MACHINE LEARNING AND PATTERN RECOGNITION

Fall 2004, Lecture 4

Gradient-Based Learning III: Architectures

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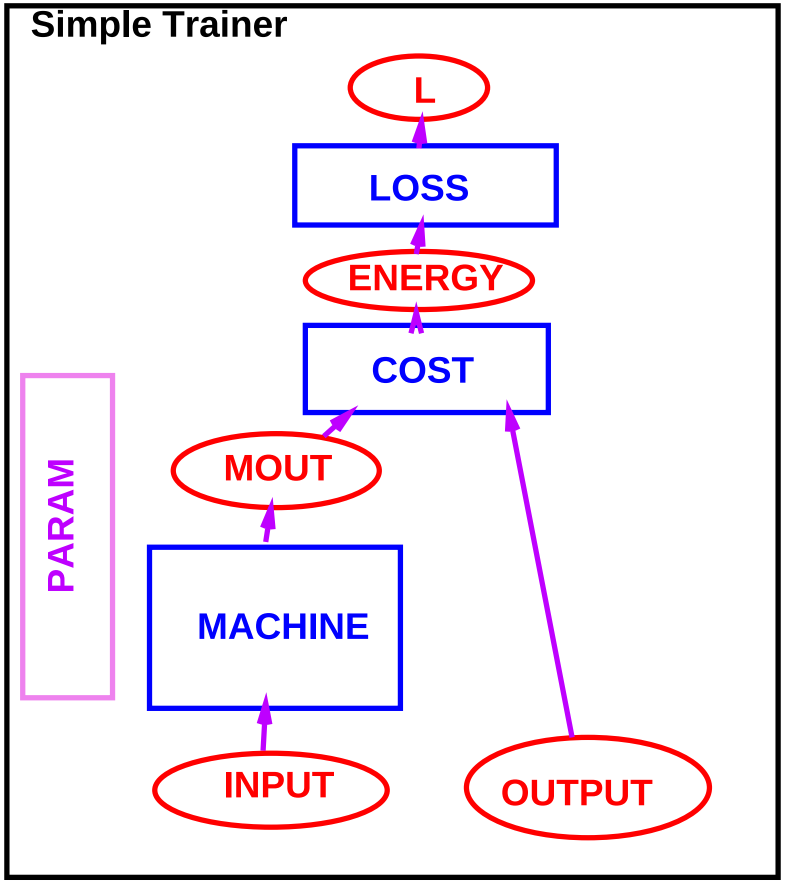
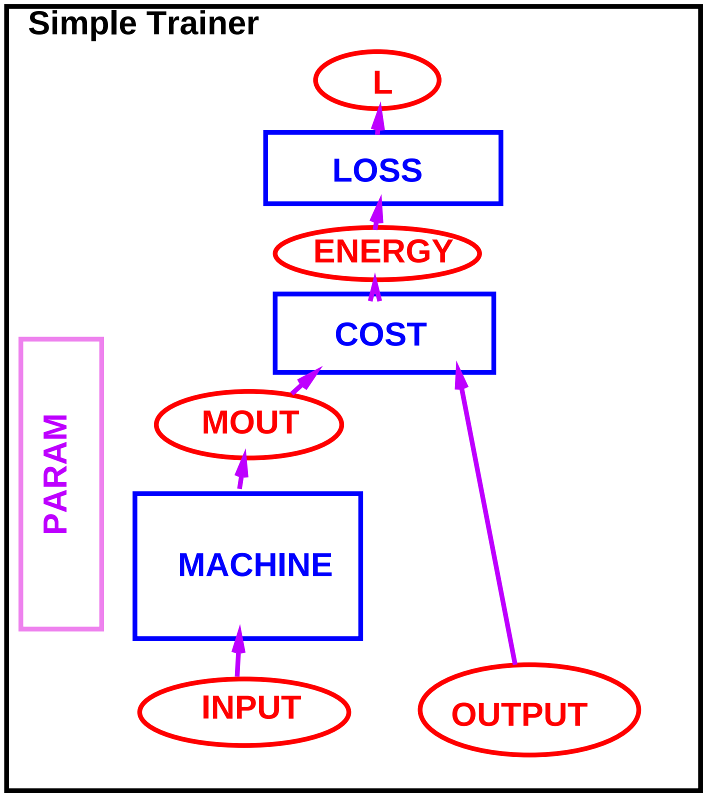
A Trainer class



The trainer object is designed to train a particular machine with a given energy function and loss. The example below uses the simple energy loss.

```
(defclass simple-trainer object
  input ; the input state
  output ; the output/label state
  machin ; the machine
  mout ; the output of the machine
  cost ; the cost module
  energy ; the energy (output of the cost) and
  param ; the trainable parameter vector
  )
```

