NEW YORK UNIVERSITY

Energy-Based Models (part 4)

http://bit.ly/DLSP20

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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 on training set
- **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

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

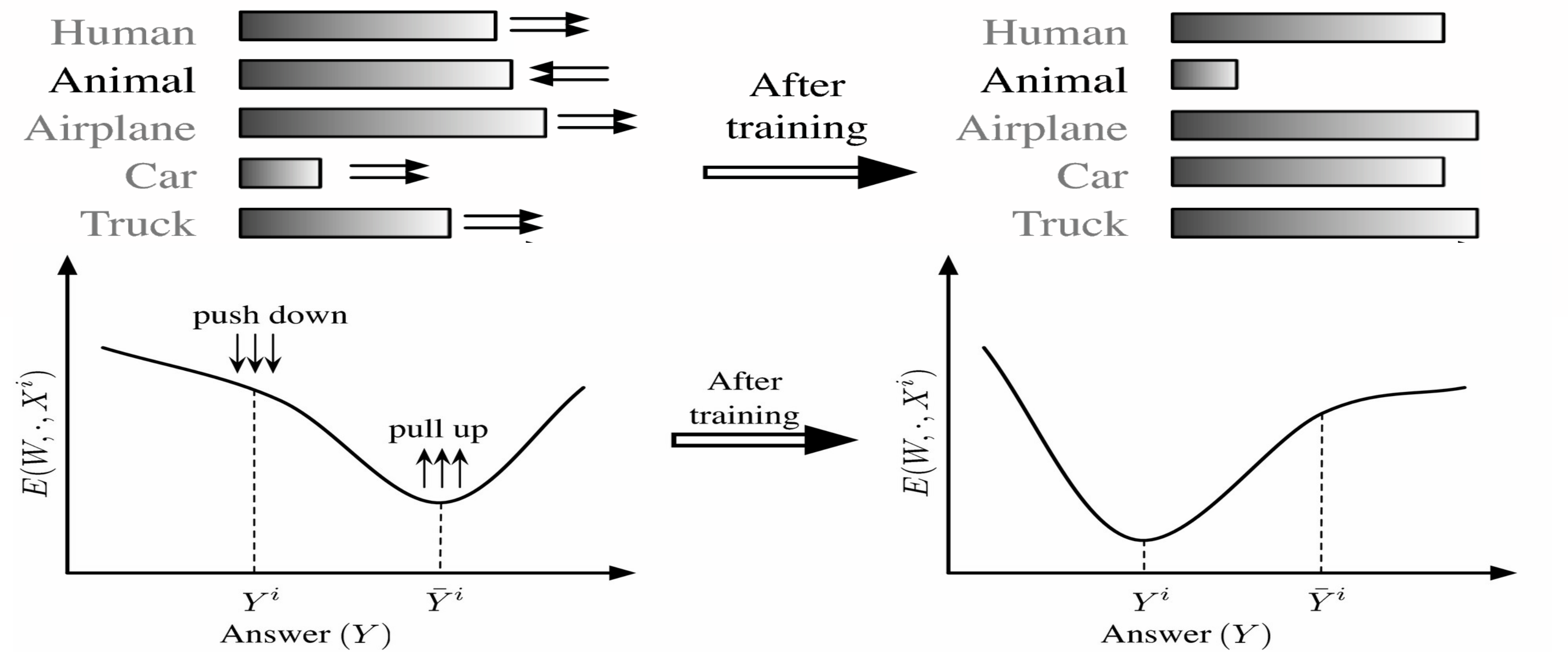
Per-sample loss

Desired answer

Energy surface for a given Xi as Y varies

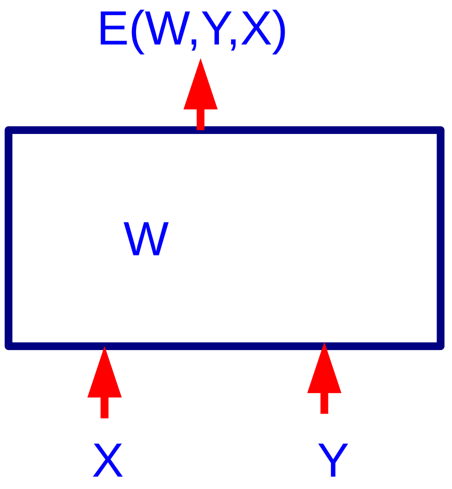
Regularizer

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



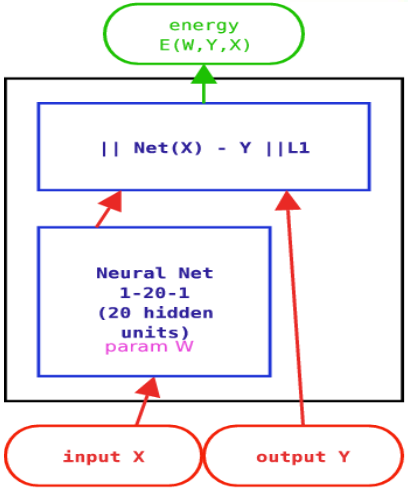
- **1. Design an architecture:** a particular form for E(W,Y,X).
- **2. Pick an inference algorithm for Y:** MAP or conditional distribution, belief prop, min cut, variational methods, gradient descent, MCMC, HMC.....
- **3. Pick a loss function:** in such a way that minimizing it with respect to W over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

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

WORKS!!!



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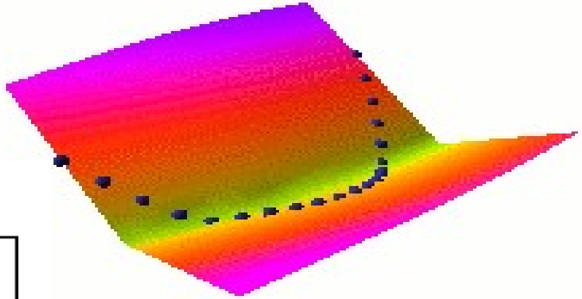
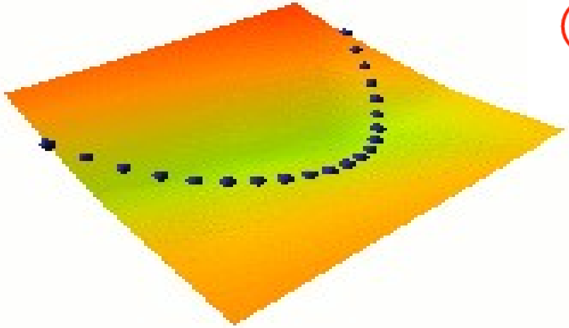
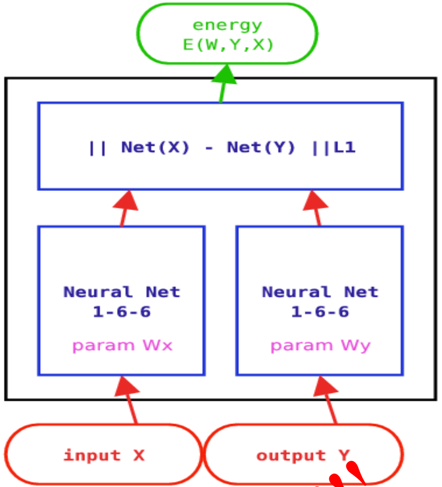






(b)

COLLAPSES!!!

