From Information Theory to Machine Learning Algorithms: A Few Vignettes

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Ph.D. final defense

June 3, 2022



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Q. How can we use tools and lessons from information theory to develop machine learning algorithms?

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- A few information-theoretic strategies to approach to a learning problem:
 - abstract out the gist from it in the infinite-sample limit;
 - reduce it to a probability estimation problem and plug-in a "good" probability;
 - adapt and apply relevant ideas from information theory,
 e.g., Wyner's common information, context-tree weighting, mixture probability, ...

Representation learning

Nonparametric methods for large-scale data

S Assumption-free data processing

Representation learning

- learning a generative model with succinct representation learning [Ryu+21];
- a fast kernel embedding without matrix eigendecomposition [RHK21];
- unifying and generalizing contrastive representation learning methods [in progress]
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 - optimal classification, regression [RK22], and density estimation [in progress] with 1-nearest neighbors;
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Part I

From Wyner's Common Information to Learning with Succinct Common Representation

• Data: $\{(\mathbf{X}_i, \mathbf{Y}_i)\}$ i.i.d. $\sim q(\mathbf{x}, \mathbf{y})$; high. dim., many-to-many relations

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- **Examples**: {(story_i, illustration_i)},

Alice was beginning to get very tired of sitting ...when suddenly a White Rabbit with pink eyes ran close by her ...see it pop down a large rabbit-hole under the hedge.





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the bird has a white body, black wings, and webbed orange feet



a blue bird with gray primaries and secondaries and white breast and throat

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 - Conditional generation: Learn $q(\mathbf{y}|\mathbf{x})$ and generate \mathbf{Y} given $\mathbf{x} \sim q(\mathbf{x})$

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 - Conditional generation: Learn $q(\mathbf{y}|\mathbf{x})$ and generate \mathbf{Y} given $\mathbf{x} \sim q(\mathbf{x})$
 - Cross-domain retrieval: Given a query x, retrieve relevant y's from a pool $\{y_i\}_{i=1}^n$

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 - a.k.a. cross-domain disentanglement problem



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 - Q. Under which criterion should we disentangle?



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 - **Q**. What is an optimal common representation?
- A. Use information theory to learn disentangled representations!



Motivation

• Cooperative game between Alice and Bob

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- Cooperative game between Alice and Bob
- Alice and Bob wish to draw a nice portrait of adulthood from a child's photo





Child's photo





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- Alice can maximally help Bob by providing the most "succinct" description!





• **Problem**: simulate a channel $q(\mathbf{y}|\mathbf{x})$ by communicating nR bits

$$\mathbf{X}^n \xrightarrow{\text{Encoder}} \underbrace{ \begin{array}{c} \mathbf{M} essage \\ \mathbf{M}(\mathbf{x}^n) \end{array}}_{\mathbf{M} \in \{1, \dots, 2^{nR}\}} \xrightarrow{\mathbf{V}^n} \mathbf{Y}^n$$

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minimize	$I(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$
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- Single-letter characterization





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Distributed simulation (Wyner 1975)

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- Distributed simulation \rightarrow joint generation

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Definition

minimize	$I(\mathbf{X},\mathbf{Y};\mathbf{Z})$
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 - Fit the generative models to data based on Wyner's optimization problem









- Decoders: $\mathbf{x}_{\theta}(\mathbf{z}, \mathbf{u}), \mathbf{y}_{\theta}(\mathbf{z}, \mathbf{v})$
- Priors (source of randomness): common $p_{\theta}(\mathbf{z})$, local $p_{\theta}(\mathbf{u}), p_{\theta}(\mathbf{v})$



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model θ

variational ϕ

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• The variational Wyner model induces four distributions:

joint cond. $(x \rightarrow y)$ cond. $(y \rightarrow x)$ variational

Jon Ryu (UCSD)

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joint	$p_{\rightarrow xy}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{u}, \mathbf{v}) \triangleq p_{\theta}(\mathbf{z}) p_{\theta}(\mathbf{u}) p_{\theta}(\mathbf{v}) \delta(\mathbf{x} - \mathbf{x}_{\theta}(\mathbf{z}, \mathbf{u})) \delta(\mathbf{y} - \mathbf{y}_{\theta}(\mathbf{z}, \mathbf{v}))$
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cond. (x $ ightarrow$ y)	$p_{x \to y}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{v}) \triangleq q(\mathbf{x})q_{\theta}(\mathbf{z} \mathbf{x})p_{\theta}(\mathbf{v})\delta(\mathbf{y} - \mathbf{y}_{\theta}(\mathbf{z}, \mathbf{v}))$
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variational	$q_{\mathbf{x}\mathbf{y}\rightarrow}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}) \triangleq q(\mathbf{x},\mathbf{y})q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y})q_{\phi}(\mathbf{u} \mathbf{z},\mathbf{x})q_{\phi}(\mathbf{v} \mathbf{z},\mathbf{y})$



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Recall Wyner's optimization problem: .

