Energy-Based Models: Structured Learning Beyond Likelihoods

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Two Big Problems in Machine Learning

1. The "Deep Learning Problem"

"Deep" architectures are necessary to solve the invariance problem in vision (and perception in general)

2. The "Partition Function Problem"

- Give high probability (or low energy) to good answers
- Give low probability (or high energy) to bad answers
- There are too many bad answers!

This tutorial discusses problem #2

- The partition function problem arises with probabilistic approaches
- Non-probabilistic approaches may allow us to get around it.
- Energy-Based Learning provides a framework in which to describe probabilistic and non-probabilistic approaches to learning
- Paper: LeCun et al. : "A tutorial on energy-based learning"
 - http://yann.lecun.com/exdb/publis
 - http://www.cs.nyu.edu/~yann/research/ebm

Plan of the Tutorial

Introduction to Energy-Based Models

- Energy-Based inference
- Examples of architectures and applications, structured outputs

Training Energy-Based Models

- Designing a loss function. Examples of loss functions
- Which loss functions work, and which ones don't work
- Getting around the partition function problem with EB learning

2. Architectures for Structured Outputs

- Energy-Based Graphical Models (non-probabilistic factor graphs)
- Latent variable models
- Linear factors: Conditional Random Fields and Maximum Margin Markov Nets
- Gradient-based learning with non-linear factors

Applications: supervised and unsupervised learning

- Integrated segmentation/recognition in vision, speech, and OCR.
- Invariant feature learning, manifold learning

Energy-Based Model for Decision-Making



Model: Measures the compatibility between an observed variable X and a variable to be predicted Y through an energy function E(Y,X).

 $Y^* = \operatorname{argmin}_{Y \in \mathcal{Y}} E(Y, X).$

- Inference: Search for the Y that minimizes the energy within a set y
- If the set has low cardinality, we can use exhaustive search.

Complex Tasks: Inference is non-trivial



What Questions Can a Model Answer?

1. Classification & Decision Making:

- "which value of Y is most compatible with X?"
- Applications: Robot navigation,.....
- Training: give the lowest energy to the correct answer

2. Ranking:

- "Is Y1 or Y2 more compatible with X?"
- Applications: Data-mining....
- Training: produce energies that rank the answers correctly

3. Detection:

- "Is this value of Y compatible with X"?
- Application: face detection....
- Training: energies that increase as the image looks less like a face.

4. Conditional Density Estimation:

- "What is the conditional distribution P(Y|X)?"
- Application: feeding a decision-making system
- Training: differences of energies must be just so.

Decision-Making versus Probabilistic Modeling

Energies are uncalibrated

- The energies of two separately-trained systems cannot be combined
- The energies are uncalibrated (measured in arbitrary untis)

How do we calibrate energies?

- We turn them into probabilities (positive numbers that sum to 1).
- Simplest way: Gibbs distribution
- Other ways can be reduced to Gibbs by a suitable redefinition of the energy.

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

Partition function Inverse temperature

Architecture and Loss Function

- Family of energy functions $\mathcal{E} = \{E(W, Y, X) : W \in \mathcal{W}\}.$ Training set $\mathcal{S} = \{(X^i, Y^i) : i = 1 \dots P\}.$
- Loss functional / Loss function $\mathcal{L}(E, \mathcal{S})$ $\mathcal{L}(W, \mathcal{S})$

Measures the quality of an energy function

Training
$$W^* = \min_{W \in \mathcal{W}} \mathcal{L}(W, \mathcal{S}).$$

Form of the loss functional

invariant under permutations and repetitions of the samples

$$\mathcal{L}(E, S) = \frac{1}{P} \sum_{i=1}^{P} L(Y^{i}, E(W, \mathcal{Y}, X^{i})) + R(W).$$

Per-sample Desired for a given Xi
loss answer as Y varies Regularizer

Designing a Loss Functional



Correct answer has the lowest energy -> LOW LOSS

Lowest energy is not for the correct answer -> HIGH LOSS

Designing a Loss Functional



Push down on the energy of the correct answer

Pull up on the energies of the incorrect answers, particularly if they are smaller than the correct one

Architecture + Inference Algo + Loss Function = Model



- **1. Design an architecture:** a particular form for E(W,Y,X).
- 2. Pick an inference algorithm for Y: MAP or conditional distribution, belief prop, min cut, variational methods, gradient descent, MCMC, HMC.....
- **3. Pick a loss function:** in such a way that minimizing it with respect to W over a training set will make the inference algorithm find the correct Y for a given X.

4. Pick an optimization method.

PROBLEM: What loss functions will make the machine approach the desired behavior?

Several Energy Surfaces can give the same answers



Both surfaces compute Y=X^2

 $\blacksquare MINy E(Y,X) = X^2$

Minimum-energy inference gives us the same answer

Simple Architectures



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$$E(W, X, Y) = ||G_{1_{W_1}}(X) - G_{2_{W_2}}(Y)||_1,$$

The Implicit Regression architecture

- allows multiple answers to have low energy.
- Encodes a constraint between X and Y rather than an explicit functional relationship
- This is useful for many applications
- Example: sentence completion: "The cat ate the {mouse,bird,homework,...}"
- [Bengio et al. 2003]
- But, inference may be difficult.



