SELF-SUPERVISED REPRESENTATION LEARNING

Jonathan Gordon and Javier Antorán

Self Supervised Learning (SSL)

Unsupervised Learning:

Learning to Model the Observed Data

Self Supervised Learning:

Learning by Predicting Proxy Targets **Extracted From Unlabelled Data**





[Larsson et. al.]





But Why Self Supervised Learning?

How Much Information is the Machine Given during Learning?

- "Pure" Reinforcement Learning (cherry)
- The machine predicts a scalar reward given once in a while.
- A few bits for some samples

Supervised Learning (icing)

- The machine predicts a category or a few numbers for each input
- Predicting human-supplied data
- > 10 \rightarrow 10,000 bits per sample

Self-Supervised Learning (cake génoise)

- The machine predicts any part of its input for any observed part.
- Predicts future frames in videos
- Millions of bits per sample



Y. LeCun



But Why Self Supervised Learning?





[D. MacKay]

[Y. LeCun]

In Other Words:

THE REVOLUTIO ILL NOT BE SUPERVISED (nor purely reinforced

Talk Layout

- 1. Examples of Self Supervised Learning (SSL) Approaches
 - Information Theoretic Interpretation
- 2. Mutual Information (MI) Motivated SSL approaches
 - Deep InfoMax
 - Contrastive Predictive Coding
- 3. Is MI the real reason behind the success of SSL?
- 4. Generative Models for Representation Learning
- 5. Self Supervised Learning for Identifiability in Non-Linear ICA

Typical SSL Approaches:

- Predict Future From Past
- Predict Adjacent Sections in Structured Data
- Predict Occluded Area from Non-Occluded One
- **Undo Data-Augmentation Transformations** \bullet

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Obtain gains in downstream tasks (usually classification)

Predicting Rotations

CNNs are not rotation invariant. Will need to learn part-whole relationships.

Representation **z**

Input **x**

Encoder

Classifier

Supervised Attention Self-Supervised Attention

Rotation? {0, 90, 180, 270}

Video x v

Audio **x_a**

Separate $p(\mathbf{a}, \mathbf{v})$ from $p(\mathbf{a})p(\mathbf{v})$

Multimodal SSL: Audio + Video

[Arandjelovic et. al.]

Word Embeddings

Unsupervised Analogical Reasoning

	Newspaper	S				
	New York Times	Baltimore	Baltimore Sun			
	San Jose Mercury News	Cincinnati	Cincinnati Enquirer			
	NHL Team	S				
	Boston Bruins	Montreal	Montreal Canadiens			
	Phoenix Coyotes	Nashville	Nashville Predators			
	NBA Team	S				
	Detroit Pistons	Toronto	Toronto Raptors			
	Golden State Warriors	Memphis	Memphis Grizzlies			
	Airlines	•				
	Austrian Airlines	Spain	Spainair			
	Brussels Airlines	Greece	Aegean Airlines			
	Company exect	cutives				
	Microsoft	Larry Page	Google			
0	IBM 🗖	Werner Vogels	Amazon 🗖			

Skip Gram Model: Separating $p(\mathbf{x}^{(t)}, \mathbf{x}^{(t+k)})$ from $p(\mathbf{x}^{(t)})p(\mathbf{x}^{(t+k)})$

[Mikolov et. al.]

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Maximise Mutual Information Between Inputs and Representations?

But What is Mutual Information?

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- Invariant to Reparametrisations!

Here: $I(\mathbf{x}, \mathbf{z}) = H(\mathbf{x}) = H(\mathbf{z}) \longrightarrow$

• Symmetric, Bounded: $0 \le I(\mathbf{x}, \mathbf{y}) = I(\mathbf{y}, \mathbf{x}) \le \min(H(\mathbf{x}), H(\mathbf{y}))$

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ISSUE: No closed form for distributions. Only have samples!

