Estimating the Information Flow in Deep Neural Networks

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MIT

IT Forum, Information Systems Laboratory, Stanford University

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MIT-IBM Watson AI Lab

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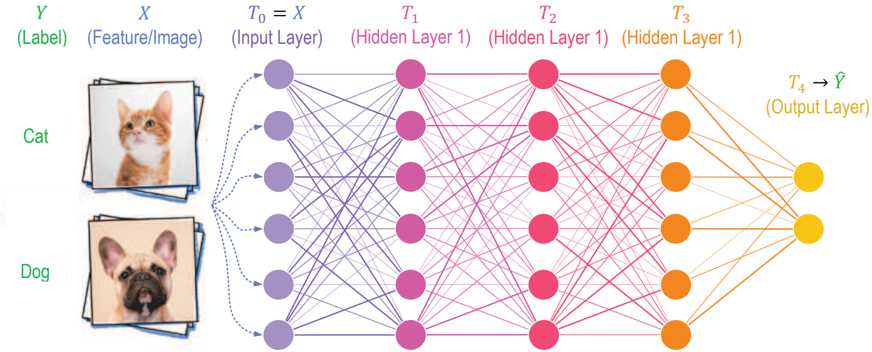
★ **Goal:** Explain 'compression' in Information Bottleneck framework

Setup and Preliminaries

Feedforward DNN for Classification:



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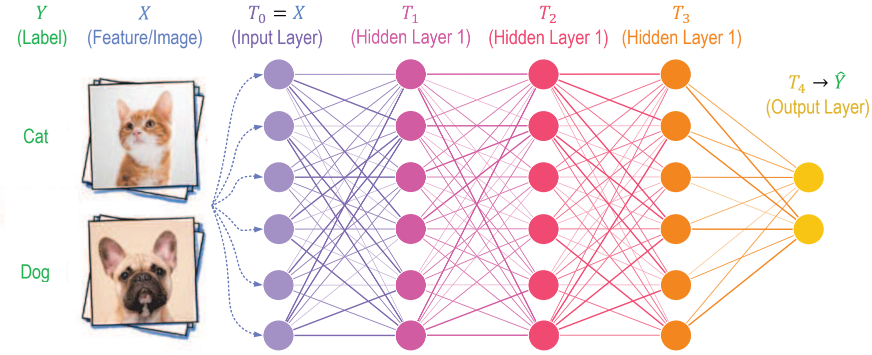

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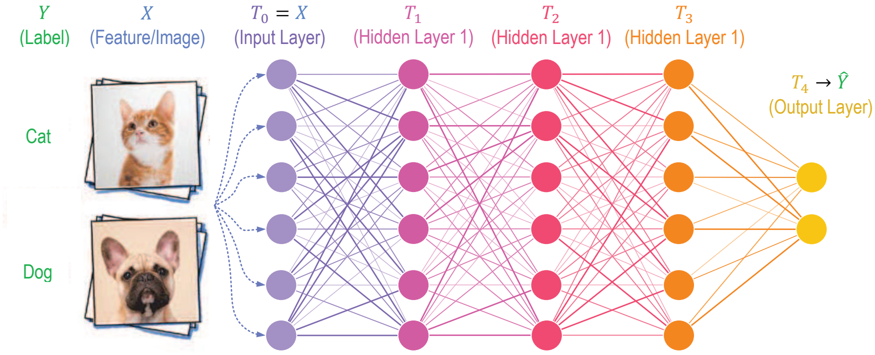

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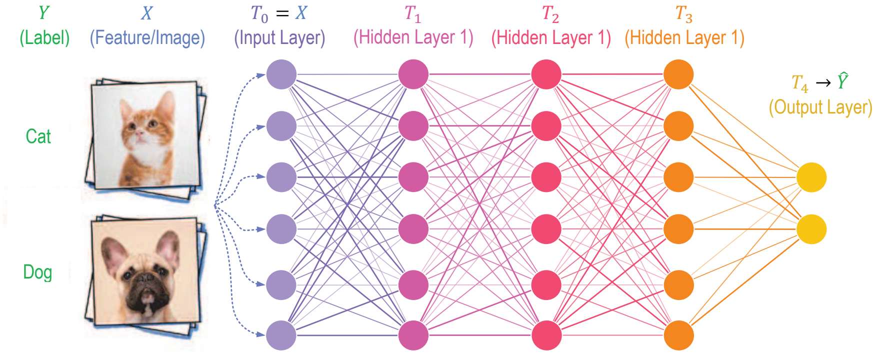

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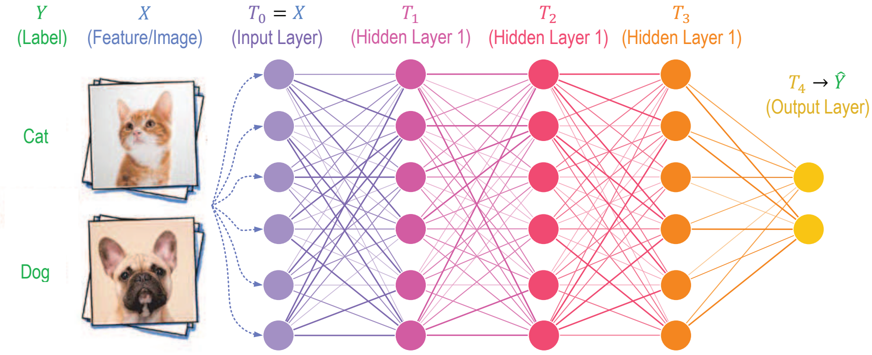

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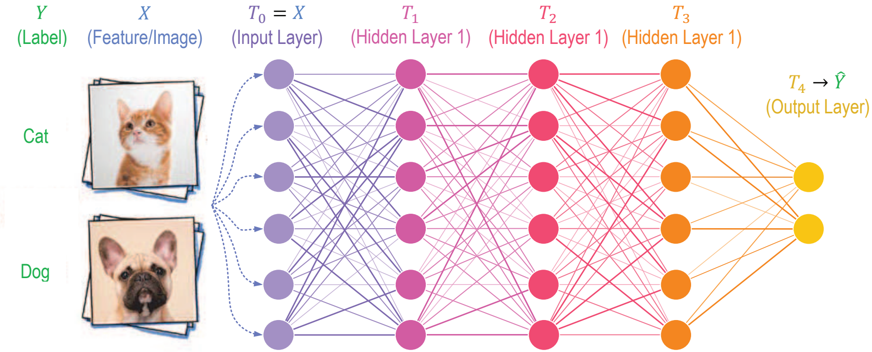