Examples of Loss Functions: Energy Loss

Energy Loss Lenergy (Yⁱ, E(W, Y, Xⁱ)) = E(W, Yⁱ, Xⁱ).
 Simply pushes down on the energy of the correct answer



$$L_{perceptron}(Y^{i}, E(W, \mathcal{Y}, X^{i})) = E(W, Y^{i}, X^{i}) - \min_{Y \in \mathcal{Y}} E(W, Y, X^{i}).$$

Perceptron Loss [LeCun et al. 1998], [Collins 2002]

- Pushes down on the energy of the correct answer
- Pulls up on the energy of the machine's answer
- Always positive. Zero when answer is correct
- No "margin": technically does not prevent the energy surface from being almost flat.
- Works pretty well in practice, particularly if the energy parameterization does not allow flat surfaces.

$$L_{perceptron}(Y^{i}, E(W, \mathcal{Y}, X^{i})) = E(W, Y^{i}, X^{i}) - \min_{Y \in \mathcal{Y}} E(W, Y, X^{i}).$$

• Energy:
$$E(W, Y, X) = -YG_W(X),$$

Inference: $Y^* = \operatorname{argmin}_{Y \in \{-1,1\}} - YG_W(X) = \operatorname{sign}(G_W(X)).$

Loss:
$$\mathcal{L}_{\text{perceptron}}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \left(\text{sign}(G_W(X^i)) - Y^i \right) G_W(X^i).$$

Learning Rule:
$$W \leftarrow W + \eta \left(Y^i - \operatorname{sign}(G_W(X^i)) \right) \frac{\partial G_W(X^i)}{\partial W},$$

• If Gw(X) is linear in W: $E(W, Y, X) = -YW^T \Phi(X)$

$$W \leftarrow W + \eta \left(Y^i - \operatorname{sign}(W^T \Phi(X^i)) \right) \Phi(X^i)$$

First, we need to define the Most Offending Incorrect Answer

Most Offending Incorrect Answer: discrete case

Definition 1 Let Y be a discrete variable. Then for a training sample (X^i, Y^i) , the **most offending incorrect answer** \overline{Y}^i is the answer that has the lowest energy among all answers that are incorrect:

$$\bar{Y}^{i} = \operatorname{argmin}_{Y \in \mathcal{Y}^{and} Y \neq Y^{i}} E(W, Y, X^{i}).$$
(8)

Most Offending Incorrect Answer: continuous case

Definition 2 Let Y be a continuous variable. Then for a training sample (X^i, Y^i) , the most offending incorrect answer \overline{Y}^i is the answer that has the lowest energy among all answers that are at least ϵ away from the correct answer:

$$\bar{Y}^{i} = \operatorname{argmin}_{Y \in \mathcal{Y}, \|Y - Y^{i}\| > \epsilon} E(W, Y, X^{i}).$$
(9)

$$L_{\text{margin}}(W, Y^i, X^i) = Q_m\left(E(W, Y^i, X^i), E(W, \bar{Y}^i, X^i)\right).$$



Examples of Generalized Margin Losses

$$L_{\text{hinge}}(W, Y^{i}, X^{i}) = \max\left(0, m + E(W, Y^{i}, X^{i}) - E(W, \bar{Y}^{i}, X^{i})\right)$$

Hinge Loss

- [Altun et al. 2003], [Taskar et al. 2003]
- With the linearly-parameterized binary classifier architecture, we get linear SVMs



$$L_{\log}(W, Y^{i}, X^{i}) = \log\left(1 + e^{E(W, Y^{i}, X^{i}) - E(W, \bar{Y}^{i}, X^{i})}\right)$$

Log Loss

- "soft hinge" loss
- With the linearly-parameterized binary classifier architecture, we get linear Logistic Regression



Examples of Margin Losses: Square-Square Loss

$$L_{\rm sq-sq}(W, Y^{i}, X^{i}) = E(W, Y^{i}, X^{i})^{2} + \left(\max(0, m - E(W, \bar{Y}^{i}, X^{i}))\right)^{2}.$$

Square-Square Loss

- [LeCun-Huang 2005]
- Appropriate for positive energy functions





LVQ2 Loss [Kohonen, Oja], Driancourt-Bottou 1991]

$$L_{\text{lvq2}}(W, Y^i, X^i) = \min\left(1, \max\left(0, \frac{E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)}{\delta E(W, \bar{Y}^i, X^i)}\right)\right),$$

Minimum Classification Error Loss [Juang, Chou, Lee 1997]

$$L_{\rm mce}(W, Y^{i}, X^{i}) = \sigma \left(E(W, Y^{i}, X^{i}) - E(W, \bar{Y}^{i}, X^{i}) \right),$$
$$\sigma(x) = (1 + e^{-x})^{-1}$$

Square-Exponential Loss [Osadchy, Miller, LeCun 2004] $L_{sq-exp}(W, Y^{i}, X^{i}) = E(W, Y^{i}, X^{i})^{2} + \gamma e^{-E(W, \bar{Y}^{i}, X^{i})},$ Conditional probability of the samples (assuming independence)

$$P(Y^{1}, \dots, Y^{P} | X^{1}, \dots, X^{P}, W) = \prod_{i=1}^{P} P(Y^{i} | X^{i}, W).$$
$$-\log \prod_{i=1}^{P} P(Y^{i} | X^{i}, W) = \sum_{i=1}^{P} -\log P(Y^{i} | X^{i}, W).$$
Gibbs distribution:
$$P(Y | X^{i}, W) = \frac{e^{-\beta E(W, Y, X^{i})}}{\int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^{i})}}.$$
$$-\log \prod_{i=1}^{P} P(Y^{i} | X^{i}, W) = \sum_{i=1}^{P} \beta E(W, Y^{i}, X^{i}) + \log \int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^{i})}.$$

• We get the NLL loss by dividing by P and Beta: $\mathcal{L}_{nll}(W, S) = \frac{1}{P} \sum_{i=1}^{P} \left(E(W, Y^i, X^i) + \frac{1}{\beta} \log \int_{u \in \mathcal{V}} e^{-\beta E(W, y, X^i)} \right).$