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• Lets write $\mathbf{a} = (\mathbf{x}, \mathbf{z}); \quad p(\mathbf{a} \mid b = 1) = p(\mathbf{x})p(\mathbf{z}); \quad p(\mathbf{a} \mid b = 0) = p(\mathbf{x}, \mathbf{z})$

$$r(\mathbf{a}) = \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{x})p(\mathbf{z})} = \frac{p(\mathbf{a} \mid b = 0)}{p(\mathbf{a} \mid b = 1)}$$

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 $\frac{p(b=1)}{p(b=0)} = \frac{p(b=0|\mathbf{a})}{p(b=1|\mathbf{a})} = \frac{p(b=0|\mathbf{a})}{1 - p(b=0|\mathbf{a})}$

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We often model conditional probabilities with parametric functions:

$$f_{NN}(\mathbf{a}) = p(b = 0 \,|\, \mathbf{a})$$

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We can learn a parametric function that estimates log density ratios from samples!

$$f_{NN}(\mathbf{a}) = \log r(\mathbf{a}) = \log \frac{p(b=0|\mathbf{a})}{1 - p(b=0|\mathbf{a})} =$$

• Lets write $\mathbf{a} = (\mathbf{x}, \mathbf{z}); \quad p(\mathbf{a} | b = 1) = p(\mathbf{x})p(\mathbf{z}); \quad p(\mathbf{a} | b = 0) = p(\mathbf{x}, \mathbf{z})$

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Representation Learning through Maximising I(x, z)

- 1. Sample from joint distribution: $(\mathbf{x}, \mathbf{z}) \sim p(\mathbf{x}, \mathbf{z})$ as $\mathbf{x} \sim p_{\mathcal{D}}(\mathbf{x});$ $\mathbf{z} = f_{\phi}(\mathbf{x})$
- 2. <u>Negative sample</u> from factorised distribution: $(\mathbf{x}, \mathbf{z}) \sim p(\mathbf{x})p(\mathbf{z})$ as $\mathbf{x}, \mathbf{x}' \sim p_{\mathcal{D}}(\mathbf{x});$ $\mathbf{z} = f_{\phi}(\mathbf{x}')$
- 3. Estimate $I(\mathbf{x}, \mathbf{z})$ with $T_{\theta}(\mathbf{x}, \mathbf{z})$
- 4.Optimise $arg max_{\theta,\phi} I(\mathbf{x}, \mathbf{z})$

Encoder f(x) Critic T(x,z) $\mathbf{t}_{\theta}(\mathbf{x}, \mathbf{z}) \approx \log \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{x})p(\mathbf{z})}$

Deep InfoMax

[Hjelm et. al.]

Deep InfoMax (DIM)

- Max MI between Local and Global Representations
- Critic is an **MLP**:

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						-	

Input \rightarrow Linear lay Linear layer Linear layer

Linear SVM **Classification Results:**

	CIFAR10			CIFAR100			
Model	conv	$f_{c}(1024)$	V(64)	conv	$f_{c}(1024)$	V(64)	
	COIIV	10 (1024)	1 (04)	COIIV	10 (1024)	1 (04)	
Fully supervised	75.39			42.27			
VAE	60.71	60.54	54.61	37.21	34.05	24.22	
AE	62.19	55.78	54.47	31.50	23.89	27.44	
β -VAE	62.4	57.89	55.43	32.28	26.89	28.96	
AAE	59.44	57.19	52.81	36.22	33.38	23.25	
BiGAN	62.57	62.74	52.54	37.59	33.34	21.49	
NAT	56.19	51.29	31.16	29.18	24.57	9.72	
DIM(G)	52.2	52.84	43.17	27.68	24.35	19.98	
DIM(L) (DV)	72.66	70.60	64.71	48.52	44.44	39.27	
DIM(L) (JSD)	73.25	73.62	66.96	48.13	45.92	39.60	
DIM(L) (infoNCE)	75.21	75.57	69.13	49.74	47.72	41.61	

	Size	Activation
yer	512	ReLU
	512	ReLU
	1	

X

Local Encoder

Zlocal

Global Encoder

Zglobal

MLP Critic

MI Max [Hjelm et. al.]