Negative Log-Likelihood Loss

- **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:**

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

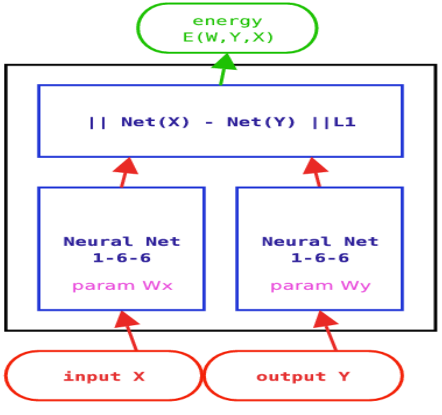
- **Reduces to the perceptron loss when Beta->infinity**

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**

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

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



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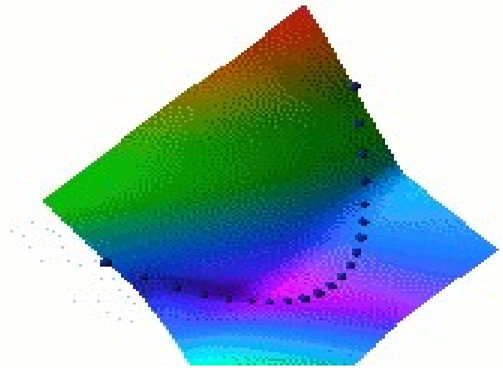


Negative Log-Likelihood Loss

- **A probabilistic model is an EBM in which:**
  - The energy can be integrated over Y (the variable to be predicted)
  - The loss function is the negative log-likelihood
- **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.

A Simpler Loss Functions:Perceptron Loss

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

- **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.
  - This is often called **“discriminative Viterbi training”** in the speech and handwriting literature

Perceptron Loss for Binary Classification

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

- **Energy:** $E(W, Y, X) = -Y G_W(X),$
- **Inference:** $Y^* = \text{argmin}_{Y \in \{-1,1\}} - Y G_W(X) = \text{sign}(G_W(X)).$
- **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:** $W \leftarrow W + \eta \left(Y^i - \text{sign}(G_W(X^i))\right) \frac{\partial G_W(X^i)}{\partial W},$
- **If Gw(X) is linear in W:** $E(W, Y, X) = -Y W^T \Phi(X)$

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

A Better Loss Function: Generalized Margin Losses

- 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** $\bar{Y}^i$ is the answer that has the lowest energy among all answers that are incorrect:*

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

- Most Offending Incorrect Answer: continuous case

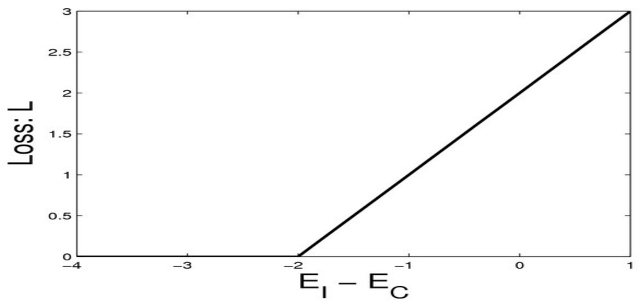
Definition 2 *Let Y be a continuous variable. Then for a training sample (X^i, Y^i), the **most offending incorrect answer** $\bar{Y}^i$ is the answer that has the lowest energy among all answers that are at least ϵ away from the correct answer:*

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

Examples of Generalized Margin Losses

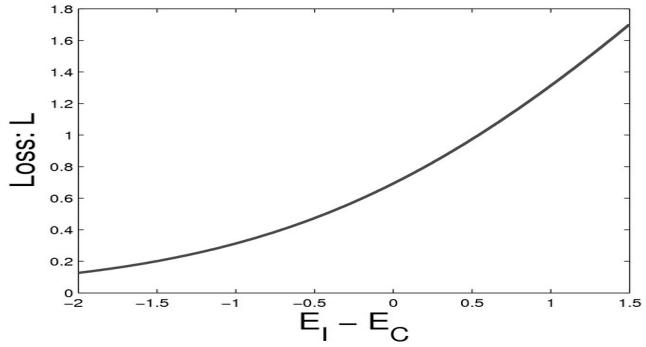
$$L_{\text{hinge}}(W, Y^i, X^i) = \max\left(0, m + E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right),$$

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



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

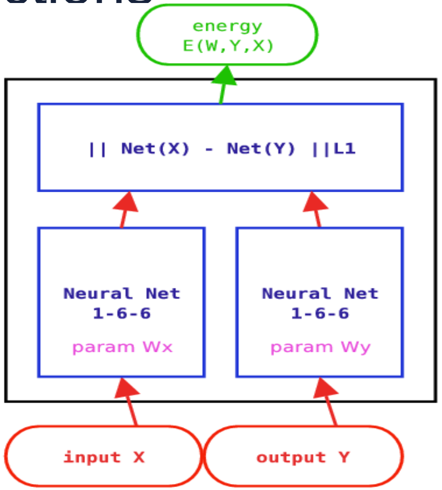
- **Log Loss**
  - "soft hinge" loss
  - With the linearly-parameterized binary classifier architecture, we get linear Logistic Regression



Examples of Margin Losses: Square-Square Loss

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

- **Square-Square Loss**
  - [LeCun-Huang 2005]
  - Appropriate for positive energy functions



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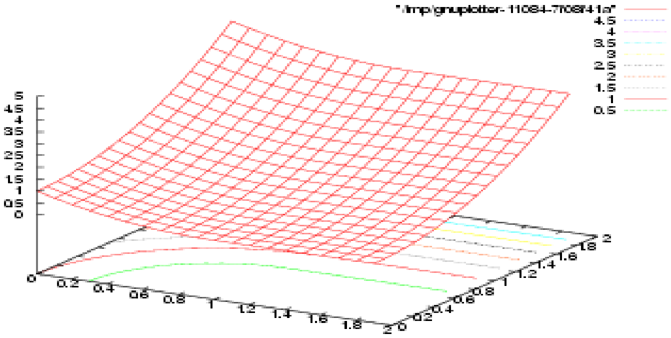
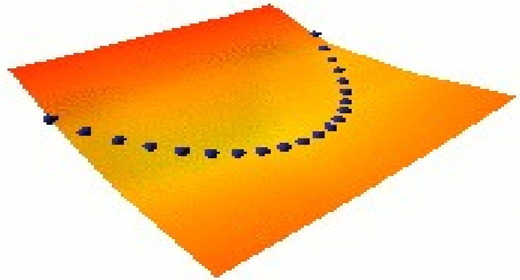


Learning Y = X^2



NO COLLAPSE!!!

Other Margin-Like Losses

- **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]

$$L_{\text{mce}}(W, Y^i, X^i) = \sigma\left(E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right),$$

$$\sigma(x) = (1 + e^{-x})^{-1}$$

- **Square-Exponential Loss** [Osadchy, Miller, LeCun 2004]

$$L_{\text{sq-exp}}(W, Y^i, X^i) = E(W, Y^i, X^i)^2 + \gamma e^{-E(W, \bar{Y}^i, X^i)},$$

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	$E(W, Y^i, X^i)^2 - \left(\max(0, m - E(W, \bar{Y}^i, X^i))\right)^2$	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

