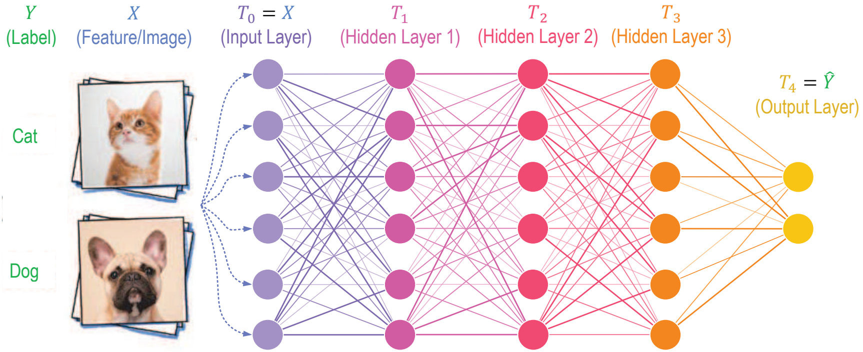

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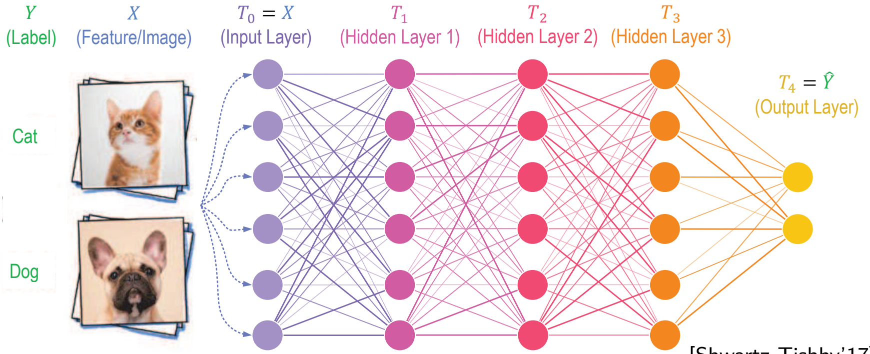

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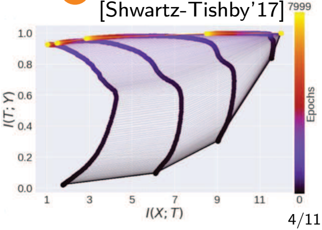
[Shwartz-Tishby'17]



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Proposition (Informal)

Det. DNNs with strictly monotone nonlinearities (e.g., tanh or sigmoid)

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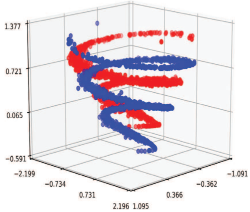

$X \sim \text{Unif}(\mathcal{X})$

$|\mathcal{X}| = 3000$

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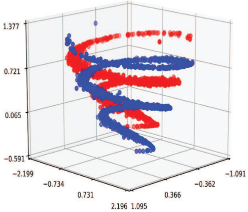
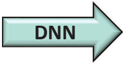
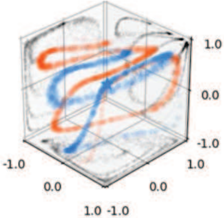




Internal Rep. Space ($T_\ell = \tilde{f}_\ell(X)$)



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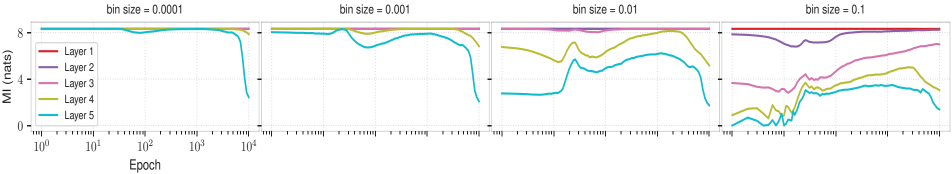

