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Energy-Based Unsupervised Learning

Energy-Based Unsupervised Learning

Learning an energy function (or contrast function) that takes

- Low values on the data manifold
- Higher values everywhere else



Capturing Dependencies Between Variables with an Energy Function

The energy surface is a "contrast function" that takes low values on the data manifold, and higher values everywhere else

- Special case: energy = negative log density
- Example: the samples live in the mapping $(Y_1)^2$



Transforming Energies into Probabilities (if necessary)

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Ι

The energy can be interpreted as an unnormalized negative log density

- Gibbs distribution: Probability proportional to exp(-energy)
 - Beta parameter is akin to an inverse temperature
 - Don't compute probabilities unless you absolutely have to
 - Because the denominator is often intractable

$$P(Y|W) = \frac{e^{-\beta E(Y,W)}}{\int_{y} e^{-\beta E(y,W)}}$$

$$E(Y,W) \propto -\log P(Y|W)$$

$$E(Y,W) \propto -\log P(Y|W)$$

Learning the Energy Function

parameterized energy function E(Y,W)

- Make the energy low on the samples
- Make the energy higher everywhere else
- Making the energy low on the samples is easy
- But how do we make it higher everywhere else?



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Seven Strategies to Shape the Energy Function

- 1. build the machine so that the volume of low energy stuff is constant
 PCA, K-means, GMM, square ICA
- 2. push down of the energy of data points, push up everywhere else
 Max likelihood (needs tractable partition function)
- 3. push down of the energy of data points, push up on chosen locations
 - contrastive divergence, Ratio Matching, Noise Contrastive Estimation, Minimum Probability Flow
- 4. minimize the gradient and maximize the curvature around data points
 score matching
- 5. train a dynamical system so that the dynamics goes to the manifold
 denoising auto-encoder
- 6. use a regularizer that limits the volume of space that has low energy
 Sparse coding, sparse auto-encoder, PSD
- 7. if E(Y) = IIY G(Y)II^2, make G(Y) as "constant" as possible.
 - Contracting auto-encoder, saturating auto-encoder

#1: constant volume of low energy

1. build the machine so that the volume of low energy stuff is constant
 PCA, K-means, GMM, square ICA...

PCA

 $E(Y) = \|W^T WY - Y\|^2$



K-Means, Z constrained to 1-of-K code $E(Y) = min_z \sum_i ||Y - W_i Z_i||^2$



#2: push down of the energy of data points, push up everywhere else

Max likelihood (requires a tractable partition function)



#2: push down of the energy of data points, push up everywhere else

Gradient of the negative log-likelihood loss for one sample Y:



#3. push down of the energy of data points, push up on chosen locations

Contrastive divergence, Ratio Matching, Noise Contrastive Estimation, Minimum Probability Flow

Contrastive divergence: basic idea

- Pick a training sample, lower the energy at that point
- From the sample, move down in the energy surface with noise
- Stop after a while
- Push up on the energy of the point where we stopped
- This creates grooves in the energy surface around data manifolds
- CD can be applied to any energy function (not just RBMs)

Persistent CD: use a bunch of "particles" and remember their positions

- Make them roll down the energy surface with noise
- Push up on the energy wherever they are
- Faster than CD

🗾 RBM

$$E(Y, Z) = -Z^T WY$$
 $E(Y) = -\log \sum_z e^{Z^T WY}$

#6. use a regularizer that limits the volume of space that has low energy

Sparse coding, sparse auto-encoder, Predictive Saprse Decomposition



Sparse Modeling, Sparse Auto-Encoders, Predictive Sparse Decomposition LISTA

How to Speed Up Inference in a Generative Model?

