Smoothing Probability Distributions for High Dimensional Learning and Inference

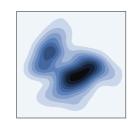
Ziv Goldfeld

Cornell University

CS Brown Bag Talk

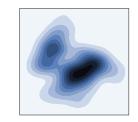
December 1st, 2020

Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$



Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

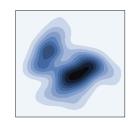
'Learning' Objective: Loss, info. measure, distance...



Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...

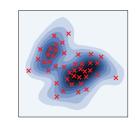
Estimation: We don't have P but i.i.d. data $\{X_i\}_{i=1}^n$



Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...

Estimation: We don't have P but i.i.d. data $\{X_i\}_{i=1}^n$

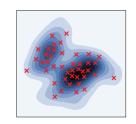


Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...

Estimation: We don't have P but i.i.d. data $\{X_i\}_{i=1}^n$

 \implies Estimate objective based on $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$



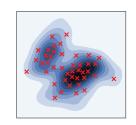
Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...

Estimation: We don't have P but i.i.d. data $\{X_i\}_{i=1}^n$

 \implies Estimate objective based on $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$

***** Estimation error is typically $n^{-1/d}$



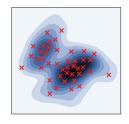
Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...

Estimation: We don't have P but i.i.d. data $\{X_i\}_{i=1}^n$

 \implies Estimate objective based on $P_n:=rac{1}{n}\sum\limits_{i=1}^n \delta_{X_i}$

***** Estimation error is typically $n^{-1/d}$





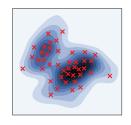
Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...

Estimation: We don't have P but i.i.d. data $\{X_i\}_{i=1}^n$

 \implies Estimate objective based on $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$

***** Estimation error is typically $n^{-1/d}$





Smoothing: Use $P*\mathcal{N}_{\sigma}$ and $P_n*\mathcal{N}_{\sigma}$, $\mathcal{N}_{\sigma} = \mathcal{N}(0, \sigma^2 I_d)$ (X+Z replaces X)

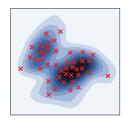
Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...

Estimation: We don't have P but i.i.d. data $\{X_i\}_{i=1}^n$

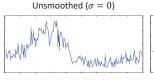
 \implies Estimate objective based on $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$

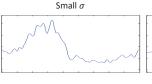
 ${f \$}$ Estimation error is typically $n^{-1/d}$

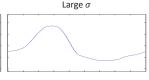




Smoothing: Use $P*\mathcal{N}_{\sigma}$ and $P_n*\mathcal{N}_{\sigma}$, $\mathcal{N}_{\sigma} = \mathcal{N}(0, \sigma^2 I_d)$ (X+Z replaces X)

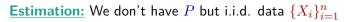






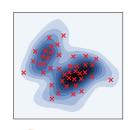
Data Distribution: $P \in \mathcal{P}(\mathbb{R}^d)$ where $d \gg 1$

'Learning' Objective: Loss, info. measure, distance...



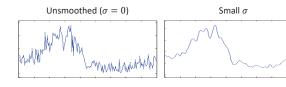
$$\implies$$
 Estimate objective based on $P_n:=\frac{1}{n}\sum_{i=1}^n \delta_{X_i}$

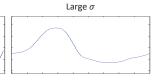
 \circledast Estimation error is typically $n^{-1/d}$





Smoothing: Use $P*\mathcal{N}_{\sigma}$ and $P_n*\mathcal{N}_{\sigma}$, $\mathcal{N}_{\sigma} = \mathcal{N}(0, \sigma^2 \mathbf{I}_d)$ (X+Z replaces X)





Alleviates CoD: Enhancing empirical convergence to $n^{-1/2} \ \forall d$

Part I:

Measuring Information Flows in Smoothed Deep Neural Networks

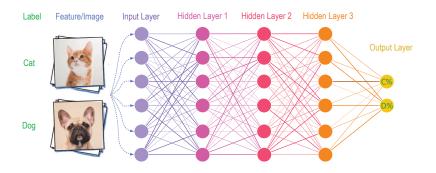
Unprecedented practical success

Unprecedented practical success

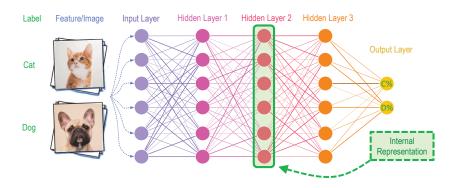


- Unprecedented practical success
- Lacking Theory: Macroscopic understanding of deep learning

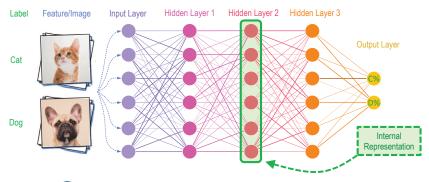
- Unprecedented practical success
- Lacking Theory: Macroscopic understanding of deep learning



- Unprecedented practical success
- Lacking Theory: Macroscopic understanding of deep learning

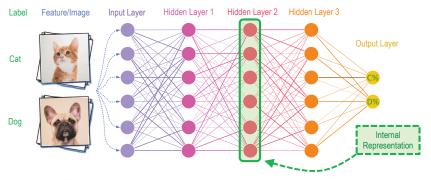


- Unprecedented practical success
- Lacking Theory: Macroscopic understanding of deep learning



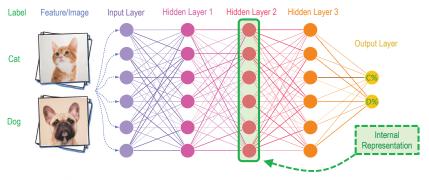
What drives the evolution of internal representations?

- Unprecedented practical success
- Lacking Theory: Macroscopic understanding of deep learning



- What drives the evolution of internal representations?
- What are properties of learned representations?

- Unprecedented practical success
- Lacking Theory: Macroscopic understanding of deep learning



- What drives the evolution of internal representations?
- What are properties of learned representations?
- ? How fully trained networks process information?

Trying to Understand Effectiveness of DL:

• Statistical learning theory: Over-parametrization and double descent [Belkin-Hsu-Ma'18, Liang-Rakhlin'18, Bartlett-Long-Lugosi-Tsiglera'20]

- Statistical learning theory: Over-parametrization and double descent [Belkin-Hsu-Ma'18, Liang-Rakhlin'18, Bartlett-Long-Lugosi-Tsiglera'20]
- Optimization theory: Dynamics in parameter space [Saxe-McClelland-Ganguli'14, Foster-Sekhari-Sridharan'18, Li-Liang'18]

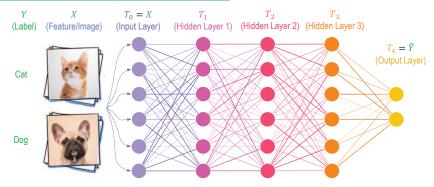
- Statistical learning theory: Over-parametrization and double descent [Belkin-Hsu-Ma'18, Liang-Rakhlin'18, Bartlett-Long-Lugosi-Tsiglera'20]
- Optimization theory: Dynamics in parameter space
 [Saxe-McClelland-Ganguli'14, Foster-Sekhari-Sridharan'18, Li-Liang'18]
- Approximation theory: Efficiently representable functions
 [Hajnal-et al'93, Delalleau-Bengio'11, Eldan-Shamir'15, Telgarsky'16, Poggio-et al'17]