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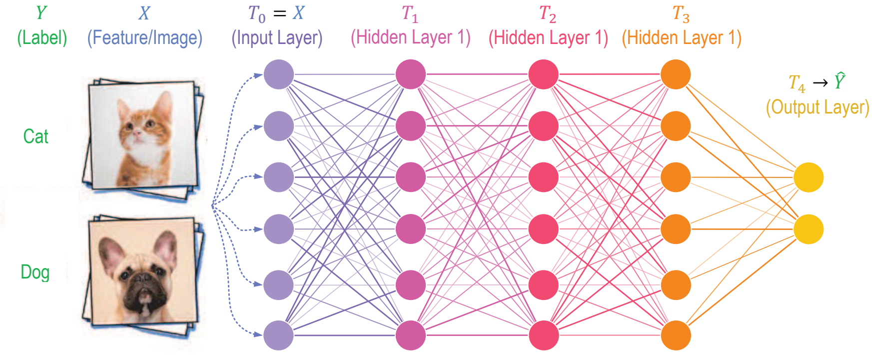

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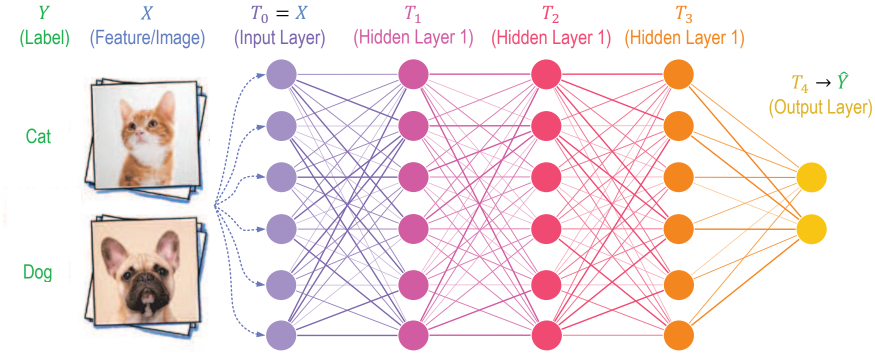

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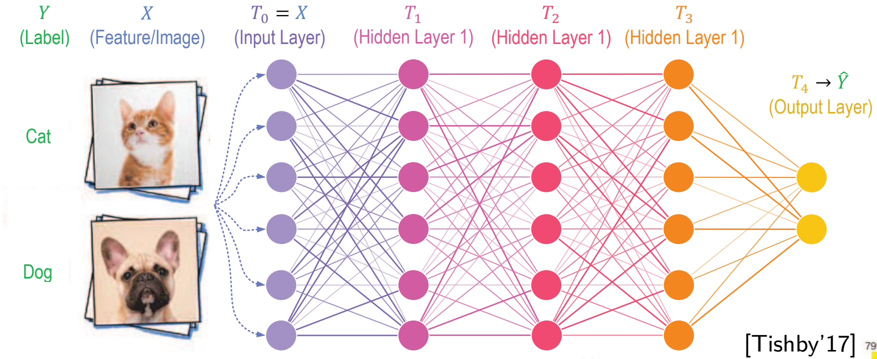

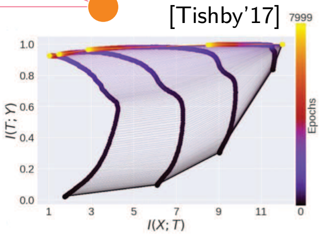

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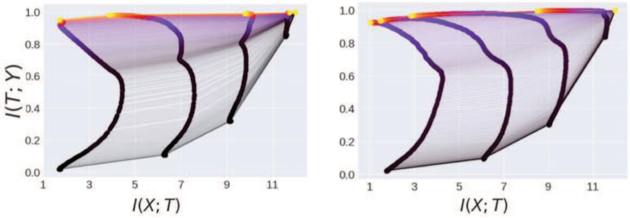
Past Works:

[Schwartz-Ziv&Tishby'17, Saxe *et al. '18]*



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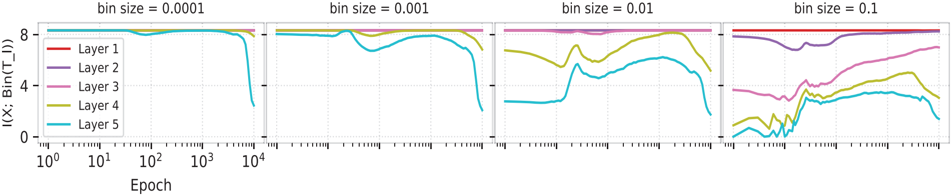

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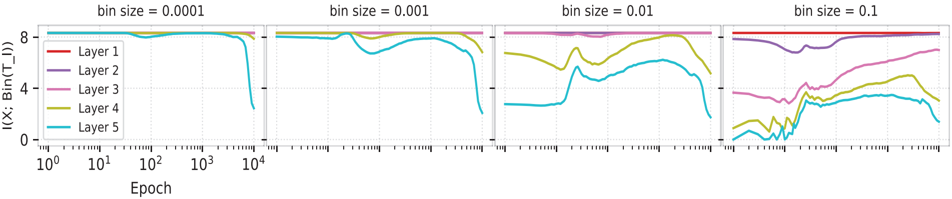

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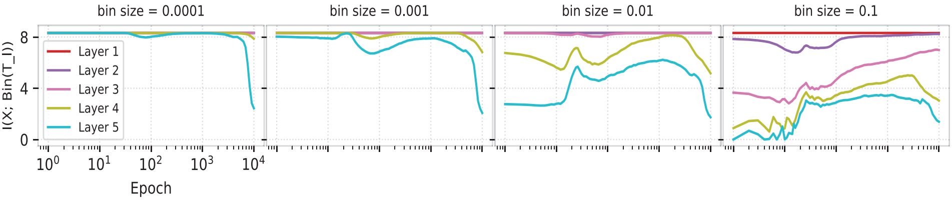

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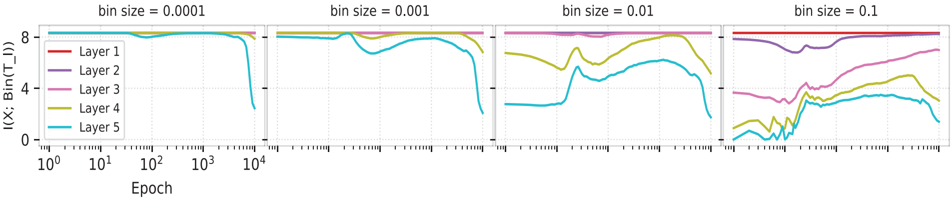

