Information Bottleneck:
Theory, Application, and Controversy

Summarized by Ziyu Ye

Agenda

- Opening the Black-Box of Deep Neural Networks via Information. Tishby and Schwartz-Ziv (2017).
- On the Information Bottleneck Theory of Deep Learning. Saxe et al (2017).
- Deep Variational Information Bottleneck. Alemi et al (2017).

Opening the Black Box of Deep Neural Networks via Information

Agenda

- Overview
- Primer on Information Theory
- The Information Plane
- Optimization v.s. Information Plane
- Rethinking Learning Theory with Information
- Conclusions

Very High-Level Idea of The Paper

1. Information compression can provide a generalization bound in learning theory.

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3. The above two phases matches the 2-stage behavior of SGD optimization:
   - Stage 1: Gradient drift
   - Stage 2: Gradient diffusion

Information Bottleneck: An Illustrative Example

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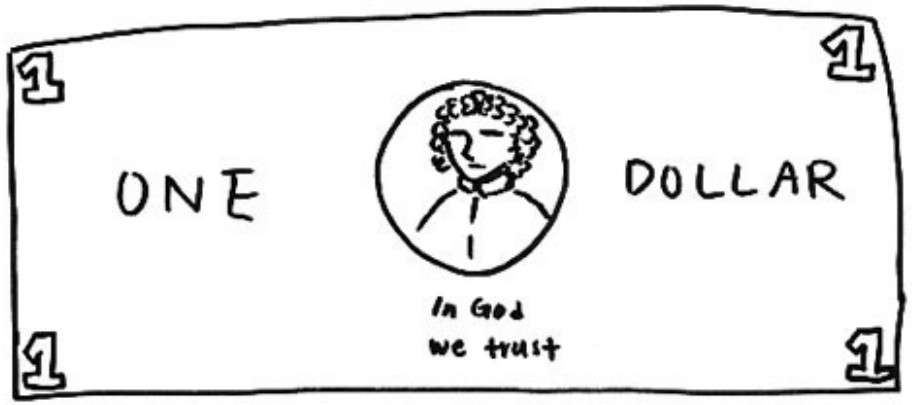

Fig 1a. Drawing of a dollar bill from memory

Fig 1b. How a dollar bill in fact looks like*

* Image source: Epstein, 2016

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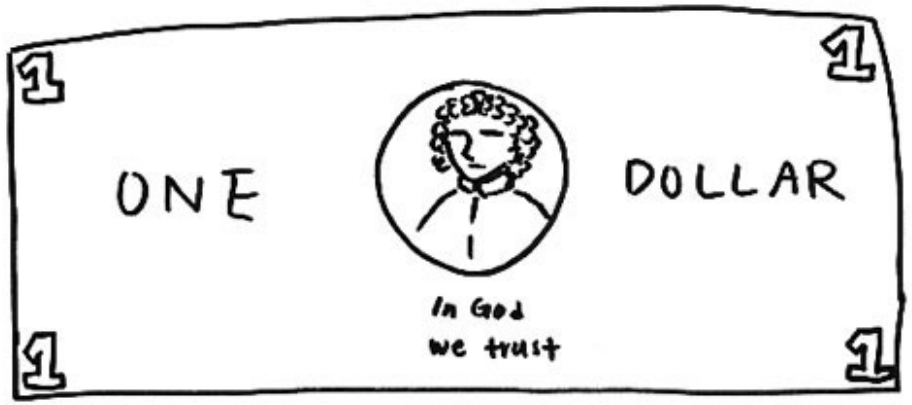

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Goal Find the most relevant features.

Shortcut Forgetting the irrelevant by constraining the information flow.

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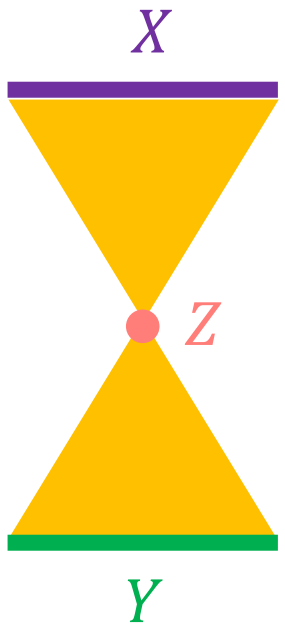

$$\max_{\boldsymbol{\theta}} I(Z, Y; \boldsymbol{\theta})$$

$$\text{s.t. } I(X, Z; \boldsymbol{\theta}) \leq I_c$$

By constraining the information flow, the neural network is forced to learn the most representative features.

Shannon's Information Measure

Entropy

$$H(X) = -\int p(x) \log p(x) dx$$

Joint Entropy

$$H(X,Y) = -\int p(x,y) \log p(x,y) dx dy$$

Conditional Entropy

$$H(X|Y) = -\int p(x,y) \log p(x|y) dx dy$$

KL Divergence

$$KL(X||Y) = \int p(x) \log \frac{p(x)}{p(y)} dx dy$$

Mutual Information

$$I(X;Y) = \int p(x,y) \log \frac{p(x|y)}{p(x,y)} dx dy$$

$$= KL(p(x,y)||p(x)p(y))$$

Properties of Mutual Information

Data Processing Inequality $\forall\, X \to Y \to Z: \;\; I(X;Y) \geq I(X;Z)$

Re-parametrization Invariance $\forall \phi, \psi: \;\; I(X;Y) = I(\phi(X);\psi(Y))$

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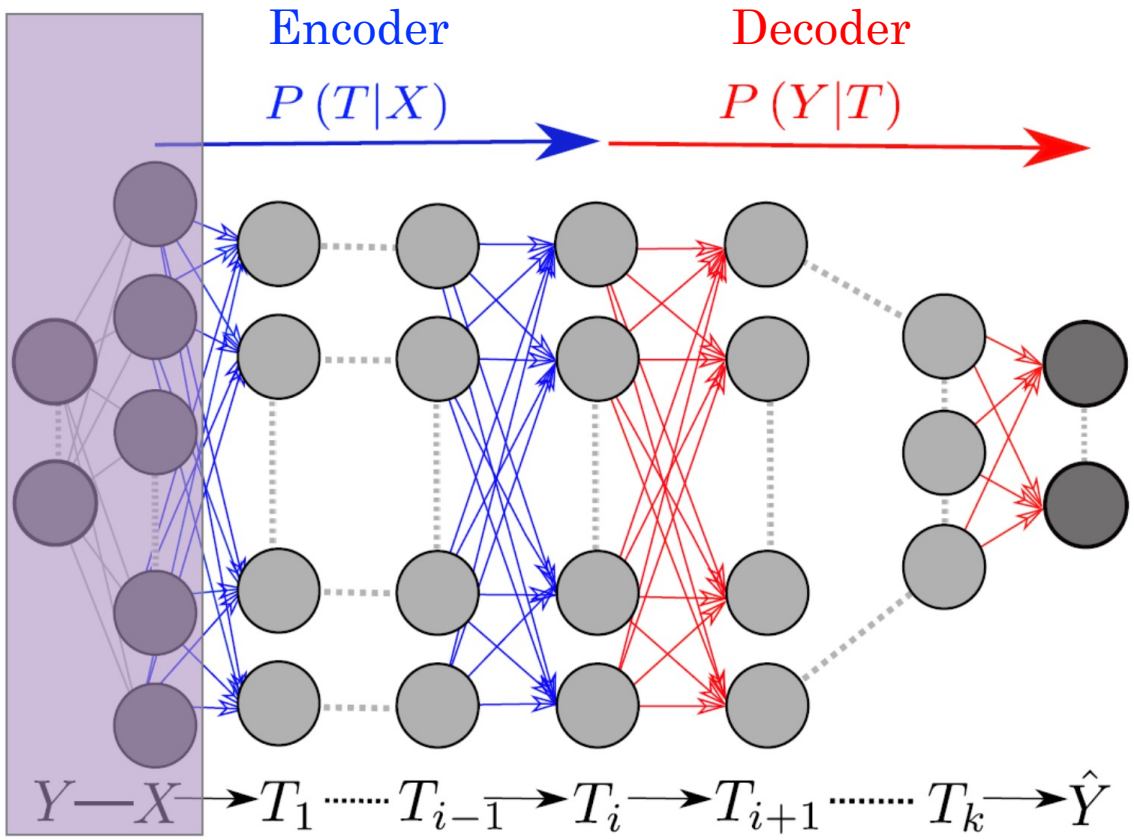
DNN as Markov Chain of Random Variables



$$I(X;Y) \geq I(T_1;Y) \geq I(T_2;Y) \geq \ldots \geq I(T_k;Y) \geq I(\hat{Y};Y)$$

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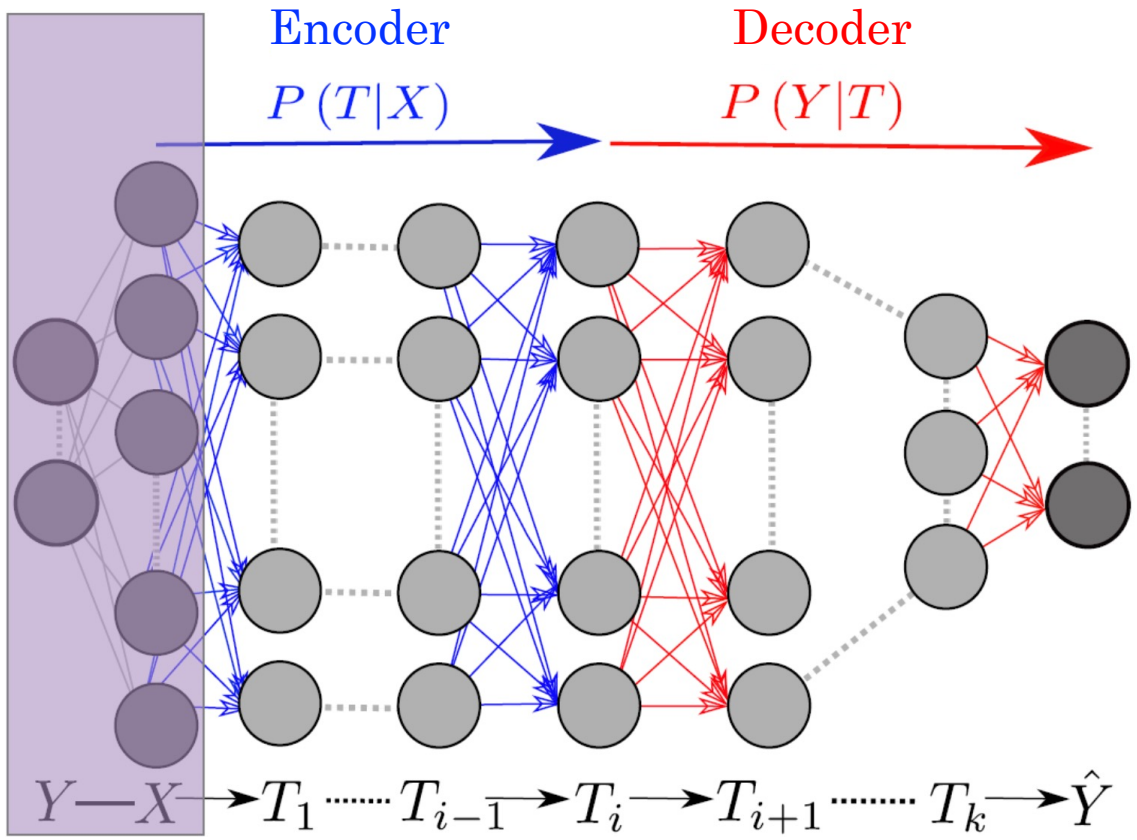

Theorem (Information Plane):

*For large typical **X**, the sample complexity of a DNN is completely determined by the encoder mutual information, **I(X;T)**, of the last hidden layer; the accuracy (generalization error) is determined by the decoder information, **I(T;Y)**, of the last hidden layer.*

$$I(X;Y) \geq I(T_1;Y) \geq I(T_2;Y) \geq \ldots \geq I(T_k;Y) \geq I(\hat{Y};Y)$$

Optimal Representation: Minimal Sufficient Statistics $S(X)$

What is the optimal representation of X w.r.t Y?