- Statistical learning theory: Over-parametrization and double descent [Belkin-Hsu-Ma'18, Liang-Rakhlin'18, Bartlett-Long-Lugosi-Tsiglera'20]
- Optimization theory: Dynamics in parameter space
 [Saxe-McClelland-Ganguli'14, Foster-Sekhari-Sridharan'18, Li-Liang'18]
- Approximation theory: Efficiently representable functions
 [Hajnal-et al'93, Delalleau-Bengio'11, Eldan-Shamir'15, Telgarsky'16, Poggio-et al'17]
- Information theory: Track information flows through the network [Tishby-Zaslavsky'15, Shwartz-Tishby'17, Saxe et al.'18, Goldfeld et al.'19]

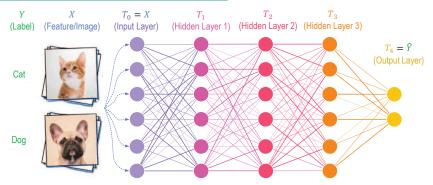
- Statistical learning theory: Over-parametrization and double descent [Belkin-Hsu-Ma'18, Liang-Rakhlin'18, Bartlett-Long-Lugosi-Tsiglera'20]
- Optimization theory: Dynamics in parameter space
 [Saxe-McClelland-Ganguli'14, Foster-Sekhari-Sridharan'18, Li-Liang'18]
- Approximation theory: Efficiently representable functions
 [Hajnal-et al'93, Delalleau-Bengio'11, Eldan-Shamir'15, Telgarsky'16, Poggio-et al'17]
- Information theory: Track information flows through the network [Tishby-Zaslavsky'15, Shwartz-Tishby'17, Saxe et al.'18, Goldfeld et al.'19]
 - Information-theoretic complexity measures of representations

- Statistical learning theory: Over-parametrization and double descent [Belkin-Hsu-Ma'18, Liang-Rakhlin'18, Bartlett-Long-Lugosi-Tsiglera'20]
- Optimization theory: Dynamics in parameter space
 [Saxe-McClelland-Ganguli'14, Foster-Sekhari-Sridharan'18, Li-Liang'18]
- Approximation theory: Efficiently representable functions
 [Hajnal-et al'93, Delalleau-Bengio'11, Eldan-Shamir'15, Telgarsky'16, Poggio-et al'17]
- Information theory: Track information flows through the network [Tishby-Zaslavsky'15, Shwartz-Tishby'17, Saxe et al.'18, Goldfeld et al.'19]
 - Information-theoretic complexity measures of representations
 - New generalization bounds, architectures, and algorithms

- Statistical learning theory: Over-parametrization and double descent [Belkin-Hsu-Ma'18, Liang-Rakhlin'18, Bartlett-Long-Lugosi-Tsiglera'20]
- Optimization theory: Dynamics in parameter space
 [Saxe-McClelland-Ganguli'14, Foster-Sekhari-Sridharan'18, Li-Liang'18]
- Approximation theory: Efficiently representable functions
 [Hajnal-et al'93, Delalleau-Bengio'11, Eldan-Shamir'15, Telgarsky'16, Poggio-et al'17]
- Information theory: Track information flows through the network [Tishby-Zaslavsky'15, Shwartz-Tishby'17, Saxe et al.'18, Goldfeld et al.'19]
 - Information-theoretic complexity measures of representations
 - New generalization bounds, architectures, and algorithms
 - Visualization and interpertability

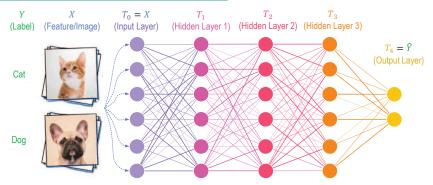


(Deterministic) Feedforward DNN: Each layer $T_{\ell} = f_{\ell}(T_{\ell-1})$

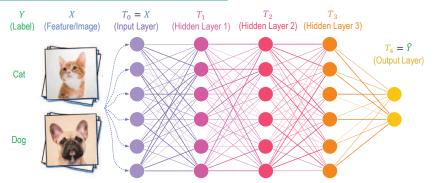


• Joint Distribution: $P_{X,Y}$

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



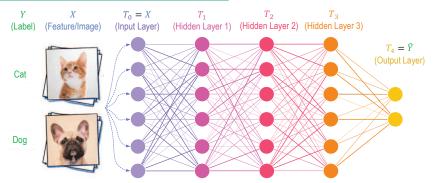
• Joint Distribution: $P_{X,Y} \implies P_{X,Y} \cdot P_{T_1,\dots,T_L|X}$



- Joint Distribution: $P_{X,Y} \implies P_{X,Y} \cdot P_{T_1,\dots,T_L|X}$
- Information Flows: $I(X;T_{\ell})$, $I(Y;T_{\ell})$, and $I(T_k;T_{\ell})$.

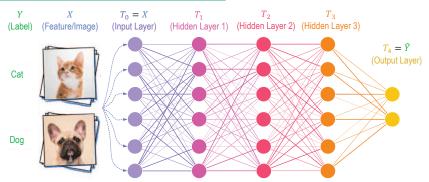
- Joint Distribution: $P_{X,Y} \implies P_{X,Y} \cdot P_{T_1,\dots,T_L|X}$
- Information Flows: $I(X;T_{\ell})$, $I(Y;T_{\ell})$, and $I(T_k;T_{\ell})$.

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



- Joint Distribution: $P_{X,Y} \implies P_{X,Y} \cdot P_{T_1,\dots,T_L|X}$
- Information Flows: $I(X; T_{\ell})$, $I(Y; T_{\ell})$, and $I(T_k; T_{\ell})$.

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

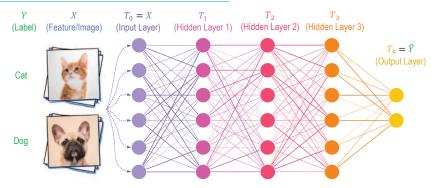


- Joint Distribution: $P_{X,Y} \implies P_{X,Y} \cdot P_{T_1,\dots,T_L|X}$
- Information Flows: $I(X; T_{\ell})$, $I(Y; T_{\ell})$, and $I(T_k; T_{\ell})$.