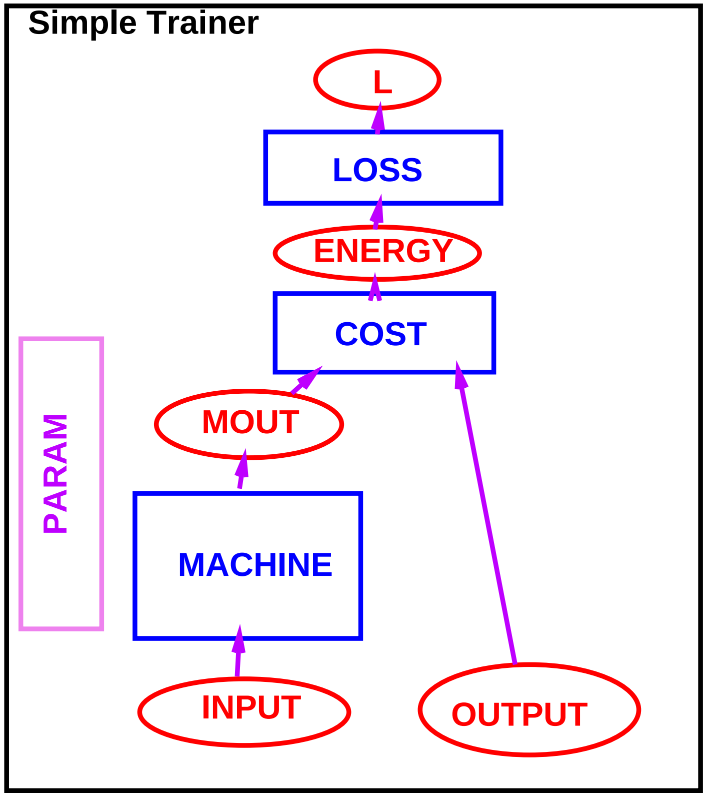
A Trainer class: running the machine



Takes an input and a vector of possible labels (each of which is a vector, hence <label-set> is a matrix) and returns the index of the label that minimizes the energy. Fills up the vector <energies> with the energy produced by each possible label.

```
(defmethod simple-trainer run
      (sample label-set energies)
  (==> input resize (idx-dim sample 0))
  (idx-copy sample :input:x)
  (==> machine fprop input mout)
  (idx-bloop ((label label-set) (e energies))
    (==> output resize (idx-dim label 0))
    (idx-copy label :output:x)
    (==> cost fprop mout output energy)
    (e (:energy:x)))
  ;; find index of lowest energy
  (idx-d1indexmin energies))
```

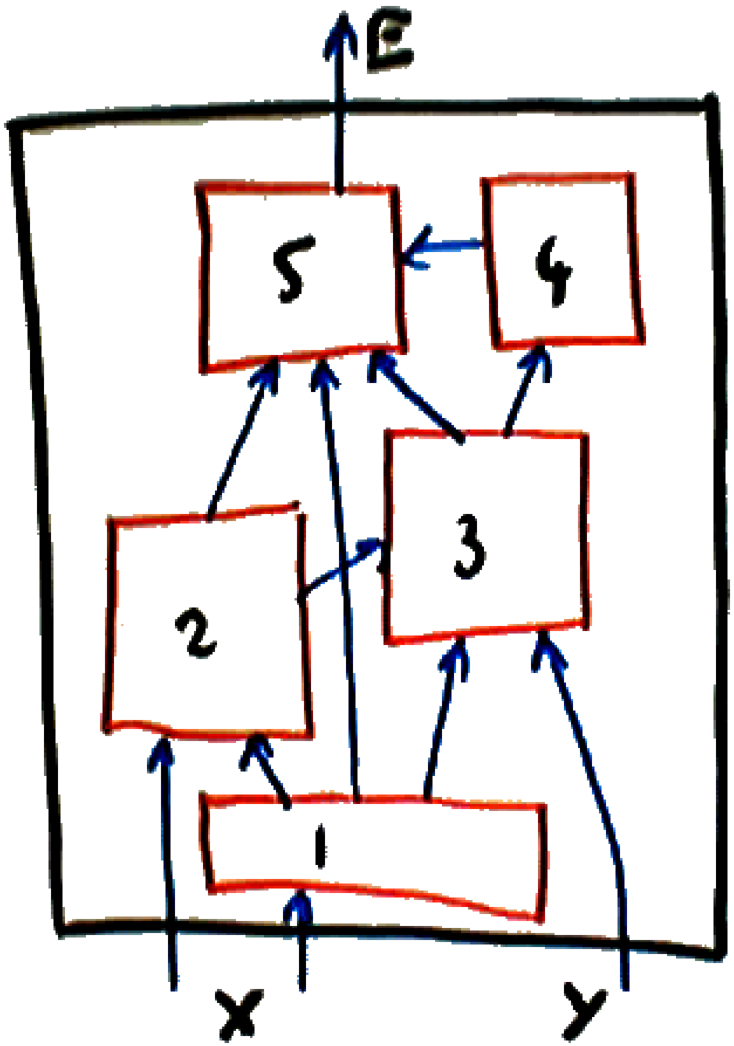
A Trainer class: training the machine



Performs a learning update on one sample. <sample> is the input sample, <label> is the desired category (an integer), <label-set> is a matrix where the i-th row is the desired output for the i-th category, and <update-args> is a list of arguments for the parameter update method (e.g. learning rate and weight decay).

```
(defmethod simple-trainer learn-sample
     (sample label label-set update-args)
  (==> input resize (idx-dim sample 0))
  (idx-copy sample :input:x)
  (==> machine fprop input mout)
  (==> output resize (idx-dim label-set 1))
  (idx-copy (select label-set 0 (label 0)) :outpu
  (==> cost fprop mout output energy)
  (==> cost bprop mout output energy)
  (==> machine bprop input mout)
  (==> param update update-args)
  (:energy:x))
```