Contrastive Predictive Coding

- Max MI between representations of spatially/temporally similar inputs

Audio-Video matching and **Word2Vec** fit within this framework!

• max $I(\mathbf{z}^{(t)}, \mathbf{z}^{(t+k)})$ with (AR NN + Bilinear) Critic $T(\mathbf{z}^{(1...k)}, \mathbf{z}^{(k+j)}) = g_{AR}(\mathbf{z}^{(1...k)})^{\mathsf{T}} W^{(j)} \mathbf{z}^{(k+j)}$

[van den Oord et. al.]

Better Contrastive Predictive Coding

- Large Batch Sizes
- Heavy Patch Augmentation
- Predict in every direction (not just forward)
- Larger Capacity NNs than when using labels
- Layer Norm (Not Batch Norm)

Text Document	Classificatio
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	Method	MR	CR	Subj
	Paragraph-vector [40] Skip-thought vector [26] Skip-thought + LN [41]	74.8 75.5 79.5	78.1 79.3 82.6	90.5 92.1 93.4
FLI / CC I I I	CPC	76.9	80.1	91.2
[He naff et. al.]				

[Chen et. al.]

Use ~InfoNCE to max MI between augmented inputs

$$\ell_{i,j} = -\log \frac{\exp(\sin(\boldsymbol{z}_i, \boldsymbol{z}_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\sin(\boldsymbol{z}_i, \boldsymbol{z}_k)/\tau)}$$

[Chen et. al.]

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Random Crop + Color Distortion Augmentation •

(a) Global and local views.

(b) Adjacent views.

(a) Without color distortion.

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Random Crop + Color Distortion Augmentation ullet

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Big Batches, Big Computers

¹With 128 TPU v3 cores, it takes ~ 1.5 hours to train our ResNet-50 with a batch size of 4096 for 100 epochs.

[Chen et. al.]

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Random Crop + Color Distortion Augmentation lacksquare

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Mutual Information Neural Estimation (Deep InfoMax)

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$$I(\mathbf{x}, \mathbf{z}) = E_{p(\mathbf{x}, \mathbf{z})} \left[\log \frac{p(\mathbf{x} \mid \mathbf{z}) q(\mathbf{x} \mid \mathbf{z})}{p(\mathbf{x}) q(\mathbf{x} \mid \mathbf{z})} \right] = E_{p(\mathbf{x}, \mathbf{z})} \left[\log \frac{q(\mathbf{x} \mid \mathbf{z})}{p(\mathbf{x})} \right] + E_{p(\mathbf{z})} [KL(p(\mathbf{x} \mid \mathbf{z}) \mid |q(\mathbf{x} \mid \mathbf{z})]]$$

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$$I(\mathbf{x}, \mathbf{z}) \ge H(x) + E_{p(\mathbf{x}, \mathbf{z})} [\log q(\mathbf{x} \mid \mathbf{z})]$$

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$$I(\mathbf{x}, \mathbf{z}) \ge H(x) + E_{p(\mathbf{x}, \mathbf{z})} [\log q(\mathbf{x} \mid \mathbf{z})]$$
We choose $q(\mathbf{x} \mid \mathbf{z}) = \frac{p(\mathbf{x})}{E_{p(\mathbf{x})} [e^{T(\mathbf{x}, \mathbf{z})}]} e^{T(\mathbf{x}, \mathbf{z})}$



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$$I(\mathbf{x}, \mathbf{z}) = E_{p(\mathbf{x}, \mathbf{z})} \left[\log \frac{p(\mathbf{x} \mid \mathbf{z}) q(\mathbf{x} \mid \mathbf{z})}{p(\mathbf{x}) q(\mathbf{x} \mid \mathbf{z})} \right] = E_{p(\mathbf{x}, \mathbf{z})} \left[\log \frac{q(\mathbf{x} \mid \mathbf{z})}{p(\mathbf{x})} \right] + E_{p(\mathbf{z})} [KL(p(\mathbf{x} \mid \mathbf{z}) \mid |q(\mathbf{x} \mid \mathbf{z})]]$$