Data Processing Inequality: $I(Y;T_\ell) \leq I(X;T_\ell)$

Information Flows in DNNs: Empirical Observations

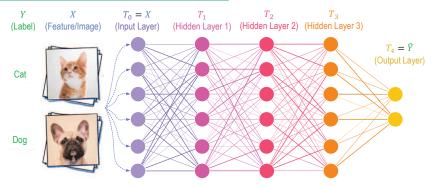
(Deterministic) Feedforward DNN: Each layer $T_{\ell} = f_{\ell}(T_{\ell-1})$



Training: Track $(I(Y;T_{\ell}),I(X;T_{\ell}))$ dynamics

Information Flows in DNNs: Empirical Observations

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

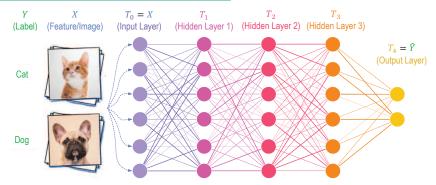


Training: Track $(I(Y;T_{\ell}),I(X;T_{\ell}))$ dynamics

• Fitting: $I(Y;T_{\ell})$ & $I(X;T_{\ell})$ rise (short)

Information Flows in DNNs: Empirical Observations

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



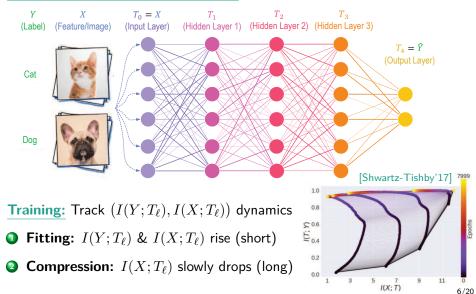
Training: Track $(I(Y;T_{\ell}),I(X;T_{\ell}))$ dynamics

• Fitting: $I(Y;T_{\ell})$ & $I(X;T_{\ell})$ rise (short)

2 Compression: $I(X;T_{\ell})$ slowly drops (long)

Information Flows in DNNs: Empirical Observations

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



Deterministic DNNs: MI degenerates or has $n^{-1/d}$ sample complexity

Deterministic DNNs: MI degenerates or has $n^{-1/d}$ sample complexity

Past methods are heuristic and w/o accuracy guarantees

Deterministic DNNs: MI degenerates or has $n^{-1/d}$ sample complexity

Past methods are heuristic and w/o accuracy guarantees

Goal: Meaningful MI & Accurate and scalable (in d) estimators

Deterministic DNNs: MI degenerates or has $n^{-1/d}$ sample complexity

Past methods are heuristic and w/o accuracy guarantees

Goal: Meaningful MI & Accurate and scalable (in d) estimators

Smoothing Inject (small) Gaussian noise to neurons' output

[Goldfeld-Berg-Greenewald-Melnyk-Nguyen-Kingsbury-Polyanskiy'19]

Deterministic DNNs: MI degenerates or has $n^{-1/d}$ sample complexity

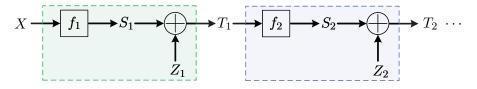
• Past methods are heuristic and w/o accuracy guarantees

Goal: Meaningful MI & Accurate and scalable (in d) estimators

Smoothing Inject (small) Gaussian noise to neurons' output

[Goldfeld-Berg-Greenewald-Melnyk-Nguyen-Kingsbury-Polyanskiy'19]

• Formally: $T_\ell = S_\ell + Z_\ell$, where $S_\ell := f_\ell(T_{\ell-1})$ and $Z_\ell \sim \mathcal{N}(0, \sigma^2 \mathrm{I}_d)$



Deterministic DNNs: MI degenerates or has $n^{-1/d}$ sample complexity

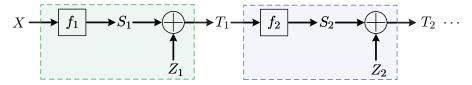
• Past methods are heuristic and w/o accuracy guarantees

Goal: Meaningful MI & Accurate and scalable (in d) estimators

Smoothing Inject (small) Gaussian noise to neurons' output

[Goldfeld-Berg-Greenewald-Melnyk-Nguyen-Kingsbury-Polyanskiy'19]

• Formally: $T_\ell = S_\ell + Z_\ell$, where $S_\ell := f_\ell(T_{\ell-1})$ and $Z_\ell \sim \mathcal{N}(0, \sigma^2 \mathrm{I}_d)$



⇒ Good proxy of det. DNN wrt performance & learned representations

Deterministic DNNs: MI degenerates or has $n^{-1/d}$ sample complexity

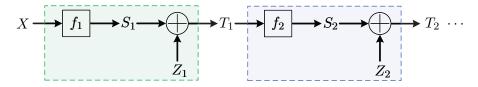
• Past methods are heuristic and w/o accuracy guarantees

Goal: Meaningful MI & Accurate and scalable (in d) estimators

Smoothing Inject (small) Gaussian noise to neurons' output

[Goldfeld-Berg-Greenewald-Melnyk-Nguyen-Kingsbury-Polyanskiy'19]

• Formally: $T_\ell = S_\ell + Z_\ell$, where $S_\ell := f_\ell(T_{\ell-1})$ and $Z_\ell \sim \mathcal{N}(0, \sigma^2 \mathrm{I}_d)$



- ⇒ Good proxy of det. DNN wrt performance & learned representations
- ⇒ Mutual information can be efficiently estimated over noisy DNN!

Theorem (Goldfeld-Greenewald-Weed-Polyanskiy'20)

For a DNN w/ bdd. activations (tanh/sigmoid), $\sigma>0$, and $\ell=1,\ldots,L$: $\inf_{\text{estimator } \hat{I}_{\sigma}}\sup_{P_X\in\mathcal{P}(\mathbb{R}^d)}\mathbb{E}\left|I(X;T_{\ell})-\hat{I}_{\sigma}(X^n,f_1,\ldots,f_{\ell})\right|\leq C_{\sigma,d_{\ell}}\cdot n^{-\frac{1}{2}}$

where
$$X^n := (X_1, \dots, X_n) \stackrel{\text{i.i.d.}}{\sim} P_X$$
 and $C_{\sigma, d_\ell} = e^{\Theta(d_\ell)}$.

Theorem (Goldfeld-Greenewald-Weed-Polyanskiy'20)

For a DNN w/ bdd. activations (tanh/sigmoid), $\sigma>0$, and $\ell=1,\ldots,L$: $\inf_{\text{estimator }\hat{I}_{\sigma}}\sup_{P_X\in\mathcal{P}(\mathbb{R}^d)}\mathbb{E}\left|I(X;T_{\ell})-\hat{I}_{\sigma}(X^n,f_1,\ldots,f_{\ell})\right|\leq C_{\sigma,d_{\ell}}\cdot n^{-\frac{1}{2}}$ where Y^n is $(Y_{\sigma},Y_{\sigma})^{i.i.d.}$ P_{σ} and C_{σ} $P(d_{\ell})$

where $X^n := (X_1, \dots, X_n) \stackrel{i.i.d.}{\sim} P_X$ and $C_{\sigma, d_\ell} = e^{\Theta(d_\ell)}$.