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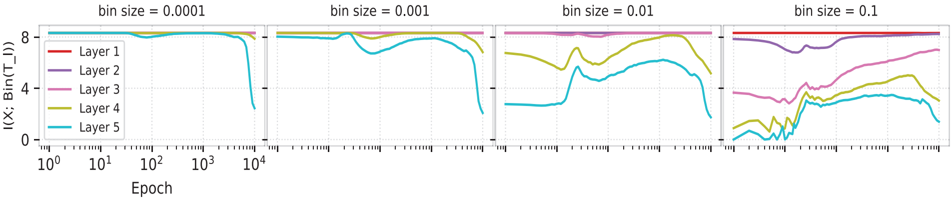

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⊛ **Real Problem:** $I(X;T_\ell)$ is meaningless in det. DNNs

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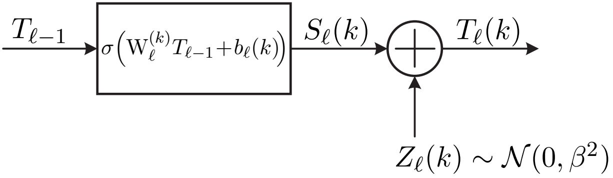

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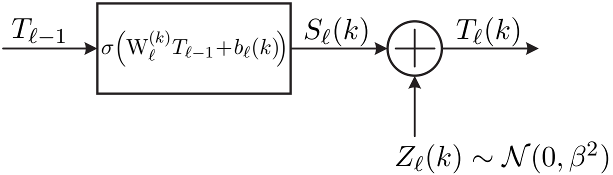

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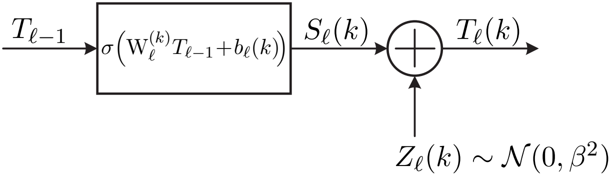

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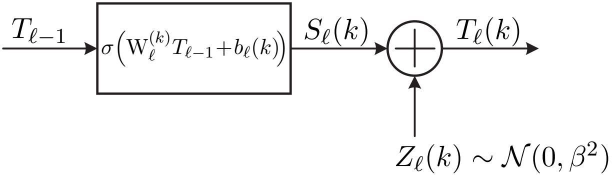

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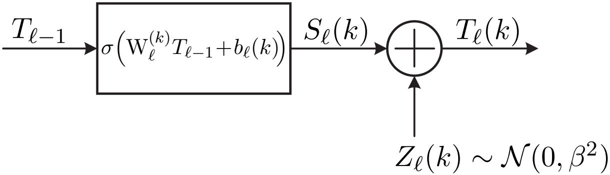

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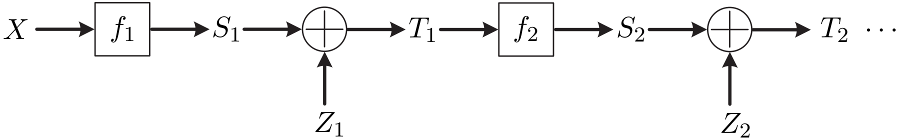

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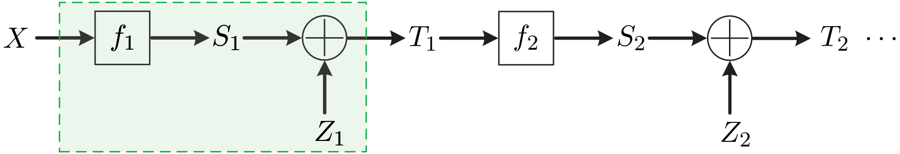

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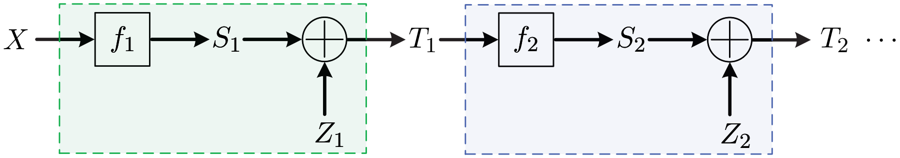

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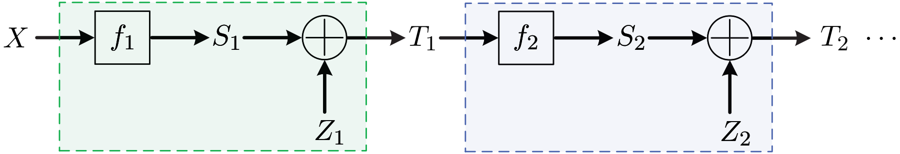

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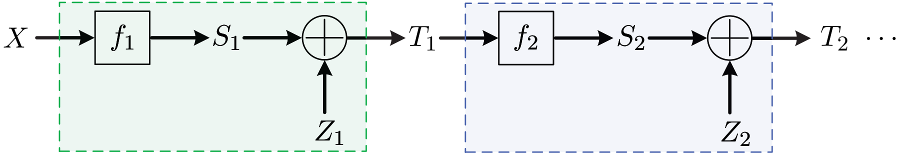

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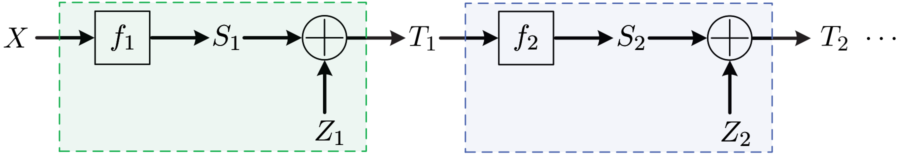

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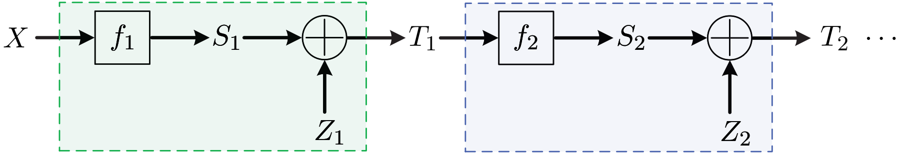