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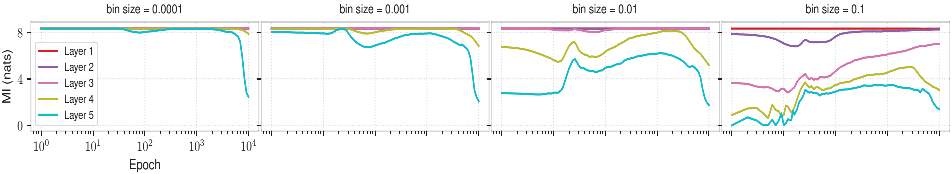

⊛ **Real Problem:** Mismatch between $I(X;T_\ell)$ measurement and model

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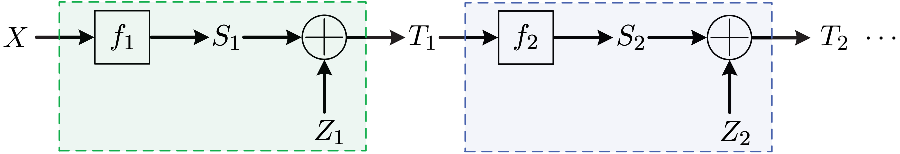

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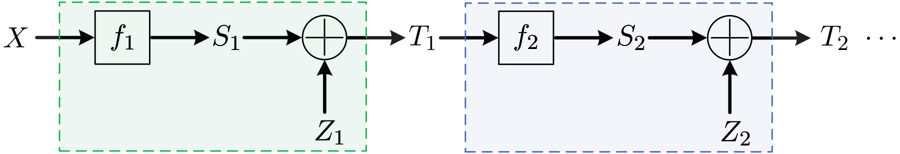

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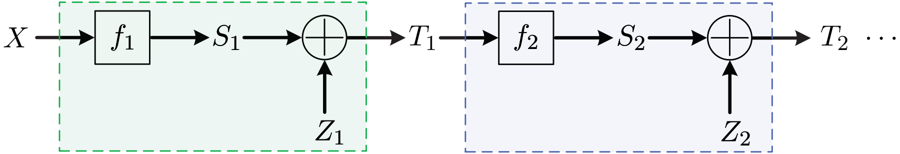

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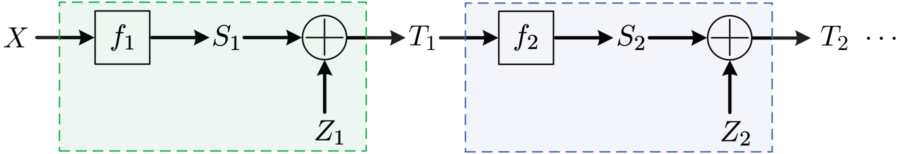

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⊛ **Challenge:** How to accurately track $I(X;T_\ell)$?

High-Dim. & Nonparametric Functional Estimation

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Distill $I(X;T_\ell)$ Estimation into Noisy Differential Entropy Estimation:

Estimate $h(P * \mathcal{N}_\sigma)$ from n i.i.d. samples $S^n \triangleq (S_i)_{i=1}^n$ of $P \in \mathcal{F}_d$ (non-parametric class) and knowledge of $\mathcal{N}_\sigma$ (Gaussian measure $\mathcal{N}(0, \sigma^2 \mathrm{I}_d)$).

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$\star$ Efficient and parallelizable

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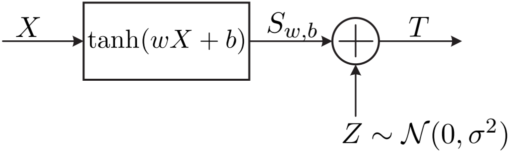
Optimality: $\hat{h}(S^n, \sigma)$ attains sharp dependence on both n and d!