Reduces to the perceptron loss when Beta->infinity

Negative Log-Likelihood Loss

Pushes down on the energy of the correct answer

Pulls up on the energies of all answers in proportion to their probability

$$\mathcal{L}_{nll}(W, S) = \frac{1}{P} \sum_{i=1}^{P} \left(E(W, Y^{i}, X^{i}) + \frac{1}{\beta} \log \int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^{i})} \right).$$

$$\frac{\partial L_{nll}(W, Y^{i}, X^{i})}{\partial W} = \frac{\partial E(W, Y^{i}, X^{i})}{\partial W} - \int_{Y \in \mathcal{Y}} \frac{\partial E(W, Y, X^{i})}{\partial W} P(Y|X^{i}, W),$$

$$(b)$$

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Negative Log-Likelihood Loss: Binary Classification

Binary Classifier Architecture:

$$\mathcal{L}_{\mathrm{nll}}(W,\mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \left[-Y^{i} G_{W}(X^{i}) + \log \left(e^{Y^{i} G_{W}(X^{i})} + e^{-Y^{i} G_{W}(X^{i})} \right) \right].$$
$$\mathcal{L}_{\mathrm{nll}}(W,\mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \log \left(1 + e^{-2Y^{i} G_{W}(X^{i})} \right),$$

Linear Binary Classifier Architecture:

$$\mathcal{L}_{\mathrm{nll}}(W,\mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \log\left(1 + e^{-2Y^{i}W^{T}\Phi(X^{i})}\right).$$

Learning Rule: logistic regression

What Makes a "Good"

Loss Function

Good loss functions make the machine produce the correct

answer

Avoid collapses and flat energy surfaces



Sufficient Condition on the Loss

Let (X^i, Y^i) be the i^{th} training example and m be a positive margin. Minimizing the loss function L will cause the machine to satisfy $E(W, Y^i, X^i) < E(W, Y, X^i) - m$ for all $Y \neq Y^i$, if there exists at least one point (e_1, e_2) with $e_1 + m < e_2$ such that for all points (e'_1, e'_2) with $e'_1 + m \ge e'_2$, we have

$$Q_{[E_y]}(e_1, e_2) < Q_{[E_y]}(e'_1, e'_2),$$

where $Q_{[E_y]}$ is given by

 $L(W, Y^{i}, X^{i}) = Q_{[E_{y}]}(E(W, Y^{i}, X^{i}), E(W, \bar{Y}^{i}, X^{i})).$

What Make a "Good" Loss Function

Good and bad loss functions

Loss (equation $\#$)	Formula	Margin
energy loss	$E(W, Y^i, X^i)$	none
perceptron	$E(W, Y^i, X^i) - \min_{Y \in \mathcal{Y}} E(W, Y, X^i)$	0
hinge	$\max\left(0, m + E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right)$	m
\log	$\log\left(1+e^{E(W,Y^i,X^i)-E(W,\bar{Y}^i,X^i)}\right)$	> 0
LVQ2	$\min\left(M, \max(0, E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right)$	0
MCE	$\left(1 + e^{-\left(E(W,Y^{i},X^{i}) - E(W,\bar{Y}^{i},X^{i})\right)}\right)^{-1}$	> 0
square-square	$E(W, Y^{i}, X^{i})^{2} - (\max(0, m - E(W, \bar{Y}^{i}, X^{i})))^{2}$	m
square-exp	$E(W, Y^i, X^i)^2 + \beta e^{-E(W, \bar{Y}^i, X^i)}$	> 0
NLL/MMI	$E(W, Y^i, X^i) + \frac{1}{\beta} \log \int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^i)}$	> 0
MEE	$1 - e^{-\beta E(W,Y^i,X^i)} / \int_{y \in \mathcal{Y}} e^{-\beta E(W,y,X^i)}$	> 0

Advantages/Disadvantages of various losses

- Loss functions differ in how they pick the point(s) whose energy is pulled up, and how much they pull them up
- Losses with a log partition function in the contrastive term pull up all the bad answers simultaneously.
 - This may be good if the gradient of the contrastive term can be computed efficiently
 - This may be bad if it cannot, in which case we might as well use a loss with a single point in the contrastive term
- Variational methods pull up many points, but not as many as with the full log partition function.
- Efficiency of a loss/architecture: how many energies are pulled up for a given amount of computation?
 - The theory for this is does not exist. It needs to be developed

The energy includes "hidden" variables Z whose value is never given to us

We can minimize the energy over those latent variables

We can also "marginalize" the energy over the latent variables

Minimization over latent variables:

$$E(Y,X) = \min_{Z \in \mathcal{Z}} E(Z,Y,X).$$

Marginalization over latent variables:

$$E(X,Y) = -\frac{1}{\beta} \log \int_{z \in \mathcal{Z}} e^{-\beta E(z,Y,X)}$$



Estimation this integral may require some approximations

(sampling, variational methods,....)

The energy includes "hidden" variables Z whose value is never given to us



What can the latent variables represent?

- Variables that would make the task easier if they were known:
 - Face recognition: the gender of the person, the orientation of the face.
 - Object recognition: the pose parameters of the object (location, orientation, scale), the lighting conditions.
 - Parts of Speech Tagging: the segmentation of the sentence into syntactic units, the parse tree.
 - Speech Recognition: the segmentation of the sentence into phonemes or phones.
 - Handwriting Recognition: the segmentation of the line into characters.
- In general, we will search for the value of the latent variable that allows us to get an answer (Y) of smallest energy.

