





Minimalistic Unsupervised Representation Learning with the Sparse Manifold Transform

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heoretical Neuroscience



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What is an unsupervised representation?

A general goal: transform raw data into a new space such that "similar" things are placed closer and meanwhile the new space is not collapsed.

Where does "similarity" come from?

Three similarities:

Spatial co-occurrence

Temporal co-occurrence

Euclidean neighborhoods





(Rumelhart, Hinton and Williams, 1986) (Roweis and Lawrence, 2000) (Tenenbaum, Silva and Langford, 2000) (Wiskott and Sejnowski, 2002) (Dumais, 2004) (Mikolov et al., 2012)

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How to establish a minimalistic unsupervised representation?

An unsupervised representation transform derived from neural and statistical principles

Neural principle: sparse coding



Neural principle: sparse coding



Sparse coding image model



Optimization:

$$\min_{\Phi, \vec{\alpha}_i, i \in 1, \dots, N} \quad \frac{1}{N} \sum_{i=1}^N \|\vec{x}_i - \Phi \vec{\alpha}_i\|_2^2 + S(\vec{\alpha}_i)$$

Learned features

Sparse encoding of a time-varying image



Sparse encoding of a time-varying image



But something is missing here: "similar" things are not placed closer

Statistical principle: manifold learning



Manifold hypothesis

(Roweis and Saul, 2000) (Tenenbaum, Silva and Langford, 2000) (Saul and Roweis, 2002)

Natural signals can be highly nonlinear

Manifold interpolation



Natural signals can be highly nonlinear

Manifold interpolation



Linear interpolation

Natural signals can be highly nonlinear

Manifold interpolation



Linear interpolation













SMT formulation



Manifold embedding

 $\vec{x}_{t} = \Phi \vec{\alpha}_{t} + \vec{n}_{t}$ $P \vec{\alpha}_{t} = \frac{1}{2} P(\vec{\alpha}_{t-1} + \vec{\alpha}_{t+1})$ $\ddot{\vec{\alpha}}_{t} = \vec{\alpha}_{t} - \frac{1}{2} (\vec{\alpha}_{t-1} + \vec{\alpha}_{t+1})$

 $\Phi \alpha$

Optimization:

$$\min_{P} tr P \sum_{t=1}^{T} (\ddot{\vec{\alpha}}_{t} \ddot{\vec{\alpha}}_{t}^{T}) P^{T}$$

s.t. $PVP^T = I$, (unit variance & decorrelation) V is covariance matrix of $\vec{\alpha}$

(Chen et al. NeurIPS'18)

 $P\alpha$

Encoding of a natural video sequence



Let's generalize the formulation a little bit



$$\begin{split} P\vec{\alpha}_{t} &= \frac{1}{2}P(\vec{\alpha}_{t-1} + \vec{\alpha}_{t+1}) & \begin{array}{c} \text{Temporal linearity} \\ (\text{second-order derivative}) \\ P\vec{\alpha}_{i} &- \sum_{j \in n(i)} w(i,j) P\vec{\alpha}_{j} = 0 & \begin{array}{c} \text{General linearity} \\ (\text{second-order derivative}) \\ (\text{second-order derivative}) \\ P\vec{\alpha}_{i} &- P\vec{\alpha}_{j} = 0 & \begin{array}{c} \text{Similarity} \\ (\text{first-order derivative}) \end{array} \end{split}$$

Let's generalize the formulation a little bit



Manifold embedding

Graph embedding

$$\begin{split} P\vec{\alpha}_{t} &= \frac{1}{2}P(\vec{\alpha}_{t-1} + \vec{\alpha}_{t+1}) & \begin{array}{c} \text{Temporal linearity} \\ (\text{second-order derivative}) \\ P\vec{\alpha}_{i} &- \sum_{j \in n(i)} w(i,j) P\vec{\alpha}_{j} = 0 & \begin{array}{c} \text{General linearity} \\ (\text{second-order derivative}) \\ (\text{second-order derivative}) \\ P\vec{\alpha}_{i} &- P\vec{\alpha}_{j} = 0 & \begin{array}{c} \text{Similarity} \\ (\text{first-order derivative}) \end{array} \end{split}$$

The similarity is better reflected in the representation space



Sensory signal neighborhood

Representation neighborhood

Our goal: transform raw data into a new space such that similar things are placed closer and meanwhile the new space is not collapsed.



Sparse coding tiles the data manifold and provides a support in the data space.



Spectral embedding establishes similarity on the support.



Spectral embedding establishes similarity on the support. Each embedding dimension is a low-frequency function on the support.



2nd embedding dim

1st embedding dim

3rd embedding dim









SMT is a local distance manipulation



MNIST

CIFAR10

	Co-Occurrence Context Range SMT-VQ (16384) SMT-VQ (65536) SMT-VQ (GloVe, 100K)					
MNIST:	Whole Image 3 Pixels	99 99	.0% 9 .2% 9	8.9% 9.3%	98.8% 99.0%	
	Color Augmentation	SMT-VQ (100K)	SMT-GQ (8192)	SMT-GQ (65536)	SimCLR (ResNet18)	VICReg (ResNet18)
CIFAR10:	Original Image Grayscale Image Only Original + Grayscale Full (ColorJitter etc.)	78.4%	79.2% 77.5% 81.4%	81.1% 78.9% 83.2%	68.3% 80.6% 85.7% 90.1%	70.2% 81.3% 83.7% 91.1%
	Color Augmentation	SMT-VQ (100K)	SMT-GQ (8192)	SMT-GQ (65536)	SimCLR (ResNet18)	VICReg (ResNet18)
CIFAR100:	Original Image Grayscale Image Original + Grayscale Full (ColorJitter etc.)	46.6% 	50.8% 45.8% 53.7%	53.2% 48.9% 57.0%	32.4% 43.0% 48.9% 63.7%	32.6% 43.9% 46.0% 65.4%

Deep SSL: 18 layers 1000 training epochs

SMT: 2 layers 1 training epoch

The convergence



(Bardes et al., ICLR'22) (Chen et al., arXiv'22) (Tong et al., arXiv'23)



Main points

Poster: **#163 (last row)** 16:30 CAT – 18:30 CAT

Unsupervised representation from neural and statistical principles

- · Sparse coding tiles the data space and provides the support
- Spectral embedding establishes similarity and linearity on the support