$I(X;T_\ell)$ Dynamics - Illustrative Minimal Example

Single Neuron Classification:



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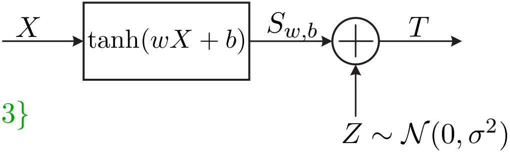

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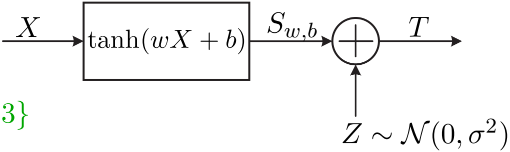

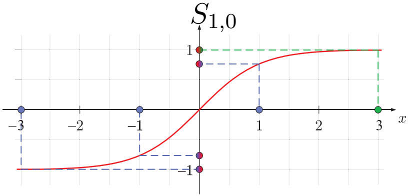

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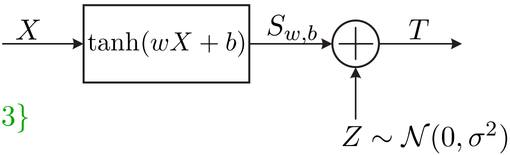

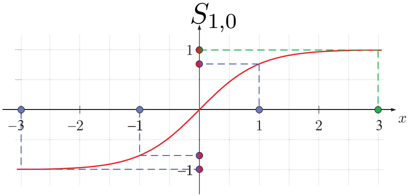

⊛ Center & sharpen transition ($\iff$ increase w and keep $b=-2w$)

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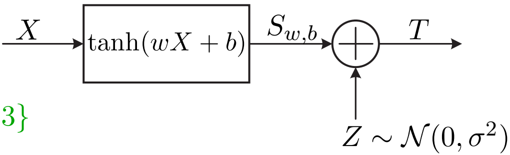

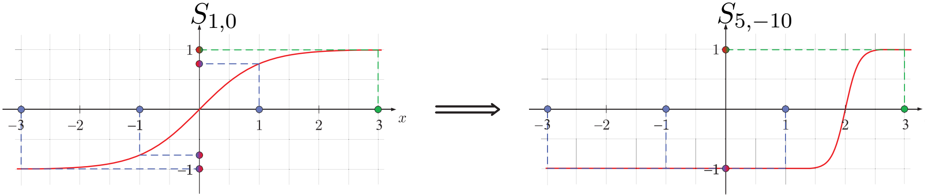

$I(X;T_\ell)$ Dynamics - Illustrative Minimal Example

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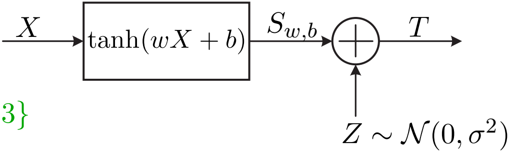
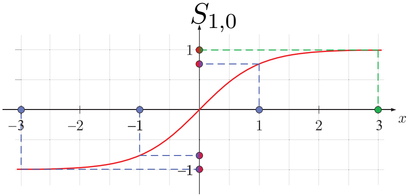
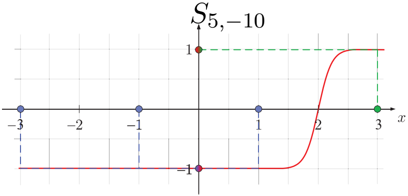




$\Longrightarrow$



✓ Correct classification performance

$I(X;T_\ell)$ Dynamics - Illustrative Minimal Example

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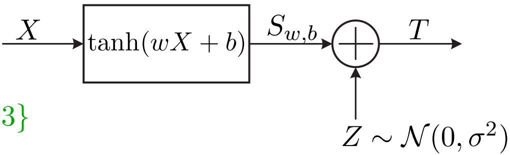

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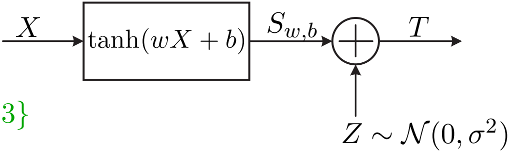

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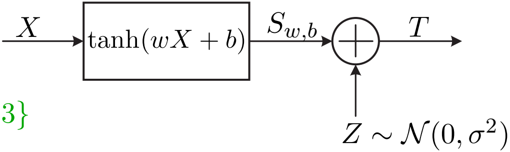