Other Topologies



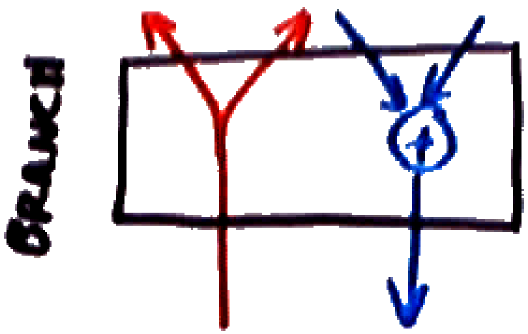
- The back-propagation procedure is not limited to feed-forward cascades.
- It can be applied to networks of module with *any* topology, as long as the connection graph is acyclic.
- If the graph is acyclic (no loops) then, we can easily find a suitable order in which to call the fprop method of each module.
- The bprop methods are called in the reverse order.
- if the graph has cycles (loops) we have a so-called *recurrent network*. This will be studied in a subsequent lecture.

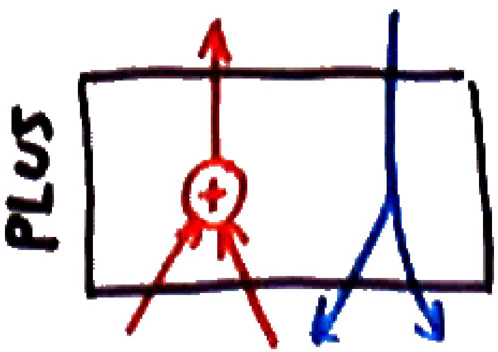
More Modules

A rich repertoire of learning machines can be constructed with just a few module types in addition to the linear, sigmoid, and euclidean modules we have already seen.
We will review a few important modules:

- The branch/plus module
- The switch module
- The Softmax module
- The logsum module

The Branch/Plus Module





- The PLUS module: a module with K inputs $X_1, \ldots, X_K$ (of any type) that computes the sum of its inputs:

$$X_{\text{out}} = \sum_k X_k$$

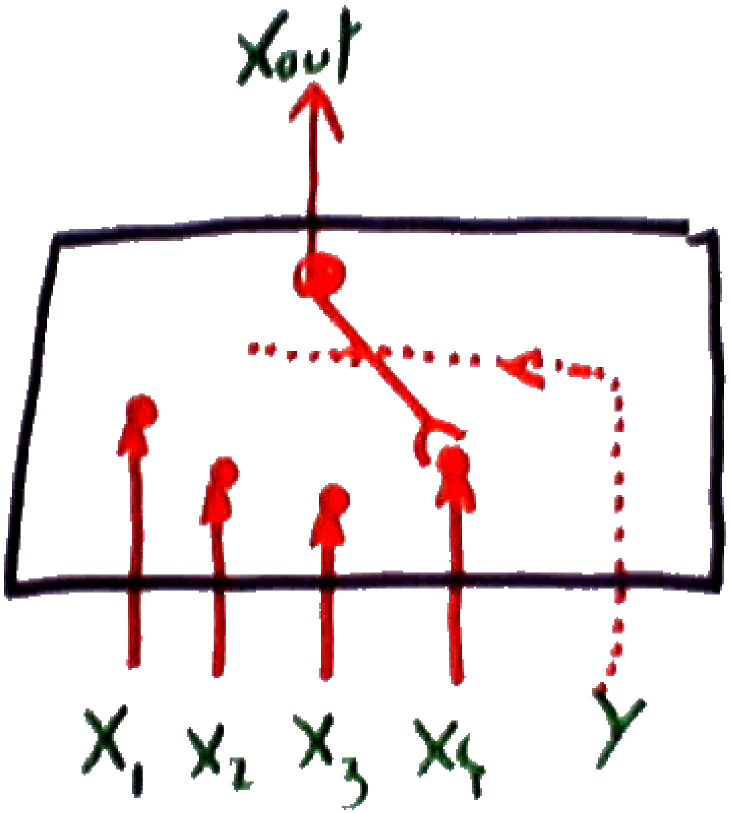
back-prop: $\frac{\partial E}{\partial X_k} = \frac{\partial E}{\partial X_{\text{out}}} \quad \forall k$

- The BRANCH module: a module with one input and K outputs $X_1, \ldots, X_K$ (of any type) that simply copies its input on its outputs:

$$X_k = X_{\text{in}} \quad \forall k \in [1..K]$$

back-prop: $\frac{\partial E}{\partial \text{in}} = \sum_k \frac{\partial E}{\partial X_k}$

The Switch Module



- A module with K inputs $X_1, \ldots, X_K$ (of any type) and one additional discrete-valued input Y.
- The value of the discrete input determines which of the N inputs is copied to the output.
- $$X_{\text{out}} = \sum_k \delta(Y - k) X_k$$

$$\frac{\partial E}{\partial X_k} = \delta(Y - k) \frac{\partial E}{\partial X_{\text{out}}}$$

the gradient with respect to the output is copied to the gradient with respect to the switched-in input. The gradients of all other inputs are zero.