Marginalizing over latent variables instead of minimizing.

$$P(Z, Y|X) = \frac{e^{-\beta E(Z, Y, X)}}{\int_{y \in \mathcal{Y}, \ z \in \mathcal{Z}} e^{-\beta E(y, z, X)}}.$$

$$P(Y|X) = \frac{\int_{z \in \mathcal{Z}} e^{-\beta E(Z,Y,X)}}{\int_{y \in \mathcal{Y}, \ z \in \mathcal{Z}} e^{-\beta E(y,z,X)}}.$$

• Equivalent to traditional energy-based inference with a redefined energy function: $Y^* = \operatorname{argmin}_{Y \in \mathcal{Y}} - \frac{1}{\beta} \log \int_{z \in \mathcal{Z}} e^{-\beta E(z,Y,X)}.$

Reduces to minimization when Beta->infinity

Face Detection and Pose Estimation with a Convolutional EBM

- **Training:** 52,850, 32x32 grey-level images of faces, 52,850 selected non-faces.
- Each training image was used 5 times with random variation in scale, in-plane rotation, brightness and contrast.
- 2nd phase: half of the initial negative set was replaced by false positives of the initial version of the detector.

 $E^{*}(W, X) = \min_{Z} ||G_{W}(X) - F(Z)||$

$$Z^* = \operatorname{argmin}_Z ||G_W(X) - F(Z)||$$



Face Manifold



Probabilistic Approach: Density model of joint P(face,pose)

Probability that image
X is a face with pose Z
$$P(X, Z) = \frac{\exp(-E(W, Z, X))}{\int_{X, Z \in \text{images, poses}} \exp(-E(W, Z, X))}$$

Given a training set of faces annotated with pose, find the W that maximizes the likelihood of the data under the model:

$$P(\text{faces} + \text{pose}) = \prod_{X,Z \in \text{faces} + \text{pose}} \frac{\exp(-E(W, Z, X))}{\int_{X,Z \in \text{images}, \text{poses}} \exp(-E(W, Z, X))}$$

Equivalently, minimize the negative log likelihood:

$$\mathcal{L}(W, \text{faces} + \text{pose}) = \sum_{X, Z \in \text{faces} + \text{pose}} E(W, Z, X) + \log \left[\int_{X, Z \in \text{images}, \text{poses}} \exp(-E(W, Z, X)) \right]$$

$$COMPLICATED$$

Energy-Based Contrastive Loss Function

$$\mathcal{L}(W) = \frac{1}{|\mathbf{f} + \mathbf{p}|} \sum_{X, Z \in \text{faces+pose}} \left[L^+ \left(E(W, Z, X) \right) \right] + L^- \left(\min_{X, Z \in \text{bckgnd,poses}} E(W, Z, X) \right)$$

$$L^{+}(E(W, Z, X)) = E(W, Z, X)^{2} = ||G_{W}(X) - F(Z)||^{2}$$



Attract the network output Gw(X) to the location of the desired pose F(Z) on the manifold

$$L^{-}\left(\min_{X,Z\in \text{bckgnd,poses}} E(W,Z,X)\right) = K\exp\left(-\min_{X,Z\in \text{bckgnd,poses}} ||G_W(X) - F(Z)||\right)$$



Repel the network output Gw(X) away from the face/pose manifold
Convolutional Network Architecture

[LeCun et al. 1988, 1989, 1998, 2005]



Hierarchy of local filters (convolution kernels),sigmoid pointwise non-linearities, and spatial subsamplingAll the filter coefficients are learned with gradient descent (back-prop)

Alternated Convolutions and Pooling/Subsampling

- Local features are extracted everywhere.
- pooling/subsampling layer builds robustness to variations in feature locations.
- Long history in neuroscience and computer vision:
 - Hubel/Wiesel 1962,
 - 🤜 Fukushima 1971-82,
 - LeCun 1988-06
 - Poggio, Riesenhuber, Serre 02-06
 - Ullman 2002-06
 - Triggs, Lowe,....



Face Detection: Results

Data Set->	TILTED		PROFILE		MIT+CMU	
False positives per image->	4.42	26.9	0.47	3.36	0.5	1.28
Our Detector	90%	97%	67%	83%	83%	88%
Jones & Viola (tilted)	90%	95%	x		X	
Jones & Viola (profile)	x		70%	83%		X





Face Detection and Pose Estimation: Results



















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Face Detection with a Convolutional Net



Efficient Inference: Energy-Based Factor Graphs

- Graphical models have given us efficient inference algorithms, such as belief propagation and its numerous variations.
- Traditionally, graphical models are viewed as probabilistic models
- At first glance, is seems difficult to dissociate graphical models (Bayesian networks) from the probabilistic view.
- Energy-Based Factor Graphs are an extension of graphical models to non-probabilistic settings.
- An EBFG is an energy function that can be written as a sum of "factor" functions that take different subsets of variables as inputs.
- Basically, most algorithms for probabilistic factor graphs (such as belief prop) have a counterpart for EBFG:
 - Operations are performed in the log domain
 - The normalization steps are left out.

Energy-Based Factor Graphs

When the energy is a sum of partial energy functions (or when the probability is a product of factors):

- An EBM can be seen as an unnormalized factor graph in the log domain
- Our favorite efficient inference algorithms can be used for inference (without the normalization step).
- Min-sum algorithm (instead of max-product), Viterbi for chain graphs
- (Log/sum/exp)-sum algorithm (instead of sum-product), Forward algorithm in the log domain for chain graphs



EBFG for Structured Outputs: Sequences, Graphs, Images

Structured outputs

When Y is a complex object with components that must satisfy certain constraints.

Typically, structured outputs are sequences of symbols that must satisfy

"grammatical" constraints

- spoken/handwritten word recognition
- spoken/written sentence recognition
- DNA sequence analysis
- Parts of Speech tagging
- Automatic Machine Translation

In General, structured outputs are collections of variables in which

subsets of variables must satisfy constraints

- Pixels in an image for image restoration
- Labels of regions for image segmentations

We represent the constraints using an Energy-Based Factor Graph.