Factor Graph with an asymmetric factor

- Inference $Z \rightarrow Y$ is easy
 - Run Z through deterministic decoder, and sample Y

Inference $Y \rightarrow Z$ is hard, particularly if Decoder function is many-to-one

- MAP: minimize sum of two factors with respect to Z
- Z* = argmin_z Distance[Decoder(Z), Y] + FactorB(Z)

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Examples: K-Means (1of K), Sparse Coding (sparse), Factor Analysis



Sparse Coding & Sparse Modeling

[Olshausen & Field 1997]

Sparse linear reconstruction

Energy = reconstruction_error + code_prediction_error + code_sparsity

$$E(Y^{i}, Z) = ||Y^{i} - W_{d}Z||^{2} + \lambda \sum_{j} |z_{j}|$$





Examples: most ICA models, Product of Experts



Encoder-Decoder Architecture

[Kavukcuoglu, Ranzato, LeCun, rejected by every conference, 2008-2009]

Train a "simple" feed-forward function to predict the result of a complex optimization on the data points of interest



1. Find optimal Zi for all Yi; 2. Train Encoder to predict Zi from Yi

- Training sample
- Input vector which is NOT a training sample
- Feature vector





- Training sample
- Input vector which is NOT a training sample
- Feature vector

Training based on minimizing the reconstruction error over the training set



- Training sample
- Input vector which is NOT a training sample

• Feature vector BAD: machine does not learn structure from training data!! It just copies the data. Y LeCun



- Training sample
- Input vector which is NOT a training sample
- Feature vector

IDEA: reduce number of available codes.





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IDEA: reduce number of available codes.



- Training sample
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IDEA: reduce number of available codes.



Predictive Sparse Decomposition (PSD): sparse auto-encoder Y LeCun

[Kavukcuoglu, Ranzato, LeCun, $2008 \rightarrow arXiv:1010.3467$], Prediction the optimal code with a trained encoder

Energy = reconstruction_error + code_prediction_error + code_sparsity

$$E(Y^{i}, Z) = ||Y^{i} - W_{d}Z||^{2} + ||Z - g_{e}(W_{e}, Y^{i})||^{2} + \lambda \sum_{j} |z_{j}|$$

$$g_{e}(W_{e}, Y^{i}) = shrinkage(W_{e}Y^{i})$$



PSD: Basis Functions on MNIST

Basis functions (and encoder matrix) are digit parts

5	2	2	2	5	8	>	0	1	1	2	1	2	6	1	9	1	3	1	0
0	1	5	1	3	7	6	C	1	1	•	1	3	.7	3	1	1	1	3	2
1	3	6	0	2	3	1	5	6	2	٢,	5	3	3	9	\$	ð	6	2	3
6	E	1		6	0	3	3	2	2	10	5	6	12	9	5	5	3	1	1
6	2	٩.	3	2	6	5	3	5	6	7	2	é	1	S	1	2	6	1	0
1	0	1	•	5	3	1	5	2	4	1	0	-	30	9	5)	3		-
6	•	9	9	0	6	0	3	2	1	0	-	1	1	7	3	1	2	3	2
2	1	9	3	•	9	-	2	0	0	0	2	0	2	1	9	7	0	3	1
9	0	3	3	7	3	2	9	5	3	•	0	6	0	0	8		•	0	5
1	0	e	4	-	5	5	2	7	5	0	-	9	1	-	2	0	2	-	1

Predictive Sparse Decomposition (PSD): Training

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Learned Features on natural patches: V1-like receptive fields

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Better Idea: Give the "right" structure to the encoder

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ISTA/FISTA: iterative algorithm that converges to optimal sparse code [Gregor & LeCun, ICML 2010], [Bronstein et al. ICML 2012], [Rolfe & LeCun ICLR 2013]

INPUT
$$Y \rightarrow W_e \rightarrow + sh() \rightarrow z \rightarrow S$$

Lateral Inhibition

$$Z(t+1) = \text{Shrinkage}_{\lambda/L} \left[Z(t) - \frac{1}{L} W_d^T (W_d Z(t) - Y) \right]$$

 $Z(t+1) = \text{Shrinkage}_{\lambda/L} \left[W_e^T Y + SZ(t) \right]; \quad W_e = \frac{1}{L} W_d; \quad S = I - \frac{1}{L} W_d^T W_d$

LISTA: Train We and S matrices to give a good approximation quickly

Ζ

Think of the FISTA flow graph as a recurrent neural net where We and S are trainable parameters

S

sh

S

sh

Time-Unfold the flow graph for K iterations

INPUT

Y

- Learn the We and S matrices with "backprop-through-time"
- Get the best approximate solution within K iterations

sh

Learning ISTA (LISTA) vs ISTA/FISTA



Number of LISTA or FISTA iterations

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LISTA with partial mutual inhibition matrix



