Energy-Based Models: The Cure Against Bayesian Fundamentalism



See: [LeCun et al. 2006]: "A Tutorial on Energy-Based Learning" [Ranzato et al. AI-Stats 2007], [Ranzato et al. NIPS 2006] http://yann.lecun.com/exdb/publis/

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 talk discusses problem #2 first and #1 second.

- 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 Yann LeCun

Plan of the Talks

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.
- Getting around the partition function problem with EB learning

Architectures for structured outputs and sequence labeling

- Energy-Based Graphical Models (non-probabilistic factor graphs)
- Latent variable models
- Conditional Random Fields, Maximum Margin Markov Nets, Graph Transformer Networks

Applications in vision

- Hierarchical models of vision and object recognition
- Unsupervised learning of invariant feature hierarchies.

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.

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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 units)

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



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 $L_{energy}(Y^i, E(W, \mathcal{Y}, X^i)) = E(W, Y^i, X^i).$ • 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 SVN



E_correct - E_incorrect

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

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] <- speech recognition</p>

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

Minimum Classification Error Loss [Juang, Chou, Lee 1997] <- speech r.

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

Square-Exponential Loss [Osadchy, Miller, LeCun 2004] <- face detection $L_{sq-exp}(W, Y^{i}, X^{i}) = E(W, Y^{i}, X^{i})^{2} + \gamma e^{-E(W, \bar{Y}^{i}, X^{i})},$ 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

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

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

$$(e^{(W, Y, X)})$$

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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 in the linear case: logistic regression

 NLL is used by lots of speech recognition systems (they call it Maximum Mutual Information), lots of handwriting recognition systems (e.g. Bengio, LeCun 94] [LeCun et al. 98]), CRF [Lafferty et al 2001]

Negative Log-Likelihood Loss

Negative Log Likelihood Loss has been used for a long time in many communities for discriminative learning with structured outputs

- Speech recognition: many papers going back to the early 90's [Bengio 92], [Bourlard 94]. They call "Maximum Mutual Information"
- Handwriting recognition [Bengio LeCun 94], [LeCun et al. 98]
- Bio-informatics [Haussler]
- Conditional Random Fields [Lafferty et al. 2001]
- Lots more.....
- In all the above cases, it was used with non-linearly parameterized energies.

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

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

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 from the probabilistic view (think "Bayesian networks").
- 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 fon 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, Energy: E(Z,Y,X)

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) is a "free energy")

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

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



Energy-Based Factor Graphs: simple graphs

V

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 subsequences of output symbols
- The graph is generally simple (chain or tree)/
- Inference is easy (dynamic programming)



Energy-Based Factor Graphs: complex/loopy graphs

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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

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



Y

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





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), without the 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
 -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 without the 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]

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



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

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

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

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

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

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

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)



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 procedurally
- 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.

Graph Transformer Networks

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.



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 [Hinton 2000]

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



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

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

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



Wide auto-encoder with sparse code

Sparse Codes

- Limiting the information content of the code prevents flat energy surfaces, without the need to explicitly push up the bad points
- Idea is to make the high dimensional code sparse by forcing each variable to be zero most of the time


Challenges of Visual Neuroscience (and Computer Vision)

The recognition of everyday objects is a very fast process.

- Experiments by Simon Thorpe and others have shown that the recognition of common object is essentially "feed forward."
- Not all of vision is feed forward (what would all those feed-back connection be there for?).

How much of the visual system is the result of learning?

- How much prior structure must be built into the visual system to enable it to learn to see?
- Are V1/V2/V4 neurons learned or hard-wired?

If the visual system is learned, what is the learning algorithm?

What learning algorithm can train neural network as "deep" as the visual system (10 layers?).

Let's try to train an artificial vision system from end to end and see what it can do.

Questions?

Is there a magic bullet for visual learning?

- Is there a general principle, or should we just resort to a bunch of tricks?
- Is there a universal learning algorithm/architecture which, given a small amount of appropriate prior structure, can produce an intelligent vision system?
- Or do we need to accumulate a large repertoire of "modules" to solve each specific problem an intelligent vision system must solve. How would we assemble those modules?

How far can we get by training a vision system end to end

Let us train a complete vision system from raw pixels to object categories, or to robot actions.

An Old Idea for Local Shift Invariance

[Hubel & Wiesel 1962]:

- simple cells detect local features
- complex cells "pool" the outputs of simple cells within a retinotopic neighborhood.