Energy-Based Factor Graphs: Three Inference Problems

X: input, Y: output, Z: latent variables

Minimization over Y and Z

$$E(Y,X) = \min_{Z \in \mathcal{Z}} E(Z,Y,X). \quad Y^* = \operatorname{argmin}_{Y \in \mathcal{Y}} E(Y,X).$$

Min over Y, marginalization over Z

$$E(X,Y) = -\frac{1}{\beta} \log \int_{z \in \mathbb{Z}} e^{-\beta E(z,Y,X)} Y^* = \operatorname{argmin}_{Y \in \mathcal{Y}} E(Y,X).$$

$$\operatorname{Marginal Distribution over Y} P(Y|X) = \frac{e^{-\beta E(Y,X)}}{\int_{y \in \mathcal{Y}} e^{-\beta E(y,X)}},$$

E1(X,Z1) E2(Z1,Z2) E3(Z2,Z3) E4(Z3,Y)
X
$$71$$
 72 73 Y

Energy-Based Factor Graphs: simple graphs

Y

Sequence Labeling

* =
$$\operatorname{argmin}_{Y \in \mathcal{Y}, Z \in \mathcal{Z}} E(Z, Y, X).$$

- Output is a sequence Y1,Y2,Y3,Y4.....
- NLP parsing, MT, speech/handwriting recognition, biological sequence analysis
- The factors ensure grammatical consistency
- They give low energy to consistent sub– sequences of output symbols
- The graph is generally simple (chain or tree)/
- Inference is easy (dynamic programming)



Energy-Based Factor Graphs: complex/loopy graphs

Image restoration

- The factors ensure local consistency on small overlapping patches
- They give low energy to "clean" patches, given the noisy versions
- The graph is loopy when the patches overlap.
- Inference is difficult, particularly when the patches are large,and when the number of greyscale values is large

$$Y^* = \operatorname{argmin}_{Y \in \mathcal{Y}} E(Y, X).$$



Efficient Inference in simple EBFG

The energy is a sum of "factor" functions, the graph is a chain

Example:

- Z1, Z2, Y1 are binary
- Z2 is ternary
- A naïve exhaustive inference would require 2x2x2x3 energy evaluations (= 96 factor evaluations)
- BUT: Ea only has 2 possible input configurations, Eb and Ec have 4, and Ed 6.
- Hence, we can precompute the 16 factor values, and put them on the arcs in a graph.
- A path in the graph is a config of variable
- The cost of the path is the energy of the config





Energy-Based Belief Prop: Minimization over Latent Variables

- The previous picture shows a chain graph of factors with 2 inputs.
- The extension of this procedure to trees, with factors that can have more than 2 inputs is the "min-sum" algorithm (a non-probabilistic form of belief propagation)
- Basically, it is the sum-product algorithm with a different semi-ring algebra (min instead of sum, sum instead of product), and no normalization step.
 - [Kschischang, Frey, Loeliger, 2001][McKay's book]



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Energy-Based Belief Prop:

Marginalization over Latent Variables

The previous picture shows a chain graph of factors with 2 inputs.

- Going along a path: add up the energies
- When several paths meet: compute

$$-\frac{1}{\beta}\log\sum_{i}e^{-\beta E_{ji}}$$

- The extension of this procedure to trees, with factors that can have more than 2 inputs is the "[log/sum/exp]-sum" algorithm (a non-probabilistic form of belief propagation)
- Basically, it is the sum-product algorithm with a different semiring algebra (log/sum/exp instead of sum, sum instead of product), and no normalization step.
 [Kschischang, Frey, Loeliger, 2001][McKay's book]

A Simple Case: Linearly Parameterized Factors: CRF, MMMN



Linearly Parameterized Factors + Negative Log Likelihood Loss = Conditional Random Fields



Linearly Parameterized Factors + NLL loss = CRF
 [Lafferty, McCallum, Pereira, 2001]

$$\begin{aligned} \mathcal{L}_{\mathrm{nll}}(W) &= \frac{1}{P} \sum_{i=1}^{P} W^{T} F(X^{i}, Y^{i}) + \frac{1}{\beta} \log \sum_{y \in \mathcal{Y}} e^{-\beta W^{T} F(X^{i}, y)} \\ \frac{\partial \mathcal{L}_{\mathrm{nll}}(W)}{\partial W} &= \frac{1}{P} \sum_{i=1}^{P} F(X^{i}, Y^{i}) - \sum_{y \in \mathcal{Y}} F(X^{i}, y) P(y | X^{i}, W), \\ P(y | X^{i}, W) &= \frac{e^{-\beta W^{T} F(X^{i}, y)}}{\sum_{y' \in \mathcal{Y}} e^{-\beta W^{T} F(X^{i}, y')}} \cdot \begin{array}{l} \text{simplest/best learning} \\ \text{procedure:} \\ \text{stochastic gradient} \end{array}$$



$$\mathcal{L}_{\text{perceptron}}(W) = \frac{1}{P} \sum_{i=1}^{P} E(W, Y^i, X^i) - E(W, Y^{*i}, X^i),$$

$$\frac{1}{P} \sum_{i=1}^{P} W^T \left(P(W^i, W^i) - P(W^i, W^i) \right)$$

$$\mathcal{L}_{\text{perceptron}}(W) = \frac{1}{P} \sum_{i=1}^{P} W^T \left(F(X^i, Y^i) - F(X^i, Y^{*i}) \right).$$

$$W \leftarrow W - \eta \left(F(X^i, Y^i) - F(X^i, Y^{*i}) \right).$$

(LeCun 1998 used non-linear factors)