- **Slightly more general form:**

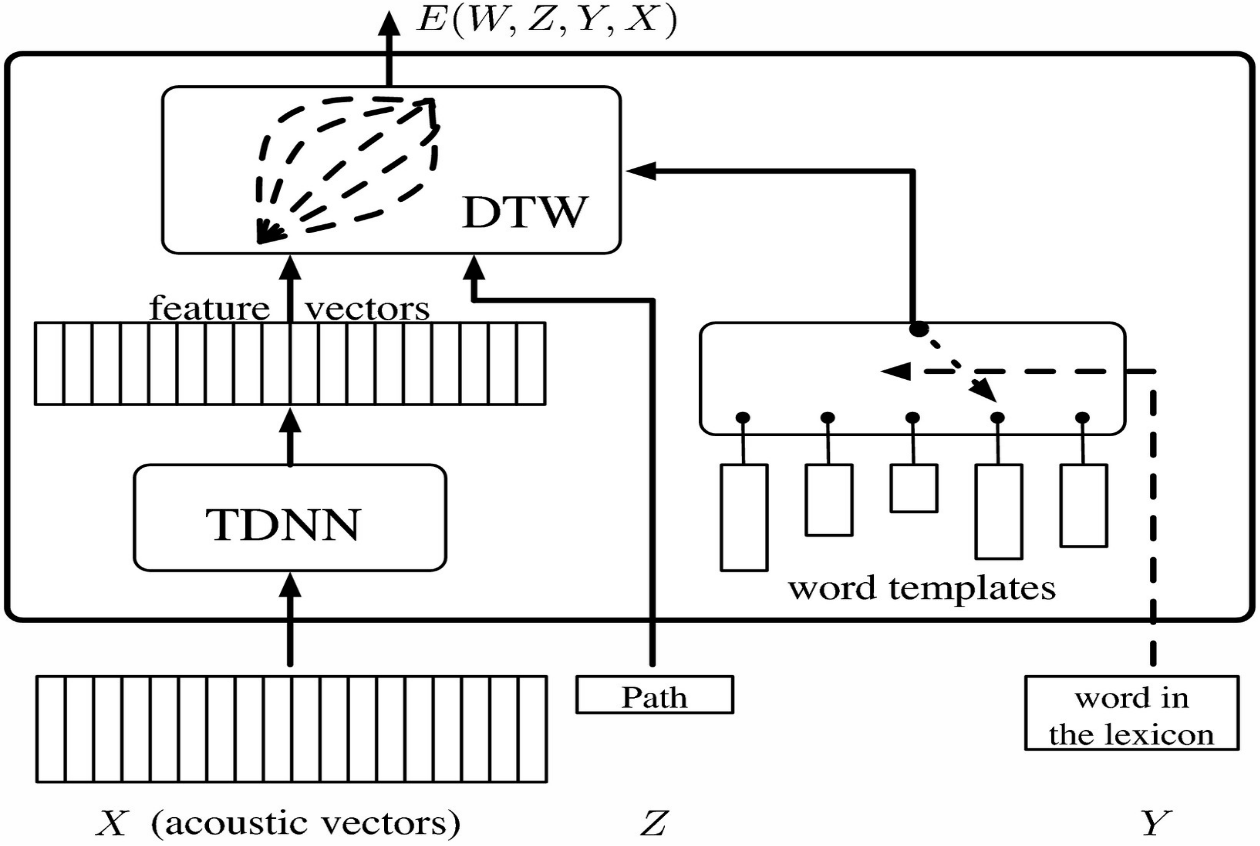
$$L(W, X^i, Y^i) = \sum_y H\left(E(W, Y^i, X^i) - E(W, y, X^i) + C(Y^i, y)\right)$$

Structured Prediction

A particular type of latent variable models

The Oldest Example of Structured Prediction

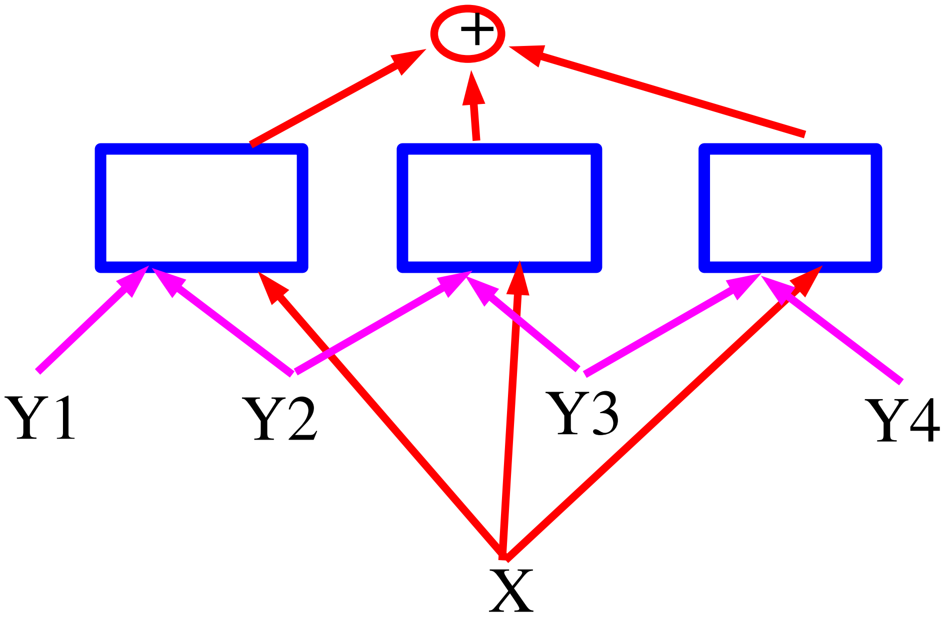
- **Trainable Automatic Speech Recognition system with a convolutional net (TDNN) and dynamic time warping (DTW)**
- **The feature extractor and the structured classifier are trained simultanesously in an integrated fashion.**
- **with the LVQ2 Loss :**
  - Driancourt and Bottou's speech recognizer (1991)
- **with NLL:**
  - Bengio's speech recognizer (1992)



Energy-Based Factor Graphs: Energy = Sum of “factors”

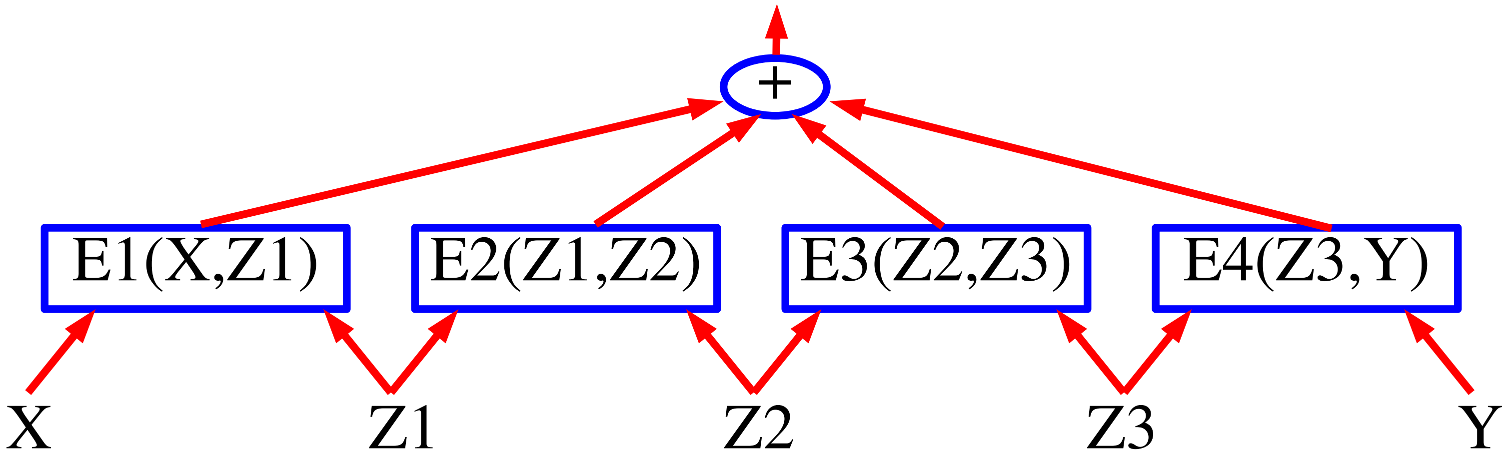
- **Sequence Labeling**
  - Output is a sequence Y1,Y2,Y3,Y4......
  - NLP parsing, MT, speech/handwriting recognition, biological sequence analysis
  - The factors ensure grammatical consistency
  - They give low energy to consistent sub-sequences of output symbols
  - The graph is generally simple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

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



Energy-Based Factor Graphs

- **When the energy is a sum of partial energy functions (or when the probability is a product of factors):**
  - Efficient inference algorithms can be used for inference (without the normalization step).