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cond. (x $ ightarrow$ y)	$p_{x \to y}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{v}) \triangleq q(\mathbf{x})q_{\theta}(\mathbf{z} \mathbf{x})p_{\theta}(\mathbf{v})\delta(\mathbf{y} - \mathbf{y}_{\theta}(\mathbf{z}, \mathbf{v}))$
cond. (y \rightarrow x)	$p_{y \to x}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{u}) \triangleq q(\mathbf{y}) q_{\theta}(\mathbf{z} \mathbf{y}) p_{\theta}(\mathbf{u}) \delta(\mathbf{x} - \mathbf{x}_{\theta}(\mathbf{z}, \mathbf{u}))$
variational	$q_{xy\to}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}) \triangleq q(\mathbf{x},\mathbf{y})q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y})q_{\phi}(\mathbf{u} \mathbf{z},\mathbf{x})q_{\phi}(\mathbf{v} \mathbf{z},\mathbf{y})$

Recall Wyner's optimization problem:

minimize	$I(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$	
subject to	$\mathbf{X} - \mathbf{Z} - \mathbf{Y}$	
variables	$q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y})$	

• For each model $p_{\text{model}} \in \{p_{\rightarrow xy}, p_{x \rightarrow y}, p_{y \rightarrow x}\}$, we can relax the problem as

 $\label{eq:minimize} \begin{array}{c} \text{minimize} \quad D(p_{\text{model}}, q_{\text{xy} \rightarrow}) + \lambda_{\text{model}}^{\text{Cl}} I_{\text{model}}(\mathbf{X}, \mathbf{Y}; \mathbf{Z}) \end{array}$

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• Distribution matching with CI regularization

Jon Ryu (UCSD)

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 - In practice, weights including $\lambda_{\text{model}}^{\text{CI}}$ can be chosen by trial and error

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- Plug-in deep neural networks for encoders, decoders, discriminators

Jon Ryu (UCSD)

• $(\mathbf{X}, \mathbf{Y}) = (\mathsf{MNIST}, \mathsf{SVHN})$ with label(SVHN)=label(MNIST)+1



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• **Z**=label, $(\mathbf{U},\mathbf{V})\approx$ (style of MNIST, style of SVHN)



- $\bullet\,$ Generated samples: same z across the rows; same u,v across the columns
- A red box highlights inputs; a yellow box highlight style references



- Numerical evaluation: $\lambda_{\rm model}^{\rm CI}$ vs. quality of generated samples
- Frechet distance: measures a distance between generated samples and test dataset
- Digit classification error: computed by pretrained MNIST/SVHN classifiers



• (X, Y)=(photo, human sketch)



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 - Given a sketch \mathbf{y}_o , retrieve the K-nearest neighbors of $\mathbf{z}_o \sim q_{\theta}(\mathbf{z}|\mathbf{y}_o)$ from $\{\mathbf{z}_j\}_{j \in [n]}$

- Zero-shot: training set has no overlapping classes with test set
- Examples: correct retrievals (left) / wrong retrievals (right)



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• Numerical evaluation: precision@K (P@K), mean average precision (mAP)

Models	P@100	mAP
LCALE [Lin+20]	0.583	0.476
IIAE [Hwa+20]	0.659	0.573
Variational Wyner	0.703	0.629

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 $\min_{q(\mathbf{z}|\mathbf{x},\mathbf{y}):\mathbf{X}-\mathbf{Z}-\mathbf{Y}} I(\mathbf{Z};\mathbf{X},\mathbf{Y})$

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- Q2. More than two variables?

Part II

From the Power of Random Guessing to Scalable Nearest-Neighbor Algorithms

Nearest-neighbor classification

• Data: Let $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ be i.i.d. samples over $\mathcal{X} \times \mathcal{Y}$
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Q. Can we make the k-NN-based algorithms viable in the realm of big data?