Linearly Parameterized Factors + Hinge Loss = Max Margin Markov Networks



Linearly Parameterized Factor + Hinge loss

• [Altun et a. 2003, Taskar et al. 2003] $\mathcal{L}_{hinge}(W) = \frac{1}{P} \sum_{i=1}^{P} \max(0, m + E(W, Y^{i}, X^{i}) - E(W, \bar{Y}^{i}, X^{i})) + \gamma ||W||^{2}.$ $\mathcal{L}_{hinge}(W) = \frac{1}{P} \sum_{i=1}^{P} \max\left(0, m + W^{T} \Delta F(X^{i}, Y^{i})\right) + \gamma ||W||^{2},$

$$\Delta F(X^{i}, Y^{i}) = F(X^{i}, Y^{i}) - F(X^{i}, \overline{Y^{i}})$$

Simple gradient descent rule:

If $\Delta F(X^i, Y^i) > -m$ then $W \leftarrow W - \eta \Delta F(X^i, Y^i) - 2\gamma W$

Can be performed in the dual (like an SVM)

Non-Linear Factors

- Energy-Based sequence labeling systems trained discriminatively have been used since the early 1990's
- Almost all of them used non-linear factors, such as multi-layer neural nets or mixtures of Gaussians.
- They were used mostly for speech and handwriting recognition
- There is a huge literature on the subject that has been somewhat ignored or forgotten by the NIPS and NLP communities.
- Why use non linear factors?
 - :-(the loss function is non-convex
 - :-o You have to use simple gradient-based optimization algorithms, such as stochastic gradient descent (but that's what works best anyway, even in the convex case)
 - :-) linear factors simply don't cut it for speech and handwriting (including SVM-like linear combinations of kernel functions)

Deep Factors / Deep Graph: ASR with TDNN/HMM

Discriminative Automatic Speech Recognition system with HMM and

various acoustic models

Training the acoustic model (feature extractor) and a (normalized) HMM in an integrated fashion.

With Minimum Empirical Error loss

Ljolje and Rabiner (1990)

with NLL:

- Bengio (1992)
- Haffner (1993)
- Bourlard (1994)

With MCE

Juang et al. (1997)

Late normalization scheme (un-normalized HMM)

- Bottou pointed out the label bias problem (1991)
- Denker and Burges proposed a solution (1995)

Example 1: Integrated Disc. Training with Sequence Alignment

Spoken word recognition with trainable elastic templates and trainable feature extraction [Driancourt&Bottou 1991, Bottou 1991, Driancourt 1994]



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Example: 1-D Constellation Model (a.k.a. Dynamic Time Warping)

- Spoken word recognition with trainable elastic templates and trainable feature extraction [Driancourt&Bottou 1991, Bottou 1991, Driancourt 1994]
- Elastic matching using dynamic time warping (Viterbi algorithm on a trellis).
- The corresponding EBFG is implicit (it changes for every new sample).



Deep Factors / Deep Graph: ASR with TDNN/DTW

- Trainable Automatic Speech Recognition system with convolutional nets (TDNN) and dynamic time warping (DTW)
- Training the feature extractor as part of the whole process.

with the LVQ2 Loss :

Driancourt and Bottou's speech recognizer (1991)

with NLL:

- Bengio's speech recognizer (1992)
- Haffner's speech recognizer (1993)



Two types of "deep" architectures

Factors are deep / graph is deep



Complex Trellises: procedural representation of trellises

- When the trellis is too large, we cannot store it in its entirety in memory.
 - We must represent it proceduraly
- The cleanest way to represent complex graphs proceduraly is through the formalism of finite-state transducer algebra
 [Mohri 1997, Pereira et al.]



- Handwriting Recognition with Graph Transformer Networks
- Un-normalized hierarchical HMMs
 - Trained with Perceptron loss [LeCun, Bottou, Bengio, Haffner 1998]
 - Trained with NLL loss [Bengio, LeCun 1994], [LeCun, Bottou, Bengio, Haffner 1998]
- Answer = sequence of symbols
- Latent variable = segmentation



End-to-End Learning.



Making every single module in the system trainable.

Every module is trained simultaneously so as to optimize a global loss function.

Using Graphs instead of Vectors.



Whereas traditional learning machines manipulate fixed-size vectors, Graph Transformer Networks manipulate graphs.



Variables:

- X: input image
- Z: path in the interpretation graph/segmentation
- Y: sequence of labels on a path
- Loss function: computing the energy of the desired answer:

E(W, Y, X)







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Variables:

- X: input image
- Z: path in the interpretation graph/segmentation
- Y: sequence of labels on a path
- Loss function: computing the constrastive term:

$$E(W, \check{Y}, X)$$





- Example: Perceptron loss
- Loss = Energy of desired answer – Energy of best answer.

(no margin)





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Graph Composition, Transducers.

- The composition of two graphs can be computed, the same way the dot product between two vectors can be computed.
- General theory: semi-ring algebra on weighted finitestate transducers and acceptors.



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Check Reader

- Graph transformer network trained to read check amounts.
- Trained globally with Negative-Log-Likelihood loss.
- 50% percent corrent, 49% reject, 1% error (detectable later in the process.
- Fielded in 1996, used in many banks in the US and Europe.
- Processes an estimated 10% of all the checks written in the US.



Learning when the space of Y is huge

- learning when Y is in a high-dimensional continuous spaces
- Image restoration, Image segmentation
- Unsupervised learning in high-dimensional space

Learning when the space of Y is huge

Solutions:

Use an energy function such that contrastive term in the loss is either constant or easy to compute

e.g. Energy is quadratic: convex (inference is easy), integral of exponential is easily computable or constant.