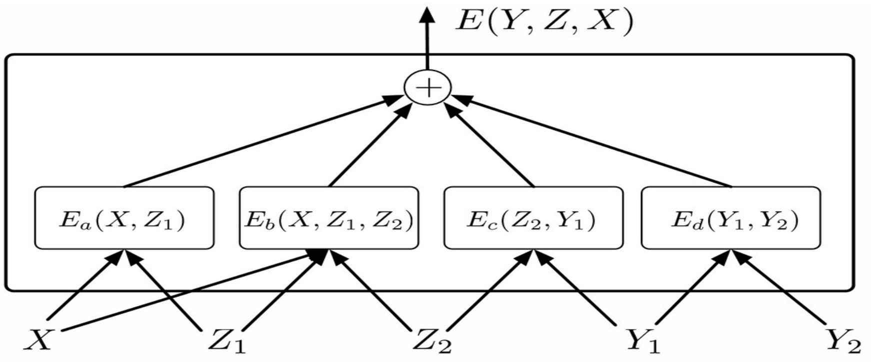


Efficient Inference: Energy-Based Factor Graphs

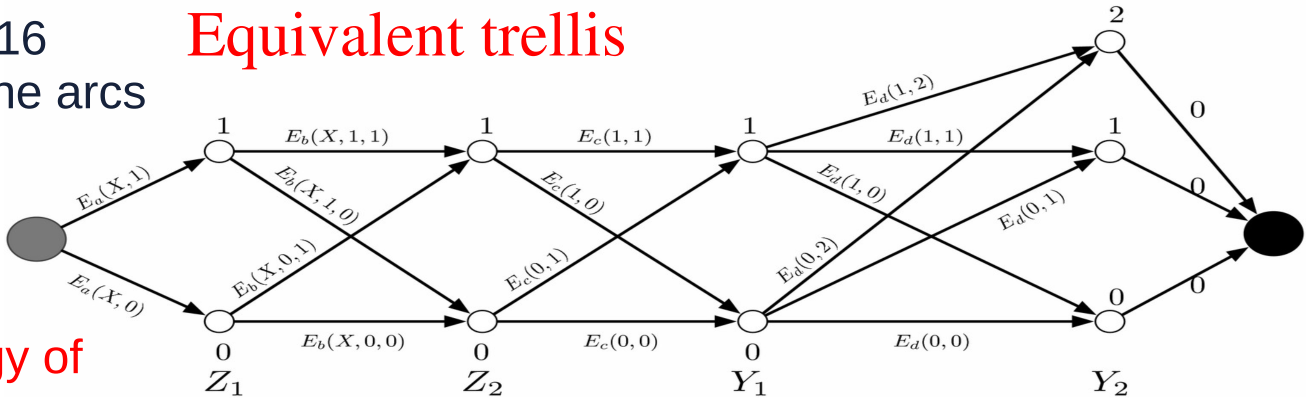
- **Example:**
  - Z1, Z2, Y1 are binary
  - Z2 is ternary
  - A naïve exhaustive inference would require 2x2x2x3=24 energy evaluations (= 96 factor evaluations)
  - BUT: Ea only has 2 possible input configurations, Eb and Ec have 4, and Ed 6.
  - Hence, we can precompute the 16 factor values, and put them on the arcs in a trellis.
  - A path in the trellis is a config of variable
  - The cost of the path is the energy of the config

- **The energy is a sum of "factor" functions**

Factor graph



Equivalent trellis



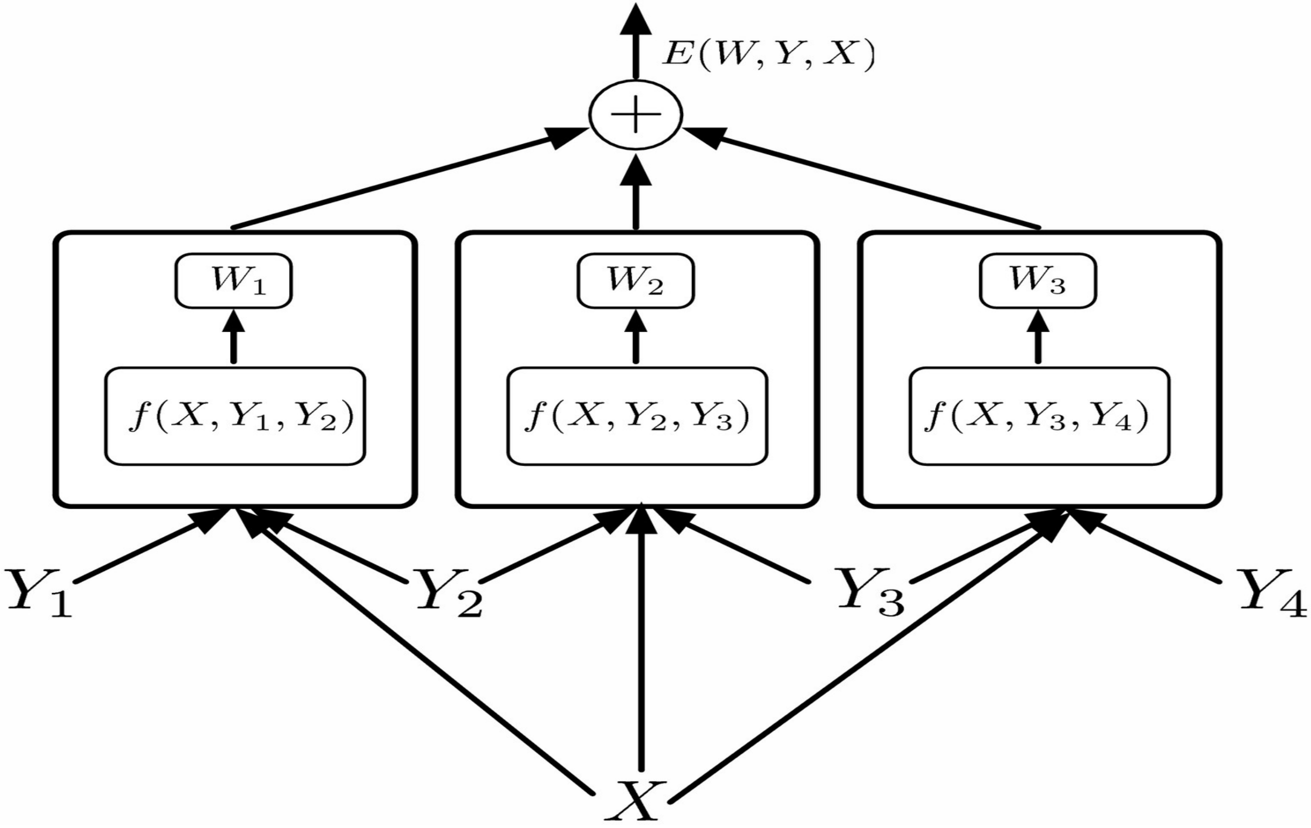
Energy-Based Belief Prop

- **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 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]