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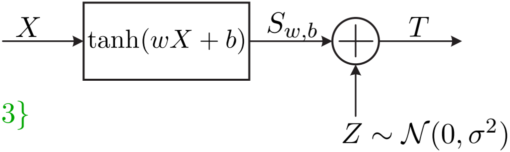

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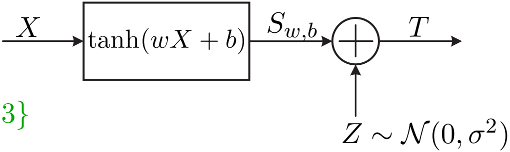

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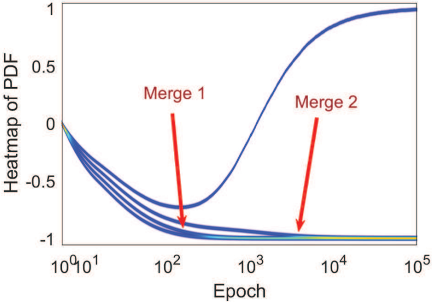

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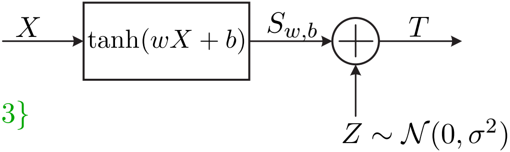

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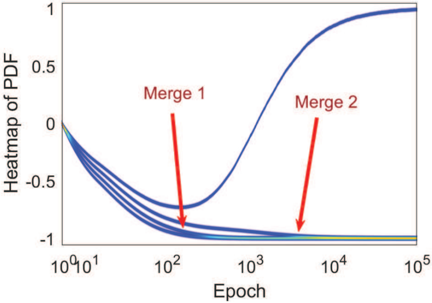

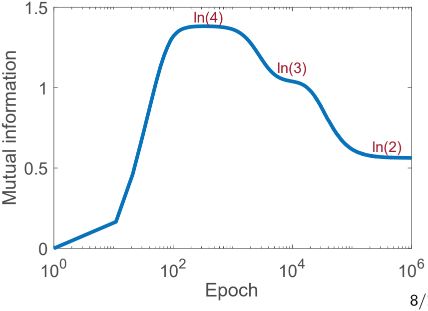

Clustering of Representations - Larger Networks

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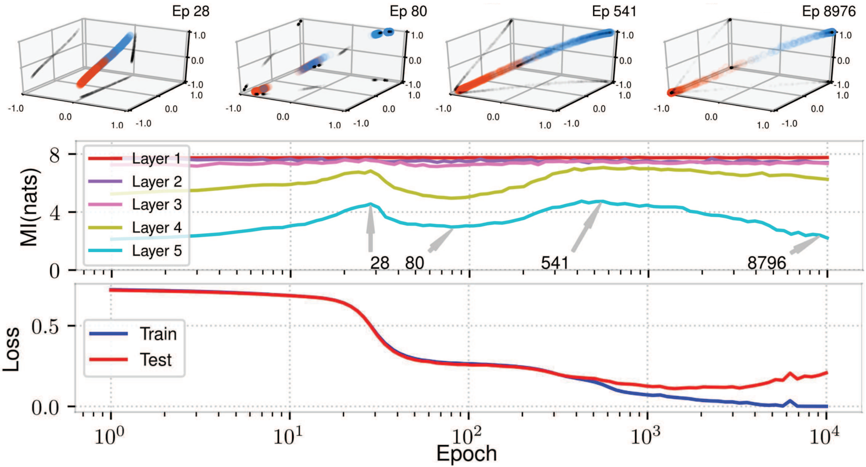

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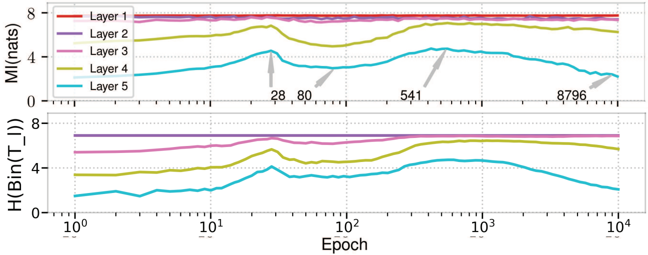

$\star$ When bin size chosen $\propto$ noise std.