Sufficient Statistics $S(X)$

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Information Bottleneck as an Approximation

$$\min_{p(t|x),p(y|t),p(t)} \{I(X;T) - \beta I(T;Y)\}$$

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$$\begin{cases} p(t|x) = \frac{p(t)}{Z(x;\beta)} \exp\left(-\beta D_{KL}\left[p(y|x) \parallel p(y|t)\right]\right) \\ p(t) = \sum_x p(t|x)\, p(x) \\ p(y|t) = \sum_x p(y|x)\, p(x|t) \ , \end{cases}$$

Information Plane: Evolution of $I(T;X)$ $v.s.$ $I(T;Y)$

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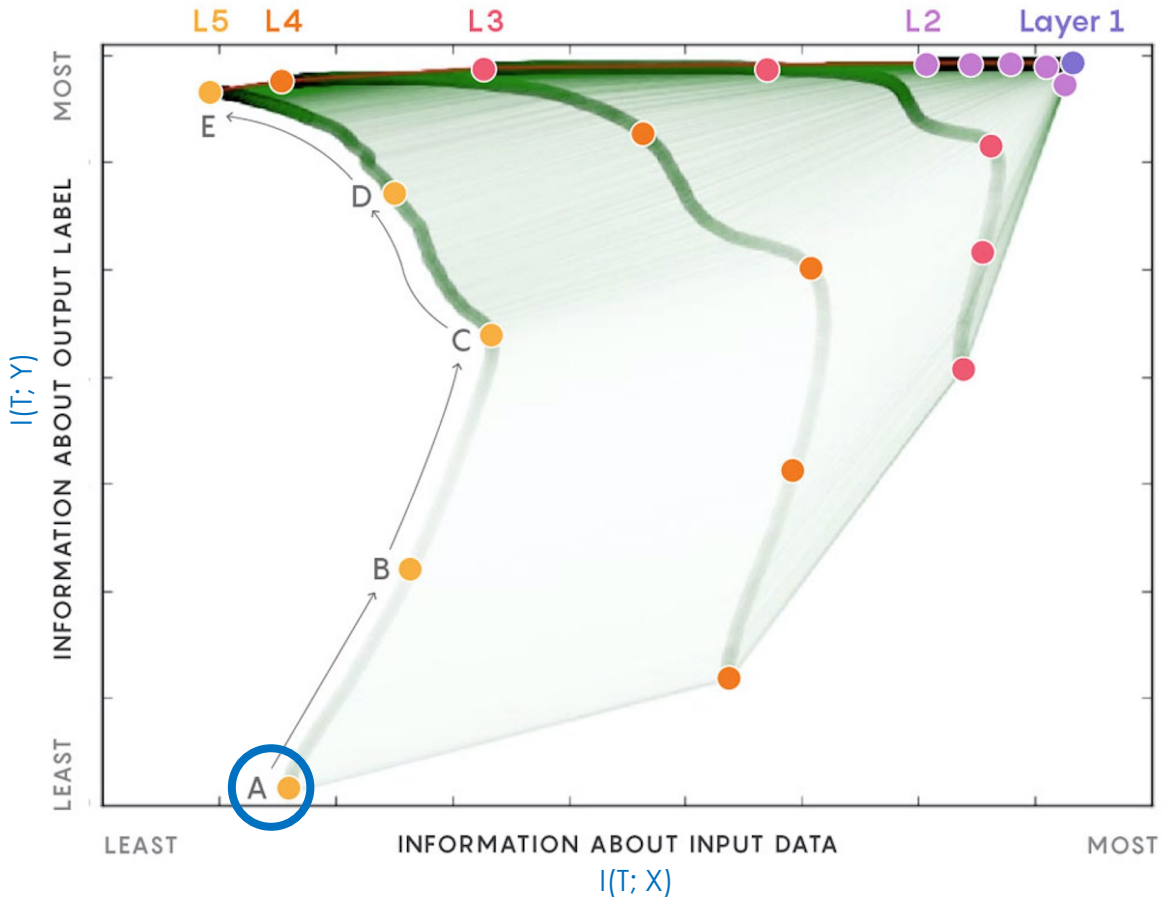
A Initial State



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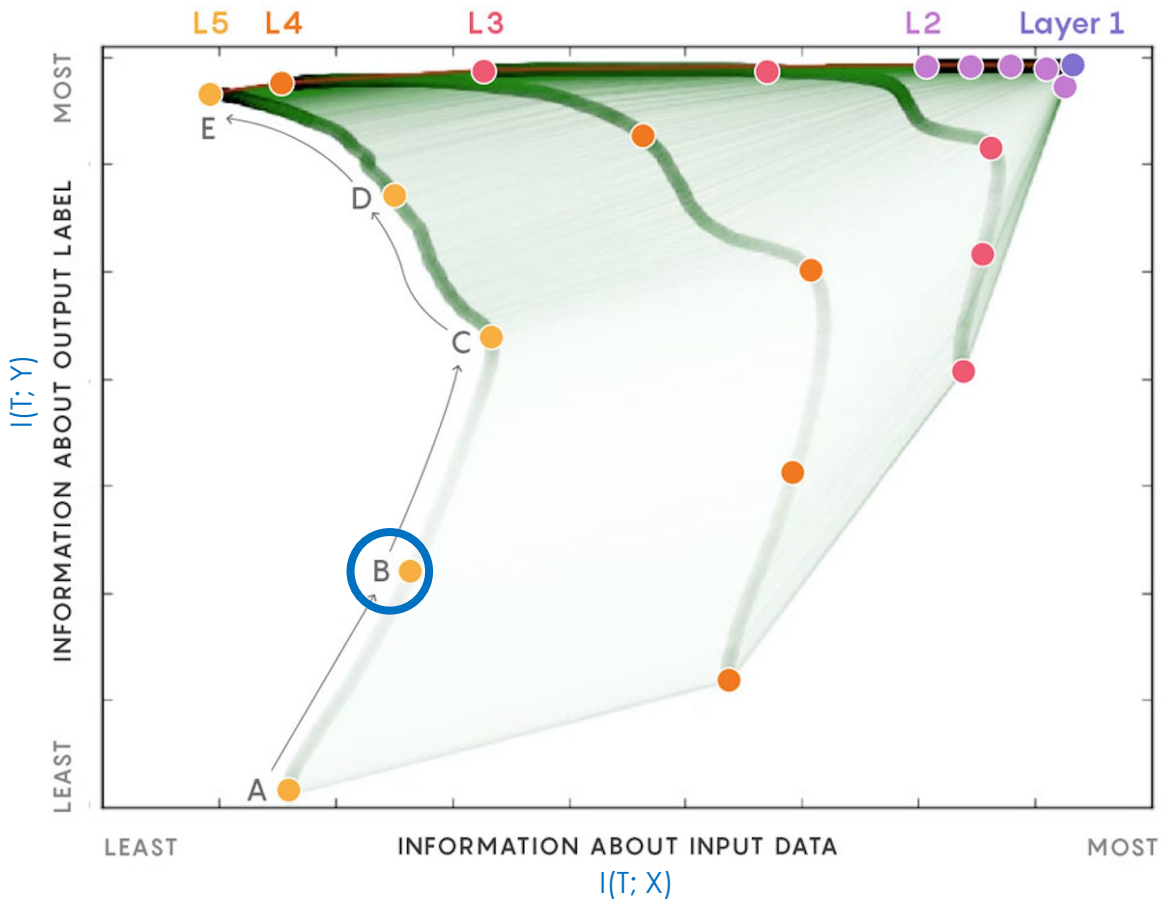
B Fitting Phase



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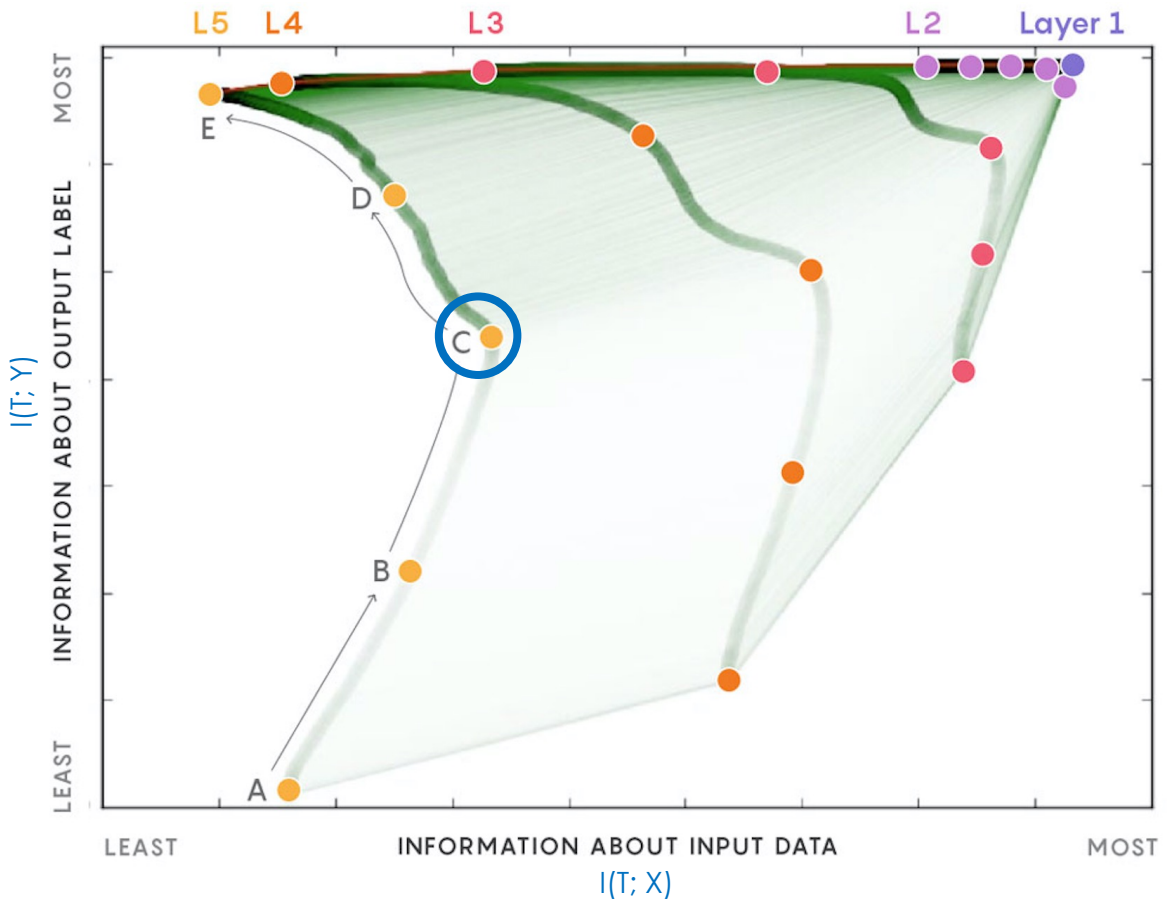
C Phase Change



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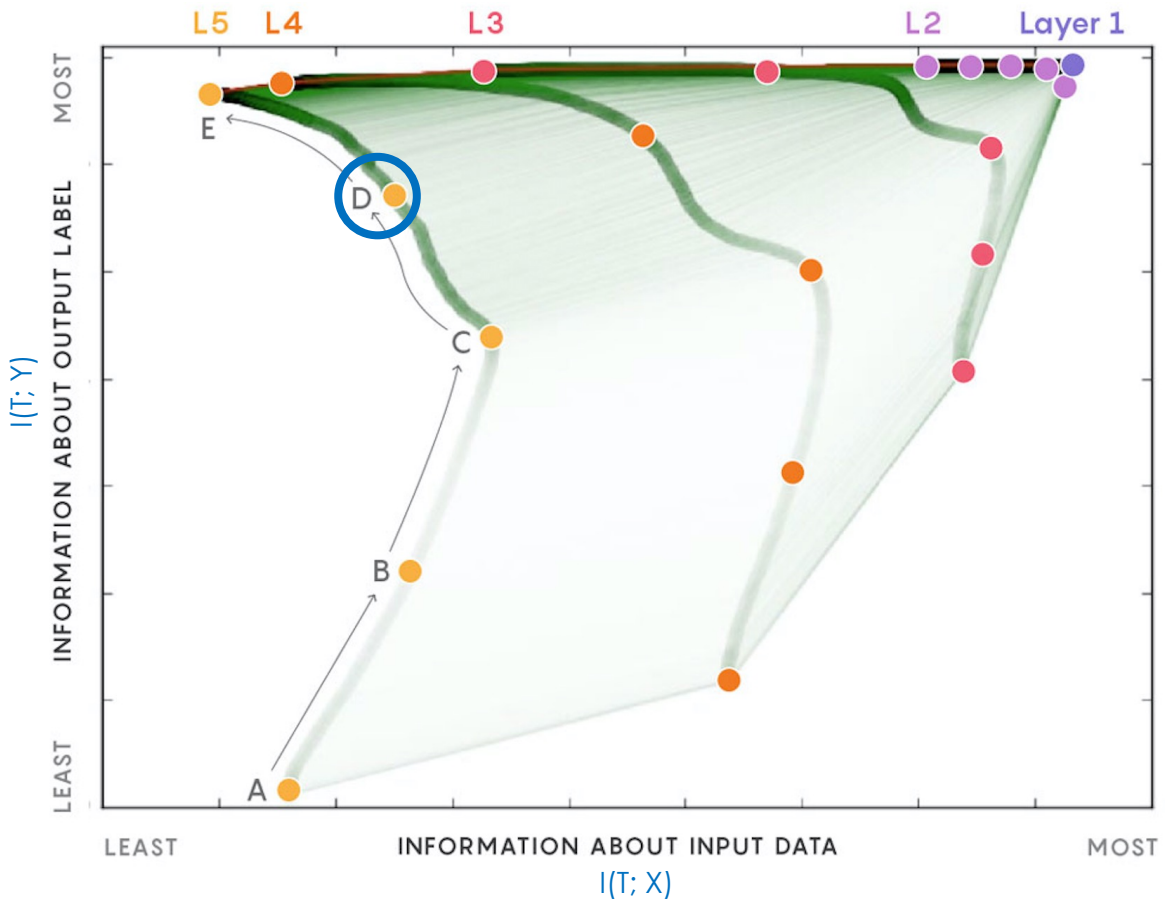
D Compression Phase