Simple Energy-Based Factor Graphs with “Shallow” Factors

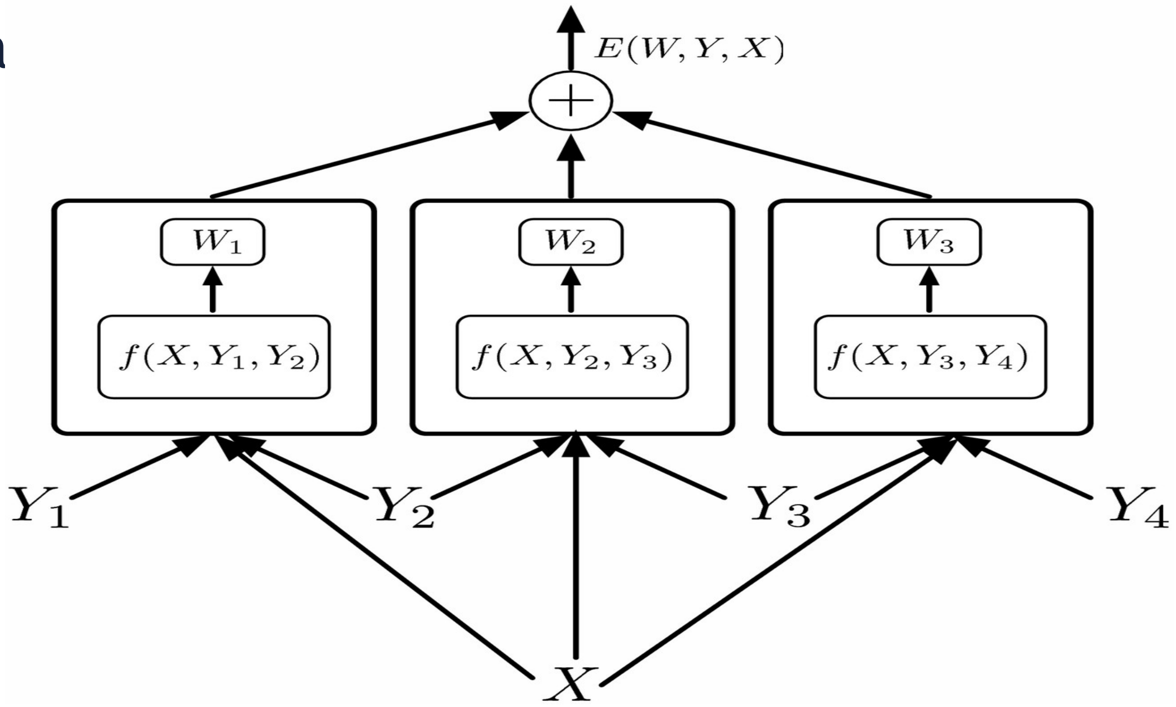
- **Linearly Parameterized Factors**

- **with the NLL Loss :**
  - Lafferty's **Conditional Random Field**
- **with Hinge Loss:**
  - Taskar and Altun/Hofmann's **Max Margin Markov Nets** and **Latent SVM**
- **with Perceptron Loss**
  - Collins's **Structured Perceptron** model



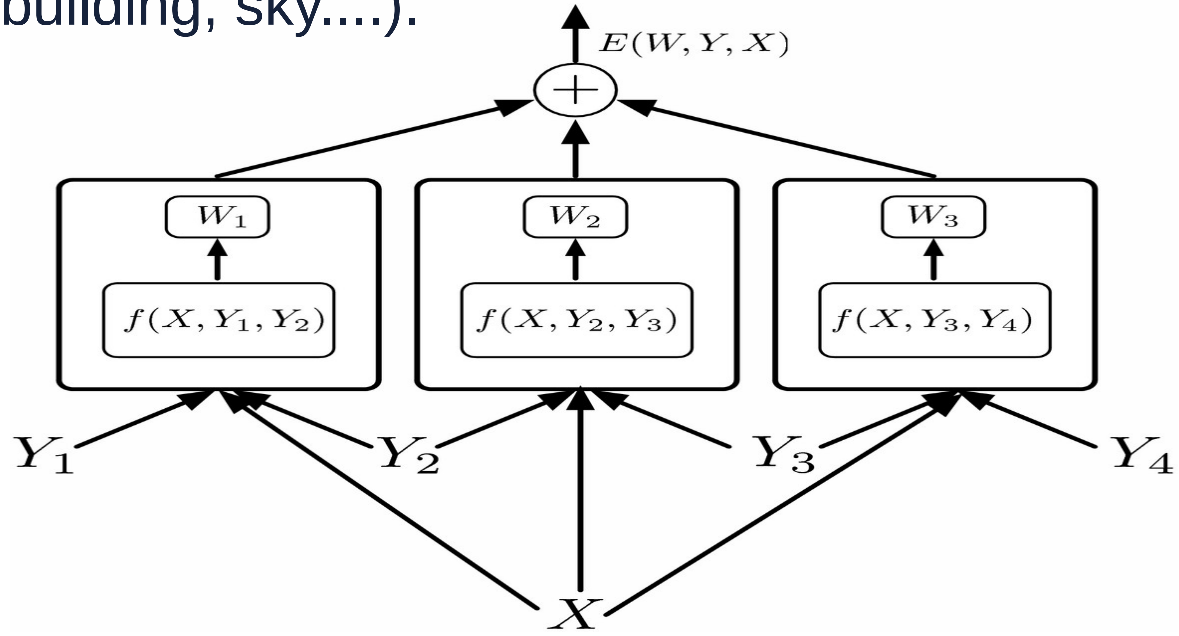
Example : The Conditional Random Field Architecture

- **A CRF is an energy-based factor graph in which:**
  - the factors are **linear in the parameters** **(shallow factors)**
  - The factors take neighboring output variables as inputs
  - The factors a



Example : The Conditional Random Field Architecture

- **Applications:**
  - X is a sentence, Y is a sequence of Parts of Speech Tags (there is one Yi for each possible group of words).
  - X is an image, Y is a set of labels for each window in the image (vegetation, building, sky....).