The Logsum Module

fprop:

$$X_{\text{out}} = -\frac{1}{\beta} \log \sum_k \exp(-\beta X_k)$$

bprop:

$$\frac{\partial E}{\partial X_k} = \frac{\partial E}{\partial X_{\text{out}}} \frac{\exp(-\beta X_k)}{\sum_j \exp(-\beta X_j)}$$

or

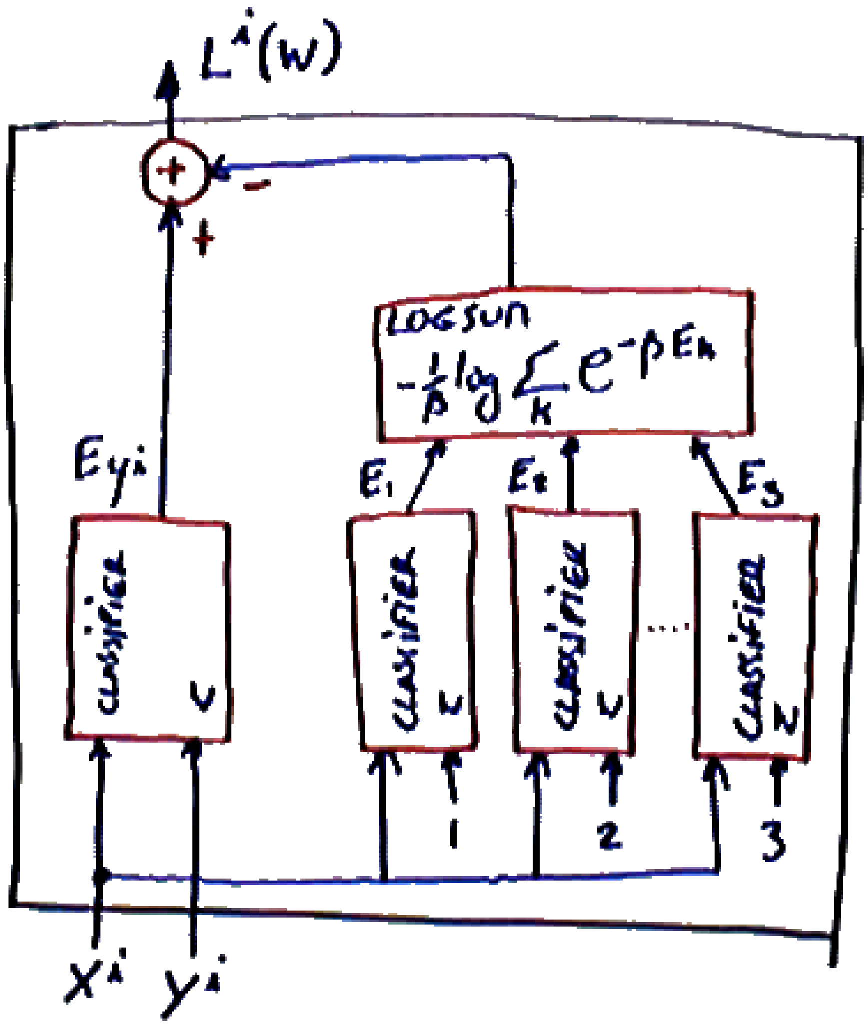
$$\frac{\partial E}{\partial X_k} = \frac{\partial E}{\partial X_{\text{out}}} P_k$$

with

$$P_k = \frac{\exp(-\beta X_k)}{\sum_j \exp(-\beta X_j)}$$

Log-Likelihood Loss function and Logsum Modules

MAP/MLE Loss $L_{\rm ll}(W, Y^i, X^i) = E(W, Y^i, X^i) + \frac{1}{\beta} \log \sum_k \exp(-\beta E(W, k, X^i))$



- A classifier trained with the Log-Likelihood loss can be transformed into an equivalent machine trained with the energy loss.
- The transformed machine contains multiple “replicas” of the classifier, one replica for the desired output, and K replicas for each possible value of Y.