The Multistage Hubel-Wiesel Architecture

Building a complete artificial vision system:

- Stack multiple stages of simple cells / complex cells layers
- Higher stages compute more global, more invariant features
- Stick a classification layer on top
- [Fukushima 1971-1982] • neocognitron
- [LeCun et al. 1988-2007]
 - convolutional net
- [Poggio et al. 2002-2006] • HMAX
- [Ullman 2002-2006]
 - fragment hierarchy
- [Lowe 2006] • HMAX

QUESTION: How do we find (or learn) the filters?



Convolutional Net Architecture, Supervised Learning



Convolutional layers (simple cells): all units in a feature plane share the same weights

- Pooling/subsampling layers (complex cells): for invariance to small distortions.
- Supervised gradient-descent learning using back-propagation
- The entire network is trained end-to-end. All the layers are trained simultaneously.

Convolutional Network for Object Recognition



96X69 input, 90,857 free parameters, 3,901,162 connections.

The architecture alternates convolutional layers (feature detectors) and subsampling layers (local feature pooling for invariance to small distortions).

The entire network is trained end-to-end (all the layers are trained simultaneously).

A gradient-based algorithm is used to minimize a supervised loss function.

Generic Object Detection and Recognition

with Invariance to Pose and Illumination

- **50** toys belonging to 5 categories: **animal, human figure, airplane, truck, car**
- **10** instance per category: **5** instances used for training, **5** instances for testing
- **Raw dataset: 972** stereo pair of each object instance. **48,600** image pairs total.

For each instance:

- 📑 18 azimuths
 - 0 to 350 degrees every 20 degrees

9 elevations

30 to 70 degrees from horizontal every 5 degrees

6 illuminations

on/off combinations of 4 lights

2 cameras (stereo)

7.5 cm apart

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Training instances

Test instances

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Data Collection, Sample Generation

Image capture setup



Objects are painted green so that:

- all features other than shape are removed
- objects can be segmented, transformed,

and composited onto various backgrounds
Original image
Object mask



Shadow factor

Composite image

Textured and Cluttered Datasets



Alternated Convolutions and Subsampling



- Local features are extracted everywhere.
- pooling/subsampling layer builds robustness to variations in feature locations.





Normalized-Uniform dataset: Test Error Rates

- Linear Classifier on raw stereo images: 30.2% error.
 K-Nearest-Neighbors on raw stereo images: 18.4% error.
 K-Nearest-Neighbors on PCA-95: 16.6% error.
 Pairwise SVM on 96x96 stereo images: 11.6% error
 - Pairwise SVM on 95 Principal Components: 13.3% error.
- Convolutional Net on 96x96 stereo images: 5.8% error.

Training instances Test instances

Jittered-Cluttered Dataset



- Jittered-Cluttered Dataset:
- **291,600** stereo pairs for training, **58,320** for testing
- Objects are jittered: position, scale, in-plane rotation, contrast, brightness, backgrounds, distractor objects,...
- Input dimension: 98x98x2 (approx 18,000)

Experiment 2: Jittered-Cluttered Dataset



291,600 training samples, **58,320** test samples

Yann LeCun

SVM with Gaussian kernel 43.3% error
Convolutional Net with binocular input: 7.8% error
Convolutional Net + SVM on top: 5.9% error
Convolutional Net with monocular input: 20.8% error
Smaller mono net (DEMO): 26.0% error
Dataset available from http://www.cs.nyu.edu/~yann

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Examples (Monocular Mode)



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 Net Architecture for Face Detection

[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)

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



















FLUIDE GLACIAL



Face Detection with a Convolutional Net



Training The Layers of a Convolutional Net Unsupervised

Supervised training of convolutional nets requires too labeled many training samples

- Extract windows from the images
- Train an unsupervised feature extractor on those windows
- Use the resulting features as the convolution kernels of a convolution network
- Repeat the process for the second layer
- Train the resulting network supervised.