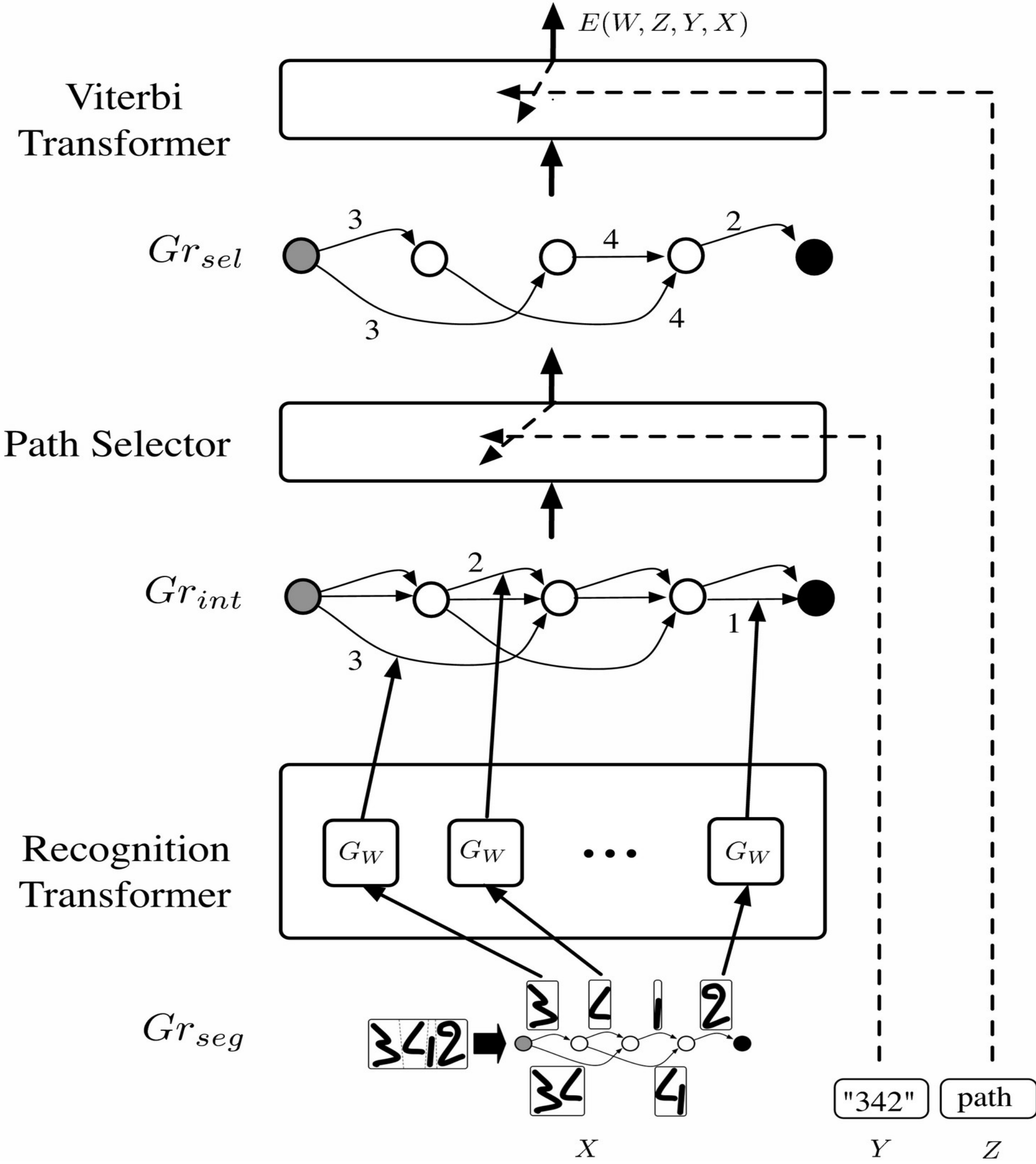


Deep/non-linear Factors for Speech and Handwriting

- **Trainable Speech/Handwriting Recognition systems that integrate Neural Nets (or other "deep" classifiers) with dynamic time warping, Hidden Markov Models, or other graph-based hypothesis representations**
- **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)
- **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)

Deep Factors & implicit graphs: GTN

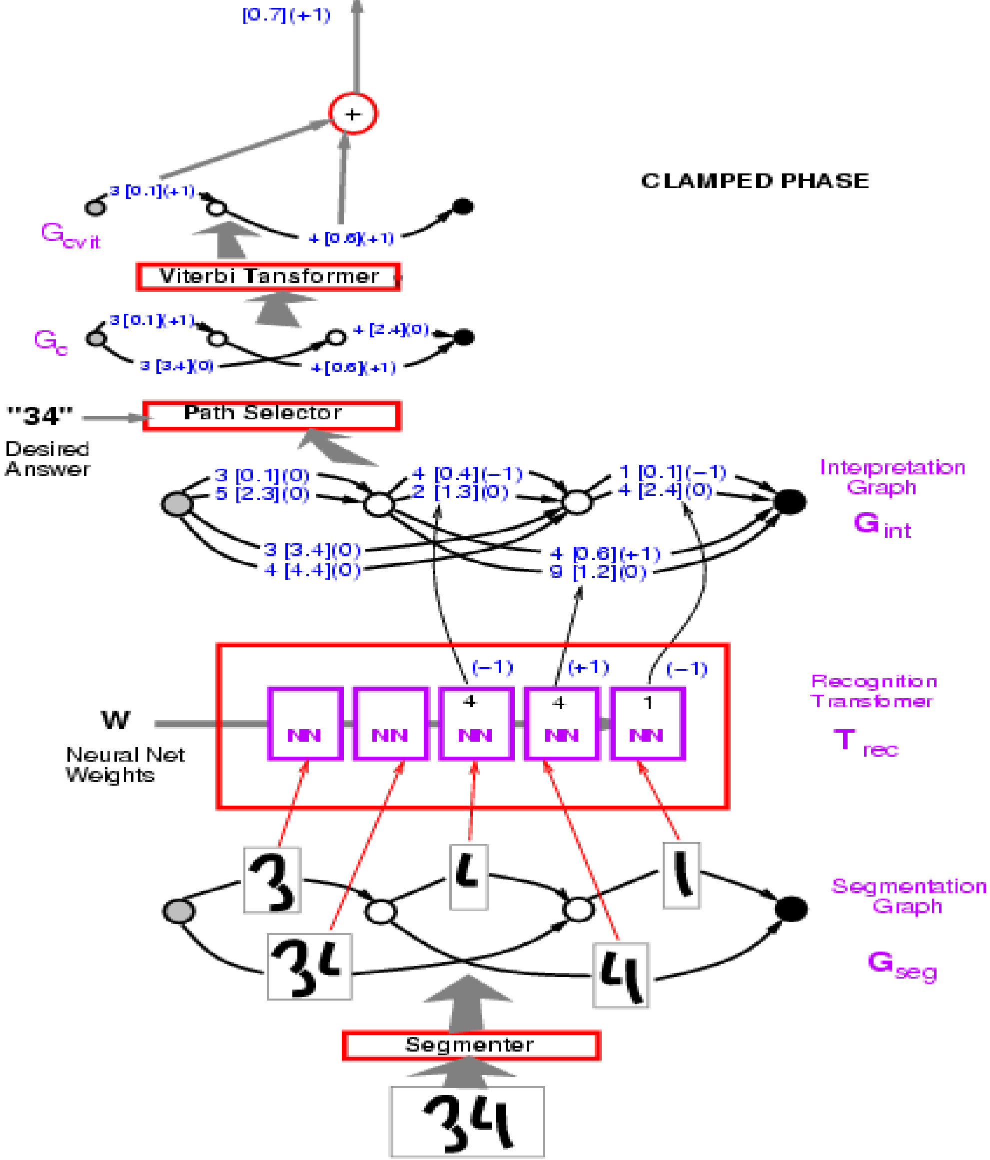
- **Handwriting Recognition with Graph Transformer Networks**
- **Un-normalized hierarchical HMMs**
  - Trained with Perceptron loss [LeCun, Bottou, Bengio, Haffner 1998]
  - Trained with NLL loss [Bengio, LeCun 1994], [LeCun, Bottou, Bengio, Haffner 1998]
- **Answer = sequence of symbols**
- **Latent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