Estimator: Propagate samples & Gaussian conv. w/ empirical measure

Theorem (Goldfeld-Greenewald-Weed-Polyanskiy'20)

For a DNN w/ bdd. activations (tanh/sigmoid), $\sigma > 0$, and $\ell = 1, \ldots, L$:

$$\inf_{\textit{estimator } \hat{I}_{\sigma}} \sup_{P_{X} \in \mathcal{P}(\mathbb{R}^{d})} \mathbb{E} \left| I(X; T_{\ell}) - \hat{I}_{\sigma}(X^{n}, f_{1}, \ldots, f_{\ell}) \right| \leq C_{\sigma, d_{\ell}} \cdot n^{-\frac{1}{2}}$$

where
$$X^n:=(X_1,\ldots,X_n)\stackrel{\text{i.i.d.}}{\sim} P_X$$
 and $C_{\sigma,d_\ell}=e^{\Theta(d_\ell)}$.

Estimator: Propagate samples & Gaussian conv. w/ empirical measure

• Optimal & explicit: Parametric rate $n^{-1/2}$ & concrete error bounds

Theorem (Goldfeld-Greenewald-Weed-Polyanskiy'20)

For a DNN w/ bdd. activations (tanh/sigmoid), $\sigma>0$, and $\ell=1,\ldots,L$:

$$\inf_{\textit{estimator } \hat{I}_{\sigma}} \sup_{P_{X} \in \mathcal{P}(\mathbb{R}^{d})} \mathbb{E} \left| I(X; T_{\ell}) - \hat{I}_{\sigma}(X^{n}, f_{1}, \ldots, f_{\ell}) \right| \leq C_{\sigma, d_{\ell}} \cdot n^{-\frac{1}{2}}$$

where
$$X^n:=(X_1,\ldots,X_n)\stackrel{\text{i.i.d.}}{\sim} P_X$$
 and $C_{\sigma,d_\ell}=e^{\Theta(d_\ell)}$.

Estimator: Propagate samples & Gaussian conv. w/ empirical measure

- **Optimal & explicit:** Parametric rate $n^{-1/2}$ & concrete error bounds
- Extensions: Readily adapted for $I(Y;T_\ell)$ and $I(T_k;T_\ell)$ estimation

Theorem (Goldfeld-Greenewald-Weed-Polyanskiy'20)

For a DNN w/ bdd. activations (tanh/sigmoid), $\sigma > 0$, and $\ell = 1, \dots, L$:

$$\inf_{\textit{estimator } \hat{I}_{\sigma}} \sup_{P_X \in \mathcal{P}(\mathbb{R}^d)} \mathbb{E} \left| I(X; T_{\ell}) - \hat{I}_{\sigma}(X^n, f_1, \dots, f_{\ell}) \right| \leq C_{\sigma, d_{\ell}} \cdot n^{-\frac{1}{2}}$$

where
$$X^n:=(X_1,\ldots,X_n)\stackrel{{\scriptscriptstyle i.i.d.}}{\sim} P_X$$
 and $C_{\sigma,d_\ell}=e^{\Theta(d_\ell)}.$

Estimator: Propagate samples & Gaussian conv. w/ empirical measure

- Optimal & explicit: Parametric rate $n^{-1/2}$ & concrete error bounds
- Extensions: Readily adapted for $I(Y;T_\ell)$ and $I(T_k;T_\ell)$ estimation

Future Goals: Improve scalability in d_ℓ & fast computational algorithm

Theorem (Goldfeld-Greenewald-Weed-Polyanskiy'20)

For a DNN w/ bdd. activations (tanh/sigmoid), $\sigma>0$, and $\ell=1,\ldots,L$:

$$\inf_{\textit{estimator } \hat{I}_{\sigma}} \sup_{P_{X} \in \mathcal{P}(\mathbb{R}^{d})} \mathbb{E} \left| I(X; T_{\ell}) - \hat{I}_{\sigma}(X^{n}, f_{1}, \ldots, f_{\ell}) \right| \leq C_{\sigma, d_{\ell}} \cdot n^{-\frac{1}{2}}$$

where
$$X^n := (X_1, \dots, X_n) \stackrel{\text{i.i.d.}}{\sim} P_X$$
 and $C_{\sigma, d_\ell} = e^{\Theta(d_\ell)}$.

Estimator: Propagate samples & Gaussian conv. w/ empirical measure

- Optimal & explicit: Parametric rate $n^{-1/2}$ & concrete error bounds
- Extensions: Readily adapted for $I(Y;T_\ell)$ and $I(T_k;T_\ell)$ estimation

Future Goals: Improve scalability in d_ℓ & fast computational algorithm

♦ Scalability: Manifold hypothesis and/or lower dimensional embeddings

Theorem (Goldfeld-Greenewald-Weed-Polyanskiy'20)

For a DNN w/ bdd. activations (tanh/sigmoid), $\sigma>0$, and $\ell=1,\ldots,L$: $\inf_{\substack{\text{estimator } \hat{I}_{\sigma} \ P_X \in \mathcal{P}(\mathbb{R}^d)}} \mathbb{E} \left| I(X;T_{\ell}) - \hat{I}_{\sigma}(X^n,f_1,\ldots,f_{\ell}) \right| \leq C_{\sigma,d_{\ell}} \cdot n^{-\frac{1}{2}}$ where $X^n := (X_1,\ldots,X_n) \stackrel{\text{i.i.d.}}{\sim} P_X$ and $C_{\sigma,d_{\ell}} = e^{\Theta(d_{\ell})}$.

Estimator: Propagate samples & Gaussian conv. w/ empirical measure

- Optimal & explicit: Parametric rate $n^{-1/2}$ & concrete error bounds
- Extensions: Readily adapted for $I(Y;T_\ell)$ and $I(T_k;T_\ell)$ estimation

Future Goals: Improve scalability in d_ℓ & fast computational algorithm

- **⊗** Scalability: Manifold hypothesis and/or lower dimensional embeddings
- **Algorithms:** Integrate high dimensional Gaussian conv. into DNN arch.

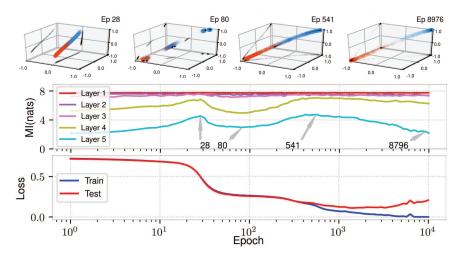
Noisy version of DNN from [Shwartz-Tishby'17]:

Noisy version of DNN from [Shwartz-Tishby'17]:

• Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP

Noisy version of DNN from [Shwartz-Tishby'17]:

Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP

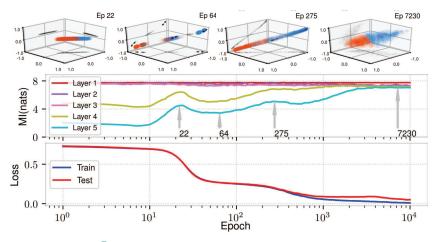


Noisy version of DNN from [Shwartz-Tishby'17]:

• Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP

Noisy version of DNN from [Shwartz-Tishby'17]:

Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP



weight orthonormality regularization

Noisy version of DNN from [Shwartz-Tishby'17]:

- Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP
- Verified in multiple experiments

Noisy version of DNN from [Shwartz-Tishby'17]:

- Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP
- Verified in multiple experiments
- \implies Compression of $I(X;T_{\ell})$ driven by clustering of representations