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Proportion of S matrix elements that are non zero

Learning Coordinate Descent (LcoD): faster than LISTA

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Number of LISTA or FISTA iterations

Reconstruction Error

Discriminative Recurrent Sparse Auto-Encoder (DrSAE)

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- Rectified linear units
- Classification loss: cross-entropy

[Rolfe & LeCun ICLR 2013]

- Reconstruction loss: squared error
- Sparsity penalty: L1 norm of last hidden layer
- Rows of Wd and columns of We constrained in unit sphere

DrSAE Discovers manifold structure of handwritten digits

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Image = prototype + sparse sum of "parts" (to move around the manifold)



Convolutional Sparse Coding

Replace the dot products with dictionary element by convolutions.

- Input Y is a full image
- Each code component Zk is a feature map (an image)
- Each dictionary element is a convolution kernel

Regular sparse coding
$$E(Y,Z) = ||Y - \sum_k W_k Z_k||^2 + \alpha \sum_k |Z_k|$$

Convolutional S.C.
$$E(Y, Z) = ||Y - \sum_{k} W_k * Z_k||^2 + \alpha \sum_{k} |Z_k|$$



"deconvolutional networks" [Zeiler, Taylor, Fergus CVPR 2010]

Convolutional PSD: Encoder with a soft sh() Function

Convolutional Formulation

Extend sparse coding from PATCH to IMAGE

$$\mathcal{L}(x, z, \mathcal{D}) = \frac{1}{2} ||x - \sum_{k=1}^{K} \mathcal{D}_k * z_k||_2^2 + \sum_{k=1}^{K} ||z_k - f(W^k * x)||_2^2 + |z|_1$$



PATCH based learning

CONVOLUTIONAL learning

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Convolutional Sparse Auto-Encoder on Natural Images

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Filters and Basis Functions obtained with 1, 2, 4, 8, 16, 32, and 64 filters.



Phase 1: train first layer using PSD



FEATURES

- Phase 1: train first layer using PSD
- Phase 2: use encoder + absolute value as feature extractor



FEATURES

- Phase 1: train first layer using PSD
- Phase 2: use encoder + absolute value as feature extractor
- Phase 3: train the second layer using PSD



FEATURES

- Phase 1: train first layer using PSD
- Phase 2: use encoder + absolute value as feature extractor
- Phase 3: train the second layer using PSD
- Phase 4: use encoder + absolute value as 2nd feature extractor



FEATURES

- Phase 1: train first layer using PSD
- Phase 2: use encoder + absolute value as feature extractor
- Phase 3: train the second layer using PSD
- Phase 4: use encoder + absolute value as 2nd feature extractor
- Phase 5: train a supervised classifier on top
- Phase 6 (optional): train the entire system with supervised back-propagation



FEATURES

Pedestrian Detection: INRIA Dataset. Miss rate vs false positives



[Kavukcuoglu et al. NIPS 2010] [Sermanet et al. ArXiv 2012]

Unsupervised Learning: Invariant Features

earning Invariant Features with L2 Group Sparsity

- Unsupervised PSD ignores the spatial pooling step.
- Could we devise a similar method that learns the pooling layer as well?
- Idea [Hyvarinen & Hoyer 2001]: group sparsity on pools of features
 - Minimum number of pools must be non-zero
 - Number of features that are on within a pool doesn't matter



Learning Invariant Features with L2 Group Sparsity

Idea: features are pooled in group.

- Sparsity: sum over groups of L2 norm of activity in group.
- [Hyvärinen Hoyer 2001]: "subspace ICA"
 - decoder only, square
- [Welling, Hinton, Osindero NIPS 2002]: pooled product of experts
 - encoder only, overcomplete, log student-T penalty on L2 pooling
- [Kavukcuoglu, Ranzato, Fergus LeCun, CVPR 2010]: Invariant PSD
 - encoder-decoder (like PSD), overcomplete, L2 pooling
- [Le et al. NIPS 2011]: Reconstruction ICA
 - Same as [Kavukcuoglu 2010] with linear encoder and tied decoder
- [Gregor & LeCun arXiv:1006:0448, 2010] [Le et al. ICML 2012]
 - Locally-connect non shared (tiled) encoder-decoder



Encoder only (PoE, ICA), Decoder Only or Encoder-Decoder (iPSD, RICA)



Groups are local in a 2D Topographic Map

- The filters arrange themselves spontaneously so that similar filters enter the same pool.
- The pooling units can be seen as complex cells
- Outputs of pooling units are invariant to local transformations of the input
 - For some it's translations, for others rotations, or other transformations.