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• Randomized likelihood (RL) detector [YAG13]:

 $\hat{Y}(x) \sim p(y|x)$

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A general factor-of-two bound [Bha+18]

For any metric d(y, y') and $Y \stackrel{d}{=} Y'$,

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- Proof of the LCV lemma. Let $d(y, \hat{y}) = \mathbb{1}\{y \neq y'\}$, apply the general bound for each x, and take expectation w.r.t. X

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Let $X_{(1)}(x)$ be the nearest neighbor of x from i.i.d. samples $\{X_1,\ldots,X_n\}$ If (\mathcal{X},ρ) is a separable metric space,

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• Observation 1. (1-NN classifier \equiv RL detector) in the sample limit

• Let $\{Y_1'(x),\ldots,Y_M'(x)\}$ be a set of conditionally i.i.d. copies of $Y|\{X=x\}$ and

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Theorem [Bha+18]
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For any $\delta>0$

 $\mathsf{P}\{\hat{Y}_M(X) \neq Y\} \leq P_e^* + O(M)(e^{-\delta^2 \Omega(M)} + \mathsf{P}\{\Delta(X) \leq \delta\})$

where

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- The *M*-NN classifier is one way to emulate the power of multiple random guessing

 $\hat{g}_{M-NN}(x) = \mathsf{mode}(Y_{(1)}(x), \dots, Y_{(M)}(x))$

- Observation 1. (1-NN classifier \equiv RL detector) in the sample limit
- Observation 2. (majority vote over M random guesses \rightarrow MAP detector) as $M\rightarrow\infty$
- Proposal: aggregate multiple 1-NN classifiers with sample splitting

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Power of multiple random guessing with 1-NN classifier

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- Fully parallelizable; with S workers, query complexity becomes 1/S



Theorem (excess risk) [RK22]

For $\mathcal{X} = \mathbb{R}^d$ with metric $\rho(x, x')$, assume:

 $\begin{array}{l} \mbox{Theorem (excess risk) [RK22]} \\ \mbox{For $\mathcal{X}=\mathbb{R}^d$ with metric $\rho(x,x')$, assume:} \\ \mbox{(I)} $\eta(x)=\mathsf{P}\{Y=1|X=x\}$ is (α,A)-Hölder continuous for some $0<\alpha\leq1$ and $A>0$, i.e., $\forall x,x'\in\mathcal{X}$,} \end{array}$

 $|\eta(x) - \eta(x')| \le A\rho^{\alpha}(x, x').$

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 $\ensuremath{ @ \ } \eta \mbox{ satisfies the } \beta \mbox{-margin condition for } \beta > 0 \mbox{, i.e., } \exists \ C > 0 \mbox{ s.t.} \label{eq:gamma-state}$

$$\mathsf{P}\Big\{\Big|\eta(X) - \frac{1}{2}\Big| \le \Delta\Big\} \le C\Delta^{\beta}$$

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- Nearly minimax-optimal [AT+07]
- The *M*-split 1-NN classifier emulates a $\Theta(M)$ -NN classifier [CD14]
- Proof idea: analyze an intermediate distance-selective rule

Jon Ryu (UCSD)

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- Q. Split-and-aggregate framework for other nonparametric algorithms?

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- My wife Kyungeun
- My babies Arielle and Asher

Thank you!

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- (* and † indicate equal contribution and alphabetical ordering, respectively.)
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Backup Slides

How to use the variational Wyner model



- Variational encoders are introduced for training, but can be also used in sampling
- Local variational encoders $q_{\phi}(\mathbf{u}|\mathbf{z}, \mathbf{x}), q_{\phi}(\mathbf{v}|\mathbf{z}, \mathbf{y})$ can be viewed as style extractors

Jon Ryu (UCSD)

• For each model $p_{\text{model}} \in \{p_{\rightarrow xy}, p_{x \rightarrow y}, p_{y \rightarrow x}\}$:

minimize	$I_{xy ightarrow}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	$\mathbf{X} - \mathbf{Z} - \mathbf{Y}$
variables	$q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y})$

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 \blacksquare Replace $\mathbf{X} - \mathbf{Z} - \mathbf{Y}$ with the model consistency

• For each model $p_{\text{model}} \in \{p_{\rightarrow xy}, p_{x \rightarrow y}, p_{y \rightarrow x}\}$:

minimize	$I_{xy ightarrow}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	$p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})\equiv q_{xy ightarrow}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})$
variables	$q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y}), q_{\phi}(\mathbf{u} \mathbf{z},\mathbf{x}), q_{\phi}(\mathbf{v} \mathbf{z},\mathbf{y}), p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})$

() Replace $\mathbf{X} - \mathbf{Z} - \mathbf{Y}$ with the model consistency

• For each model $p_{\text{model}} \in \{p_{\rightarrow xy}, p_{x \rightarrow y}, p_{y \rightarrow x}\}$:

minimize	$I_{xy ightarrow}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	$D(p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}),q_{xy\to}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}))=0$
variables	$q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y}), q_{\phi}(\mathbf{u} \mathbf{z},\mathbf{x}), q_{\phi}(\mathbf{v} \mathbf{z},\mathbf{y}), p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})$