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:**

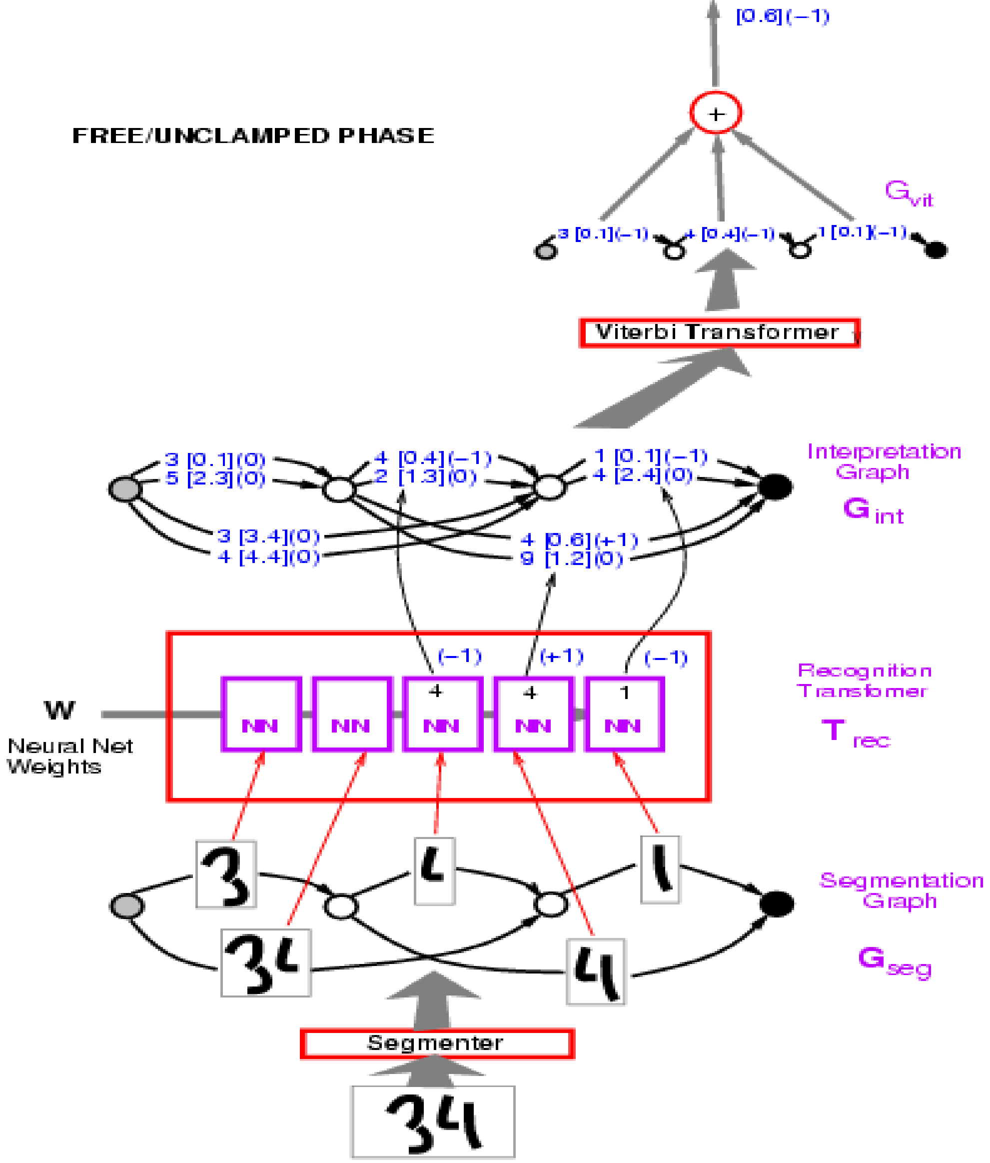
$$E(W, Y, X)$$



Graph Transformer Networks

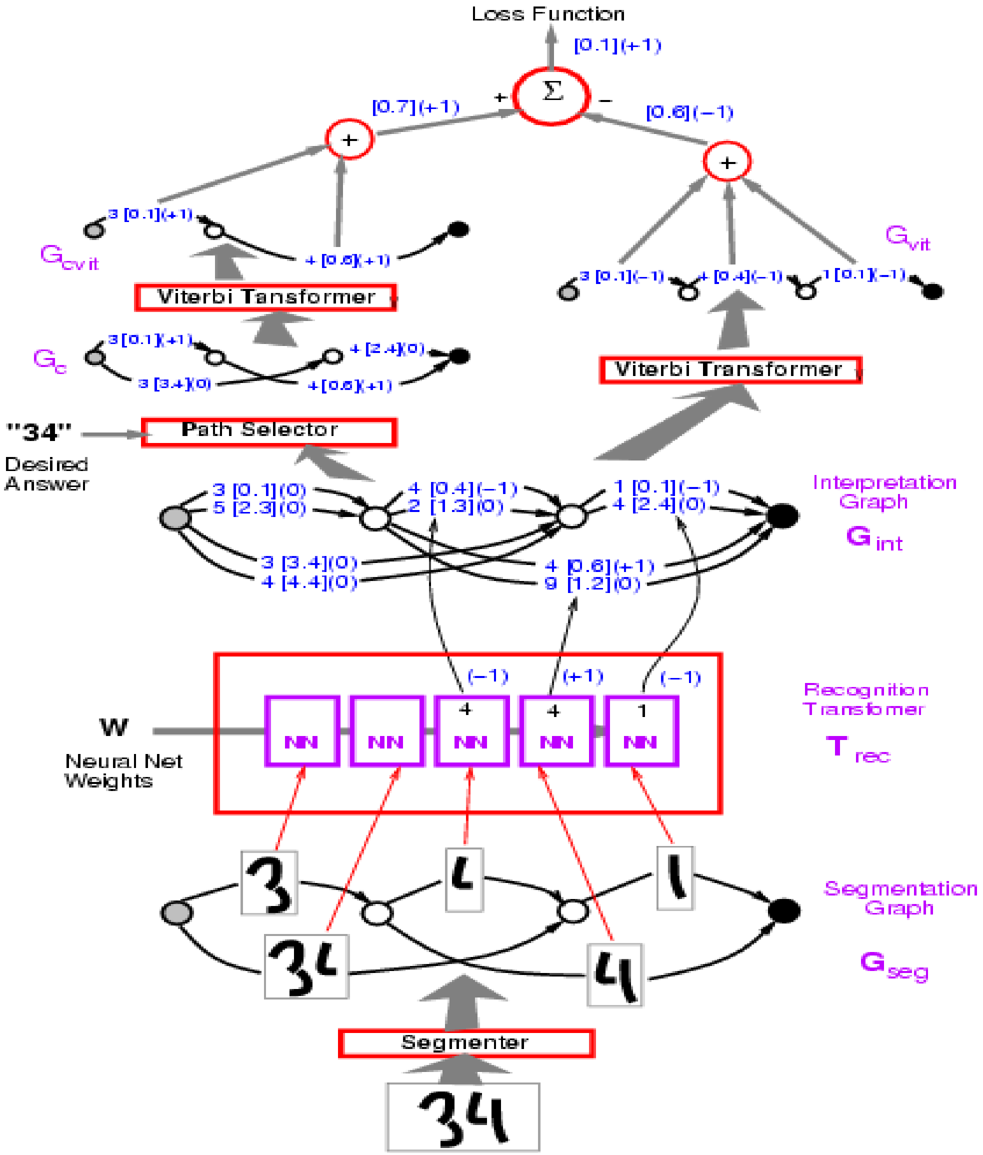
- **Variables:**
  - X: input image
  - Z: path in the interpretation graph/segmentation
  - Y: sequence of labels on a path
- **Loss function: computing the constrastive term:**