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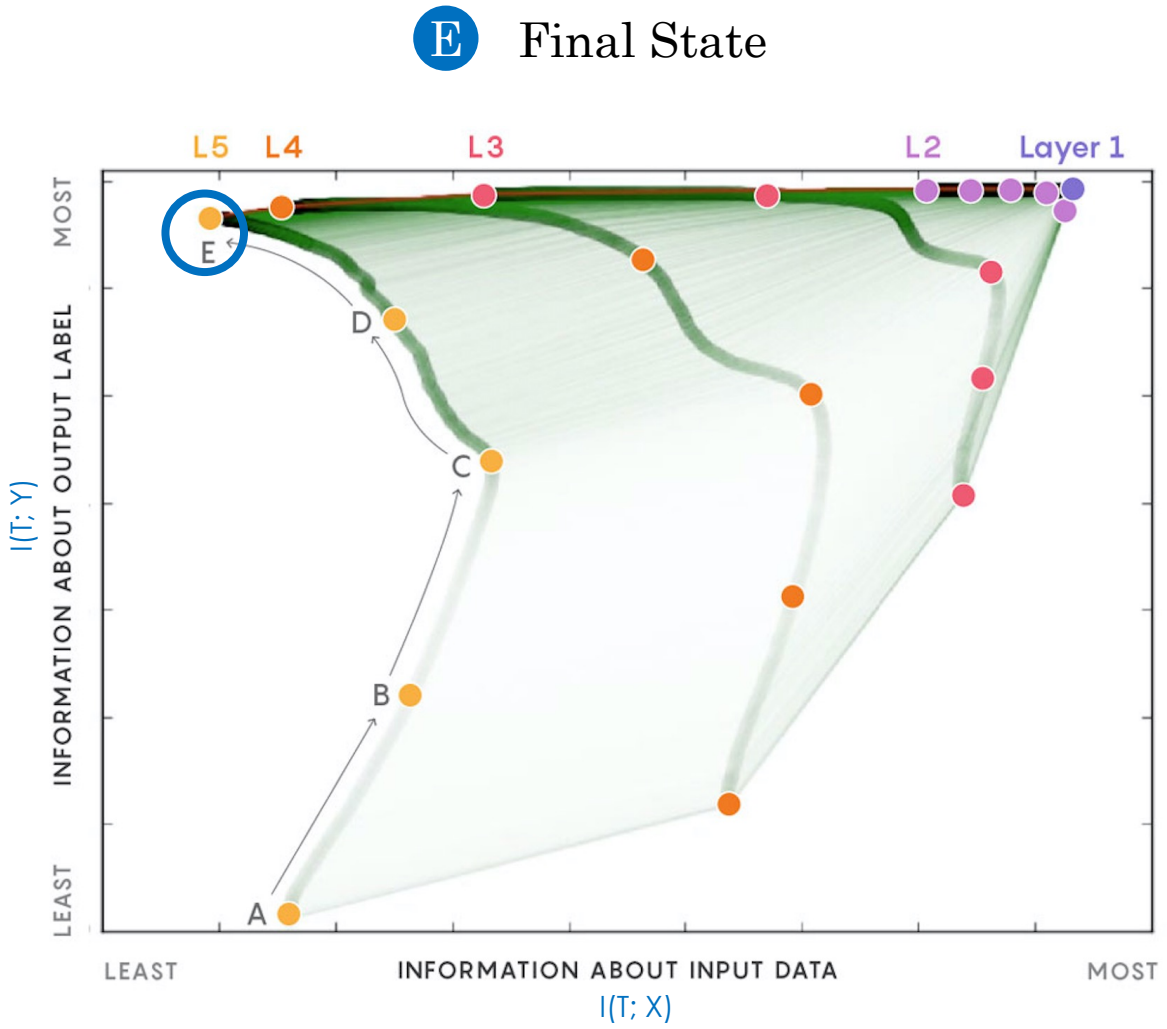

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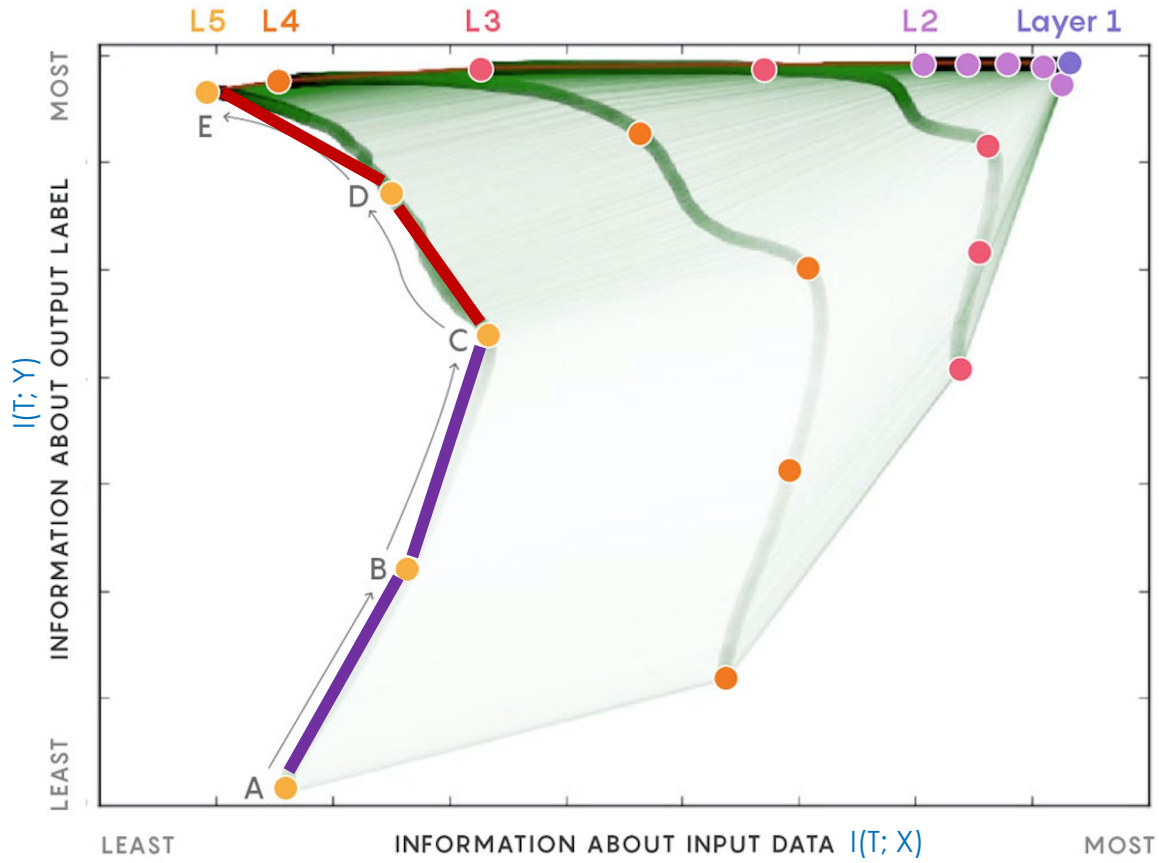

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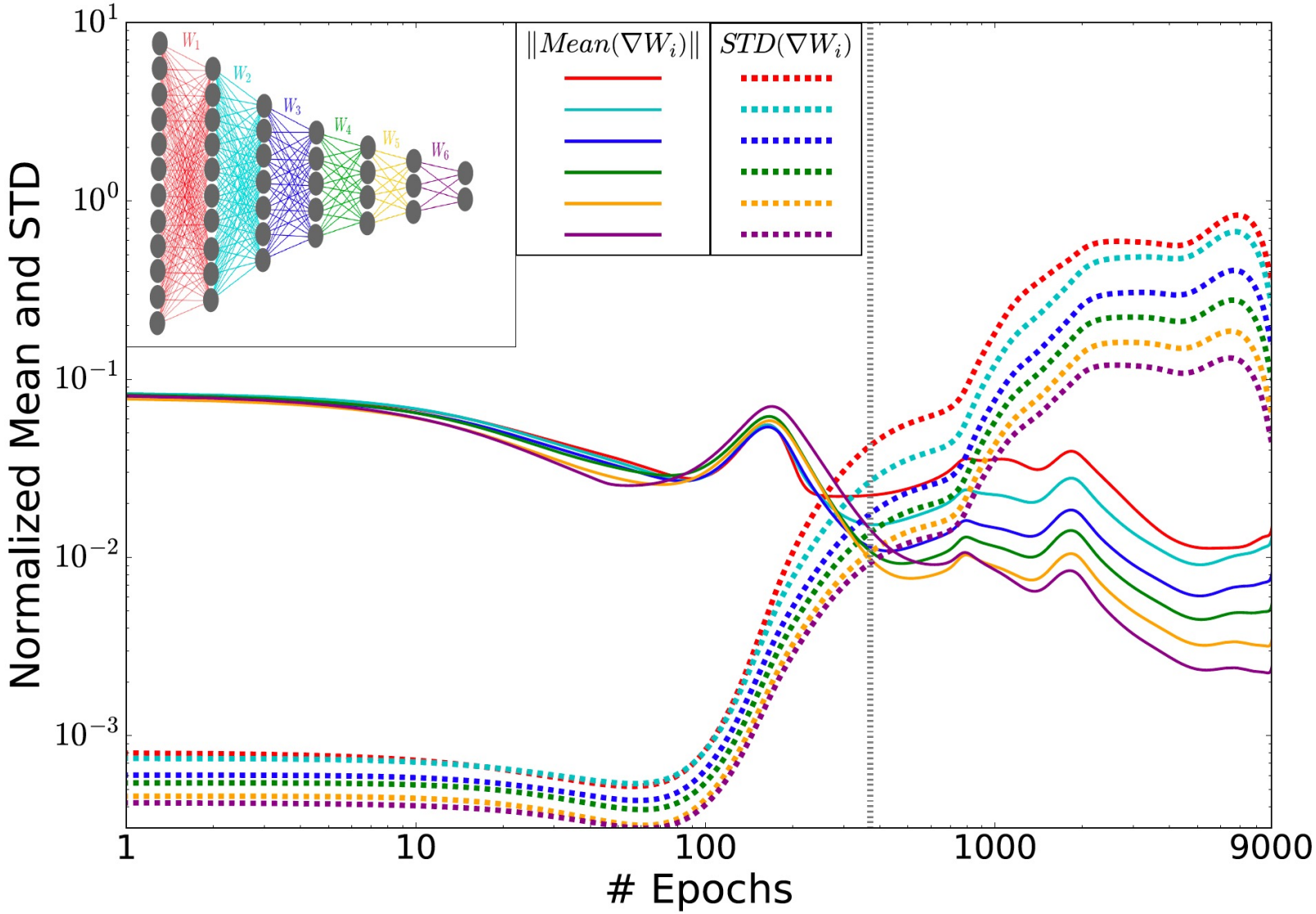
Optimization Process of SGD



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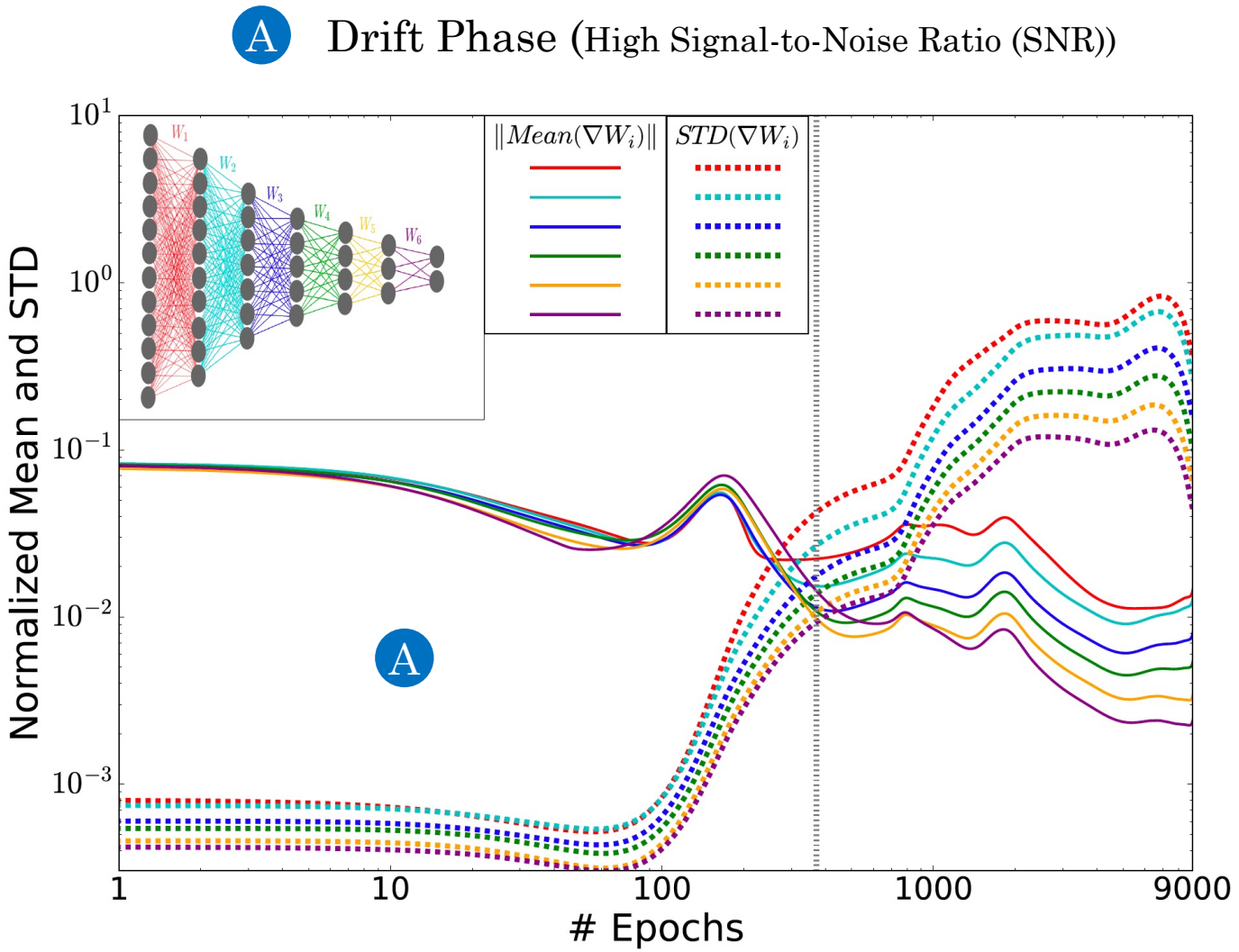