Encoder/Decoder Architecture for learning Sparse

Feature Representations

Algorithm:

- I. find the code Z that minimizes the reconstruction error AND is close to the encoder output
- 2. Update the weights of the decoder to decrease the reconstruction error
- 3. Update the weights of the encoder to decrease the prediction error



Sparsifying Logistic

- Maps a code vector into a sparse code vector with components between 0 and 1 (most of which are near zero).
 - Essentially: a sigmoid function with a large adaptive threshold.
 $Z_i = \frac{Z_i}{z}$ input unit
 - Z_i corresponding output unit

$$\overline{z}_{i}(k) = \frac{\eta e^{\beta z_{i}(k)}}{\xi_{i}(k)}, \quad i \in [1..m], k \in [1..P], \eta \in (0,1), \beta > 0$$

$$\xi_{i}(k) = \eta e^{\beta z_{i}(k)} + (1-\eta)\xi_{i}(k-1)$$

Expanding the denominator:

$$\overline{z}_{i}(k) = \frac{\eta e^{\beta z_{i}(k)}}{\eta e^{\beta z_{i}(k)} + \eta (1-\eta) e^{\beta z_{i}(k-1)} + \eta (1-\eta)^{2} e^{\beta z_{i}(k-2)} + \dots}$$

equivalent to a sigmoid with a large threshold:

$$\overline{z}_{i}(k) = \frac{1}{1 + e^{-\beta \left[z_{i}(k) - \frac{1}{\beta} \log\left(\frac{1-\eta}{\eta} \xi_{i}(k-1)\right)\right]}}$$

Sparsifying Logistic

$$\overline{z}_{i}(k) = \frac{\eta e^{\beta z_{i}(k)}}{\xi_{i}(k)}, \quad i \in [1..m], k \in [1..P]$$
$$\xi_{i}(k) = \eta e^{\beta z_{i}(k)} + (1-\eta)\xi_{i}(k-1)$$

EXAMPLE

Input: random variable uniformly distributed in [-1,1]

Output: a Poisson process with firing rate determined by $\eta \;\; {\rm and} \; \beta \;$.

• Increasing β the gain is increased and the output takes almost binary values.

• Increasing η more importance is given to the current sample, a spike will be more likely to occur.











Berkeley data set

- ✤ 100,000 12x12 patches
- 200 units in the code • $\eta_{\beta}^{\eta} 0.02$
 - 1
- learning rate 0.001
- ◆L1 regularizer 0.001
- ◆ fast convergence: < 30min.</p>



200 decoder filters (reshaped columns of matrix W_d)



test sample code word



codes are:

sparse

almost binary

quite decorrelated

 in testing codes are produced by propagating the input patch through encoder and Sparsifying Légistic

controls sparsity

controls the "bit content" in each code unit

unit activity

code words from 200 randomly selected test patches

What about an autoencoder?



MNIST Dataset



Handwritten Digit Dataset MNIST: 60,000 training samples, 10,000 test samples

Handwritten digits - MNIST



- ♦ 60,000 28x28 images
- 196 units in the code
- → η 0.01
- β 1
- learning rate 0.001
- L1, L2 regularizer 0.005

Encoder *direct* filters

Handwritten digits - MNIST



Best Results on MNIST (from raw images: no preprocessing)

CLASSIFIER	DE	EFORMATION I	ERROR	Reference				
Knowledge-free methods								
2-layer NN, 800 HU, CE			1.60	Simard et al., ICDAR 2003				
3-layer NN, 500+300 HU,	CE, reg		1.53	Hinton, in press, 2005				
SVM, Gaussian Kernel			1.40	Cortes 92 + Many others				
Unsupervised Stacked RB	M + backprop		0.95	Hinton, Neur Comp 2006				
Convolutional nets								
Convolutional net LeNet-5	, ,		0.80	Ranzato et al. NIPS 2006				
Convolutional net LeNet-6),		0.70	Ranzato et al. NIPS 2006				
Conv. net LeNet-6- + uns	up learning		0.60	Ranzato et al. NIPS 2006				
Training set augmented with Affine Distortions								
2-layer NN, 800 HU, CE	Af	fine	1.10	Simard et al., ICDAR 2003				
Virtual SVM deg-9 poly	Af	fine	0.80	Scholkopf				
Convolutional net, CE	Af	fine	0.60	Simard et al., ICDAR 2003				
Training et augmented with Elastic Distortions								
2-layer NN, 800 HU, CE	Ela	astic	0.70	Simard et al., ICDAR 2003				
Convolutional net, CE	Ela	astic	0.40	Simard et al., ICDAR 2003				
Conv. net LeNet-6- + uns	up learning Ela	astic	0.39	Ranzato et al. NIPS 2006				



CLASSIFICATION EXPERIMENTS

IDEA: improving supervised learning by pre-training with the unsupervised method (*) sparse representations & lenet6 (1->50->50->200->10)

The baseline: lenet6 initialized randomly

Test error rate: 0.70%. Training error rate: 0.01%.