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By-Product Result:

- Refute 'compression (tight clustering) improves generalization' claim

[Come see us at poster #96 for details]

Summary

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Thank you!

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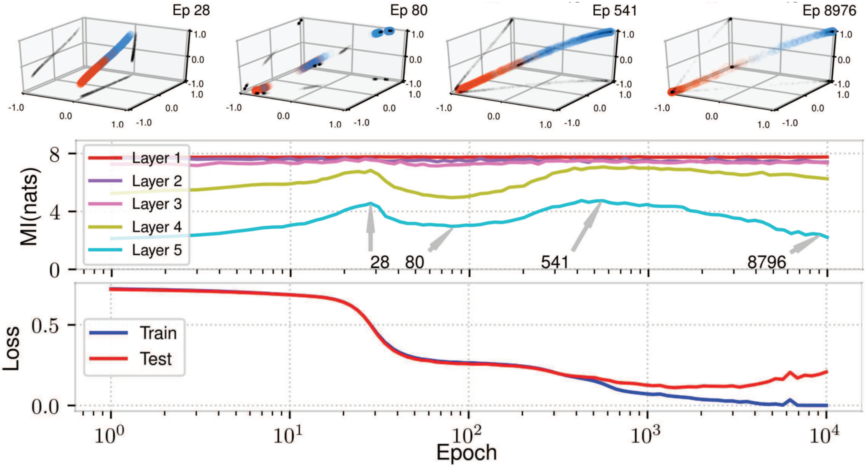

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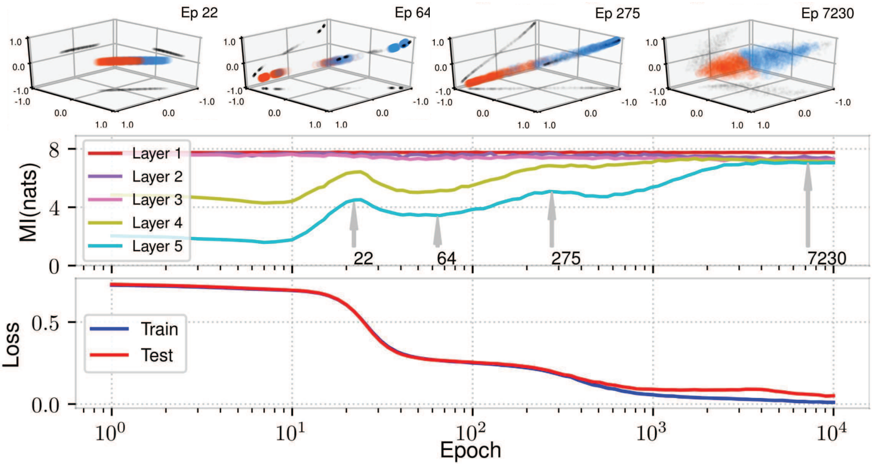

⊛ weight orthonormality regularization [Cisse *et al.*'17]

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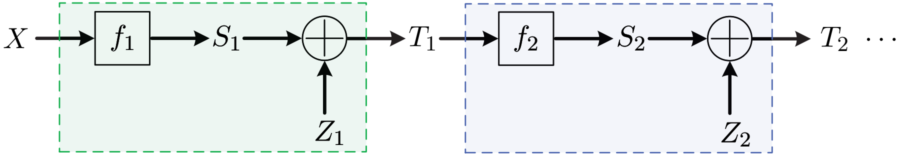