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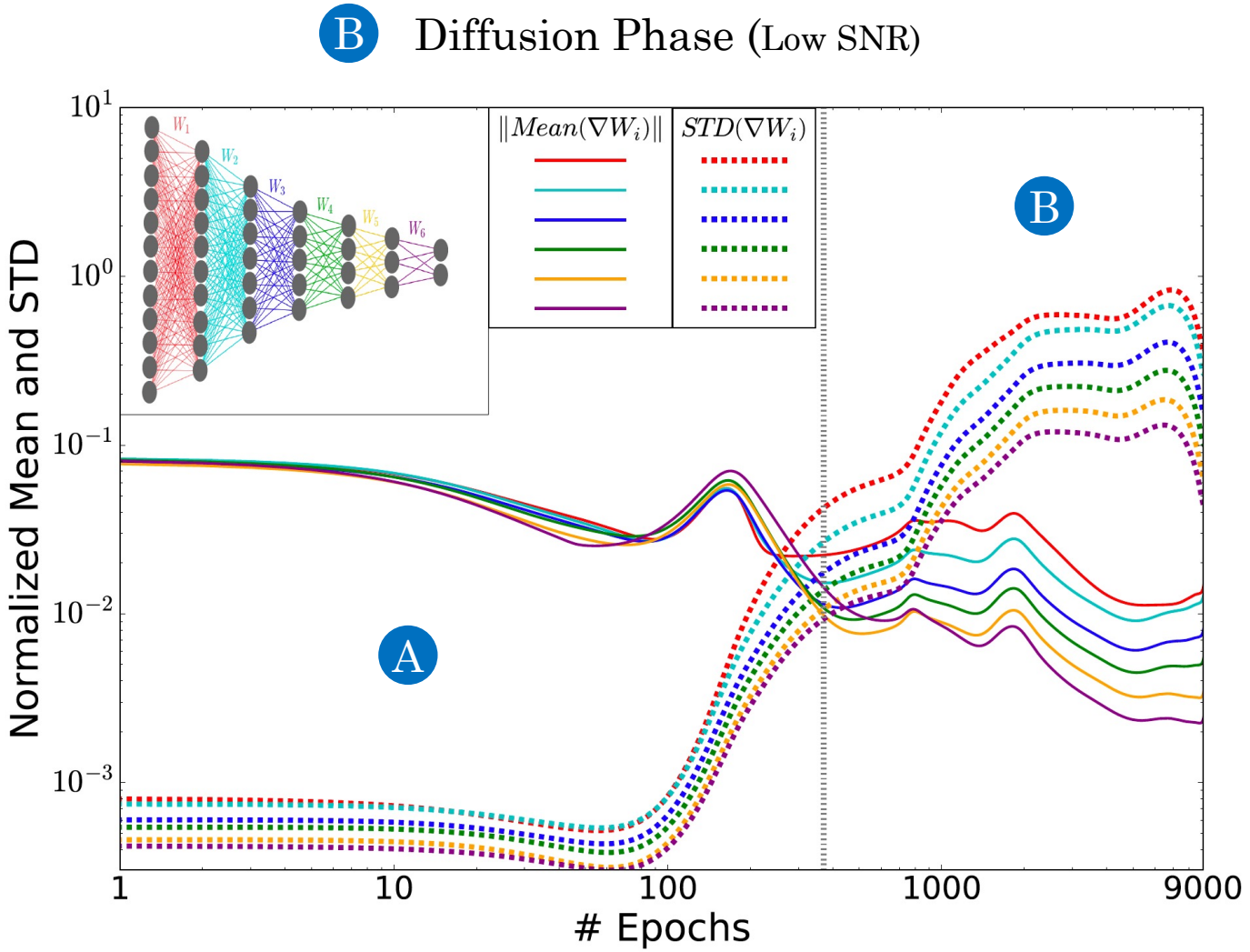
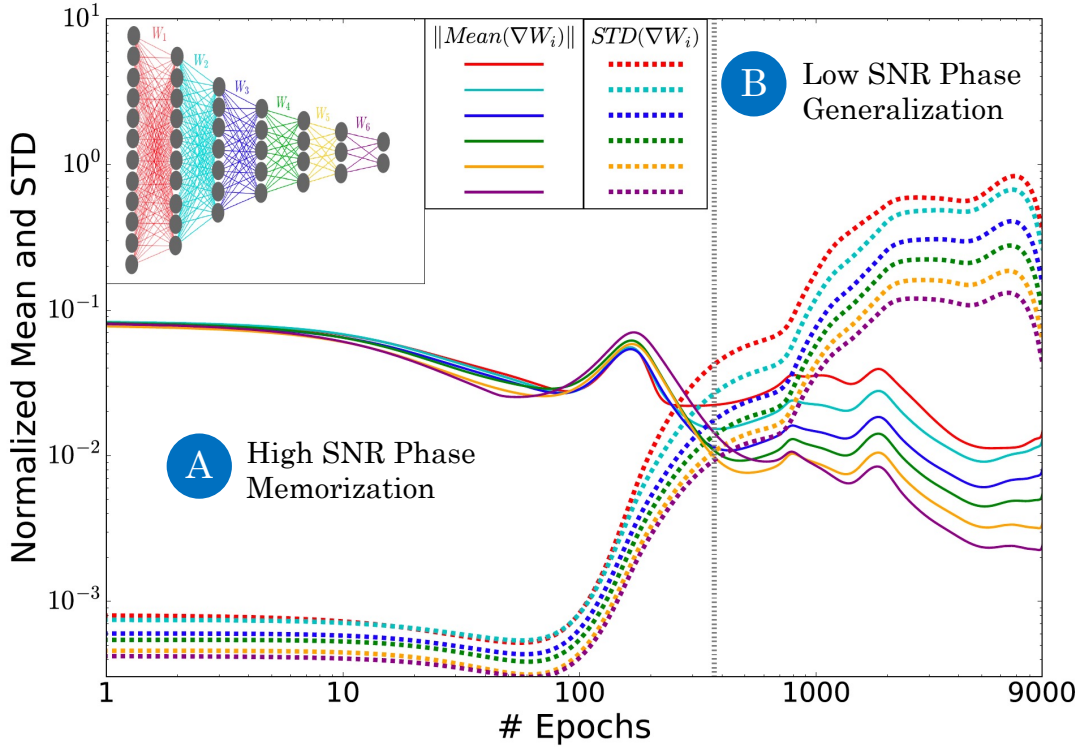
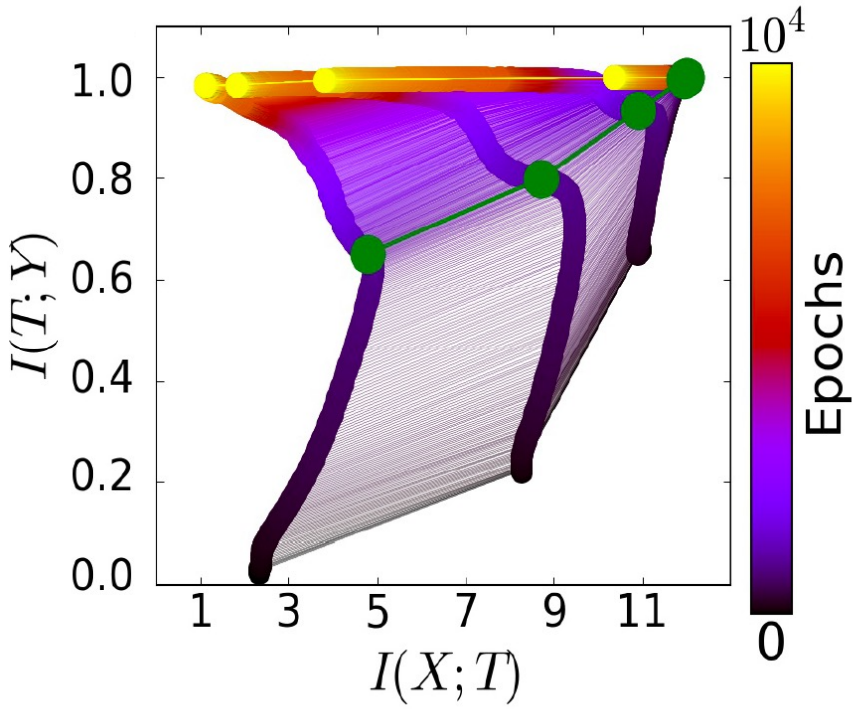
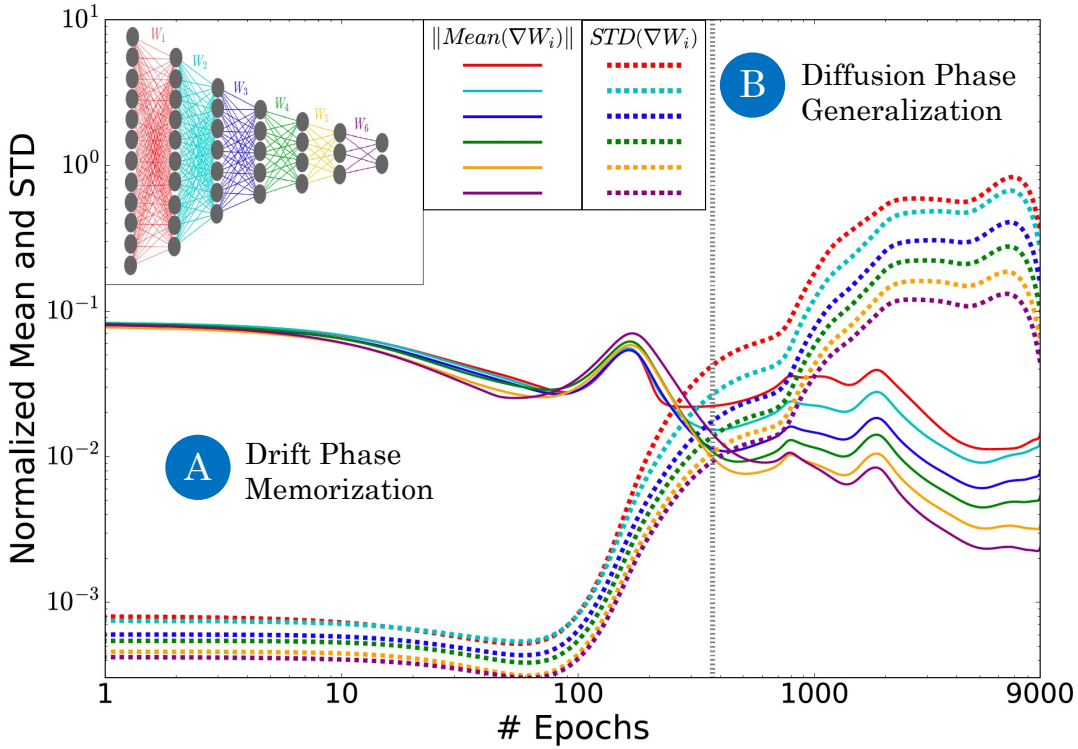


Optimization Process of SGD v.s. Information Plane





Theoretical Analysis on the Diffusion Phase



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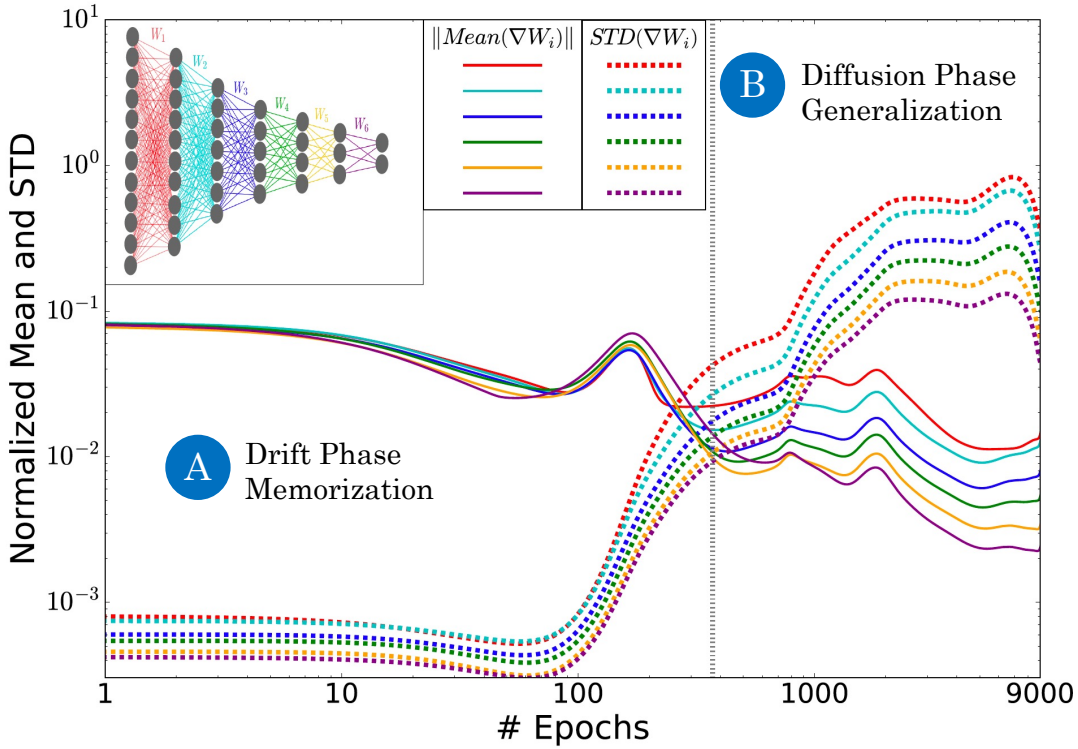