Image-level training, local filters but no weight sharing

- Training on 115x115 images. Kernels are 15x15 (not shared across space!)
 Decoder
 - [Gregor & LeCun 2010]
 - Local receptive fields
 - No shared weights
 - 4x overcomplete
 - L2 pooling
 - Group sparsity over pools



Image-level training, local filters but no weight sharing

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Training on 115x115 images. Kernels are 15x15 (not shared across

space!)



Topographic Maps

bermayer and GG Blasdel, Journal of oscience, Vol 13, 4114-4129 (Monkey)

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119x119 Image Input 100x100 Code 20x20 Receptive field size sigma=5



Michael C. Crair, et. al. The Journal of Neurophysiology Vol. 77 No. 6 June 1997, pp. 3381-3385 (**Cat**)

Image-level training, local filters but no weight sharing

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Color indicates orientation (by fitting Gabors)



Invariant Features Lateral Inhibition

Replace the L1 sparsity term by a lateral inhibition matrix
 Easy way to impose some structure on the sparsity

$$\min_{W,Z} \sum_{x \in X} ||Wz - x||^2 + |z|^T S|z|$$



Invariant Features via Lateral Inhibition: Structured Sparsity

Each edge in the tree indicates a zero in the S matrix (no mutual inhibition)Sij is larger if two neurons are far away in the tree



Invariant Features via Lateral Inhibition: Topographic Maps

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Non-zero values in S form a ring in a 2D topology

Input patches are high-pass filtered



Invariant Features through Temporal Constancy

Object is cross-product of object type and instantiation parameters
 Mapping units [Hinton 1981], capsules [Hinton 2011]



What-Where Auto-Encoder Architecture





Low-Level Filters Connected to Each Complex Cell

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C1 (where)



C2 (what)

Generating Images





Future Challenges





Integrating Feed-Forward and Feedback



- Deconvolutional networks
 - [Zeiler-Graham-Fergus ICCV 2011]

- Feed-forward/Feedback networks allow reconstruction, multimodal prediction, restoration, etc...
 - Deep Boltzmann machines can do this, but there are scalability issues with training



- Deep Learning systems can be assembled into factor graphs
 - Energy function is a sum of factors
 - Factors can embed whole deep learning systems
 - X: observed variables (inputs)
 - Z: never observed (latent variables)
 - Y: observed on training set (output variables)
- Inference is energy minimization (MAP) or free energy minimization (marginalization) over Z and Y given an X



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 - \blacktriangleright F(X,Y) = MIN_z E(X,Y,Z)
 - F(X,Y) = -log SUM_z exp[-E(X,Y,Z)]



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Integrting deep learning and structured prediction is a very old idea

- In fact, it predates structured prediction
- Globally-trained convolutional-net + graphical models
 - trained discriminatively at the word level
 - Loss identical to CRF and structured perceptron
 - Compositional movable parts model
- A system like this was reading 10 to 20% of all the checks in the US around 1998



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Future Challenges

Integrated feed-forward and feedback

- Deep Boltzmann machine do this, but there are issues of scalability.
- Integrating supervised and unsupervised learning in a single algorithm
 - Again, deep Boltzmann machines do this, but....
- Integrating deep learning and structured prediction ("reasoning")
 - This has been around since the 1990's but needs to be revived
- Learning representations for complex reasoning
 - "recursive" networks that operate on vector space representations of knowledge [Pollack 90's] [Bottou 2010] [Socher, Manning, Ng 2011]
- Representation learning in natural language processing
 - [Y. Bengio 01],[Collobert Weston 10], [Mnih Hinton 11] [Socher 12]
- Better theoretical understanding of deep learning and convolutional nets
 - e.g. Stephane Mallat's "scattering transform", work on the sparse representations from the applied math community....