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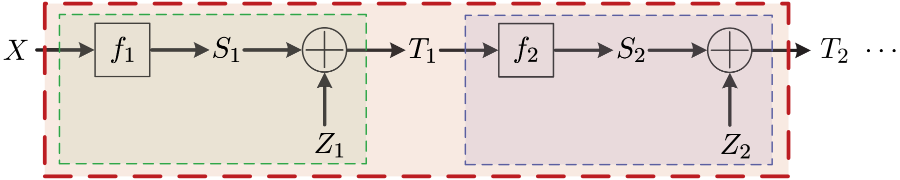

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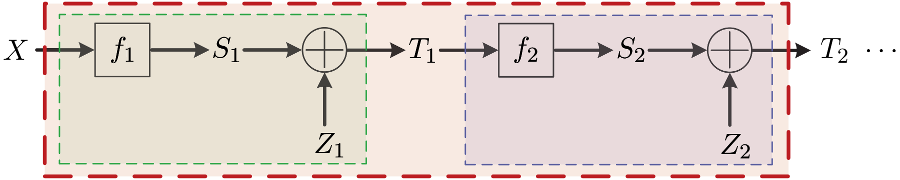

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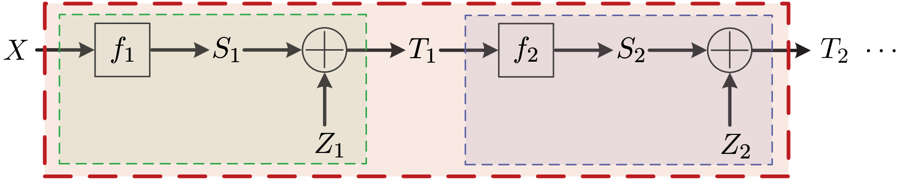

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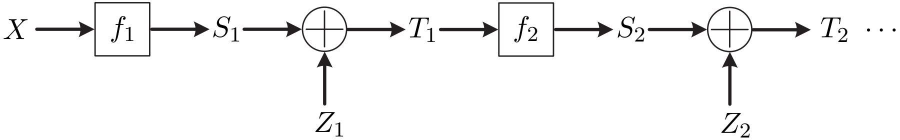

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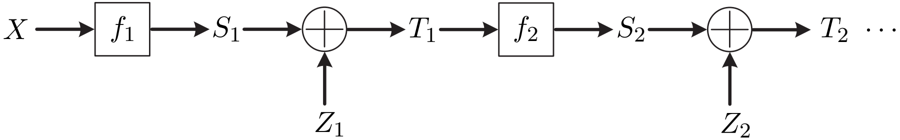

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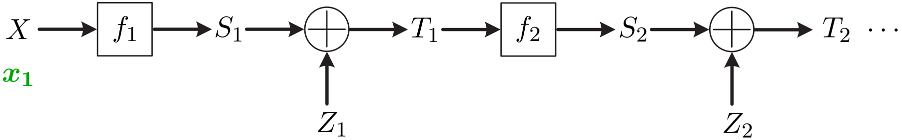

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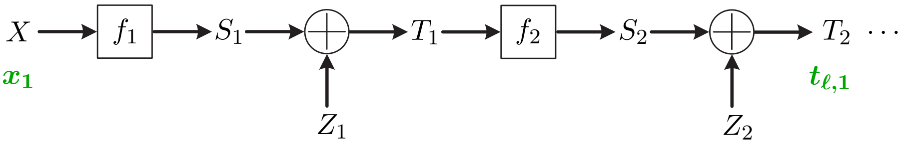

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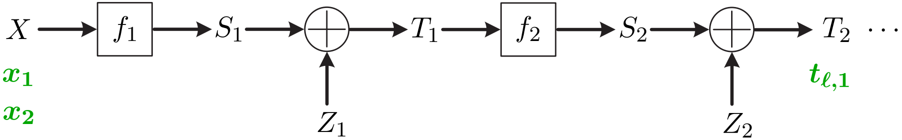

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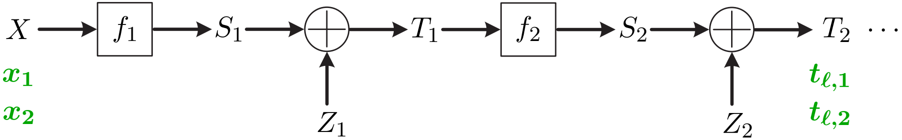

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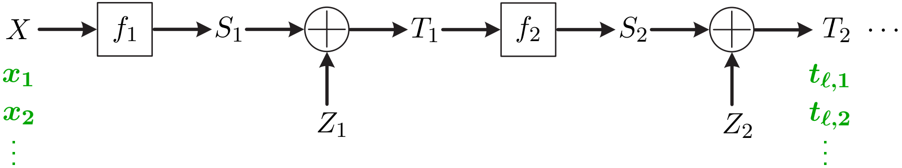

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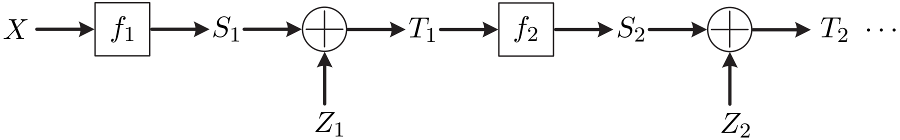

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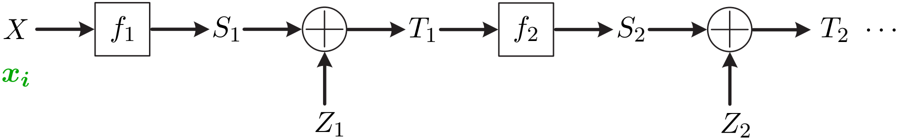

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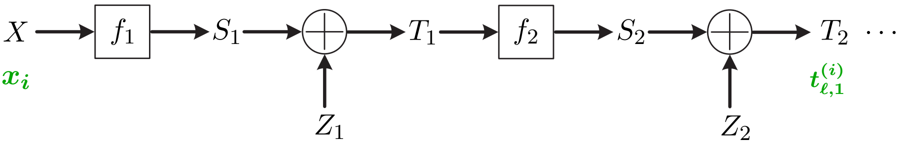

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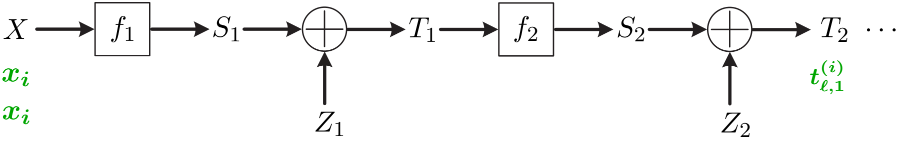