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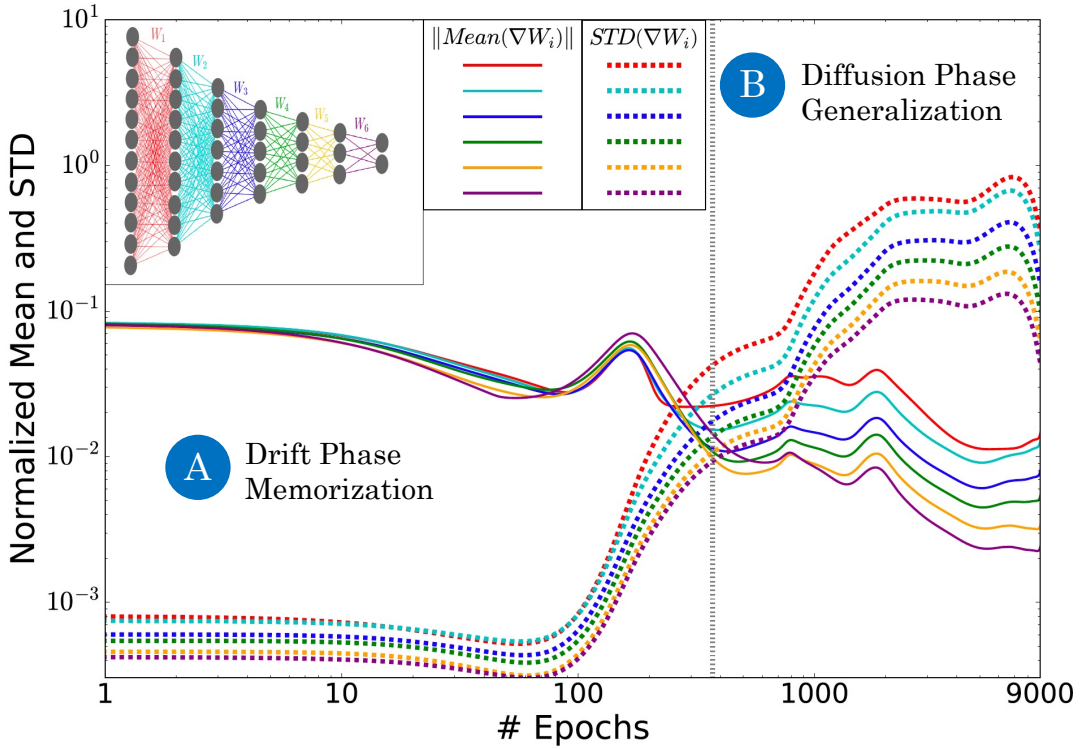

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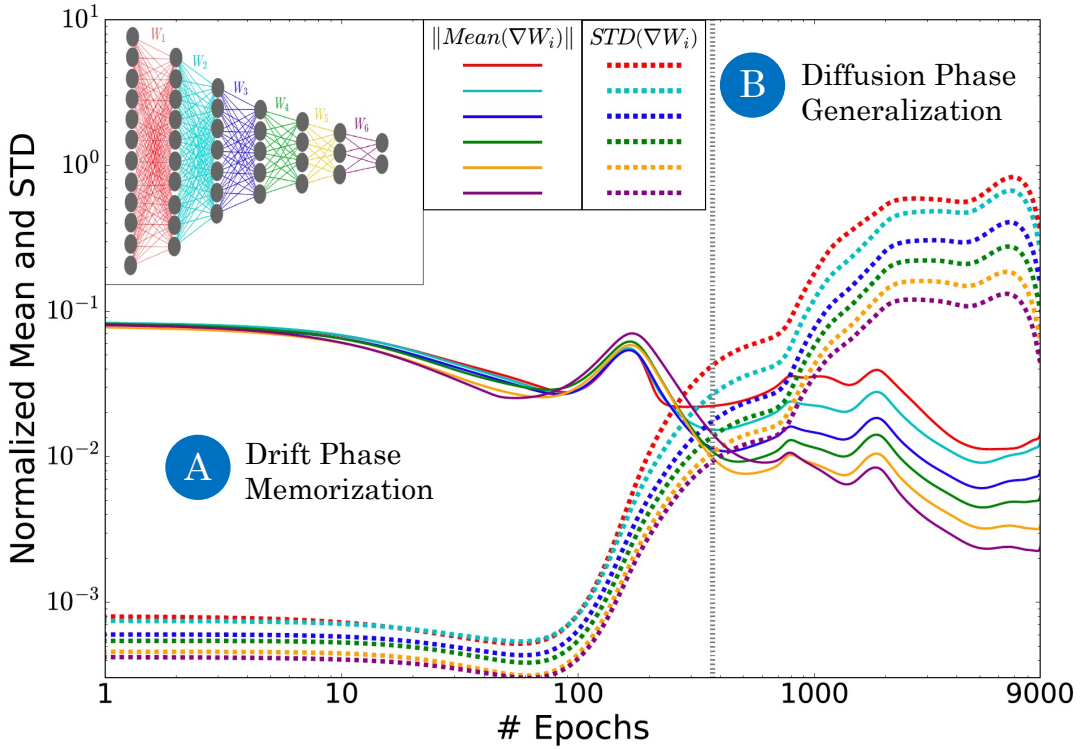

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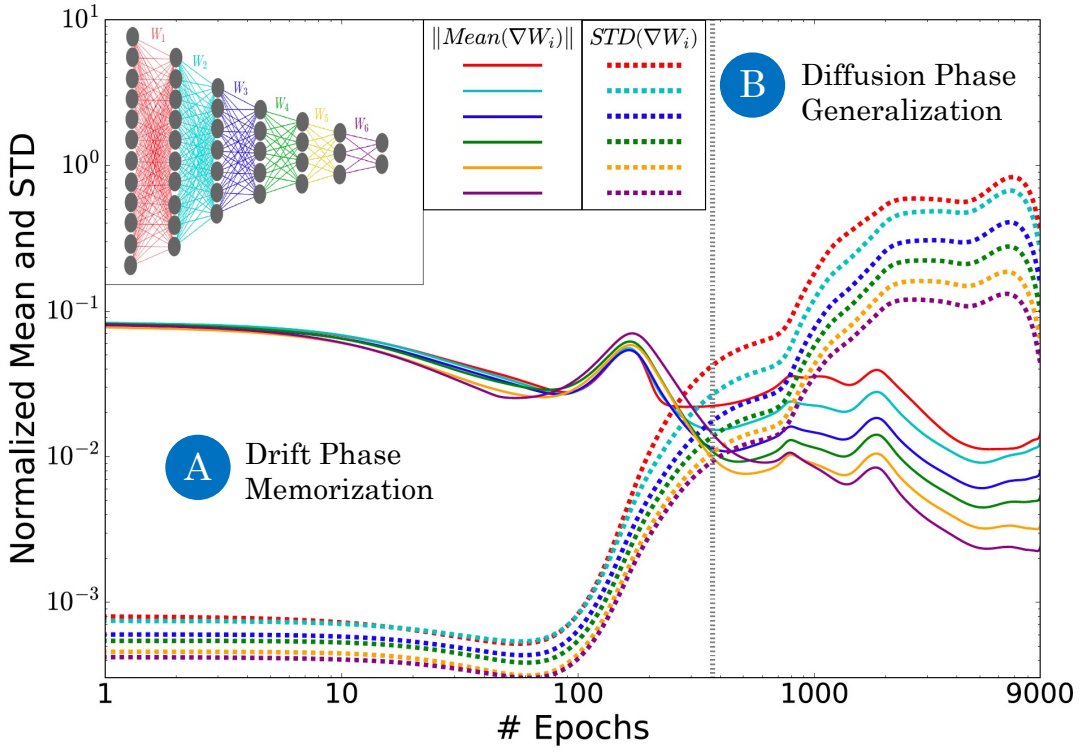

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5. As $I\left(X;T_k\right) = H(X) - H\left(X|T_k\right)$, that minimizes $I\left(X;T_k\right)$.

Rethinking Generalization Bound

1 "Old" Generalization Bound

$$\varepsilon^2 < \frac{\log|H_\varepsilon| + \log 1/\delta}{2m}$$

ε : generalization error

δ : confidence

m: number of training examples

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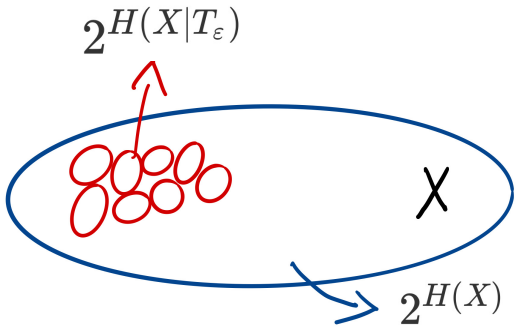

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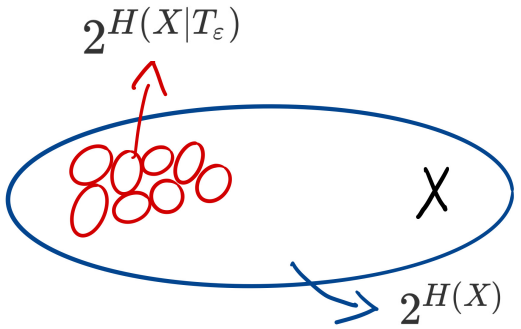

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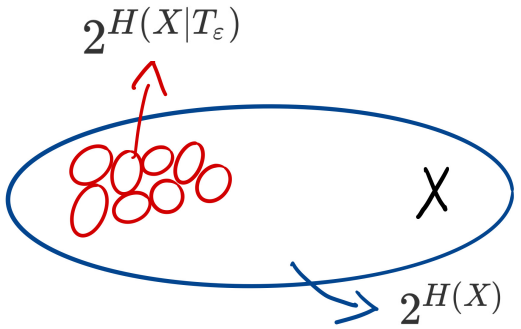

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Conclusion

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On the Information Bottleneck Theory of Deep Learning

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- Generalizability v.s. Information Plane
- Optimization v.s. Information Plane
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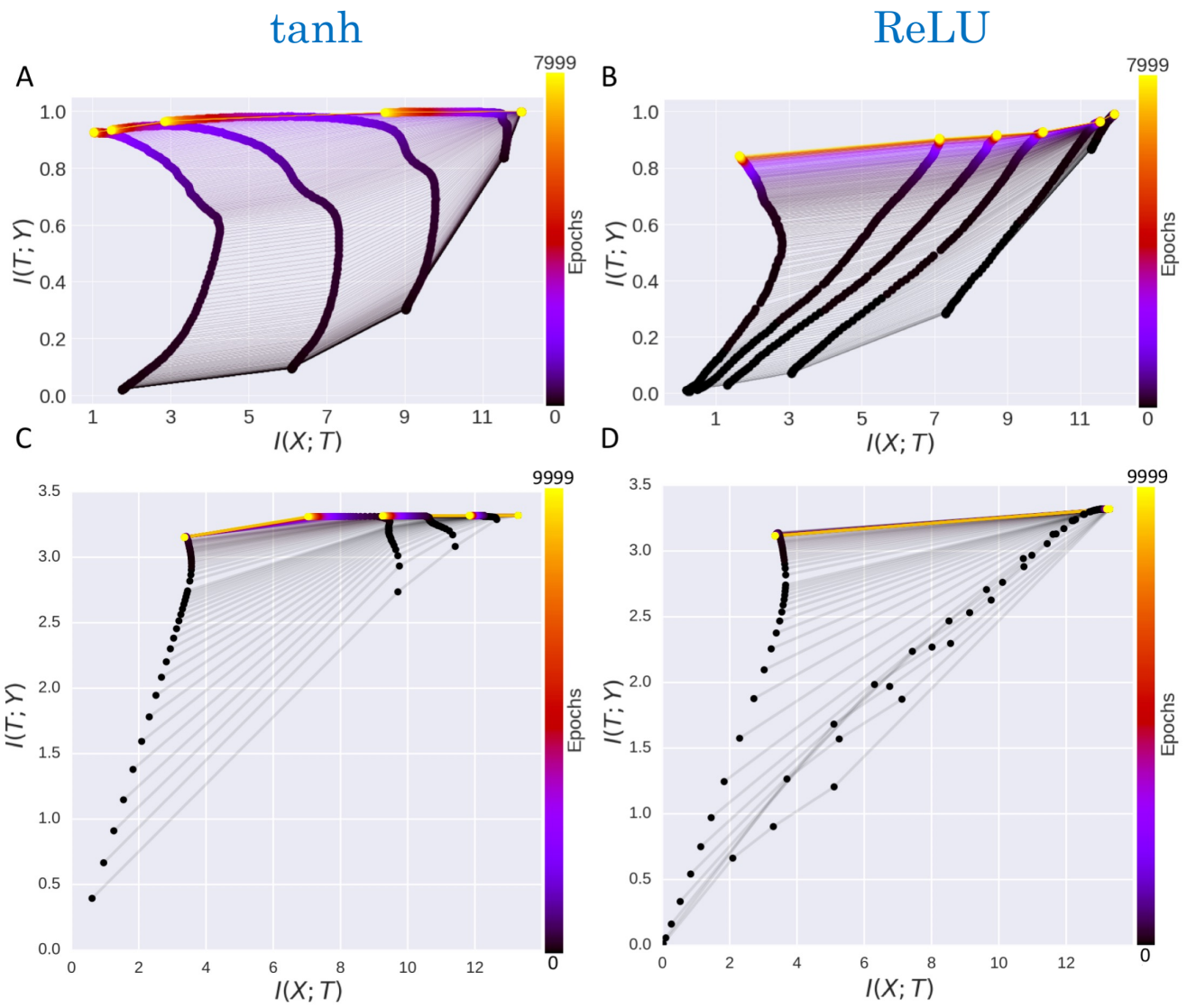
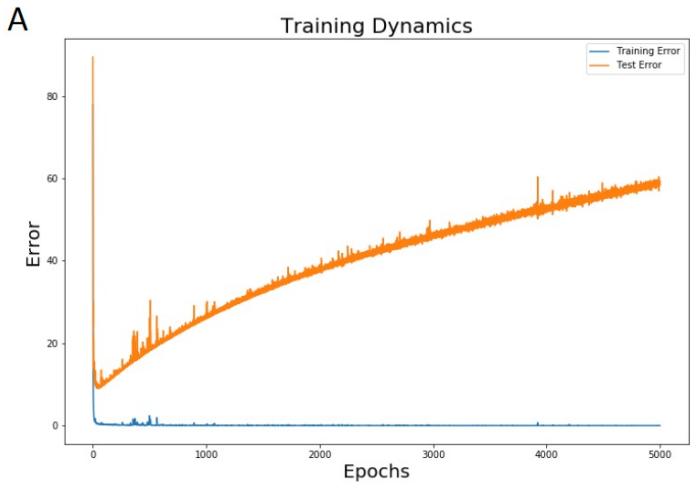
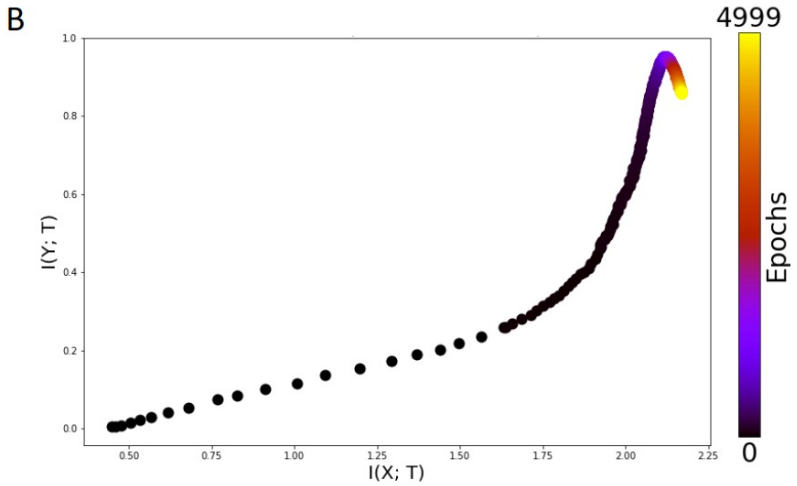
Tanh v.s. ReLU


tanh
ReLU
Synthetic Dataset
MNIST
A
B
C
D
7999
9999
Epochs
I(T; Y)
I(X; T)