Softmax Module

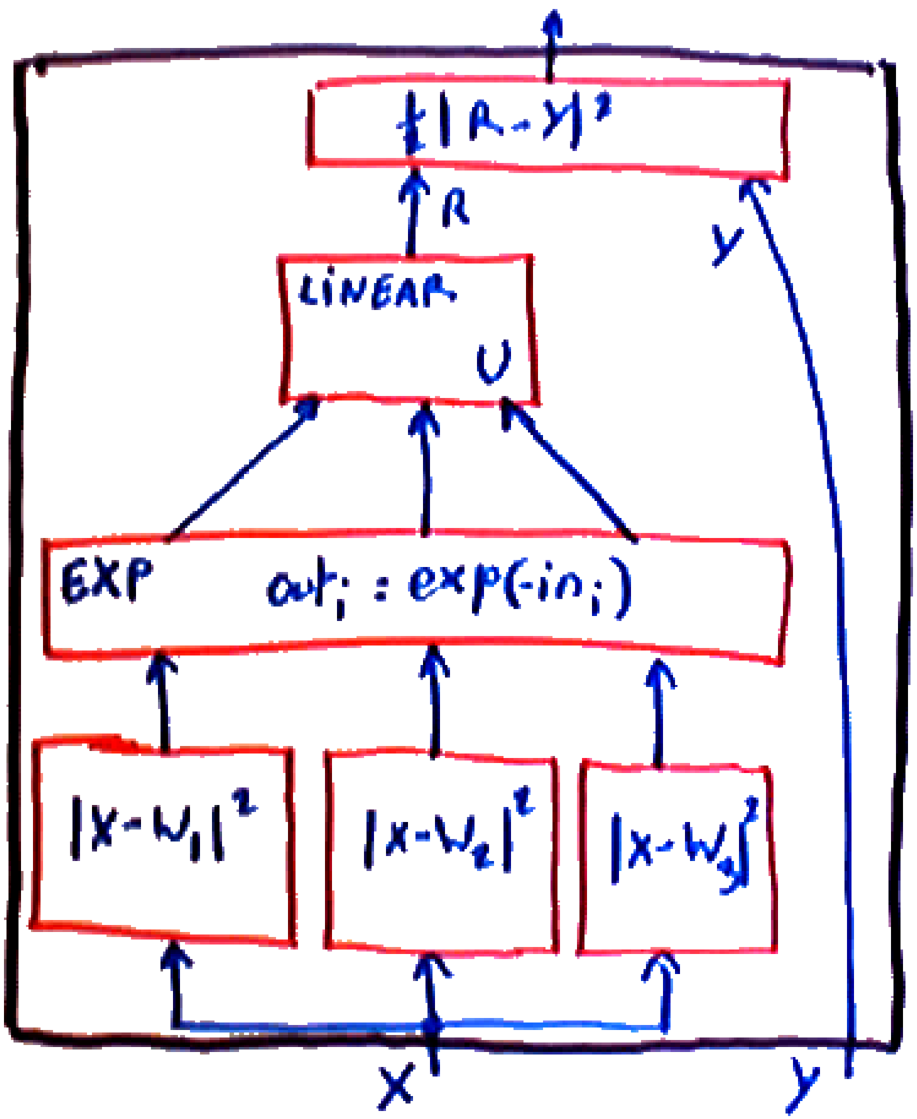
A single vector as input, and a “normalized” vector as output:

$$(X_{\rm out})_i = \frac{\exp(-\beta x_i)}{\sum_k \exp(-\beta x_k)}$$

Exercise: find the bprop

$$\frac{\partial (X_{\rm out})_i}{\partial x_j} = ???$$

Radial Basis Function Network (RBF Net)



- Linearly combined Gaussian bumps.
- $F(X, W, U) = \sum_i u_i \exp(-k_i(X - W_i)^2)$
- The centers of the bumps can be initialized with the K-means algorithm (see below), and subsequently adjusted with gradient descent.
- This is a good architecture for regression and function approximation.

MAP/MLE Loss and Cross-Entropy

- classification (y is scalar and discrete). Let's denote $E(y, X, W) = E_y(X, W)$
- MAP/MLE Loss Function:

$$L(W) = \frac{1}{P} \sum_{i=1}^{P} [E_{y^i}(X^i, W) + \frac{1}{\beta} \log \sum_k \exp(-\beta E_k(X^i, W))]$$

- This loss can be written as

$$L(W) = \frac{1}{P} \sum_{i=1}^{P} -\frac{1}{\beta} \log \frac{\exp(-\beta E_{y^i}(X^i, W))}{\sum_k \exp(-\beta E_k(X^i, W))}$$

Cross-Entropy and KL-Divergence

- let's denote $P(j|X^i,W) = \frac{\exp(-\beta E_j(X^i,W))}{\sum_k \exp(-\beta E_k(X^i,W))}$, then

$$L(W) = \frac{1}{P}\sum_{i=1}^{P}\frac{1}{\beta}\log\frac{1}{P(y^i|X^i,W)}$$

$$L(W) = \frac{1}{P}\sum_{i=1}^{P}\frac{1}{\beta}\sum_k D_k(y^i)\log\frac{D_k(y^i)}{P(k|X^i,W)}$$

with $D_k(y^i) = 1$ iff $k = y^i$, and 0 otherwise.

- example1: $D = (0,0,1,0)$ and $P(.|X_i,W) = (0.1,0.1,0.7,0.1)$. with $\beta = 1$, $L^i(W) = \log(1/0.7) = 0.3567$
- example2: $D = (0,0,1,0)$ and $P(.|X_i,W) = (0,0,1,0)$. with $\beta = 1$, $L^i(W) = \log(1/1) = 0$

