# Estimating the Information Flow in Deep Neural Networks 

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## Information in the Modern Age \& Complex Systems

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Complex System: Multi-component system driven by local interactions

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Processing
Communication

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Stabilization of written data
Model \& Study:
Interacting particle sys.

## Storage



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Emerging Networks (loT):

1) Decentralized \& ad hoc
2) Varying connectivity
3) Cooperative components

## Building Blocks:

Rich IT literature
Network Modeling:
Random graphs \& Actions based on primitives

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* Goal: Explain 'compression' in Information Bottleneck framework


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- IB Theory: Track MI pairs $\left(I\left(X ; T_{\ell}\right), I\left(Y ; T_{\ell}\right)\right)$ (information plane)


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| $Y$ | $X$ | $T_{0}=X$ | $T_{1}$ | $T_{2}$ | $T_{3}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| (Label) | (Feature/lmage) | (Input Layer) | (Hidden Layer 1) | (Hidden Layer 1) | (Hidden Layer 1) |



Dog


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$\star$ For almost all weight matrices and bias vectors


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## Past Works:

[Shwartz-Tishby'17, Saxe et al.'18]



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- Smaller bins $\Longrightarrow$ Closer to truth: $\quad I\left(X ; T_{\ell}\right)=\ln \left(2^{12}\right) \approx 8.31$


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* Real Problem: $I\left(X ; T_{\ell}\right)$ is meaningless in det. DNNs


## Auxiliary Framework - Noisy Deep Neural Networks

Modification: Inject (small) Gaussian noise to neurons' output
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Performance \& learned representations similar to det. DNNs $\left(\beta \approx 10^{-1}\right)$

Mutual Information in Noisy DNNs

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## Mutual Information Estimation in Noisy DNNs

Noisy DNN: $S_{\ell} \triangleq f_{\ell}\left(T_{\ell-1}\right) \quad \Longrightarrow \quad T_{\ell}=S_{\ell}+Z_{\ell}, \quad Z_{\ell} \sim \mathcal{N}\left(0, \beta^{2} \mathrm{I}\right)$


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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 $\varphi\left(P D F\right.$ of $\left.\mathcal{N}\left(0, \beta^{2} I_{d}\right)\right)$.

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- Guarantees: Estimation risk is $O(1 / \sqrt{n})$ (all constants explicit)*
$\star$ Exponentially large in $d$ though constants, which is provably necessary.


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Faster Rate: $\mathrm{kNN} / \mathrm{KDE}$ est. via 'noisy' samples attain $O\left(n^{-\frac{a}{b+d}}\right)$

## Back to Noisy DNNs

## $I\left(X ; T_{\ell}\right)$ Dynamics - Illustrative Minimal Example

Single Neuron Classification:

$$
\begin{aligned}
& \xrightarrow[X]{\tanh (w X+b)} \xrightarrow{S_{w, b}} \overbrace{\uparrow} \xrightarrow{T} \\
& \\
& \\
& \sim \mathcal{N}\left(0, \beta^{2}\right)
\end{aligned}
$$

## $I\left(X ; T_{\ell}\right)$ Dynamics - Illustrative Minimal Example

## Single Neuron Classification:

- Input: $X \sim \operatorname{Unif}\{ \pm 1, \pm 3\}$

$$
\begin{array}{rr|r|}
\substack{X \\
\{3\} \\
\\
\\
\\
\\
\\
\\
\\
\\
\\
\\
\\
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$\circledast$ Center \& sharpen transition $(\Longleftrightarrow$ increase $w$ and keep $b=-2 w)$

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$\checkmark$ Correct classification performance

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## Single Neuron Classification:

- Input: $X \sim \operatorname{Unif}\{ \pm 1, \pm 3\}$
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$\Longrightarrow$ Compression of $I\left(X ; T_{\ell}\right)$ driven by clustering of representations


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


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$\Longrightarrow$ 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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- Enhanced DNN training alg. (regularize intermediate layers wrt $I(Y ; T)$ )


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- Design tool for DNN architectures
- Algorithmic Perspective:

- Better understanding of internal representation evolution \& final state
- Enhanced DNN training alg. (regularize intermediate layers wrt $I(Y ; T)$ )


## References

[1] Z. Goldfeld, E. van den Berg, K. Greenewald, I. Melnyk, N. Nguyen, B. Kingsbury and Y. Polyanskiy, "Estimating information flow in neural networks," Arxiv preprint https://arxiv.org/abs/1810.05728, October 2018.
[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
[3] Z. Goldfeld, G. Bresler and Y. Polyanskiy, "Information storage in the stochastic Ising model," Submitted to the IEEE Transactions on Information Theory, May 2018.
Arxiv: https://arxiv.org/abs/1805.03027

## Information Storage in Interacting Particle Systems

Motivation: Demand for high-capacity data storage devices

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[G.-Bresler-Polyanskiy'18] Performance benchmarks \& hard-drive designs

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Q: Reliable (\& secure) information passing protocols? Fundamental limits?