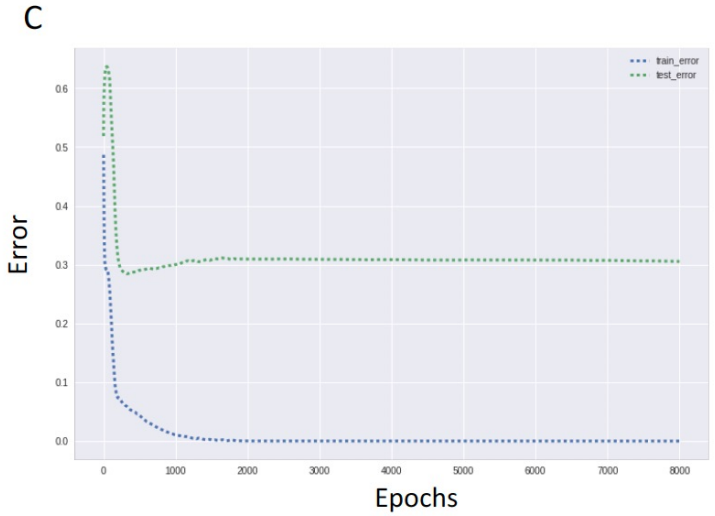
Overfitting: Linear v.s. Nonlinear

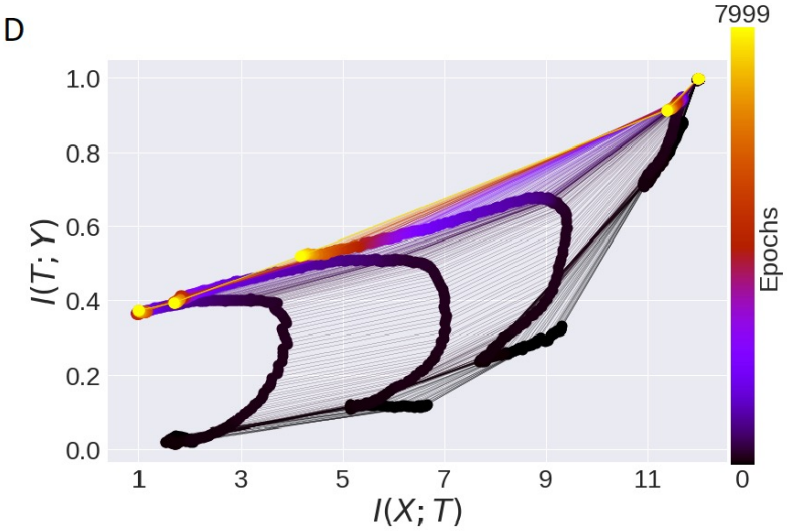
Linear



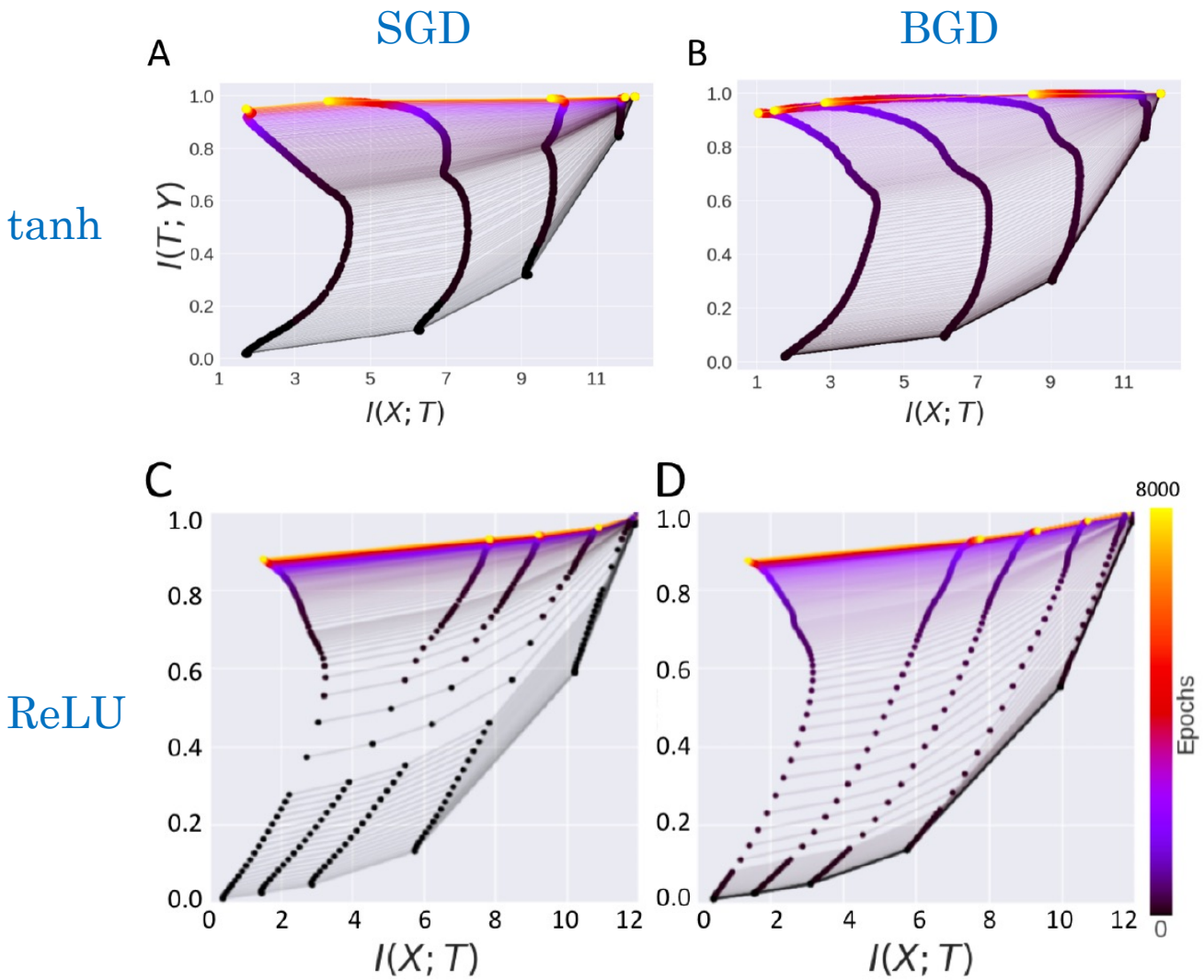


Non-Linear

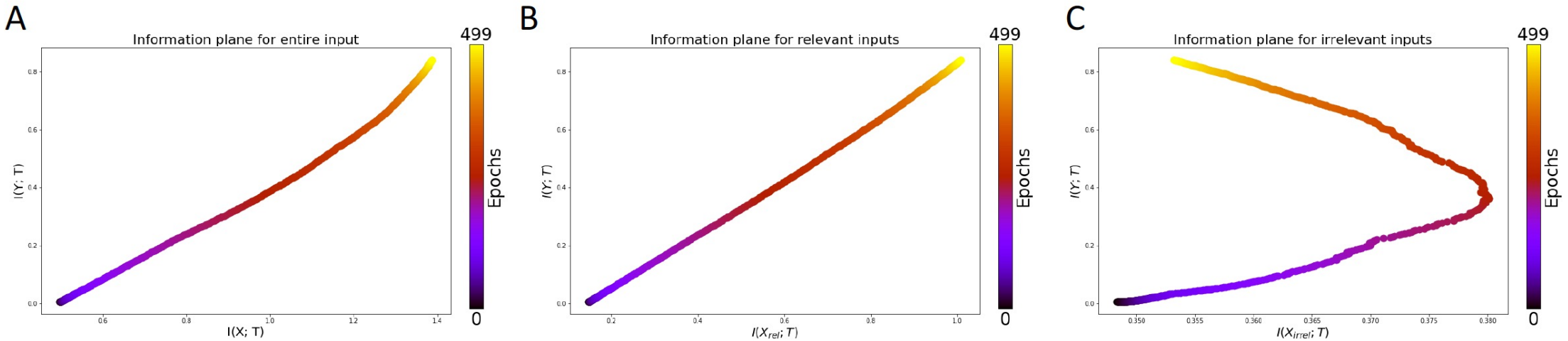


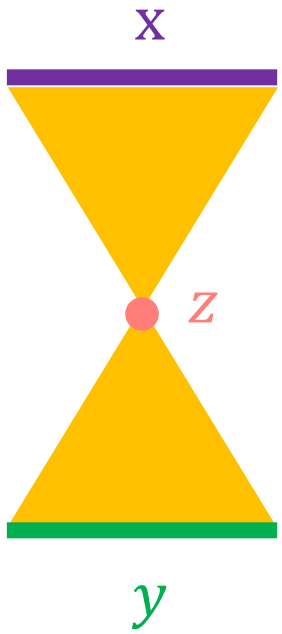


Stochastic v.s. Non-Stochastic



Compression: Relevance v.s. Irrelevant



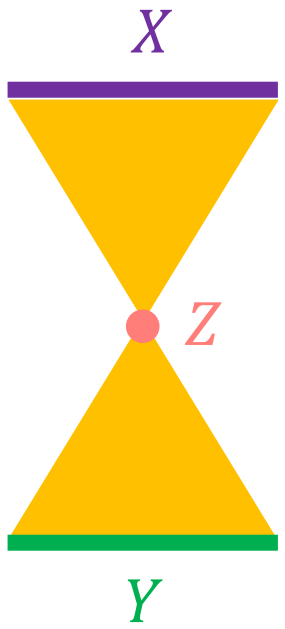


Deep Variational Information Bottleneck

Agenda

- Overview
- Primer on Variational Inference
- Variational Information Bottleneck (VIB)
- Experiment Results for VIB
- Conclusions

Information Bottleneck as a Regularizer for DNN



$$\max_{\boldsymbol{\theta}} I(Z, Y; \boldsymbol{\theta})$$

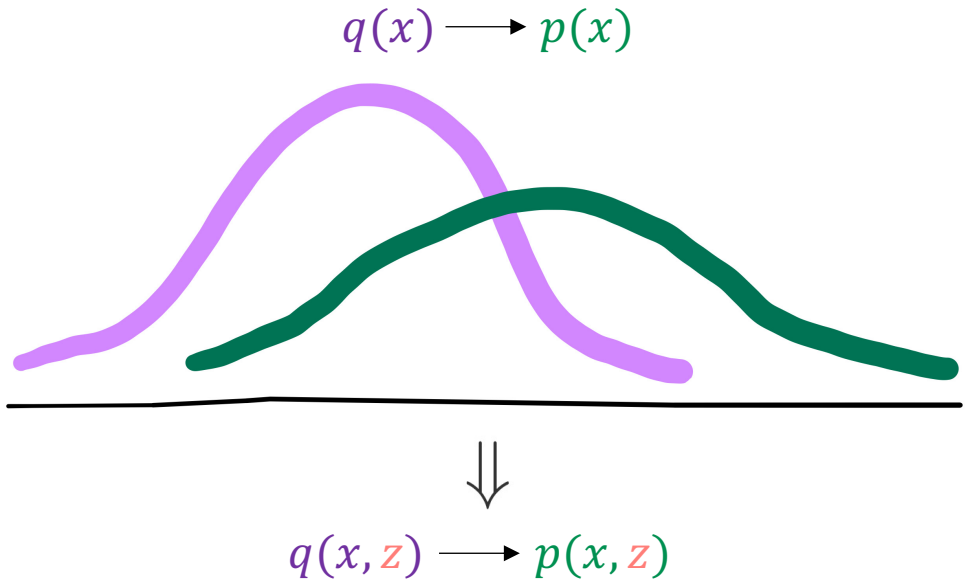
$$\text{s.t. } I(X, Z; \boldsymbol{\theta}) \leq I_c$$

By constraining the information flow, the neural network is forced to learn the most representative features.

- Better generalizability
- Robustness to attacks

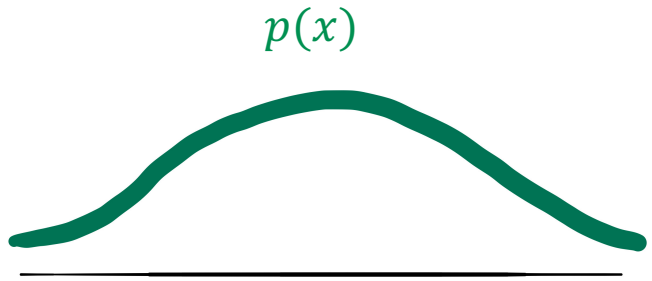
Primer on Variational Inference

Variational inference is to approximate intractable distribution with latent variables.