Cross-Entropy and KL-Divergence

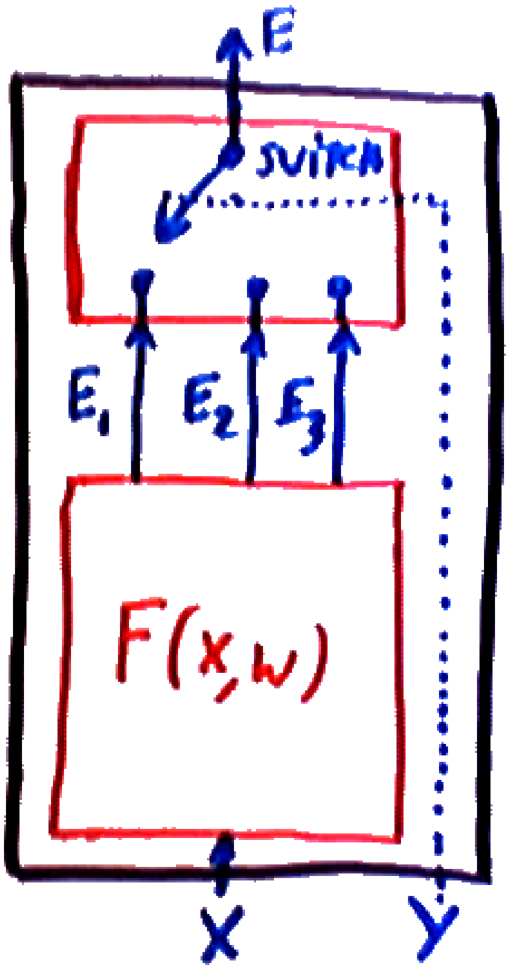
$$L(W) = \frac{1}{P}\sum_{i=1}^{P}\frac{1}{\beta}\sum_k D_k(y^i)\log\frac{D_k(y^i)}{P(k|X^i,W)}$$

- $L(W)$ is proportional to the *cross-entropy* between the conditional distribution of y given by the machine $P(k|X^i,W)$ and the *desired* distribution over classes for sample i, $D_k(y^i)$ (equal to 1 for the desired class, and 0 for the other classes).
- The cross-entropy also called *Kullback-Leibler divergence* between two distributions $Q(k)$ and $P(k)$ is defined as:

$$\sum_k Q(k)\log\frac{Q(k)}{P(k)}$$

- It measures a sort of dissimilarity between two distributions.
- the KL-divergence is not a distance, because it is not symmetric, and it does not satisfy the triangular inequality.

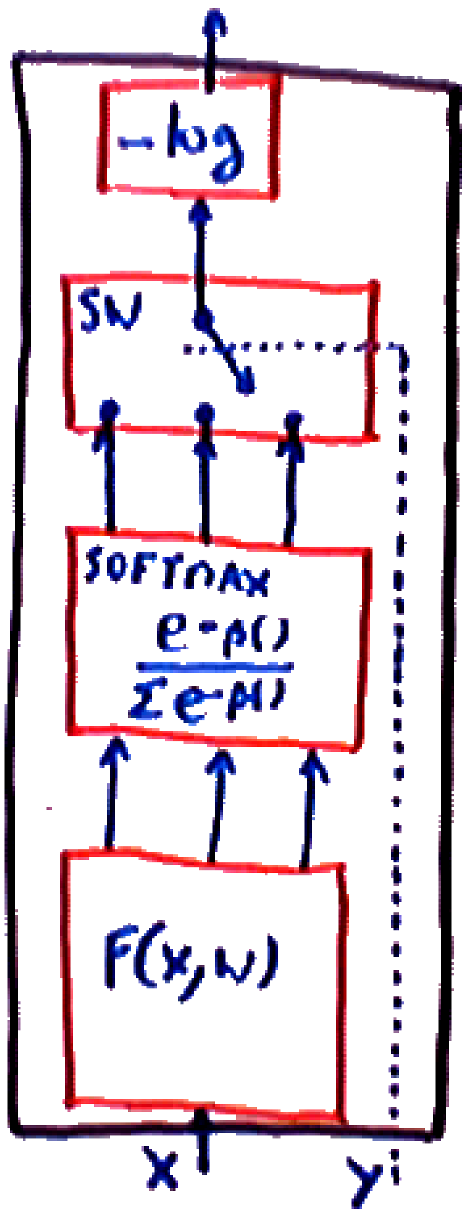
Multiclass Classification and KL-Divergence



- Assume that our discriminant module $F(X, W)$ produces a vector of energies, with one energy $E_k(X, W)$ for each class.
- A switch module selects the smallest E_k to perform the classification.
- As shown above, the MAP/MLE loss below be seen as a KL-divergence between the desired distribution for y, and the distribution produced by the machine.

$$L(W) = \frac{1}{P}\sum_{i=1}^{P}[E_{y^i}(X^i, W) + \frac{1}{\beta}\log\sum_k \exp(-\beta E_k(X^i, W))]$$