Noisy version of DNN from [Shwartz-Tishby'17]:

- Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP
- Verified in multiple experiments
- \implies Compression of $I(X;T_{\ell})$ driven by clustering of representations

Consequences and Future Goals: $I(X;T_{\ell})$ quantifies rep. complexity

Noisy version of DNN from [Shwartz-Tishby'17]:

- Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP
- Verified in multiple experiments
- \implies Compression of $I(X;T_{\ell})$ driven by clustering of representations

Consequences and Future Goals: $I(X;T_{\ell})$ quantifies rep. complexity

Noisy version of DNN from [Shwartz-Tishby'17]:

- Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP
- Verified in multiple experiments
- \implies Compression of $I(X;T_{\ell})$ driven by clustering of representations

Consequences and Future Goals: $I(X;T_{\ell})$ quantifies rep. complexity

- **ℜ** Regularization and prunning: Algorithmic & architectural advances

Noisy version of DNN from [Shwartz-Tishby'17]:

- Binary Classification: 12-bit input & 12-10-7-5-4-3-2 tanh MLP
- Verified in multiple experiments
- \implies Compression of $I(X;T_{\ell})$ driven by clustering of representations

Consequences and Future Goals: $I(X;T_{\ell})$ quantifies rep. complexity

- **ℜ** Regularization and prunning: Algorithmic & architectural advances
- **♦ Visualization and interpretability:** Heatmap of DNN neural activity

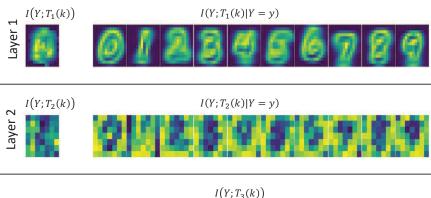
:

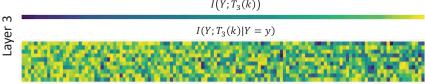
Mutual Information Heatmap Example

Noisy CNN for MNIST: Classification of hand-written digits

Mutual Information Heatmap Example

Noisy CNN for MNIST: Classification of hand-written digits





Part II:

Smooth Statistical Distances for High-Dimensional Learning and Inference

Goal: Learn a model $Q_{\theta} \approx P \in \mathcal{P}(\mathbb{R}^d)$ to approximate data distribution

Goal: Learn a model $Q_{\theta} pprox P \in \mathcal{P}(\mathbb{R}^d)$ to approximate data distribution

Method: Complicated transformation of a simple latent variable

Goal: Learn a model $Q_{\theta} pprox P \in \mathcal{P}(\mathbb{R}^d)$ to approximate data distribution

Method: Complicated transformation of a simple latent variable

• Latent variable $Z \sim Q_Z \in \mathcal{P}(\mathbb{R}^p)$, $p \ll d$

Goal: Learn a model $Q_{\theta} pprox P \in \mathcal{P}(\mathbb{R}^d)$ to approximate data distribution

Method: Complicated transformation of a simple latent variable

- Latent variable $Z \sim Q_Z \in \mathcal{P}(\mathbb{R}^p)$, $p \ll d$
- \bullet Expand Z to \mathbb{R}^d space via (random) transformation $Q_{X|Z}^{(\theta)}$

Goal: Learn a model $Q_{\theta} pprox P \in \mathcal{P}(\mathbb{R}^d)$ to approximate data distribution

Method: Complicated transformation of a simple latent variable

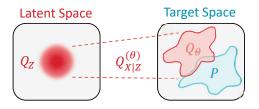
- Latent variable $Z \sim Q_Z \in \mathcal{P}(\mathbb{R}^p)$, $p \ll d$
- ullet Expand Z to \mathbb{R}^d space via (random) transformation $Q_{X|Z}^{(heta)}$
- \Longrightarrow Generative model: $Q_{\theta}(\cdot) := \int_{\mathbb{R}^p} Q_{X|Z}^{(\theta)}(\cdot|z) \, \mathrm{d}Q_Z(z)$

Implicit (Latent Variable) Generative Models

Goal: Learn a model $Q_{\theta} pprox P \in \mathcal{P}(\mathbb{R}^d)$ to approximate data distribution

Method: Complicated transformation of a simple latent variable

- Latent variable $Z \sim Q_Z \in \mathcal{P}(\mathbb{R}^p)$, $p \ll d$
- ullet Expand Z to \mathbb{R}^d space via (random) transformation $Q_{X|Z}^{(heta)}$
- \implies Generative model: $Q_{\theta}(\cdot) := \int_{\mathbb{R}^p} Q_{X|Z}^{(\theta)}(\cdot|z) \, \mathrm{d}Q_Z(z)$

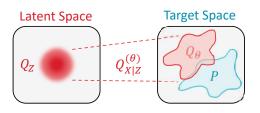


Implicit (Latent Variable) Generative Models

Goal: Learn a model $Q_{\theta} \approx P \in \mathcal{P}(\mathbb{R}^d)$ to approximate data distribution

Method: Complicated transformation of a simple latent variable

- Latent variable $Z \sim Q_Z \in \mathcal{P}(\mathbb{R}^p)$, $p \ll d$
- ullet Expand Z to \mathbb{R}^d space via (random) transformation $Q_{X|Z}^{(heta)}$
- \Longrightarrow Generative model: $Q_{\theta}(\cdot) := \int_{\mathbb{R}^p} Q_{X|Z}^{(\theta)}(\cdot|z) \, \mathrm{d}Q_Z(z)$



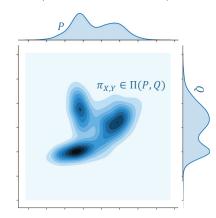
Minimum Distance Estimation: Solve $\theta^* \in \operatorname{argmin} \delta(P, Q_{\theta})$

$$\theta^{\star} \in \operatorname*{argmin}_{\theta} \delta(P, Q_{\theta})$$

Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

ullet Coupling: $\Pi(P,Q)=\left\{\pi_{X,Y}\in\mathcal{P}(\mathbb{R}^d imes\mathbb{R}^d)\;\middle| \pi_X=P\;\&\;\pi_Y=Q
ight\}$



Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

- Coupling: $\Pi(P,Q) = \left\{ \pi_{X,Y} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \ \middle| \pi_X = P \ \& \ \pi_Y = Q \right\}$
- Cost: c(x,y) = ||x-y|| for transporting x to y

Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

- Coupling: $\Pi(P,Q) = \left\{ \pi_{X,Y} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \middle| \pi_X = P \& \pi_Y = Q \right\}$
- Cost: c(x,y) = ||x y|| for transporting x to y

Definition (1-Wasserstein)

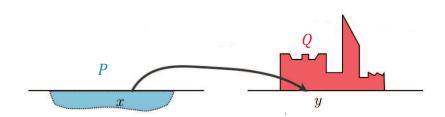
The 1-Wasserstein distance: $\mathsf{W}_1(P,Q) := \inf_{\pi_{X,Y} \in \Pi(P,Q)} \mathbb{E}_{\pi} \|X - Y\|$