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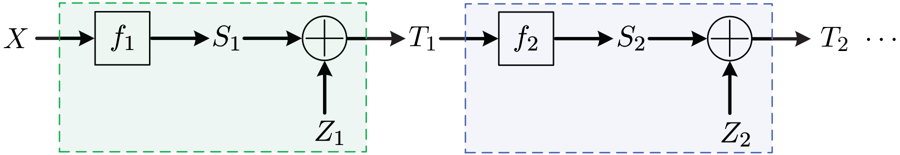

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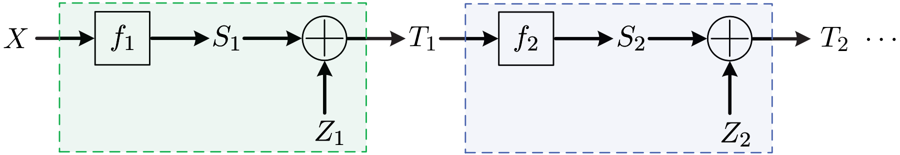

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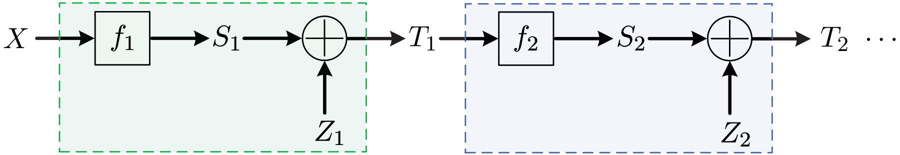

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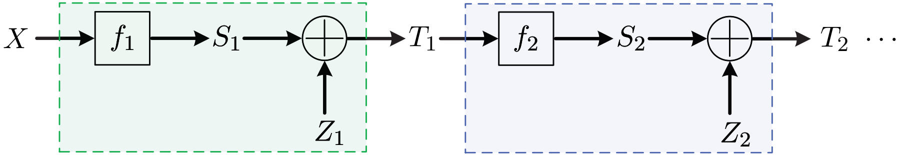

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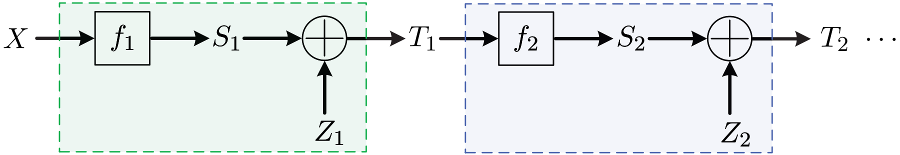

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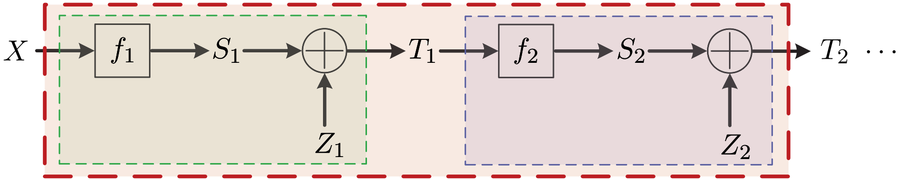

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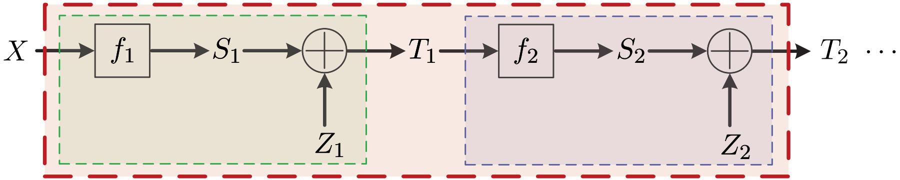

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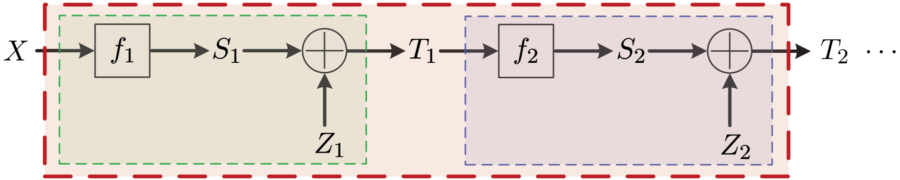