Multiclass Classification and Softmax



- The previous machine: discriminant function with one output per class + switch, with MAP/MLE loss
- It is equivalent to the following machine: discriminant function with one output per class + softmax + switch + log loss

$$L(W) = \frac{1}{P}\sum_{i=1}^{P} \frac{1}{\beta} - \log P(y^i|X, W)$$

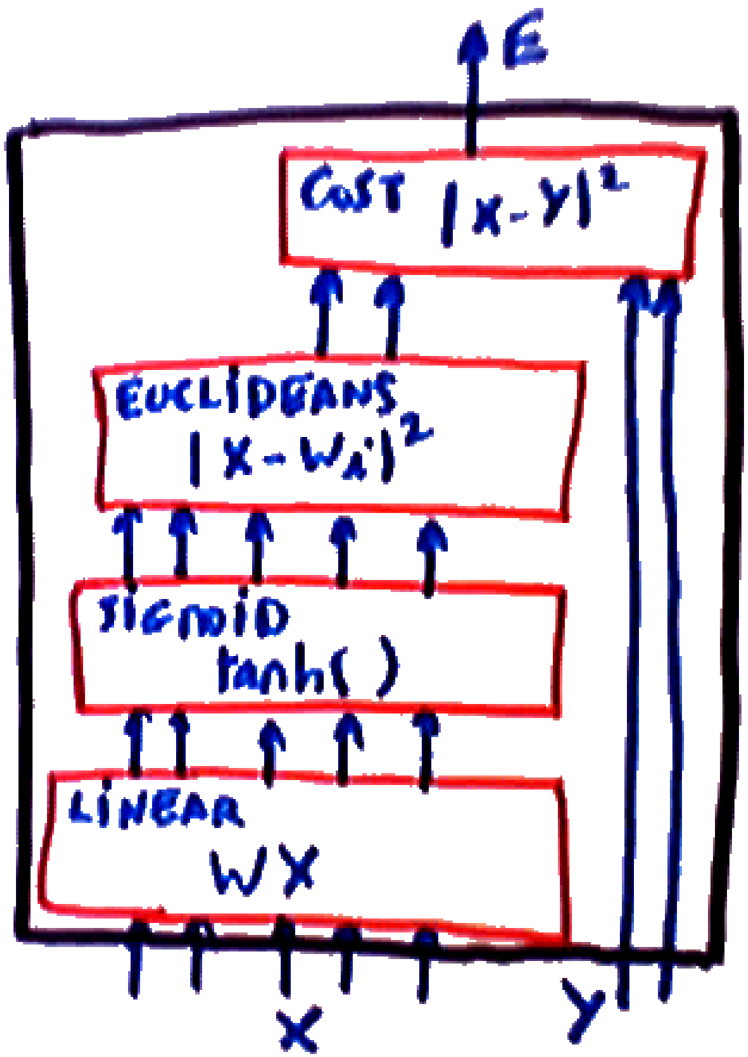
with $P(j|X^i, W) = \frac{\exp(-\beta E_j(X^i,W))}{\sum_k \exp(-\beta E_k(X^i,W))}$ (softmax of the $-E_j$'s).

- Machines can be transformed into various equivalent forms to factorize the computation in advantageous ways.

Multiclass Classification with a Junk Category

- Sometimes, one of the categories is "none of the above", how can we handle that?
- We add an extra energy wire E_0 for the "junk" category which does not depend on the input. E_0 can be a hand-chosen constant or can be equal to a trainable parameter (let's call it w_0).
- everything else is the same.

NN-RBF Hybrids

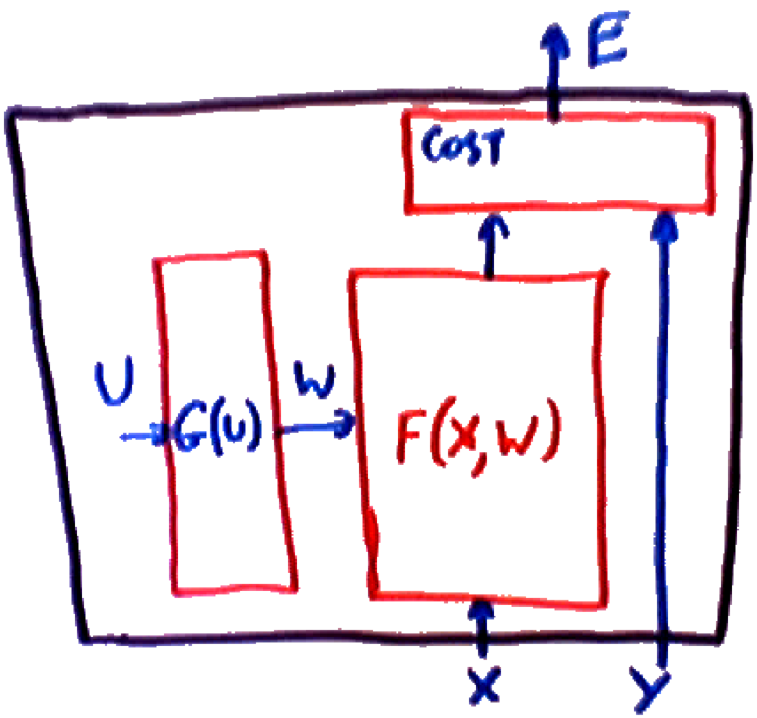


- sigmoid units are generally more appropriate for low-level feature extraction.
- Euclidean/RBF units are generally more appropriate for final classifications, particularly if there are many classes.
- Hybrid architecture for multiclass classification: sigmoids below, RBFs on top + softmax + log loss.