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



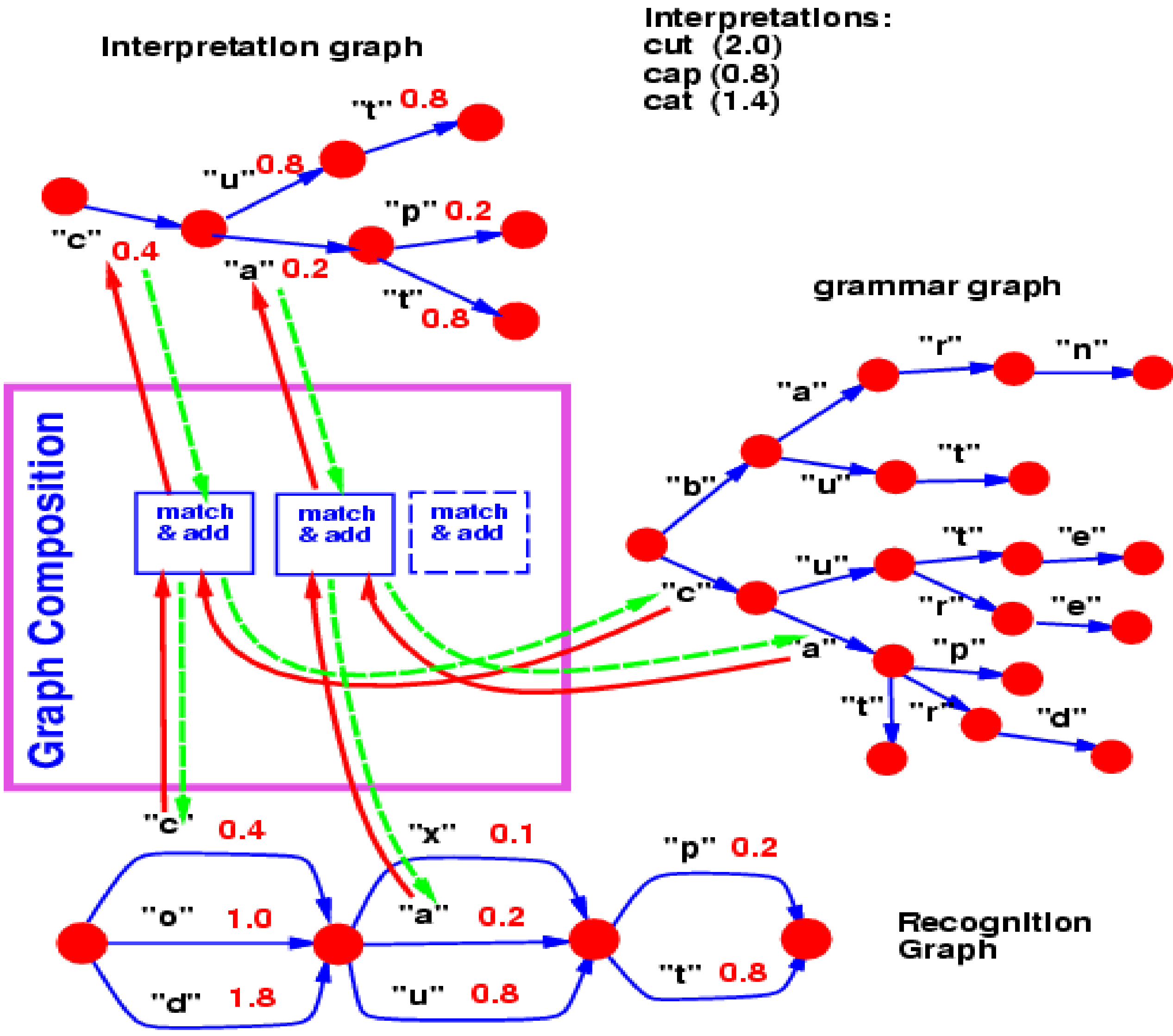
Graph Transformer Networks

- **Example: Perceptron loss**
- **Loss = Energy of desired answer – Energy of best answer.**
  - (no margin)



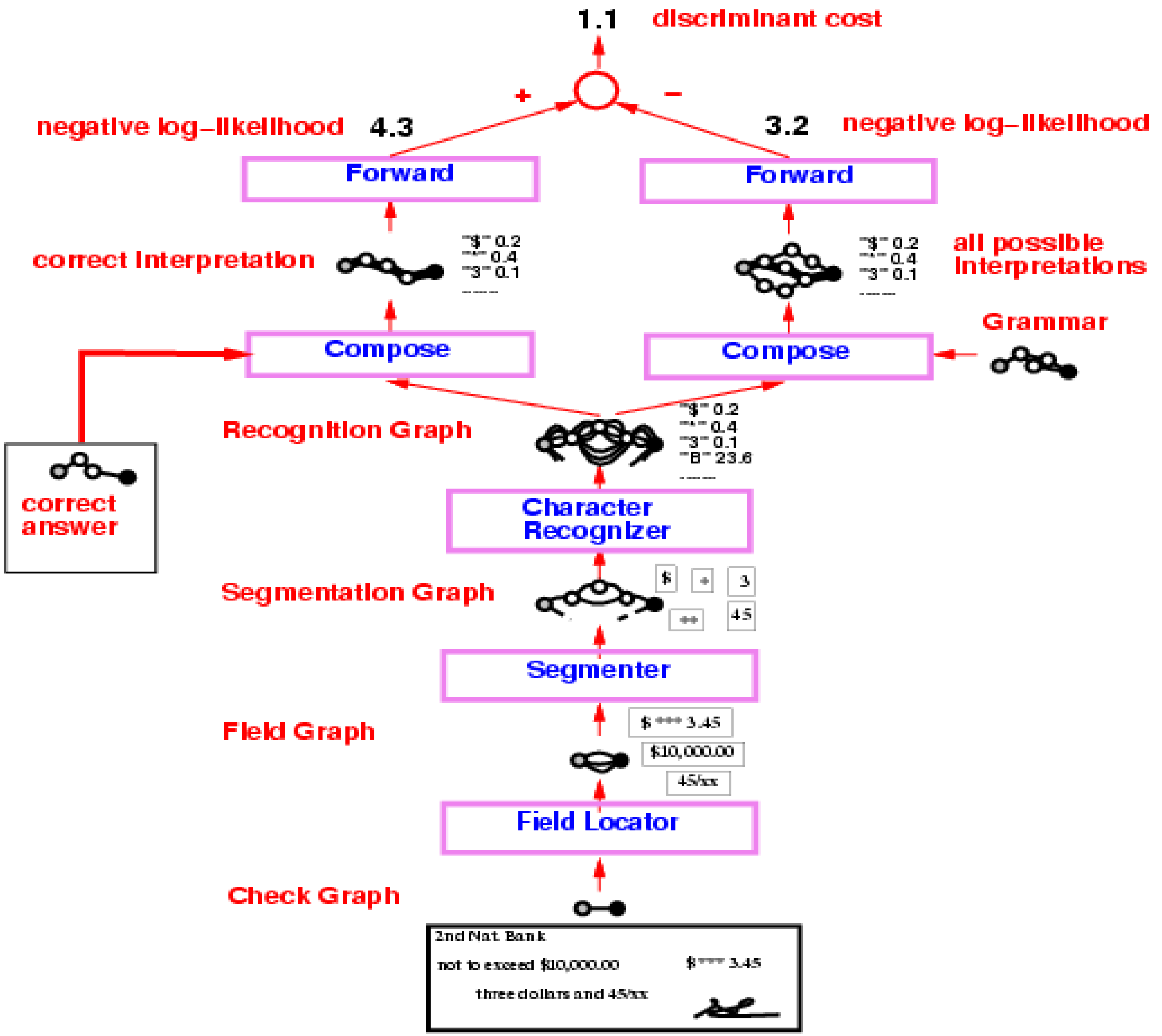
Graph Composition, Transducers.

- 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 finite-state 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.**



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)**