Setup: $P, Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

- Coupling: $\Pi(P,Q) = \left\{ \pi_{X,Y} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \ \middle| \pi_X = P \ \& \ \pi_Y = Q \right\}$
- Cost: c(x,y) = ||x y|| for transporting x to y

Definition (1-Wasserstein)

The 1-Wasserstein distance: $\mathsf{W}_1(P,Q) := \inf_{\pi_{X,Y} \in \Pi(P,Q)} \mathbb{E}_{\pi} \|X - Y\|$



Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

- Coupling: $\Pi(P,Q) = \left\{ \pi_{X,Y} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \mid \pi_X = P \ \& \ \pi_Y = Q \right\}$
- Cost: c(x,y) = ||x y|| for transporting x to y

Definition (1-Wasserstein)

The 1-Wasserstein distance: $\mathsf{W}_1(P,Q) := \inf_{\pi_{X,Y} \in \Pi(P,Q)} \mathbb{E}_{\pi} \|X - Y\|$

Comments:

Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

- Coupling: $\Pi(P,Q) = \left\{ \pi_{X,Y} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \ \middle| \pi_X = P \ \& \ \pi_Y = Q \right\}$
- Cost: c(x,y) = ||x y|| for transporting x to y

Definition (1-Wasserstein)

The 1-Wasserstein distance: $\mathsf{W}_1(P,Q) := \inf_{\pi_{X,Y} \in \Pi(P,Q)} \mathbb{E}_{\pi} \|X - Y\|$

Comments:

• Robustness to Supp. Mismatch: $W_1(P,Q) < \infty$, $\forall P,Q \in \mathcal{P}_1(\mathbb{R}^d)$

Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

- Coupling: $\Pi(P,Q) = \left\{ \pi_{X,Y} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \middle| \pi_X = P \& \pi_Y = Q \right\}$
- Cost: $c(x,y) = \|x y\|$ for transporting x to y

Definition (1-Wasserstein)

The 1-Wasserstein distance: $\mathsf{W}_1(P,Q) := \inf_{\pi_{X,Y} \in \Pi(P,Q)} \mathbb{E}_{\pi} \|X - Y\|$

Comments:

- \bullet Robustness to Supp. Mismatch: $\mathsf{W}_1(P,Q)<\infty$, $\forall P,Q\in\mathcal{P}_1(\mathbb{R}^d)$
- ullet Metric: $\left(\mathcal{P}_1(\mathbb{R}^d),\mathsf{W}_1
 ight)$ is metric space (metrizes weak convergence)

Setup: $P,Q \in \mathcal{P}_1(\mathbb{R}^d)$ (subscript for finite 1st moments)

- Coupling: $\Pi(P,Q) = \left\{ \pi_{X,Y} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \ \middle| \pi_X = P \ \& \ \pi_Y = Q \right\}$
- Cost: c(x,y) = ||x-y|| for transporting x to y

Definition (1-Wasserstein)

The 1-Wasserstein distance: $\mathsf{W}_1(P,Q) := \inf_{\pi_{X,Y} \in \Pi(P,Q)} \mathbb{E}_{\pi} \|X - Y\|$

Comments:

- Robustness to Supp. Mismatch: $W_1(P,Q) < \infty$, $\forall P,Q \in \mathcal{P}_1(\mathbb{R}^d)$
- ullet Metric: $\left(\mathcal{P}_1(\mathbb{R}^d),\mathsf{W}_1
 ight)$ is metric space (metrizes weak convergence)
- Duality: $W_1(P,Q) = \sup_{f \in \text{Lin}} \mathbb{E}_P[f] \mathbb{E}_Q[f] \implies \text{W-GAN (minimax)}$

$$\underline{ \text{Dual Representation:}} \quad \mathsf{W}_1(P,Q) = \sup_{f \in \mathsf{Lip}_1(\mathbb{R}^d)} \mathbb{E}_P f(X) - \mathbb{E}_Q f(Y)$$

GANs [Goodfellow et al'14]:

GANs [Goodfellow et al'14]:

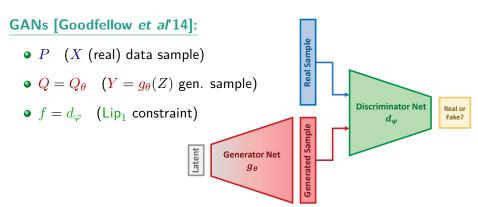
 \bullet P (X (real) data sample)

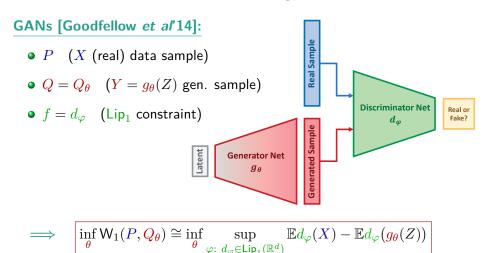
GANs [Goodfellow et al'14]:

- \bullet P (X (real) data sample)
- $Q = Q_{\theta}$ $(Y = g_{\theta}(Z) \text{ gen. sample})$

GANs [Goodfellow et al'14]:

- P (X (real) data sample)
- $ullet Q = Q_{ heta} \quad ig(Y = g_{ heta}(Z) \ ext{gen. sample}ig)$
- $f = d_{\varphi}$ (Lip₁ constraint)





Generative Adversarial Networks

NVIDIA's ProGAN 2.0 [Karras et al'19]



Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

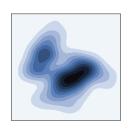
Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

Estimation: We don't have P but data

Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

Estimation: We don't have P but data

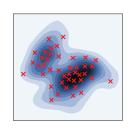
ullet $\{X_i\}_{i=1}^n$ are i.i.d. samples from $P\in\mathcal{P}(\mathbb{R}^d)$



Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

Estimation: We don't have P but data

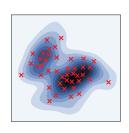
- ullet $\{X_i\}_{i=1}^n$ are i.i.d. samples from $P\in\mathcal{P}(\mathbb{R}^d)$
- Empirical distribution $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$



Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

Estimation: We don't have P but data

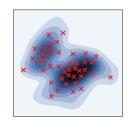
- ullet $\{X_i\}_{i=1}^n$ are i.i.d. samples from $P\in\mathcal{P}(\mathbb{R}^d)$
- Empirical distribution $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$
- \implies Inherently we work with $W_1(P_n,Q_{\theta})$



Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

Estimation: We don't have P but data

- ullet $\{X_i\}_{i=1}^n$ are i.i.d. samples from $P\in\mathcal{P}(\mathbb{R}^d)$
- Empirical distribution $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$
- \implies Inherently we work with $W_1(P_n, Q_\theta)$

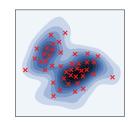


Optimization: Can solve $\inf_{\theta} W_1(P_n, Q_{\theta})$ approximately

Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

Estimation: We don't have P but data

- $\{X_i\}_{i=1}^n$ are i.i.d. samples from $P \in \mathcal{P}(\mathbb{R}^d)$
- Empirical distribution $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$
- \implies Inherently we work with $W_1(P_n, Q_\theta)$