$I(\mathbf{x}, \mathbf{z}) \geq H$

We choose $q(\mathbf{x})$

 $I(\mathbf{x}, \mathbf{z}) \ge \max_{\theta} E_{p(\mathbf{x}, \mathbf{z})}$

$$I(x) + E_{p(\mathbf{x},\mathbf{z})}[\log q(\mathbf{x} \mid \mathbf{z})]$$

$$\mathbf{x} \,|\, \mathbf{z}) = \frac{p(\mathbf{x})}{E_{p(\mathbf{x})}[e^{T(\mathbf{x}, \mathbf{z})}]} e^{T(\mathbf{x}, \mathbf{z})}$$

$$\mathbf{z}[T_{\theta}] - \log(E_{p(\mathbf{x})p(\mathbf{z})}[e^{T_{\theta}}])$$



Mutual Information Neural Estimation (Deep InfoMax)

$$I(\mathbf{x}, \mathbf{z}) = E_{p(\mathbf{x}, \mathbf{z})} \left[\log \frac{p(\mathbf{x} \mid \mathbf{z})q(\mathbf{x} \mid \mathbf{z})}{p(\mathbf{x})q(\mathbf{x} \mid \mathbf{z})} \right] = E_{p(\mathbf{x}, \mathbf{z})} \left[\log \frac{q(\mathbf{x} \mid \mathbf{z})}{p(\mathbf{x})} \right] + E_{p(\mathbf{z})} [KL(p(\mathbf{x} \mid \mathbf{z}) \mid |q(\mathbf{x} \mid \mathbf{z})]]$$

$I(\mathbf{x}, \mathbf{z}) \geq H$

We choose $q(\mathbf{x})$

 $I(\mathbf{x}, \mathbf{z}) \ge \max_{\theta} E_{p(\mathbf{x}, \mathbf{z})}$

Bound tight

$$I(x) + E_{p(\mathbf{x},\mathbf{z})}[\log q(\mathbf{x} \mid \mathbf{z})]$$

$$\mathbf{x} \,|\, \mathbf{z}) = \frac{p(\mathbf{x})}{E_{p(\mathbf{x})}[e^{T(\mathbf{x}, \mathbf{z})}]} e^{T(\mathbf{x}, \mathbf{z})}$$

$$\mathbf{z}[T_{\theta}] - \log(E_{p(\mathbf{x})p(\mathbf{z})}[e^{T_{\theta}}])$$

if
$$T = \log \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{x})p(\mathbf{z})}$$





Similar to MINE, but: We draw an additional K-1 samples from x to a normalisation constant: $E_{p(\mathbf{x})}[e^T] \approx m(\mathbf{z} \,|\, \mathbf{x}_1 \dots \mathbf{x}_k) = \frac{1}{K} \sum_{i=1}^K e^{T(\mathbf{x}_i, \mathbf{z})}$







Note that: $I(\mathbf{x}, \mathbf{z}) \ge I^{NCE} + \log K$ Larger K (batch sizes) will yield less biased estimates





Comparing MI estimators

Correlated Gaussian







$$\mathbf{z} = (W\mathbf{x})^3; \quad \mathbf{x} \sim \mathcal{N}(0,1)$$

[Poole et. al.]

Which One Should I Use?

Batch-Size: N

2N Critic Evaluations

- JSD
- MINE
- MINE-f

N^2 Critic Evaluations

- InfoNCE

* If possible use InfoNCE with large batch size



Is MI Maximisation Really the Solution?

• During training encoders become less invertible



More flexible critics can make for worse representations



Bilinear: $T(\mathbf{z}, \mathbf{x}) = \mathbf{z}^{\mathsf{T}} W \mathbf{x}$ Separable: $T(\mathbf{z}, \mathbf{x}) = \phi(\mathbf{z}^{\mathsf{T}})\phi(\mathbf{x})$

[Tschannen et. al.]