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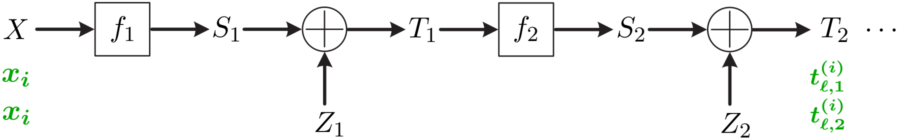

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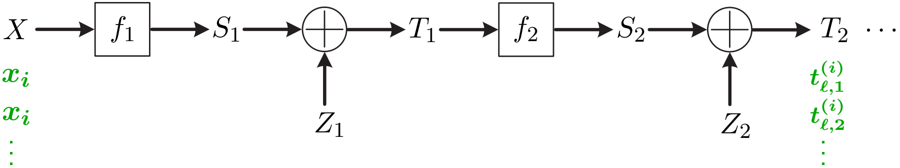

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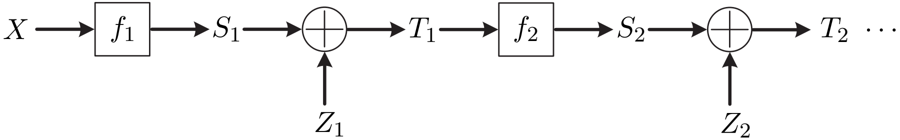

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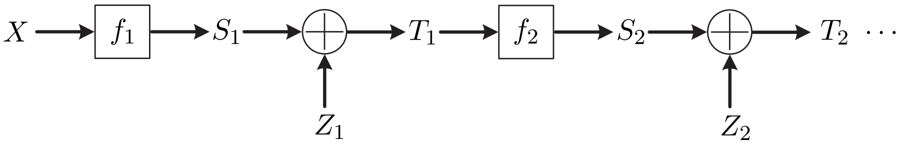

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- Most results assume lower bounded density

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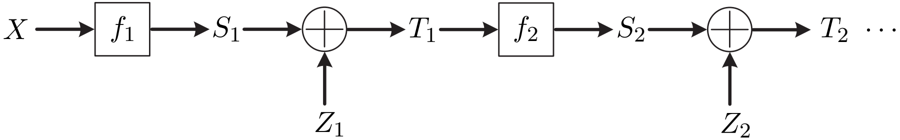

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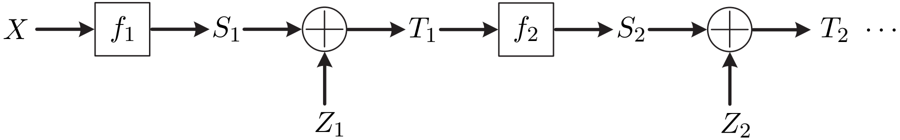

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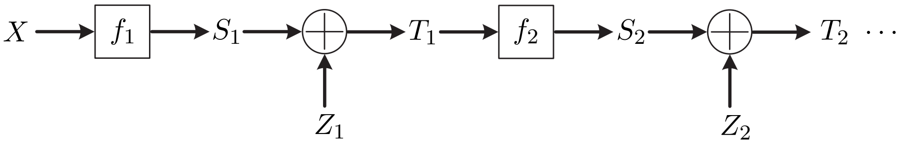

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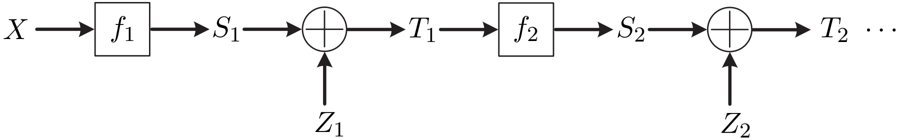

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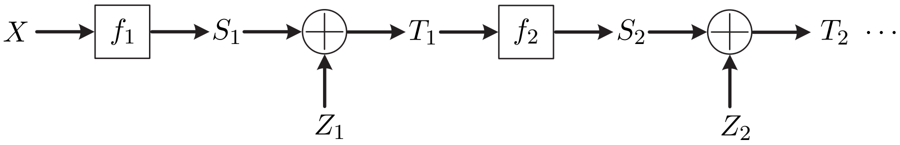

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- **Assume:** supp $= [0,1]^d$ & Periodic BC & $s \in (0,2]$

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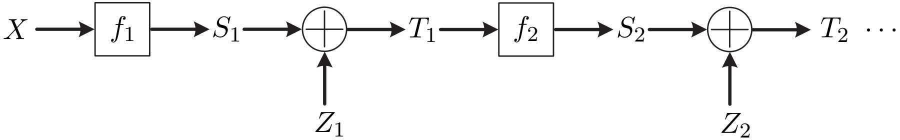

$\implies$ Estimate $I(X;T_\ell)$ from samples via **general-purpose $h(P)$ est.:**

- Most results assume lower bounded density $\implies$ **Inapplicable**
- **2 Works Drop Assumption:**
  1. KDE + Best poly. approximation [Han-Jiao-Weissman-Wu'17]
  2. Kozachenko-Leonenko (kNN) estimator [Jiao-Gao-Han'17]
- **Assume:** supp $= [0,1]^d$ & Periodic BC & $s \in (0,2] \implies$ **Inapplicable***

⋆ Except sub-Gaussian result from [Han-Jiao-Weissman-Wu'17]

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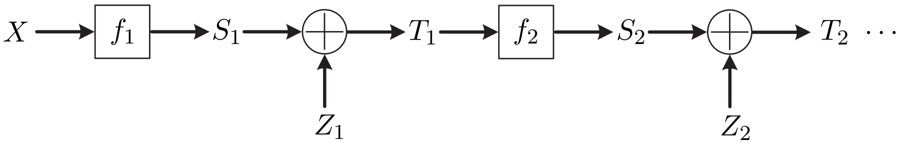

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Exploit Structure - Ad Hoc Estimation

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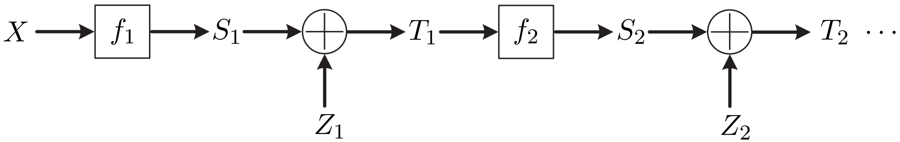