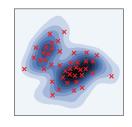
Optimization: Can solve $\inf_{\theta} W_1(P_n, Q_{\theta})$ approximately

Find $\hat{\theta}_n$ s.t. $W_1(P_n, Q_{\hat{\theta}_n}) \leq \inf_{\theta} W_1(P_n, Q_{\theta}) + \epsilon$

Goal: Solve OPT := $\inf_{\theta} W_1(P, Q_{\theta})$ exactly (find θ^*)

Estimation: We don't have P but data

- $\{X_i\}_{i=1}^n$ are i.i.d. samples from $P \in \mathcal{P}(\mathbb{R}^d)$
- Empirical distribution $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$
- \implies Inherently we work with $W_1(P_n, Q_\theta)$



Optimization: Can solve $\inf_{\theta} W_1(P_n, Q_{\theta})$ approximately

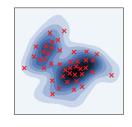
Find
$$\hat{\theta}_n$$
 s.t. $W_1(P_n, Q_{\hat{\theta}_n}) \leq \inf_{\theta} W_1(P_n, Q_{\theta}) + \epsilon$

Generalization:
$$W_1(P, Q_{\hat{\theta}_n}) - OPT \le 2W_1(P_n, P) + \epsilon$$

Goal: Solve OPT :=
$$\inf_{\theta} W_1(P, Q_{\theta})$$
 exactly (find θ^*)

Estimation: We don't have P but data

- ullet $\{X_i\}_{i=1}^n$ are i.i.d. samples from $P\in\mathcal{P}(\mathbb{R}^d)$
- Empirical distribution $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$
- \implies Inherently we work with $\mathsf{W}_1(P_n, Q_{\theta})$



Optimization: Can solve $\inf_{\theta} W_1(P_n, Q_{\theta})$ approximately

Find
$$\hat{\theta}_n$$
 s.t. $W_1(P_n, Q_{\hat{\theta}_n}) \leq \inf_{\theta} W_1(P_n, Q_{\theta}) + \epsilon$

Generalization:
$$W_1(P, Q_{\hat{\theta}_n}) - OPT \le 2W_1(P_n, P) + \epsilon$$

 \implies Boils down to empirical approximation question under W₁

Question: What can we say about $W_1(P_n, P)$?

Question: What can we say about $W_1(P_n, P)$?

Theorem (Dudley'69)

For $d \geq 3$ and $\mathcal{P}_1(\mathbb{R}^d) \ni P \ll \mathsf{Leb}(\mathbb{R}^d)$: $\mathbb{EW}_1(P_n, P) \asymp n^{-\frac{1}{d}}$

Question: What can we say about $W_1(P_n, P)$?

Theorem (Dudley'69)

For $d \geq 3$ and $\mathcal{P}_1(\mathbb{R}^d) \ni P \ll \mathsf{Leb}(\mathbb{R}^d)$: $\mathbb{E}\mathsf{W}_1(P_n, P) \asymp n^{-\frac{1}{d}}$



Question: What can we say about $W_1(P_n, P)$?

Theorem (Dudley'69)

For $d \geq 3$ and $\mathcal{P}_1(\mathbb{R}^d) \ni P \ll \mathsf{Leb}(\mathbb{R}^d)$: $\mathbb{EW}_1(P_n, P) \asymp n^{-\frac{1}{d}}$

Curse of Dimensionality

★ Implication: Too slow given dimensionality of real-world data

Question: What can we say about $W_1(P_n, P)$?

Theorem (Dudley'69)

For $d \geq 3$ and $\mathcal{P}_1(\mathbb{R}^d) \ni P \ll \mathsf{Leb}(\mathbb{R}^d)$: $\mathbb{EW}_1(P_n, P) \asymp n^{-\frac{1}{d}}$

Curse of Dimensionality

- * Implication: Too slow given dimensionality of real-world data
- **Question:** Can smoothing help alleviates CoD?

Smooth 1-Wasserstein Distance

Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma} := \mathcal{N}(0, \sigma^2 I_d)$ is a d-dimensional isotropic Gaussian.

Smooth 1-Wasserstein Distance

Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma}:=\mathcal{N}(0,\sigma^2\mathrm{I}_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

Smooth 1-Wasserstein Distance

Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma}:=\mathcal{N}(0,\sigma^2\mathrm{I}_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

$$X \perp Z_1 \implies X + Z_1 \sim P * \mathcal{N}_{\sigma}$$
 & $Y \perp Z_2 \implies Y + Z_2 \sim Q * \mathcal{N}_{\sigma}$

Definition (Goldfeld-Greenewald'19)

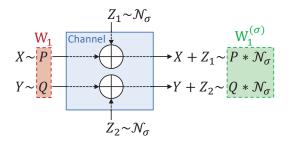
For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma}:=\mathcal{N}(0,\sigma^2\mathrm{I}_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

$$X \perp Z_1 \implies X + Z_1 \sim P * \mathcal{N}_{\sigma}$$
 & $Y \perp Z_2 \implies Y + Z_2 \sim Q * \mathcal{N}_{\sigma}$



Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma}:=\mathcal{N}(0,\sigma^2\mathrm{I}_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

$$X \perp Z_1 \implies X + Z_1 \sim P * \mathcal{N}_{\sigma} \quad \& \quad Y \perp Z_2 \implies Y + Z_2 \sim Q * \mathcal{N}_{\sigma}$$

Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma} := \mathcal{N}(0, \sigma^2 \mathrm{I}_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

$$X \perp Z_1 \implies X + Z_1 \sim P * \mathcal{N}_{\sigma}$$
 & $Y \perp Z_2 \implies Y + Z_2 \sim Q * \mathcal{N}_{\sigma}$

$$\bullet \ \ \text{Retain duality:} \ \ \mathsf{W}_1^{(\sigma)}(P,Q) = \sup_{f \in \mathsf{Lip}_1(\mathbb{R}^d)} \mathbb{E}\big[f(X+Z)\big] - \mathbb{E}\big[f(Y+Z)\big]$$

Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma} := \mathcal{N}(0, \sigma^2 I_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

$$X \perp Z_1 \implies X + Z_1 \sim P * \mathcal{N}_{\sigma}$$
 & $Y \perp Z_2 \implies Y + Z_2 \sim Q * \mathcal{N}_{\sigma}$

- $\bullet \ \ \text{Retain duality:} \ \ \mathsf{W}_1^{(\sigma)}(P,Q) = \sup_{f \in \mathsf{Lip}_1(\mathbb{R}^d)} \mathbb{E}\big[f(X+Z)\big] \mathbb{E}\big[f(Y+Z)\big]$
- Inherit metric structure: Topologically equivalent to unsmooth W₁

Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma}:=\mathcal{N}(0,\sigma^2\mathrm{I}_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

$$X \perp Z_1 \implies X + Z_1 \sim P * \mathcal{N}_{\sigma} \quad \& \quad Y \perp Z_2 \implies Y + Z_2 \sim Q * \mathcal{N}_{\sigma}$$

- $\bullet \ \ \text{Retain duality:} \ \ \mathsf{W}_1^{(\sigma)}(P,Q) = \sup_{f \in \mathsf{Lip}_1(\mathbb{R}^d)} \mathbb{E}\big[f(X+Z)\big] \mathbb{E}\big[f(Y+Z)\big]$
- Inherit metric structure: Topologically equivalent to unsmooth W₁
- Stability: $|W_1^{(\sigma)}(P,Q) W_1(P,Q)| \le 2\sigma\sqrt{d}$ for all P,Q

Definition (Goldfeld-Greenewald'19)

For $\sigma \geq 0$, the smooth 1-Wasserstein distance between P and Q is

$$\mathsf{W}_{1}^{(\sigma)}(P,Q) := \mathsf{W}_{1}(P * \mathcal{N}_{\sigma}, Q * \mathcal{N}_{\sigma}),$$

where $\mathcal{N}_{\sigma} := \mathcal{N}(0, \sigma^2 \mathrm{I}_d)$ is a d-dimensional isotropic Gaussian.