Approximate the derivative of the contrastive term in the loss with a variational approximation

Simple sampling approximation:

- Pull down on the energy of the training samples
- Pull up on the energies of other configurations that have low energy (that are threatening)
- Question: how do we pick those configurations?
- One idea: contrastive Divergence

Contrastive Divergence

- To generate the "bad" configurations:
- 1. Start from the correct value of Y
- 2. Pull down the energy of the correct value
- 3. To obtain a "bad" configuration, go down the energy surface with "some noise"
- 4. pull up the energy of the obtained configuration



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Contrastive Divergence

- To generate the "bad" configurations:
- Hybrid Monte-Carlo Sampling: simulate a ball rolling down the energy surface in Y space.
- Wick the ball in the a random direction (with a random momentum), and run the simulation for a few iterations.
- The final configuration is quite likely to have lower energy than



Energy-Based Unsupervised Learning with Margin Loss

Example: learning a spiral in 2D

Energy: || Y – F(W,Y)||^2 where F is a 2-layer neural net

 $L(Y, W) = \alpha E(Y, W) + max(0, m - E(\overline{Y}, W))$

$$\overline{Y} \! \leftarrow \! \overline{Y} \! - \! \eta \frac{\delta E(\overline{Y})}{\delta Y} \! + \! \epsilon$$



Example: Conditional Product of Experts

[Ning, Delhome, LeCun, Piano, Bottou, Barbano: "Toward Automatic Phenotyping of Developing Embryos from Videos" *IEEE Trans. Image Processing*, September 2005]

Using Energy-Based Models for image "cleanup" (segmentation, denoising,.....)



 $E(Y, X, W) = E_F(Y, X) + E_I(Y, W)$

MAP Inference: clamp X and find a Y that minimizes E(Y,X,W)

Conditional PoE: Contrastive Divergence Training



The negative log-likelihood loss has an intractable sum over all possible configurations of Y **Hinton's method:**

- use MCMC to approximate the derivative of the log partition function
- realize it takes too long. Get bored waiting.
- decide to cut the number of iterations of MCMC.
- realize that it's a sensible thing to do, and call is Contrastive Divergence
- come up with a complicated justification for it.



Conditional PoE: Training with the Linear-Exponential Loss



Energy-based loss: make the energy of the desired answer low, and make the energy of the most offending undesired answer high (forget about likelihoods altogether)

Conditional Product of Experts: Training



 $L(Y^{i}, X^{i}, W) = E(Y^{i}, X^{i}, W) - c. \exp(-\beta \min_{y, |y-Y^{i}| > \delta} E(y, X^{i}, W))$

Conditional Product of Experts



Fitting energy: summed over "sites" (e.g. pixels) Internal energy: summed over "experts" (e.g. Features) and sites.

C. Elegans Embryo Phenotyping

[Ning, Delhome, LeCun, Piano, Bottou, Barbano IEEE Trans. Image Processing, October 2005]

- Analyzing results for Gene Knock-Out Experiments
- Automatically determining if a roundworm embryo is developing normally after a gene has been knocked out.





Time-lapse movie

Architecture

Region Classification with a convolutional network

- Local Consistency with a Conditional Product of Experts
- Embryo classification with elastic model matching



Region Labeling with a Convolutional Net

- Supervised training fromhand-labeled images
- 5 categories:

nucleus, nuclear membrane, cytoplasm, cell wall, external medium



Image Segmentation with Local Consistency Constraints

[Teh, Welling, Osindero, Hinton, 2001], [Kumar, Hebert 2003], [Zemel 2004]

Learn local consistency constraints with an Energy-Based Model so as to clean up images produced by the segmentor.



Convolutional Conditional PoE



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C. Elegans Embryo Phenotyping

Analyzing results for Gene Knock-Out Experiments

Original Images

Segmentation #1

Segmentation #2

CCPoE Cleanup



C. Elegans Embryo Phenotyping

Analyzing results for Gene Knock-Out Experiments



$$L(Y^{i}, X^{i}, W) = E(Y^{i}, X^{i}, W) + c. \exp(-\beta \min_{y, |y-Y^{i}| > \delta} E(y, X^{i}, W))$$



Somewhat similar to the Field of Experts [Roth & Black CVPR 2005]





Noisy peppers PSNR=22.10

CCPoE PSNR=30.40



CCPoE PSNR=30.40

FoE PSNR=30.41 (Roth & Black report 30.58)



Random Kernels, PSNR= 29.70

CCPoE PSNR=30.40

(Gasp!)

1:7.65e+00/-7.14e+00 2:6.48e+00/-3.81e+00 3:3.46e+00/-4.98e+00 4:4.00e+00/-5.08e+00 5:6.39e+00/-6.01e+00 6:6.79e+00/-7.70e+00



7:7.77e+00/-6.80e+00 8:6.29e+00/-4.71e+00 9:9.12e+00/-6.21e+00 10:8.29e+00/-5.63e+0011:7.91e+00/-7.04e+0012:4.50e+00/-4.80e+00



13:8.77e+00/-6.64e+0014:5.52e+00/-6.27e+0015:5.90e+00/-6.29e+0016:8.16e+00/-7.56e+0017:4.20e+00/-7.06e+0018:8.72e+00/-8.13e+00



19:3.84e+00/-4.54e+0020:7.56e+00/-7.00e+0021:6.03e+00/-5.17e+0022:5.48e+00/-7.06e+0023:6.56e+00/-7.37e+0024:5.96e+00/-5.42e+00



Random Kernels, PSNR= 29.70

1:1.54e+00/-8.79e-01 2:1.71e+00/-1.57e+00 3:1.55e+00/-1.83e+00 4:1.88e+00/-1.64e+00 5:1.60e+00/-1.64e+00 6:5.74e-01/-8.86e-01



7:3.17e+00/-3.23e+00 8:3.70e-01/-3.24e-01 9:2.36e+00/-1.50e+00 10:1.64e+00/-2.71e+0011:1.38e+00/-1.30e+0012:2.02e+00/-1.82e+00



13:8.67e-01/-6.75e-0114:2.47e+00/-2.26e+0015:9.34e-01/-1.23e+0016:1.30e+00/-1.32e+0017:1.30e+00/-1.93e+0018:1.50e+00/-1.66e+00