Experiment 1

- Train on 5x5 patches to find 50 features
- Use the scaled filters in the encoder to initialize the kernels in the first convolutional layer

Test error rate: 0.60%. Training error rate: 0.00%.

Experiment 2

Same as experiment 1, but training set augmented by elastically distorted digits (random initialization gives test error rate equal to 0.49%).

Test error rate: 0.39%. Training error rate: 0.23%.

(*)[Hinton, Osindero, Teh "A fast learning algorithm for deep belief nets" Neural Computaton 2006]






MNIST Errors (0.42% error)



Learning Invariant Feature Hierarchies

Learning Shift Invariant Features



Standard Feature Extractor

Invariant Feature Extractor

Learning Invariant Feature Hierarchies

Learning Shift Invariant Features



Shift Invariant Global Features on MNIST

Learning 50 Shift Invariant Global Features on MNIST:

50 filters of size 20x20 movable in a 28x28 frame (81 positions)
 movable strokes!



Example of Reconstruction

Any character can be reconstructed as a linear combination of a small number of basis functions.





Figure 1: 50 7x7 filters in the first convolutional layer that were learned by the network trained supervised from *random* initial conditions with 600K digits.



Figure 2: 50 7x7 filters that were learned by the unsupervised method (on 60K digits), and that are used to initialize the first convoltional layer of the network.



Figure 3: 50 7x7 filters in the first convolutional layer that were learned by the network trained supervised from the initial conditions given by the *unsupervised method* (see fig.2) with 600K digits.

Influence of Number of Training Samples



New York University

Generic Object Recognition: 101 categories + background

Caltech-101 dataset: 101 categories

- accordion airplanes anchor ant barrel bass beaver binocular bonsai brain brontosaurus buddha butterfly camera cannon car_side ceiling_fan cellphone chair chandelier cougar_body cougar_face crab crayfish crocodile crocodile_head cup dalmatian dollar_bill dolphin dragonfly electric_guitar elephant emu euphonium ewer Faces Faces_easy ferry flamingo flamingo_head garfield gerenuk gramophone grand_piano hawksbill headphone hedgehog helicopter ibis inline_skate joshua_tree kangaroo ketch lamp laptop Leopards llama lobster lotus mandolin mayfly menorah metronome minaret Motorbikes nautilus octopus okapi pagoda panda pigeon pizza platypus pyramid revolver rhino rooster saxophone schooner scissors scorpion sea_horse snoopy soccer_ball stapler starfish stegosaurus stop_sign strawberry sunflower tick trilobite umbrella watch water_lilly wheelchair wild_cat windsor_chair wrench yin_yang
- Only 30 training examples per category!
- A convolutional net trained with backprop (supervised) gets 20% correct recognition.
- Training the filters with the sparse invariant unsupervised method

Training the 1st stage filters

- 12x12 input windows (complex cell receptive fields)
- 9x9 filters (simple cell receptive fields)
- 4x4 pooling



Training the 2nd stage filters

- **13x13 input windows (complex cell receptive fields on 1st features)**
- 9x9 filters (simple cell receptive fields)
- Each output feature map combines 4 input feature maps





Generic Object Recognition: 101 categories + background

9x9 filters at the first level



9x9 filters at the second level



Shift-Invariant Feature Hierarchies on Caltech-101

- 2 layers of filters trained unsupervised
- supervised classifier on top.
- 54% correct on
 Caltech-101 with
 30 examples per
 class
- 20% correct with purely supervised backprop



Another Architecture for Caltech-256



Recognition Rate on Caltech 101



Practical Conclusion

The Multi-stage Hubel-Wiesel Architecture can be trained to recognize almost any set of objects.

- Supervised gradient descent learning requires too many examples
- Unsupervised learning of each layer reduces the number of necessary training samples
- Invariant feature learning preserves the nature of each feature, but throws away the instantiation parameters (position).
- Invariant feature hierarchies can be trained unsupervised
 - on large training sets: the recognition rate is almost as good as supervised gradient descent learning
 - on small training sets: the recognition rate is much better.