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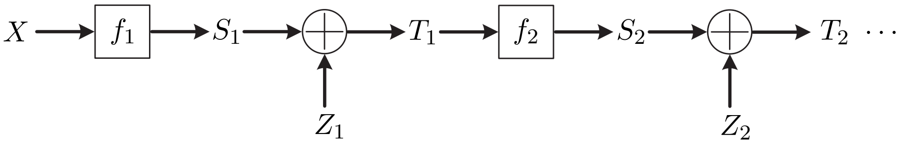

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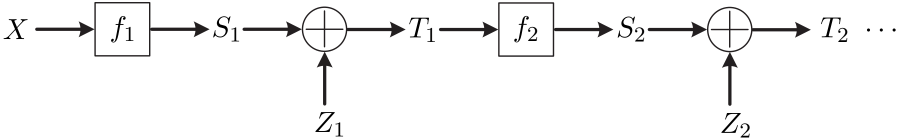

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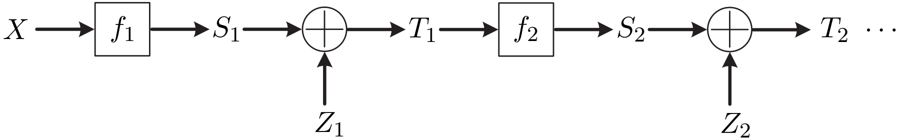

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Differential Entropy Estimation under Gaussian Convolutions

Estimate $h(P * \varphi)$ based on n i.i.d. samples from $P \in \mathcal{F}_d$ (nonparametric class) and knowledge of φ (PDF of $\mathcal{N}(0, \beta^2 \mathrm{I}_d)$).

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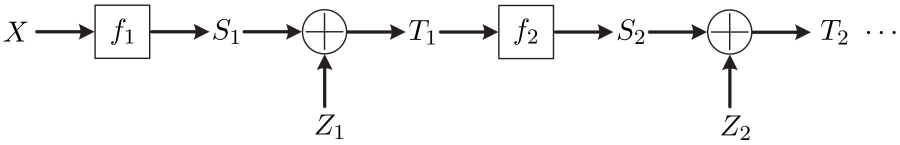

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Nonparametric Class: Depends on DNN architecture (nonlinearities)

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Abs. Error Minimax Risk: S^n are n i.i.d. samples from P, define

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The Sample Propagation Estimator - Convergence

Theorem (ZG-Greenewald-Polyanskiy '18)

For $\mathcal{F}_d \triangleq \left\{P \middle| \mathsf{supp}(P) \subseteq [-1,1]^d\right\}$ *and any* $\beta > 0$ *and* $d \geq 1$*, we have*

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$$+\left(c_{\beta,d}^2 + \frac{2c_{\beta,d}d(1+\beta^2)}{\beta^2} + \frac{8d(d+2\beta^4+d\beta^4)}{\beta^4}\right)\frac{2}{n}$$

where $c_{\beta,d} \triangleq \frac{d}{2}\log(2\pi\beta^2) + \frac{d}{\beta^2}$.

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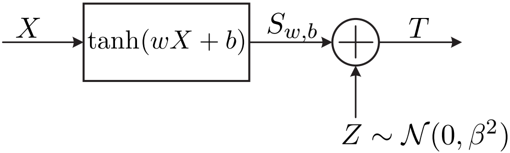
- **Extension:** P with sub-Gaussian marginals (ReLU + Weight regular.)

Back to Noisy DNNs

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

Single Neuron Classification:



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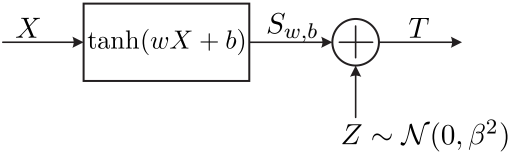

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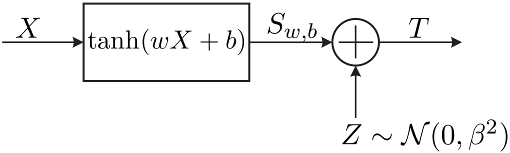

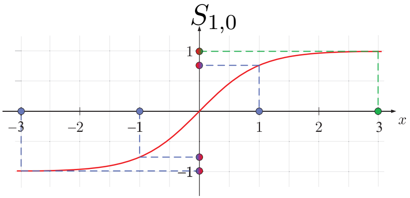

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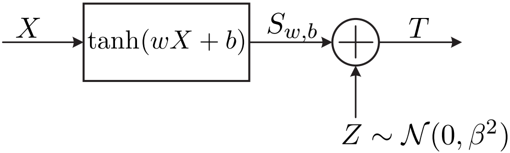

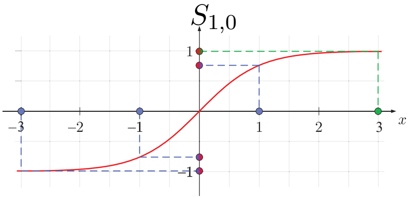

⊛ Center & sharpen transition ($\Longleftrightarrow$ increase w and keep $b = -2w$)

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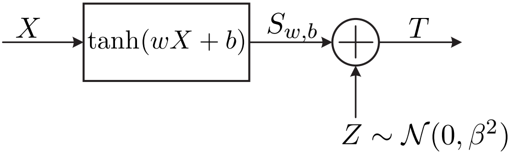

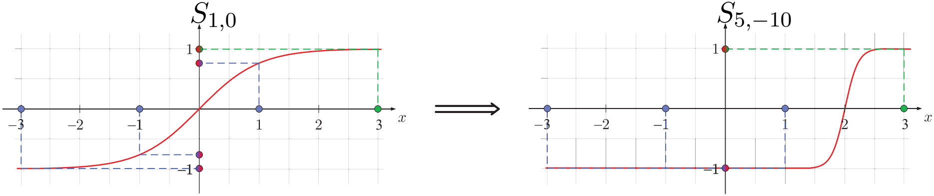

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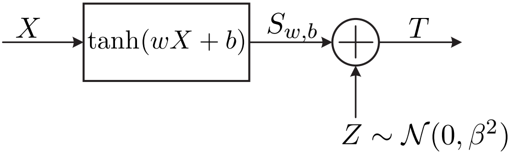