Variational Inference for Generative Models

Variational inference is to approximate intractable distribution with latent variables.



Variational Inference for Generative Models

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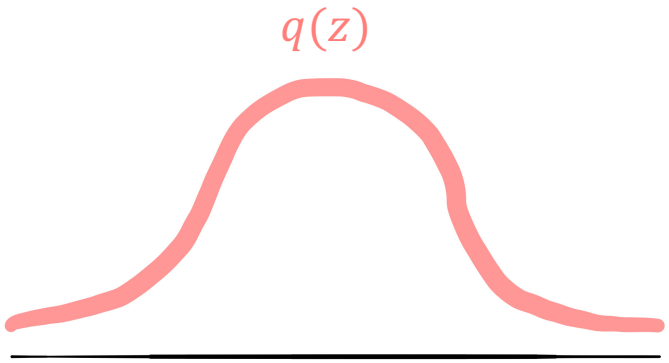

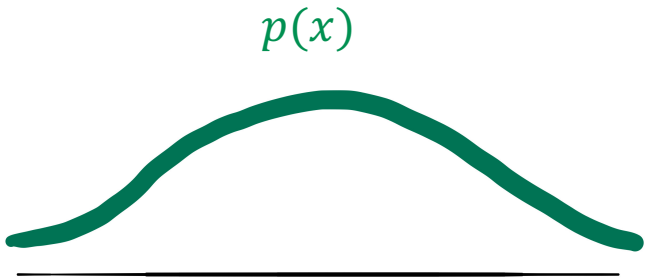

Variational Inference for Generative Models

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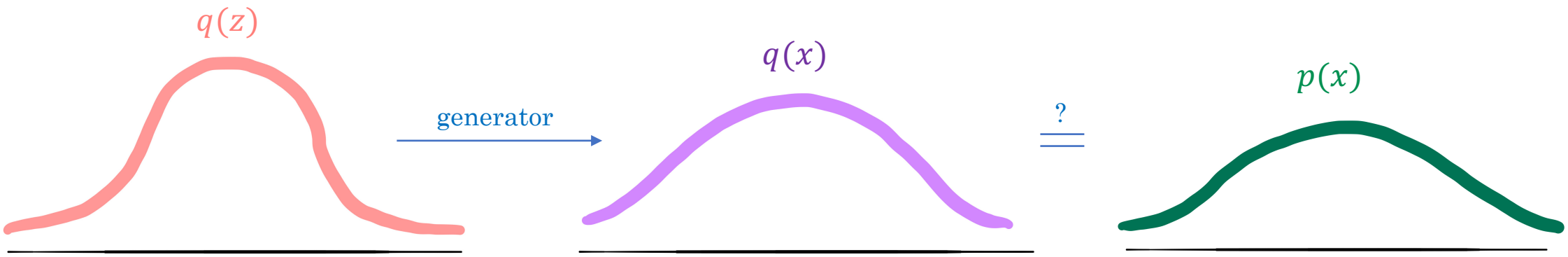

Derivation for Variational Autoencoder (VAE)

$p(x)$: Evidence probability for the sample $\{x_i\}_1^N$

$q(x)$: Proposed probability to approximate $p(x)$

Step 1: Approximating by minimizing KL divergence: $\min KL(p(x) \,||\, q(x))$

Derivation for VAE

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$q(x)$: Proposed probability to approximate $p(x)$

Step 1: Approximating by minimizing KL divergence: $\min KL(p(x) \,||\, q(x))$

Step 2: Introducing latent variable z, by defining:

$$p(x,z) = p(x)p(z|x)$$

$$q(x,z) = q(z)q(x|z)$$

Derivation for VAE

$p(x)$: Evidence probability for the sample $\{x_i\}_1^N$

$q(x)$: Proposed probability to approximate $p(x)$

$q(z)$: Pre-defined prior for the latent vector z

$p(z|x)$: Posterior of z given x.

$q(x|z)$: Posterior of x given z.

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Step 1: Approximating by minimizing KL divergence: $\min KL(p(x) \,||\, q(x))$

Step 2: Introducing latent variable z, such that $p(x,z) = p(x)p(z|x)$ and $q(x,z) = q(z)q(x|z)$.

Step 3: Show that $KL(p(x) \,||\, q(x))$ is upper bounded by $KL(p(x,z)||\, q(x,z))$:

$$KL(p(x,z)||\, q(x,z)) = KL\big(p(x) \,||\, q(x)\big) + \int p(x) KL\big(p(z|x) \,||\, q(z|x)\big) dx$$
$$\geq KL\big(p(x) \,||\, q(x)\big)$$

Derivation for VAE

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$q(x)$: Proposed probability to approximate $p(x)$

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Step 4: Reformulate the goal:

$$\min KL(p(x,z)||\, q(x,z))$$

$$\Updownarrow$$

$$\min \mathbb{E}_{x\sim p(x)}\left[\left[KL(p(z|x)\,||\,q(z)) + \mathbb{E}_{z\sim p(z|x)}[-\log q(x|z)]\right]\right]$$

Derivation for VAE *(Special Case of Information Bottleneck)*

$p(x)$: Evidence probability for the sample $\{x_i\}_1^N$

$q(x)$: Proposed probability to approximate $p(x)$

$q(z)$: Pre-defined prior for the latent vector z

$p(z|x)$: Posterior of z given x: *learned by encoder*

$q(x|z)$: Posterior of x given z: *learned by decoder*

Step 4: Reformulate the goal:

$$\min KL(p(x)||\, q(x))$$

$$\Updownarrow$$

$$\min \mathbb{E}_{x\sim p(x)}\left[\left[KL(p(z|x)\,||\,q(z)) + \mathbb{E}_{z\sim p(z|x)}[-\log q(x|z)]\right]\right]$$

$p(z|x)$: encoder; $q(z)$: pre-defined prior; $q(x|z)$: decoder

Derivation for VAE *(Special Case of Information Bottleneck)*

$p(x)$: Evidence probability for the sample $\{x_i\}_1^N$

$q(x)$: Proposed probability to approximate $p(x)$

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$$\min KL(p(x)||\, q(x))$$

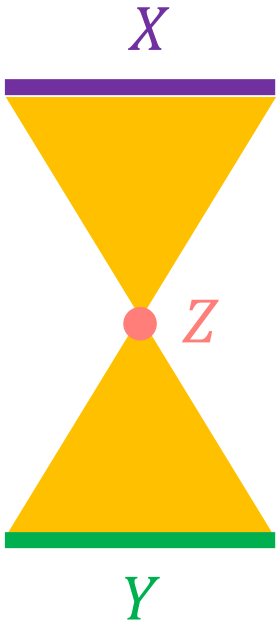
$$\Updownarrow$$

$$\min \mathbb{E}_{x\sim p(x)}\Big[KL(p(z|x)\,||\,q(z)) + \mathbb{E}_{z\sim p(z|x)}[-\log q(x|z)]\Big]$$

$KL(p(z|x)\,||\,q(z))$: *Regularizer*

$\mathbb{E}_{z\sim p(z|x)}[-\log q(x|z)]$: *Reconstruction Loss*

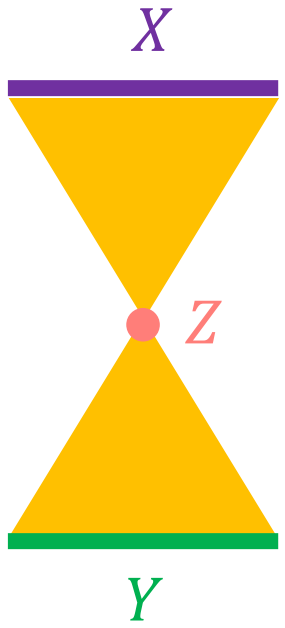
Variational Information Bottleneck (VIB)



$$\max_{\boldsymbol{\theta}} I(Z, Y; \boldsymbol{\theta})$$

$$\text{s.t. } I(X, Z; \boldsymbol{\theta}) \leq I_c$$

Variational Information Bottleneck (VIB)



$$\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Solve for $I(Z, Y)$

$$I(Z, Y) = \int p(y, z) \log \frac{p(y|z)}{p(y)} dydz$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Solve for $I(Z, Y)$

$$I(Z, Y) = \int p(y, z) \log \frac{p(y|z)}{p(y)} dy dz$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Solve for $I(Z, Y)$

$$I(Z,Y) = \int p(y,z) \log \frac{p(y|z)}{p(y)} dydz$$

$$\geq \int p(y,z) \log \frac{q(y|z)}{p(y)} dydz \longrightarrow \text{Decoder!}$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Solve for $I(Z, Y)$

$$
\begin{aligned}
I(Z, Y) &= \int p(y, z) \log \frac{p(y|z)}{p(y)} dydz \\
&\geq \int p(y, z) \log \frac{q(y|z)}{p(y)} dydz \quad \longrightarrow \text{Decoder!} \\
&= \int p(y, z) \log q(y|z) dydz - \int p(y) \log q(y) dy
\end{aligned}
$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Solve for $I(Z, Y)$

$$
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I(Z,Y) &= \int p(y,z) \log \frac{p(y|z)}{p(y)} dydz \\
&\geq \int p(y,z) \log \frac{q(y|z)}{p(y)} dydz \quad \longrightarrow \text{Decoder!} \\
&= \int p(y,z) \log q(y|z) dydz - \int p(y) \log q(y) dy \\
&\geq \int p(y,z) \log q(y|z) dydz
\end{aligned}
$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

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→ Encoder!

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→ Encoder!

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Solve for $I(Z, X)$

$$I(Z, X) = \int p(x, z) \log \frac{p(z|x)}{p(z)} dxdz \quad \rightarrow \text{Encoder!}$$

$$\leq \int p(x, z) \log \frac{p(z|x)}{q(z)} dxdz \quad \rightarrow \text{Pre-defined Prior!}$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Solve for $I(Z, X)$

$$I(Z, X) = \int p(x, z) \log \frac{p(z|x)}{p(z)} dx dz \quad \rightarrow \text{Encoder!}$$

$$\leq \int p(x, z) \log \frac{p(z|x)}{q(z)} dx dz \quad \rightarrow \text{Pre-defined Prior!}$$

$$= \int p(x) p(z|x) \log \frac{p(z|x)}{q(z)} dx dz$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Put together…

$$I(Z,Y) - \beta I(Z,X) \geq \int p(x)p(y|x)y(z|x) \log q(y|z) dx dy dz - \beta \int p(x)p(z|x) \log \frac{p(z|x)}{q(z)} dx dz$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Put together…

$$I(Z,Y) - \beta I(Z,X) \geq \int p(x)p(y|x)y(z|x) \log q(y|z) dx dy dz - \beta \int p(x)p(z|x) \log \frac{p(z|x)}{q(z)} dx dz$$

$$= \mathbb{E}_{x \sim p(x)} \left[\mathbb{E}_{z \sim p(z|x)} [-\log q(y|z)] + \beta \cdot KL(p(z|x) \| q(z)) \right]$$

Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Put together…

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Solve for $\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$

Put together…

$$I(Z,Y) - \beta I(Z,X) \geq \int p(x)p(y|x)y(z|x) \log q(y|z) dxdydz - \beta \int p(x)p(z|x) \log \frac{p(z|x)}{q(z)} dxdz$$

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$$= \mathbb{E}_{x \sim p(x)} \left[\beta \cdot KL(p(z|x) \| q(z)) + \mathbb{E}_{z \sim p(z|x)} [-\log q(y|z)] \right]$$

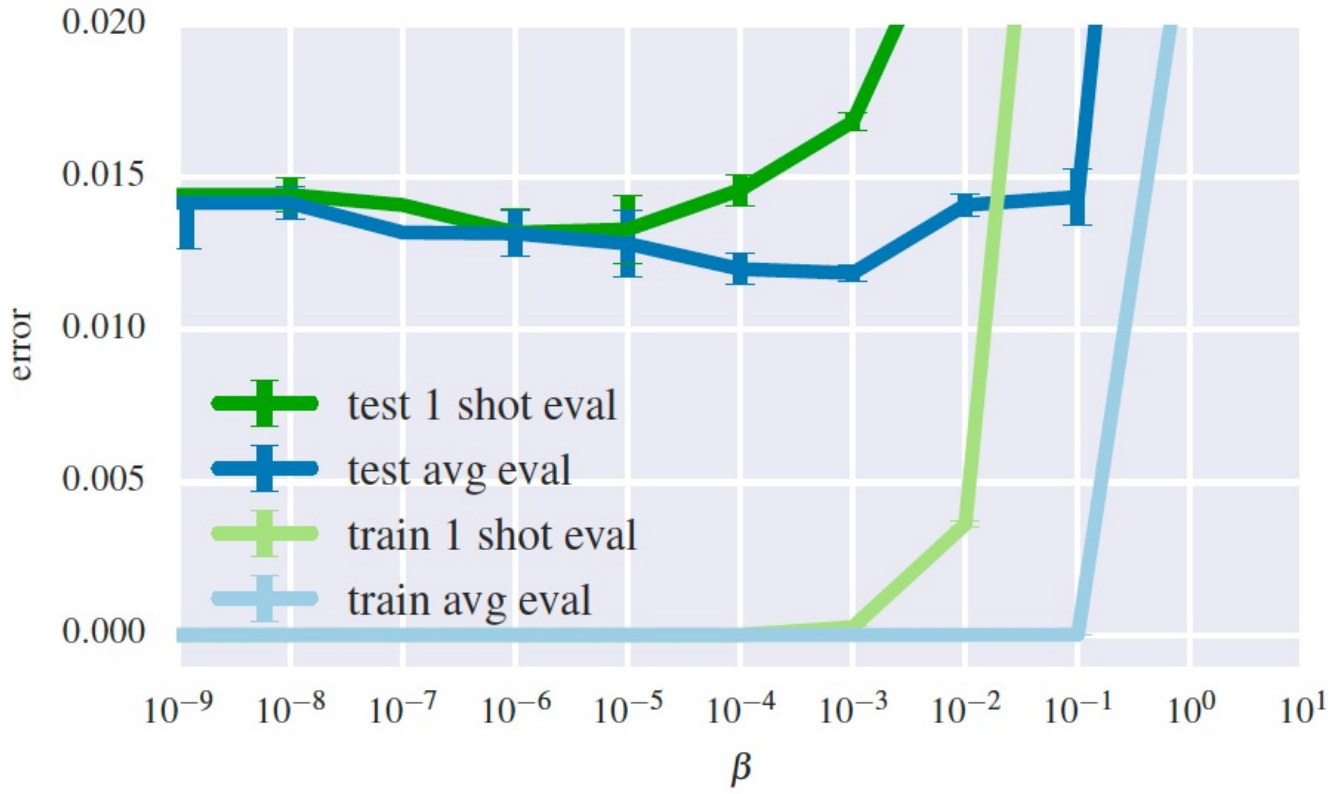
VAE as a special class for Information Bottleneck

$$\min \mathbb{E}_{x \sim p(x)} \left[KL(p(z|x) \,||\, q(z)) + \mathbb{E}_{z \sim p(z|x)} [-\log q(x|z)] \right]$$