Interpretation: $X \sim P$, $Y \sim Q$ and $Z_1, Z_2 \sim \mathcal{N}_{\sigma}$

$$X \perp Z_1 \implies X + Z_1 \sim P * \mathcal{N}_{\sigma} \quad \& \quad Y \perp Z_2 \implies Y + Z_2 \sim Q * \mathcal{N}_{\sigma}$$

- Retain duality: $W_1^{(\sigma)}(P,Q) = \sup_{f \in \text{Lin}_1(\mathbb{R}^d)} \mathbb{E}[f(X+Z)] \mathbb{E}[f(Y+Z)]$
- ullet Inherit metric structure: Topologically equivalent to unsmooth W_1
- Stability: $|W_1^{(\sigma)}(P,Q) W_1(P,Q)| \le 2\sigma\sqrt{d}$ for all P,Q
- Fast emp. convergence: $W_1^{(\sigma)}(P_n,P) \asymp n^{-1/2}$ in all dimensions!

① Generalization:
$$W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) - \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$$

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- 2 Limit distributions: Asymptotic dist. of MDE and empirical error

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- Limit distributions: Asymptotic dist. of MDE and empirical error
- Inequalities: Web of relationships between smooth distances

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- ② Limit distributions: Asymptotic dist. of MDE and empirical error
- Inequalities: Web of relationships between smooth distances
 - ⇒ Compatible for high-dimensional learning and inference!

Smooth Generative Models: MDE wrt smooth distance

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- ② Limit distributions: Asymptotic dist. of MDE and empirical error
- Inequalities: Web of relationships between smooth distances
 - ⇒ Compatible for high-dimensional learning and inference!

Future Goals: More distances, kernel, and efficient algorithms

Smooth Generative Models: MDE wrt smooth distance

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- 2 Limit distributions: Asymptotic dist. of MDE and empirical error
- Inequalities: Web of relationships between smooth distances
 - ⇒ Compatible for high-dimensional learning and inference!

Future Goals: More distances, kernel, and efficient algorithms

\$ More distances: p-Wasserstein distances, f-divergences, and IPMs

Smooth Generative Models: MDE wrt smooth distance

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- ② Limit distributions: Asymptotic dist. of MDE and empirical error
- Inequalities: Web of relationships between smooth distances
 - ⇒ Compatible for high-dimensional learning and inference!

Future Goals: More distances, kernel, and efficient algorithms

- \$ More distances: p-Wasserstein distances, f-divergences, and IPMs
- **※** More kernels: Optimize over choice of smoothing kernel

Smooth Generative Models: MDE wrt smooth distance

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- 2 Limit distributions: Asymptotic dist. of MDE and empirical error
- Inequalities: Web of relationships between smooth distances
 - ⇒ Compatible for high-dimensional learning and inference!

Future Goals: More distances, kernel, and efficient algorithms

- f 8 More distances: p-Wasserstein distances, f-divergences, and IPMs
- ★ More kernels: Optimize over choice of smoothing kernel
- * Efficient algorithms: Fast computational methods :

Smooth Generative Models: MDE wrt smooth distance

- **①** Generalization: $W_1^{(\sigma)}(P, Q_{\hat{\theta}_n}) \inf_{\theta} W_1^{(\sigma)}(P, Q_{\theta}) \lesssim n^{-\frac{1}{2}}, \quad \forall d$
- ② Limit distributions: Asymptotic dist. of MDE and empirical error
- Inequalities: Web of relationships between smooth distances
 - ⇒ Compatible for high-dimensional learning and inference!

Future Goals: More distances, kernel, and efficient algorithms

- **❀ More distances:** *p*-Wasserstein distances, *f*-divergences, and IPMs
- ★ More kernels: Optimize over choice of smoothing kernel
- **Efficient algorithms:** Fast computational methods :

 $\textbf{Next-generation systems:} \ \ \textbf{benchmark performance} \ \& \ \ \textbf{resource efficiency}$

Neural Estimation:

Neural Estimation:

• Approx. discriminator by a NN & optimize via gradient methods

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

Adapt classic learning setup to incorporate privacy constraints

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner
- Algorithms: Key-based schemes, Hadamard codes, etc.

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner
- Algorithms: Key-based schemes, Hadamard codes, etc.

Data Storage in Interacting Particle Systems:

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner
- Algorithms: Key-based schemes, Hadamard codes, etc.

Data Storage in Interacting Particle Systems:

Distill storage question from particular tech. & incorporate physics

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner
- Algorithms: Key-based schemes, Hadamard codes, etc.

Data Storage in Interacting Particle Systems:

- Distill storage question from particular tech. & incorporate physics
- Study information capacity (systems size, storage time, temp.)

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner
- Algorithms: Key-based schemes, Hadamard codes, etc.

Data Storage in Interacting Particle Systems:

- Distill storage question from particular tech. & incorporate physics
- Study information capacity (systems size, storage time, temp.)

Physical Layer Security:

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner
- Algorithms: Key-based schemes, Hadamard codes, etc.

Data Storage in Interacting Particle Systems:

- Distill storage question from particular tech. & incorporate physics
- Study **information capacity** (systems size, storage time, temp.)

Physical Layer Security:

Beneficial properties but impractical assumptions (known channel)

Neural Estimation:

- Approx. discriminator by a NN & optimize via gradient methods
- Performance guarantees? Approximation vs. estimation tradeoffs

Learning under privacy:

- Adapt classic learning setup to incorporate privacy constraints
- Theory: Bound the risk when compared to non-privatized learner
- Algorithms: Key-based schemes, Hadamard codes, etc.

Data Storage in Interacting Particle Systems:

- ullet Distill storage question from particular tech. & incorporate physics
- Study **information capacity** (systems size, storage time, temp.)

Physical Layer Security:

- Beneficial properties but impractical assumptions (known channel)
- Bridge gaps via adversarial models & connect to adversarial learning

Want to know more?

Website: http://people.ece.cornell.edu/zivg/

Email: goldfeld@cornell.edu

Office: 322 Rhodes Hall

Spring 2021: ECE 6970 Statistical Distances for Machine Learning

Thank you!