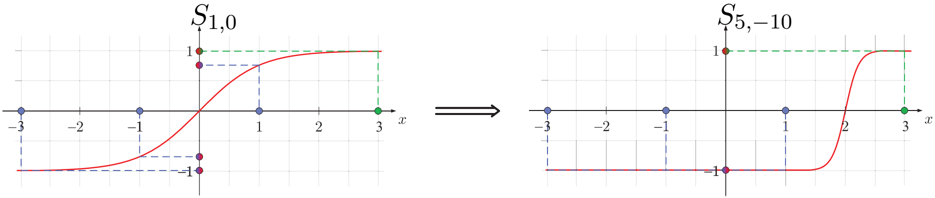

✓ Correct classification performance

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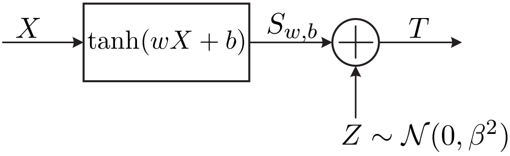

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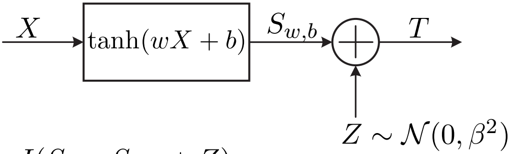

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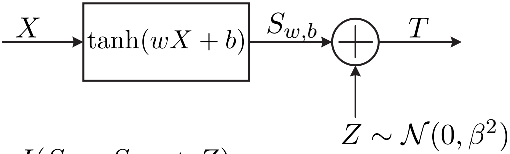

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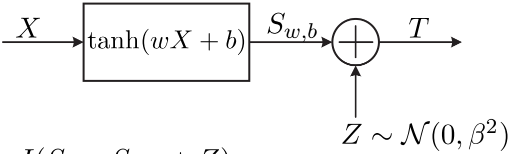

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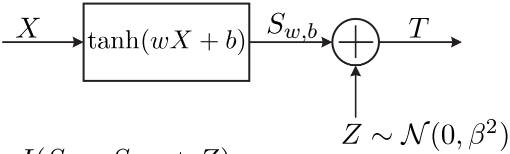

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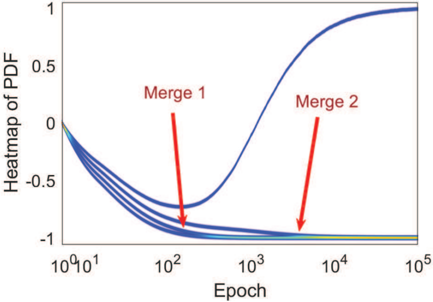

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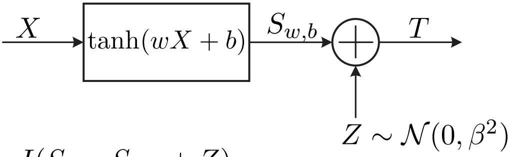

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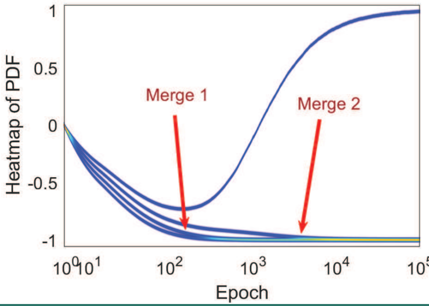

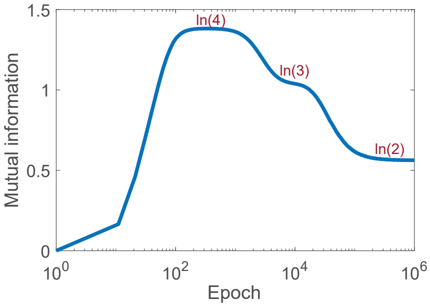

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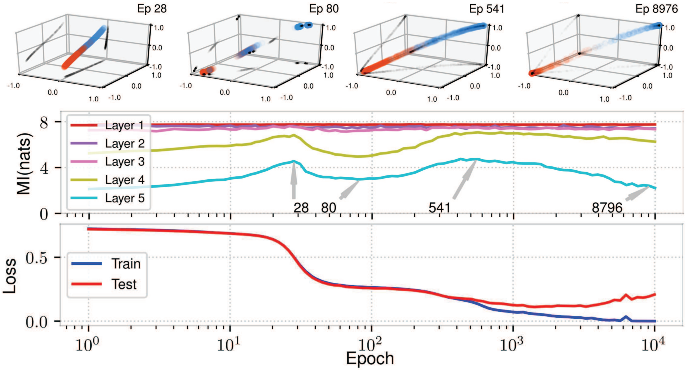

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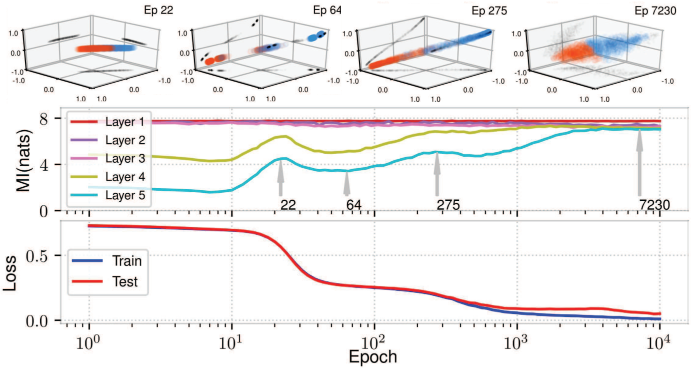

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$\Longrightarrow$ Compression of $I(X;T_\ell)$ driven by clustering of representations

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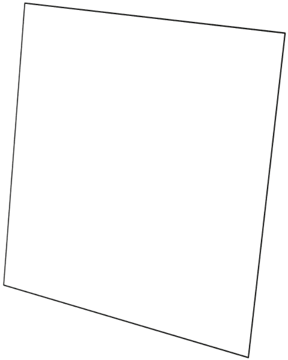

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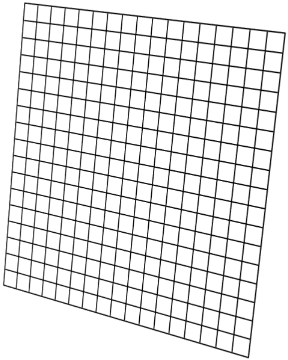

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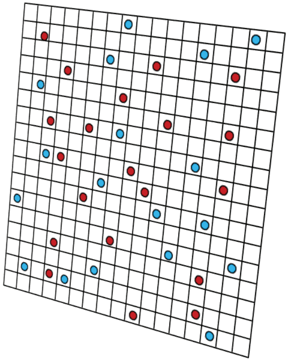

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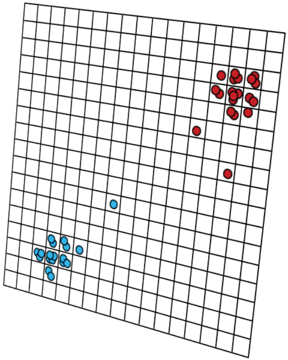

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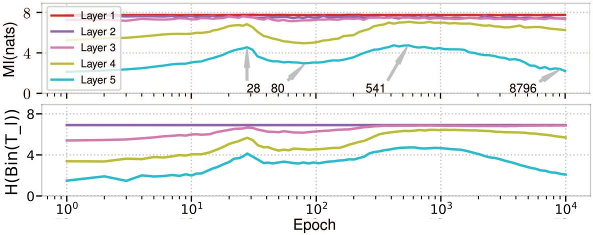

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$\implies$ Past works were not showing MI but clustering (via binned-MI)!