() Replace $\mathbf{X} - \mathbf{Z} - \mathbf{Y}$ with the model consistency
minimize	$I_{xy o}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	$D(p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}),q_{xy\to}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}))=0$
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- \blacksquare Replace $\mathbf{X} \mathbf{Z} \mathbf{Y}$ with the model consistency
- **2** Replace $I_{xy \rightarrow}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$ with $I_{model}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$

minimize	$I_{model}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	$D(p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}),q_{xy\to}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}))=0$
variables	$q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y}), q_{\phi}(\mathbf{u} \mathbf{z},\mathbf{x}), q_{\phi}(\mathbf{v} \mathbf{z},\mathbf{y}), p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})$

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minimize	$I_{model}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
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- \blacksquare Replace $\mathbf{X} \mathbf{Z} \mathbf{Y}$ with the model consistency
- O Replace $I_{xy \rightarrow}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$ with $I_{model}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$
- 8 Relax the equality constraint

minimize	$I_{model}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	$D(p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}),q_{xy\to}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})) \leq \epsilon$
variables	$q_{\phi}(\mathbf{z} \mathbf{x},\mathbf{y}), q_{\phi}(\mathbf{u} \mathbf{z},\mathbf{x}), q_{\phi}(\mathbf{v} \mathbf{z},\mathbf{y}), p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})$

- \blacksquare Replace $\mathbf{X} \mathbf{Z} \mathbf{Y}$ with the model consistency
- O Replace $I_{xy \rightarrow}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$ with $I_{model}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$
- 8 Relax the equality constraint

minimize	$I_{model}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	$D(p_{model}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}),q_{xy\to}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})) \leq \epsilon$
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- \blacksquare Replace $\mathbf{X}-\mathbf{Z}-\mathbf{Y}$ with the model consistency
- O Replace $I_{xy \rightarrow}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$ with $I_{model}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$
- 8 Relax the equality constraint
- Convert to an unconstrained Lagrangian minimization

minimize	$D(p_{\mathrm{model}}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v}),q_{\mathrm{xy}\rightarrow}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{u},\mathbf{v})) + \lambda_{\mathrm{model}}^{\mathrm{CI}}I_{\mathrm{model}}(\mathbf{X},\mathbf{Y};\mathbf{Z})$
subject to	
variables	$q_{\phi}(\mathbf{z} \mathbf{x}, \mathbf{y}), q_{\phi}(\mathbf{u} \mathbf{z}, \mathbf{x}), q_{\phi}(\mathbf{v} \mathbf{z}, \mathbf{y}), p_{model}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{u}, \mathbf{v})$

- \blacksquare Replace $\mathbf{X} \mathbf{Z} \mathbf{Y}$ with the model consistency
- O Replace $I_{xy \rightarrow}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$ with $I_{model}(\mathbf{X}, \mathbf{Y}; \mathbf{Z})$
- 8 Relax the equality constraint
- Convert to an unconstrained Lagrangian minimization

Experiment. CUB image-caption

• $(\mathbf{X}, \mathbf{Y}) = (bird images, captions)$



the bird has a white body, black wings, and webbed orange feet



a blue bird with gray primaries and secondaries and white breast and throat

Used ResNet-101 features for images

Experiment. CUB image-caption

→(image, caption)







this small bird is black white white with a small bill bill and black feet



this white bird is mostly white white with a long bill, and black feet this bird is grey with grey and has long long, pointy short pointy beak

this hird is grey

with grey and a

black beak . pointy

short pointy beak.

eak. beak.

this is a black and

white black bird

and a short black

this is a black and

white black bird

and a long long

vellow . .



this bird has a

black and and

white and white

this bird has a white and and white and white with and feet. image→caption



breast , with vellow breast and

its feathers

and and and its of

this is a very , and this bird has a very white and and , thin beak with a color with with a , breast and and a long brown beak , the blue patches . .

this bird a small , and yellow black yellow small , color with with black beak and a crown black black breast and a black and black of its feathers , the bird crown it's the borty



this bird has a red this crown and breast , red with red red red with and red and on on red

this bird is a red the bird has red red, red red color red red and a red and and and black red red.

caption→image



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Experiment. CUB image-caption

• Numerical evaluation: correlation of generated samples

Model	joint	$image{ o}caption$	$caption{\rightarrow}image$
Test set		0.273	
MMVAE [Shi+19] Variational Wyner	0.263 0.303	0.104 0.327	0.135 0.318