Is MI Maximisation Really the Solution?

- Utility of representation is a function of "decodable information", not MI
- •This depends on **inductive biases** from:
 - MI estimator
 - Critic Function + Encoder Function
 - Objects between which MI is maximised

•A bijection can be applied to a useful representation making it not useful, maintaining $I(\mathbf{x}, \mathbf{z})$



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A Generative Modelling Perspective





Goal: $\theta^* = \arg \max \log p_{\theta}(D)$ $\theta \in \Theta$



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Probabilistic PCA $p_{\theta}(s) = \mathcal{N}(s; 0, I)$ $p_{\theta}(x \mid s) = \mathcal{N}(x; Ws + \mu, \sigma^2 I)$



Goal: $\theta^* = \arg \max \log p_{\theta}(D)$ $\theta \in \Theta$

Factor Analysis

$$p_{\theta}(s) = \mathcal{N}(s; 0, I)$$

 $p_{\theta}(x | s) = \mathcal{N}(x; Ws + \mu, \Sigma)$



Goal: $\theta^* = \arg \max \log p_{\theta}(D)$ $\theta \in \Theta$

VAE

$$p_{\theta}(s) = \mathcal{N}(s; 0, I)$$

$$p_{\theta}(x \mid s) = \mathcal{N}\left(x; f_{nn}^{\mu}(s), f_{nn}^{\sigma^{2}}(s)\right)$$

I. Khemakhem, et al. 2019

Identifiability: the "true" parameters will be recovered given infinite observations

I. Khemakhem, et al. 2019



For generative models: $p_{\theta}(x) = p_{\theta'}(x) \implies \theta = \theta'$

I. Khemakhem, et al. 2019

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For generative models: $p_{\theta}(x) = p_{\theta'}(x) \implies \theta = \theta'$

Identifiable models provide:

A principled approach to representation learning (as opposed to *"just" generative modelling).*

Links to other unsupervised desiderata (e.g., "disentanglement")

I. Khemakhem, et al. 2019



PCA / Factor Analysis:

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Scaling: $WS = \frac{\alpha}{\alpha}WS = (\alpha^{-1}W)(\alpha S)$

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Scaling: $WS = \frac{\alpha}{\alpha}WS = (\alpha^{-1}W)(\alpha S)$

Rotation: $WS = WRR^{-1}S = W'S'$

F. Locatello et al. 2019.

Theorem. Let $p(s) = \prod p_d(s_d)$, then there exists an infinite family of bijections of the form $f: \mathcal{S} \to \mathcal{S}$ such that $\int p_{\theta}(x \mid s) p(s) ds = \int p_{\theta'}(x \mid f(s)) p(f(s)) ds$ for some alternative generative model with parameters θ' .

F. Locatello et al. 2019.



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 $p_{\theta}(x) \approx p_{\theta^*}(x)$

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 $p_{\theta}(s, x)$

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 $p_{\theta}(x) \approx p_{\theta*}(x)$

 $p_{\theta}(s, x) \approx p_{\theta^*}(s, x)$

J. Shlens. 2014

The Cocktail Party Problem



voice



J. Shlens. 2014

The Cocktail Party Problem

2



J. Shlens. 2014

The Cocktail Party Problem

2



The Cocktail Party Problem

2


The Cocktail Party Problem





$p_{\theta}(s) = \prod_{i=1}^{d} p_i(s_i; \theta)$



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 $x = As; \quad A \in \mathbb{R}^{d \times d}$



Goal: recover $A^{-1} \implies s = A^{-1}x$



 $x = As; \quad A \in \mathbb{R}^{d \times d}$

 $W = A^{-1};$

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D. Mackay. 2003.