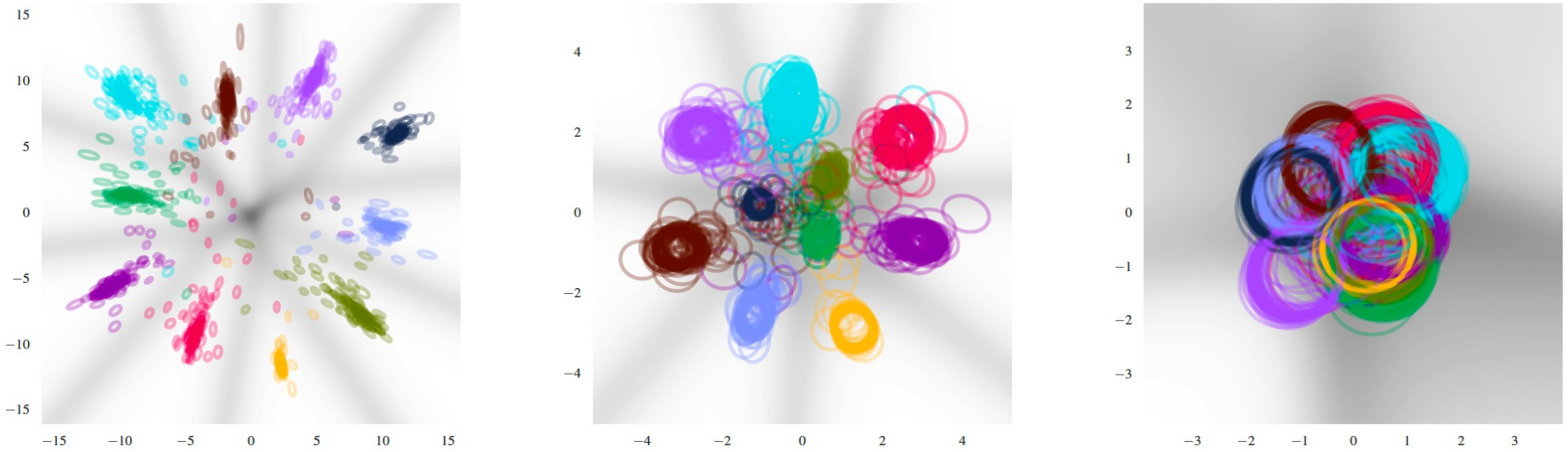
Performance on MNIST

Model	error
Baseline	1.38%
Dropout	1.34%
Dropout (Pereyra et al., 2016)	1.40%
Confidence Penalty	1.36%
Confidence Penalty (Pereyra et al., 2016)	1.17%
Label Smoothing	1.40%
Label Smoothing (Pereyra et al., 2016)	1.23%
VIB ($\beta = 10^{-3}$)	**1.13%**

Effect of β on Performance

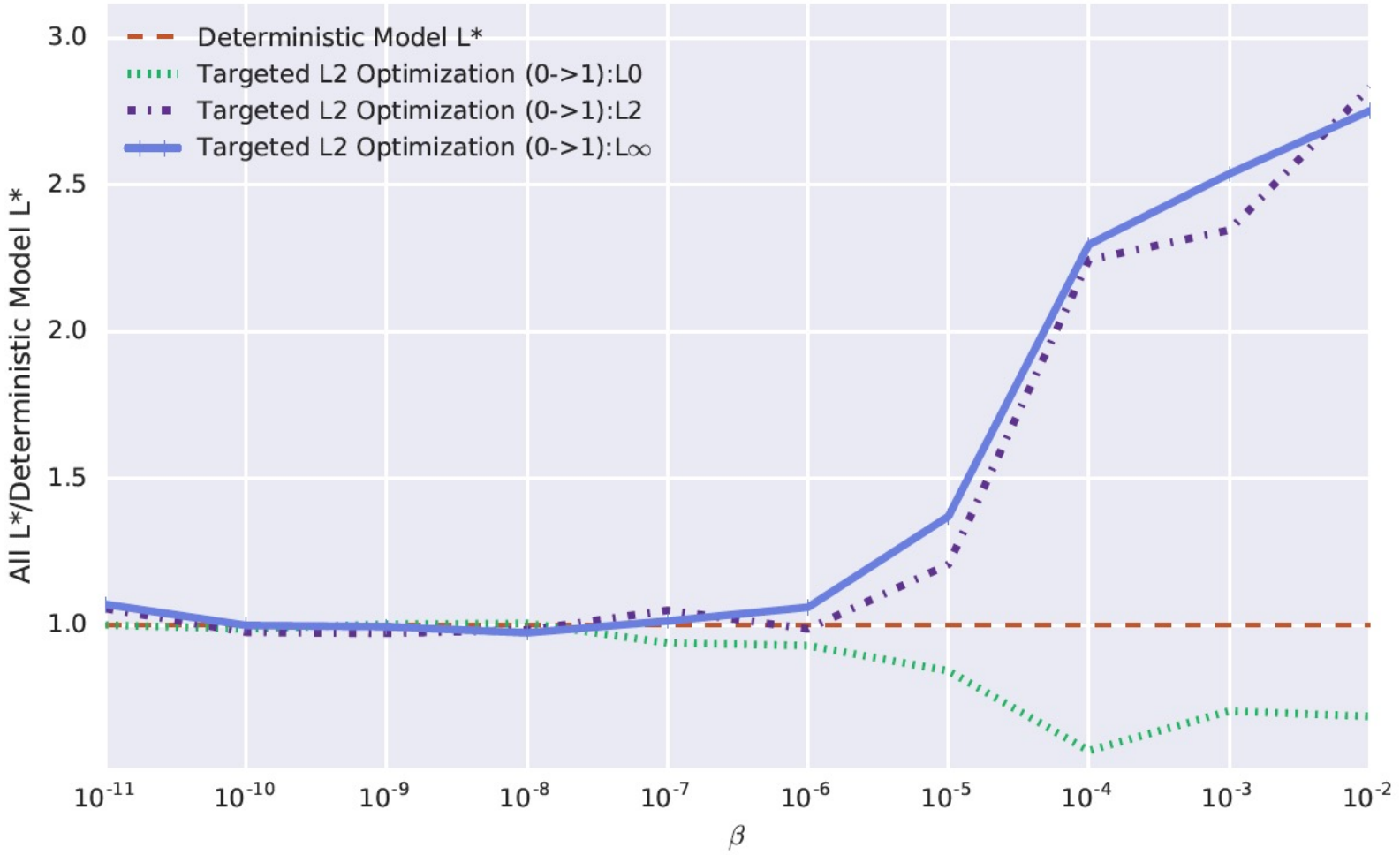


Effect of β on Representation Learning

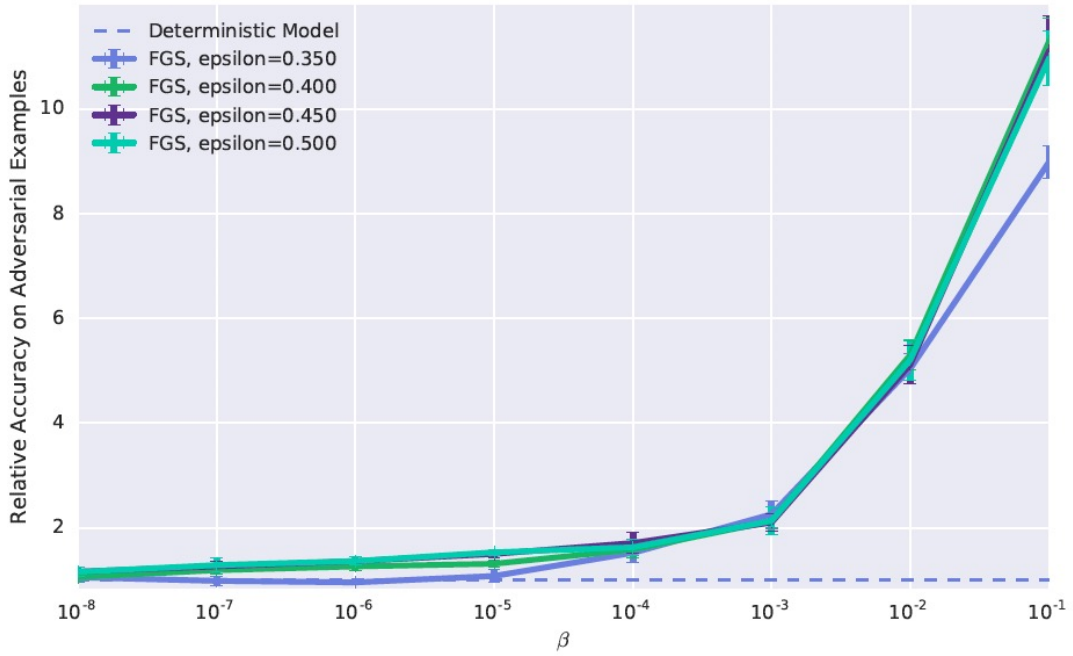


(a) $\beta = 10^{-3}$, $\text{err}_{\text{mc}} = 3.18\%$, $\text{err}_1 = 3.24\%$ (b) $\beta = 10^{-1}$, $\text{err}_{\text{mc}} = 3.44\%$, $\text{err}_1 = 4.32\%$ (c) $\beta = 10^{0}$, $\text{err}_{\text{mc}} = 33.82\%$, $\text{err}_1 = 62.81\%$.

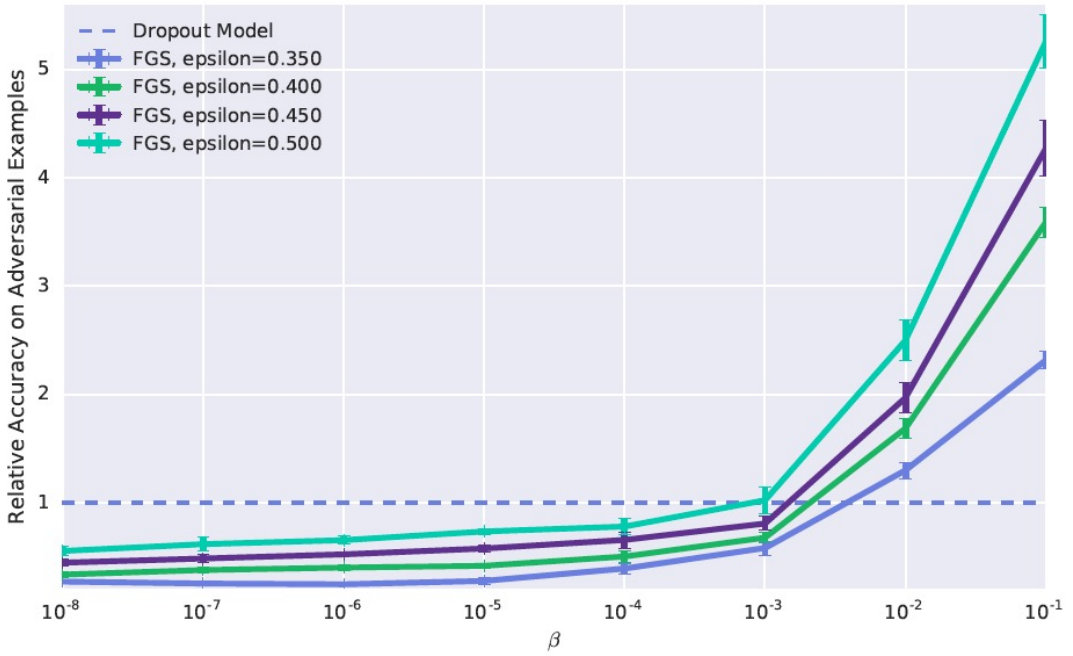
Adversarial Robustness



Effect of β on Relative Accuracy on Adversarial Examples (FGS)



(a)

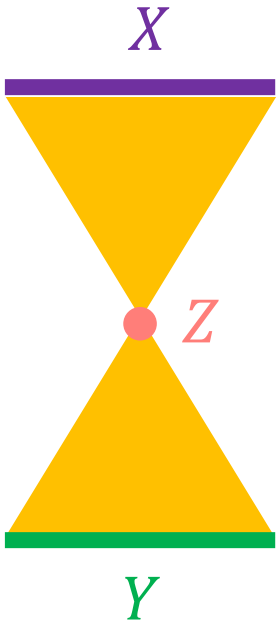


(b)

Adversarial Robustness

Metric	Determ	IRv2	VIB(0.01)
Sucessful target	1.0	1.0	**0.567**
L_2	6.45	14.43	**43.27**
L_∞	0.18	0.44	**0.92**

Conclusions



$$\max_{\theta} I(Z, Y; \theta) - \beta I(Z, X; \theta)$$