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$\Longrightarrow$ **Clustering** is the common phenomenon of interest!

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$$\sup \mathbb{E}\left|h(P*\varphi) - h(\hat{P}_n*\varphi)\right| \leq \sup \mathbb{E}\left|h_{\mathcal{R}}(P*\varphi) - h_{\mathcal{R}}(\hat{P}_n*\varphi)\right| + 2\sup\left|h_{\mathcal{R}^c}(P*\varphi)\right|$$

- **Inside R:**
  - $-t\log t$ modulus of cont. for $x \mapsto x\log x$ & Jensen's ineq.

    $\Longrightarrow$ Focus on analyzing $\mathbb{E}\left|(P*\varphi)(x) - (\hat{P}_n*\varphi)(x)\right|$
  - Bias & variance analysis

    $$\Longrightarrow \mathbb{E}\left|(P*\varphi)(x) - (\hat{P}_n*\varphi)(x)\right| \leq c_1\sqrt{\frac{(P*\tilde{\varphi})(x)}{n}}, \quad \tilde{\varphi} = \mathcal{N}\left(0, \frac{\beta^2}{2}\mathrm{I}\right)$$
  - Plug back in & Convex analysis

    $$\Longrightarrow \sup \mathbb{E}\left|h_{\mathcal{R}}(P*\varphi) - h_{\mathcal{R}}(\hat{P}_n*\varphi)\right| \leq c_2 \log\left(\frac{n\lambda(\mathcal{R})}{c_3}\right)\sqrt{\frac{\lambda(\mathcal{R})}{n}}$$

The Sample Propagation Estimator - Proof Ideas

Strategy: Split analysis to $\mathcal{R} \triangleq [-1,1]^d + \mathcal{B}(0, \sqrt{c \log n})$ and $\mathcal{R}^c$

- **Restricted Entropy:** $h_{\mathcal{R}}(p) \triangleq \mathbb{E}\left[-\log p(X) \mathbb{1}_{\{X \in \mathcal{R}\}}\right]$

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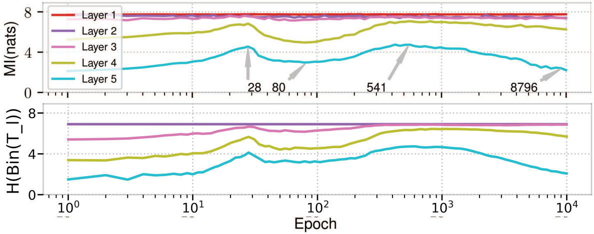
- **Outside R:** $O\left(\frac{1}{n}\right)$ decay via Chi-squared distribution tail bounds

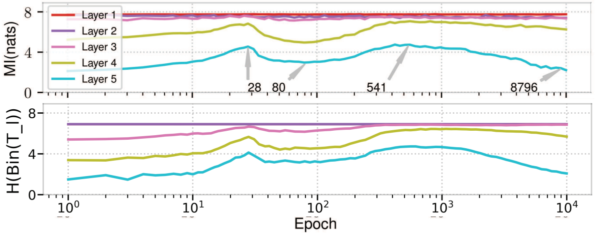
Binning vs True Mutual Information

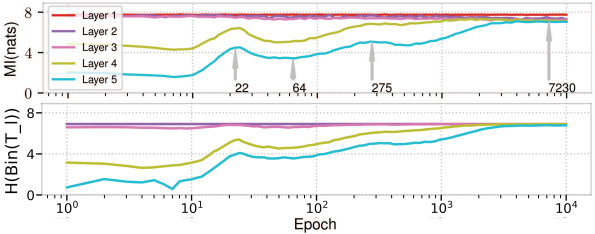
Comparing to Previously Shown MI Plots:



Binning vs True Mutual Information

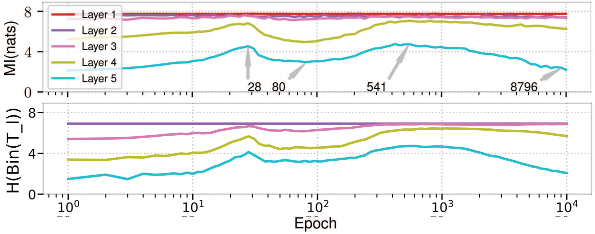
Comparing to Previously Shown MI Plots:

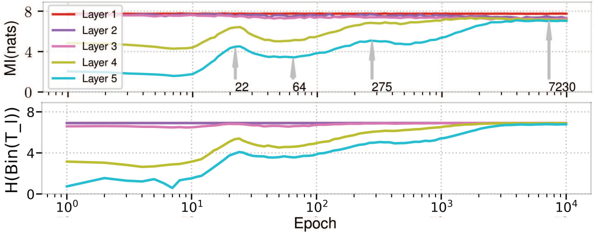




Binning vs True Mutual Information

Comparing to Previously Shown MI Plots:





$\Longrightarrow$ Past works were not showing MI but clustering (via binned-MI)!

References

[1] Z. Goldfeld, E. van den Berg, K. Greenewald, I. Melnyk, N. Nguyen, B. Kingsbury and Y. Polyanskiy, “Estimating information flow in DNNs,” Submitted to the *International Conference on Learning Representations (ICLR-2019)*, New Orleans, Louisiana, US, May 2019.
Arxiv (extended): `https://arxiv.org/abs/1810.05728`

[2] Z. Goldfeld, K. Greenewald and Y. Polyanskiy, “Estimating differential entropy under Gaussian convolutions,” Submitted to the *IEEE Transactions on Information Theory*, October 2018.
Arxiv: `https://arxiv.org/abs/1810.11589`