 $a_i = \sum W_{ij} x_j$

i

 $W = A^{-1};$

 $\phi(a_i) = \frac{\mathrm{d}}{\mathrm{d}a_i} \log p_i(a_i)$

 $a_i = \sum_j W_{ij} x_j$

Maximum Likelihood Solution $W = A^{-1};$ $a_i = \sum_i W_{ij} x_j$ $\phi(a_i) = \frac{d}{da_i} \log p_i(a_i)$

$\log p(x^{(n)} | A) = \log |\det W| + \sum_{i} \log p_i(a_i^{(n)})$

Maximum Likelihood Solution $a_i = \sum_j W_{ij} x_j$ $W = A^{-1}$:

$\log p(x^{(n)}|A) = \log |\det W| + \sum \log p_i(a_i^{(n)})$

$\frac{\partial}{\partial W_{ij}} \log p(x^{(n)} | A) = [W^T]_{ij}^{-1} + x_j^{(n)} \phi(a_i^{(n)})$

 $\phi(a_i) = \frac{d}{da_i} \log p_i(a_i)$





Choice of $p \iff \phi$



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Identifiable when:

- 1. p_i is not Gaussian (except perhaps one).
- 2. $p_i \perp p_j$ for all i, j



A. Hyvarinen and P. Pajunen. 1998.

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$$p_{\theta}(s) = \prod_{i=1}^{d} p_i(s_i; \theta)$$

 $x = f(s; \theta); \quad f: \mathbb{R}^d \to \mathbb{R}^d$

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Goal: recover f^{-1}

Non-linear ICA $p_{\theta}(s) = \prod_{i=1}^{n} p_i(s_i;\theta)$ i=1 $x = f(s; \theta); \quad f: \mathbb{R}^d \to \mathbb{R}^d$ Goal: recover f^{-1}

Existence: for any random variable $x \in \mathbb{R}^d$, there exists a function $g: \mathcal{X} \to \mathcal{S}$ such that s_1, \ldots, s_d have density $p_{\theta}(s)$ (constructive).

A. Hyvarinen and P. Pajunen. 1998.

Existence: for any random variable $x \in \mathbb{R}^d$, there exists a function $g: \mathcal{X} \to \mathcal{S}$ such that s_1, \ldots, s_d have density $p_{\theta}(s)$ (constructive).

Non-uniqueness: the number of solutions g is at least as large as the class of measurepreserving functions $h: [0,1]^n \rightarrow [0,1]^n$.

A. Hyvarinen and P. Pajunen. 1998.



 $s_t = \left(s_1(t), \dots, s_n(t)\right)$



A. Hyvarinen and H. Morioka. 2016.

$$s_t = \left(s_1(t), \dots, s_n(t)\right)$$

 $p_{i,\tau}(s_i) \propto \lambda_i(\tau) q_i(s_i)$



$$s_{t} = (s_{1}(t), \dots, s_{n}(t))$$
$$p_{i,\tau}(s_{i}) \propto \lambda_{i}(\tau)q_{i}(s_{i})$$
$$x_{t} = f(s_{t})$$





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Time (t)





Identifiability via TCL

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Theorem. Assume that (ii) TCL is applied to learn a feature extractor $h(x_t; \theta)$, and (*iii*) the parameters $\lambda_{i,v}$ are "well-behaved". Then, with infinite data we have that $q(S_{i})$

- (i) the observed data are generated from the detailed model,

$$f_t) = Ah(x; \theta) + b$$
.

A. Hyvarinen et al. 2019., Khemakhem et al., 2019



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$$p_{\theta}(s) = \prod_{i=1}^{d} p_i(s_i | u; \theta)$$
$$x = f(s; \theta); \quad f: \mathbb{R}^d \to \mathbb{R}^d$$

$$r(x, u) = \sum_{i=1}^{n} \psi_i(h(x; \theta), u)$$

 $\tilde{x} = (x, u); \quad \tilde{x}^* = (x, u^*)$
Contrastive learning —> Self-supervised "heuristics"

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Self-supervised learning $\langle - \rangle$ identifiability in generative models

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