- **Mutual Information:** $I(X;T_\ell) = h(T_\ell) - \int \mathrm{d}P_X(x) h(T_\ell | X = x)$
- **Structure:** $S_\ell \perp Z_\ell \quad \Longrightarrow \quad T_\ell = S_\ell + Z_\ell \sim P * \mathcal{N}_\sigma$

⊛ **Know** the distribution $\mathcal{N}_\sigma$ of Z_ℓ (noise injected by design)

⊛ **Extremely complicated** $P \implies$ Treat as unknown

⊛ **Easily** get i.i.d. samples from P via DNN forward pass

Structured Estimator (with Implementation in Mind)

Differential Entropy Estimation under Gaussian Convolutions

Estimate $h(P * \mathcal{N}_\sigma)$ *via* n *i.i.d. samples* $S^n \triangleq (S_i)_{i=1}^n$ *from unknown* $P \in \mathcal{F}_d$ *(nonparametric class) and knowledge of* $\mathcal{N}_\sigma$ *(noise distribution).*

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- **Plug-in:** $\hat{h}$ is plug-in est. for the functional $\mathsf{T}_\sigma(P) \triangleq h(P * \mathcal{N}_\sigma)$

Structured Estimator - Convergence Rate

Theorem (ZG-Greenewald-Weed-Polyanskiy'19)

For any $\sigma > 0,\ d \geq 1$*, we have*

$$\sup_{P \in \mathcal{F}_{d,K}^{(\mathsf{SG})}} \mathbb{E}\left| h(P * \mathcal{N}_\sigma) - h(\hat{P}_{S^n} * \mathcal{N}_\sigma) \right| \leq C_{\sigma,d,K} \cdot n^{-\frac{1}{2}}$$

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$\Longrightarrow$ Analyze empirical 1-Wasserstein distance under Gaussian convolutions

Empirical W_1 & The Magic of Gaussian Convolution

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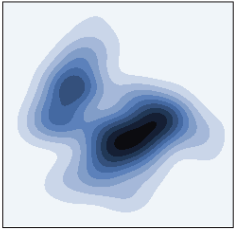

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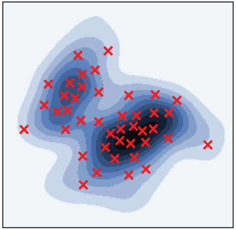

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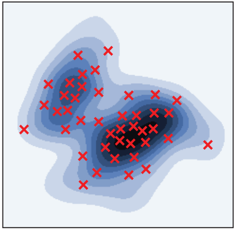

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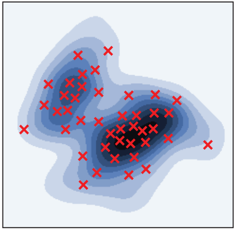

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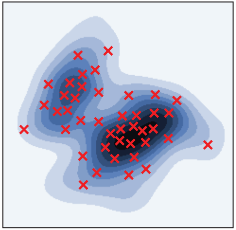

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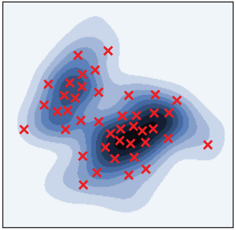

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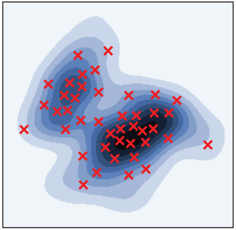

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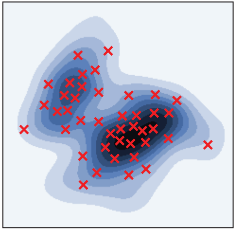

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Curse of Dimensionality

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Is Exponentiality in Dimension Necessary?

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- $H(Q)$ estimation sample complexity $\Omega\left(\frac{|\mathcal{C}_d|}{\eta \log |\mathcal{C}_d|}\right)$ [Valiant-Valiant'10]