19:8.09e-01/-6.92e-0120:7.59e-01/-9.99e-0121:1.55e+00/-1.39e+0022:9.00e-01/-1.33e+0023:2.18e+00/-1.87e+0024:2.86e+00/-2.03e+00



Roth & Black Kernels, PSNR= 30.58

1:2.01e+00/-2.09e+00 2:2.48e+00/-2.54e+00 3:4.38e-02/-4.67e-02 4:3.17e+00/-2.77e+00 5:1.85e+00/-2.20e+00 6:3.91e+00/-4.51e+00



7:1.98e+00/-1.60e+00 8:3.88e+00/-3.91e+00 9:3.24e+00/-4.38e+00 10:9.09e-01/-8.14e-0111:4.70e+00/-4.07e+0012:3.04e-02/-2.39e-02



13:2.18e+00/-2.38e+0014:5.12e+00/-5.45e+0015:1.91e+00/-1.51e+0016:5.72e-02/-5.25e-0217:4.55e-02/-4.90e-0218:1.57e+00/-1.40e+00



19:3.43e-02/-3.38e-0220:1.38e+00/-1.40e+0021:4.16e+00/-3.51e+0022:4.89e+00/-4.56e+0023:4.87e+00/-4.74e+0024:3.26e+00/-3.53e+00



CCPoE Kernels, PSNR= 30.40

EBM for Face Recognition



X and Y are images

Y is a discrete variable with many

possible values

All the people in our gallery

Example of architecture:

A function G(X) maps input images into a low-dimensional space in which the Euclidean distance measures dissemblance.

Inference:

- Find the Y in the gallery that minimizes the energy (find the Y that is most similar to X)
- Minimization through exhaustive search.

Learning an Invariant Dissimilarity Metric with EBM

[Chopra, Hadsell, LeCun CVPR 2005]
Training a parameterized, invariant dissimilarity metric may be a solution to the many-category problem.

- Find a mapping Gw(X) such that the Euclidean distance ||Gw(X1)- Gw(X2)|| reflects the "semantic" distance between X1 and X2.
- Once trained, a trainable dissimilarity metric can be used to classify new categories using a very small number of training samples (used as prototypes).
- This is an example where probabilistic models are too constraining, because we would have to limit ourselves to models that can be normalized over the space of input pairs.
- With EBMs, we can put what we want in the box (e.g. A convolutional net).

Siamese Architecture

Application: face verification/recognition



Loss Function



Siamese models: distance between the outputs of two identical copies of a model.

- **Energy function**: E(W,X1,X2) = ||Gw(X1)-Gw(X2)||
- If X1 and X2 are from the same category (genuine pair), train the two copies of the model to produce similar outputs (low energy)
- If X1 and X2 are from different categories (impostor pair), train the two copies of the model to produce different outputs (high energy)
- Loss function: increasing function of genuine pair energy, decreasing function of impostor pair energy.

Loss Function

Our Loss function for a single training pair (X1,X2):

$$\begin{split} L(W, X_{1,}X_{2}) &= (1-Y)L_{G}(E_{W}(X_{1,}X_{2})) + YL_{I}(E_{W}(X_{1,}X_{2})) \\ &= (1-Y)\frac{2}{R}(E_{W}(X_{1,}X_{2})^{2}) + (Y)2Re^{-2.77\frac{E_{W}(X_{1,}X_{2})}{R}} \end{split}$$

$$E_{W}(X_{1},X_{2}) = \|G_{W}(X_{1}) - G_{W}(X_{2})\|_{LI}$$

And R is the largest possible value of

 $E_{W}(X_{1}, X_{2})$

Y=0 for a genuine pair, and Y=1 for an impostor pair.



Face Verification datasets: AT&T, FERET, and AR/Purdue

• The AT&T/ORL dataset

- Total subjects: 40. Images per subject: 10. Total images: 400.
- Images had a moderate degree of variation in pose, lighting, expression and head position.
- Images from 35 subjects were used for training. Images from 5 remaining subjects for testing.
- Training set was taken from: 3500 genuine and 119000 impostor pairs.
- Test set was taken from: 500 genuine and 2000 impostor pairs.
- http://www.uk.research.att.com/facedatabase.html





AT&T/ORL Dataset



Face Verification datasets: AT&T, FERET, and AR/Purdue

- The FERET dataset. part of the dataset was used only for training.
- Total subjects: 96. Images per subject: 6. Total images: 1122.
- Images had high degree of variation in pose, lighting, expression and head position.
- The images were used for training only.
- http://www.itl.nist.gov/iad/humanid/feret/





FERET Dataset



Architecture for the Mapping Function Gw(X)

Convolutional net



Internal state for genuine and impostor pairs


Dataset for Verification

Verification Results



Classification Examples

Example: Correctly classified genuine pairs













energy: 0.0046

energy: 0.3159 energy: 0.0043 **Example: Correctly classified impostor pairs**



energy: 20.1259











energy: 5.7186





energy: 2.8243



energy: 10.3209



A similar idea for Learning a Manifold with Invariance Properties

Loss function:

- Pay quadratically for making outputs of neighbors far apart
- Pay quadratically for making outputs of non-neighbors smaller than a margin m



Yann LeCun

A Manifold with Invariance to Shifts



Training set: 3000 "4" and 3000 "9" from MNIST. Each digit is shifted horizontally by -6, -3, 3, and 6 pixels Neighborhood graph: 5 nearest neighbors in Euclidean distance, and shifted versions of self and nearest neighbors Output Dimension: 2 Test set (shown) 1000 "4" and 1000 "9"

Automatic Discovery of the Viewpoint Manifold with Invariant to Illumination



Yann LeCun