Communities

DeepLearning.net

- http://deeplearning.net
- Maintained by Yoshua Bengio's group
- International Conference on Learning Representations
 - https://sites.google.com/site/representationlearning2013/
 - Open review system
 - Papers and videos available online
 - Takes place in April
 - Extended version of selected papers published in JMLR
 - https://plus.google.com/communities/108755902083074010353
- "Deep Learning" community on Google+
 - https://plus.google.com/communities/112866381580457264725

SOFTWARE

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Torch7: learning library that supports neural net training

- http://www.torch.ch
- http://code.cogbits.com/wiki/doku.php (tutorial with demos by C. Farabet)
- http://eblearn.sf.net (C++ Library with convnet support by P. Sermanet)

Python-based learning library (U. Montreal)

- http://deeplearning.net/software/theano/ (does automatic differentiation)

RNN

- www.fit.vutbr.cz/~imikolov/rnnlm (language modeling)
- http://sourceforge.net/apps/mediawiki/rnnl/index.php (LSTM)

CUDAMat & GNumpy

- code.google.com/p/cudamat
- www.cs.toronto.edu/~tijmen/gnumpy.html

Misc

- www.deeplearning.net//software_links

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Convolutional Nets

 LeCun, Bottou, Bengio and Haffner: Gradient-Based Learning Applied to Document Recognition, Proceedings of the IEEE, 86(11):2278-2324, November 1998

- Krizhevsky, Sutskever, Hinton "ImageNet Classification with deep convolutional neural networks" NIPS 2012

– Jarrett, Kavukcuoglu, Ranzato, LeCun: What is the Best Multi-Stage Architecture for Object Recognition?, Proc. International Conference on Computer Vision (ICCV'09), IEEE, 2009

- Kavukcuoglu, Sermanet, Boureau, Gregor, Mathieu, LeCun: Learning Convolutional Feature Hierachies for Visual Recognition, Advances in Neural Information Processing Systems (NIPS 2010), 23, 2010

- see yann.lecun.com/exdb/publis for references on many different kinds of convnets.

 see http://www.cmap.polytechnique.fr/scattering/ for scattering networks (similar to convnets but with less learning and stronger mathematical foundations)

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Applications of Convolutional Nets

- Farabet, Couprie, Najman, LeCun, "Scene Parsing with Multiscale Feature Learning, Purity Trees, and Optimal Covers", ICML 2012
- Pierre Sermanet, Koray Kavukcuoglu, Soumith Chintala and Yann LeCun: Pedestrian Detection with Unsupervised Multi-Stage Feature Learning, CVPR 2013
- D. Ciresan, A. Giusti, L. Gambardella, J. Schmidhuber. Deep Neural Networks Segment Neuronal Membranes in Electron Microscopy Images. NIPS 2012
- Raia Hadsell, Pierre Sermanet, Marco Scoffier, Ayse Erkan, Koray Kavackuoglu, Urs Muller and Yann LeCun: Learning Long-Range Vision for Autonomous Off-Road Driving, Journal of Field Robotics, 26(2):120-144, February 2009
- Burger, Schuler, Harmeling: Image Denoisng: Can Plain Neural Networks Compete with BM3D?, Computer Vision and Pattern Recognition, CVPR 2012,

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Applications of RNNs

- Mikolov "Statistical language models based on neural networks" PhD thesis 2012
- Boden "A guide to RNNs and backpropagation" Tech Report 2002
- Hochreiter, Schmidhuber "Long short term memory" Neural Computation 1997
- Graves "Offline arabic handwrting recognition with multidimensional neural networks" Springer 2012
- Graves "Speech recognition with deep recurrent neural networks" ICASSP 2013

Deep Learning & Energy-Based Models

- Y. Bengio, Learning Deep Architectures for AI, Foundations and Trends in Machine Learning, 2(1), pp.1-127, 2009.
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- M. Ranzato Ph.D. Thesis "Unsupervised Learning of Feature Hierarchies" NYU 2009

Practical guide

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- L. Bottou, Stochastic gradient descent tricks, Neural Networks, Tricks of the Trade Reloaded, LNCS 2012.
- Y. Bengio, Practical recommendations for gradient-based training of deep architectures, ArXiv 2012