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(1) KDE + Best poly. approximation [Han-Jiao-Weissman-Wu'17]


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$\Longrightarrow$ Estimate $I\left(X ; T_{\ell}\right)$ from samples via general-purpose $\boldsymbol{h}(\boldsymbol{P})$ est.:

- Most results assume lower bounded density $\Longrightarrow$ Inapplicable
- 2 Works Drop Assumption:
(1) KDE + Best poly. approximation [Han-Jiao-Weissman-Wu'17]
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* Except sub-Gaussian result from [Han-Jiao-Weissman-Wu'17]


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- Rate: Risk $\leq O\left(n^{-\frac{\alpha s}{\beta s+d}}\right), \quad \mathrm{w} / \alpha, \beta \in \mathbb{N}, s$ smoothness, $d$ dimension


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Estimate $h(P * \varphi)$ based on $n$ i.i.d. samples from $P \in \mathcal{F}_{d}$ (nonparametric class) and knowledge of $\varphi\left(P D F\right.$ of $\left.\mathcal{N}\left(0, \beta^{2} I_{d}\right)\right)$.

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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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- Computing: Can be efficiently computed via MC integration


## The Sample Propagation Estimator - Convergence

Theorem (ZG-Greenewald-Polyanskiy '18)
For $\mathcal{F}_{d} \triangleq\left\{P \mid \operatorname{supp}(P) \subseteq[-1,1]^{d}\right\}$ and any $\beta>0$ and $d \geq 1$, we have

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\begin{array}{r}
\leq \frac{1}{2\left(4 \pi \beta^{2}\right)^{\frac{d}{4}}} \log \left(\frac{n(2+2 \beta \sqrt{(2+\epsilon) \log n})^{d}}{\left(\pi \beta^{2}\right)^{\frac{d}{2}}}\right)(2+2 \beta \sqrt{(2+\epsilon) \log n})^{\frac{d}{2}} \frac{1}{\sqrt{n}} \\
+\left(c_{\beta, d}^{2}+\frac{2 c_{\beta, d} d\left(1+\beta^{2}\right)}{\beta^{2}}+\frac{8 d\left(d+2 \beta^{4}+d \beta^{4}\right)}{\beta^{4}}\right) \frac{2}{n}
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where $c_{\beta, d} \triangleq \frac{d}{2} \log \left(2 \pi \beta^{2}\right)+\frac{d}{\beta^{2}}$.

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


## The Sample Propagation Estimator - Proof Ideas

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\Longrightarrow \mathbb{E}\left|(P * \varphi)(x)-\left(\hat{P}_{n} * \varphi\right)(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)
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$\sup \mathbb{E}\left|h(P * \varphi)-h\left(\hat{P}_{n} * \varphi\right)\right| \leq \sup \mathbb{E}\left|h_{\mathcal{R}}(P * \varphi)-h_{\mathcal{R}}\left(\hat{P}_{n} * \varphi\right)\right|+2 \sup \left|h_{\mathcal{R}^{c}}(P * \varphi)\right|$
- Inside R: $\triangleright-t \log t$ modulus of cont. for $x \mapsto x \log x \&$ Jensen's ineq.
$\Longrightarrow$ Focus on analyzing $\mathbb{E}\left|(P * \varphi)(x)-\left(\hat{P}_{n} * \varphi\right)(x)\right|$
- Bias \& variance analysis
$\Longrightarrow \mathbb{E}\left|(P * \varphi)(x)-\left(\hat{P}_{n} * \varphi\right)(x)\right| \leq c_{1} \sqrt{\frac{(P * \tilde{\varphi})(x)}{n}}, \quad \tilde{\varphi}=\mathcal{N}\left(0, \frac{\beta^{2}}{2} \mathrm{I}\right)$
- Plug back in \& Convex analysis


## The Sample Propagation Estimator - Proof Ideas

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$\Longrightarrow \sup \mathbb{E}\left|h_{\mathcal{R}}(P * \varphi)-h_{\mathcal{R}}\left(\hat{P}_{n} * \varphi\right)\right| \leq c_{2} \log \left(\frac{n \lambda(\mathcal{R})}{c_{3}}\right) \sqrt{\frac{\lambda(\mathcal{R})}{n}}$


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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:



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## Binning vs True Mutual Information

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