Parameter-Space Transforms

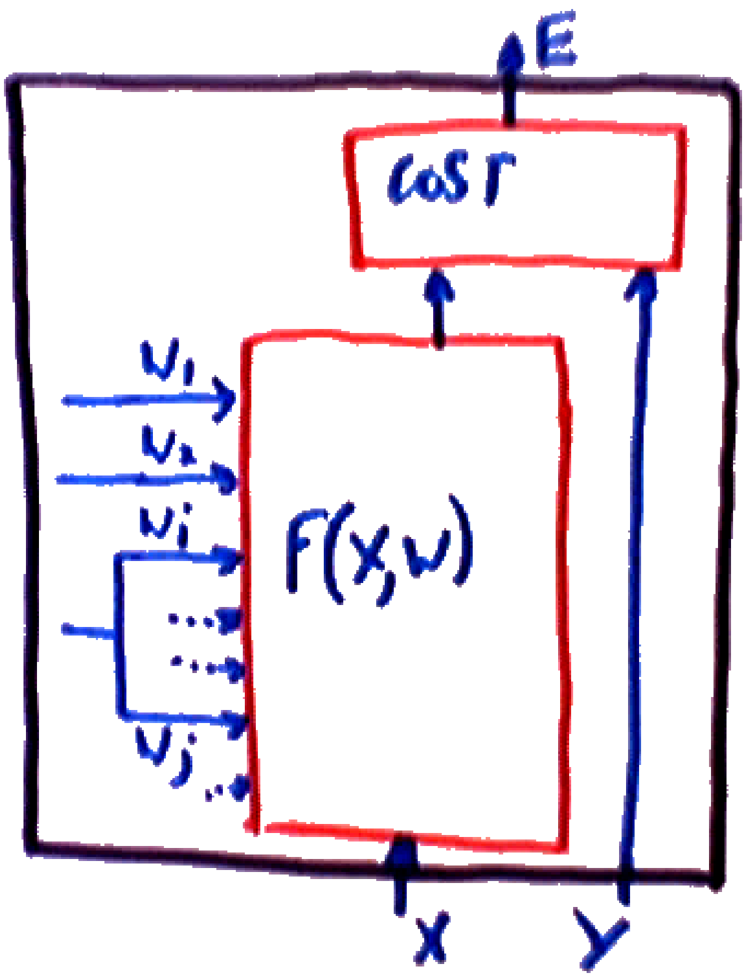
Reparameterizing the function by transforming the space

$$E(Y, X, W) \rightarrow E(Y, X, G(U))$$



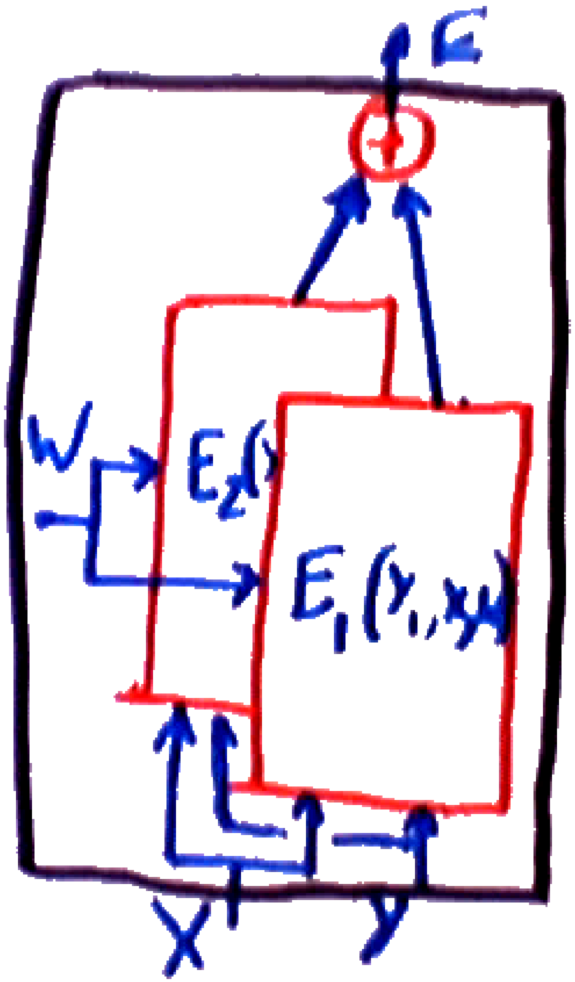
- gradient descent in U space: $U \leftarrow U - \eta \frac{\partial G}{\partial U}' \frac{\partial E(Y,X,W)}{\partial W}'$
- equivalent to the following algorithm in W space: $W \leftarrow W - \eta \frac{\partial G}{\partial U} \frac{\partial G}{\partial U}' \frac{\partial E(Y,X,W)}{\partial W}'$
- dimensions: $[N_w \times N_u][N_u \times N_w][N_w]$

Parameter-Space Transforms: Weight Sharing



- A single parameter is replicated multiple times in a machine
- $E(Y, X, w_1, \ldots, w_i, \ldots, w_j, \ldots) \rightarrow E(Y, X, w_1, \ldots, u_k, \ldots, u_k, \ldots)$
- gradient: $\frac{\partial E()}{\partial u_k} = \frac{\partial E()}{\partial w_i} + \frac{\partial E()}{\partial w_j}$
- w_i and w_j are tied, or equivalently, u_k is shared between two locations.

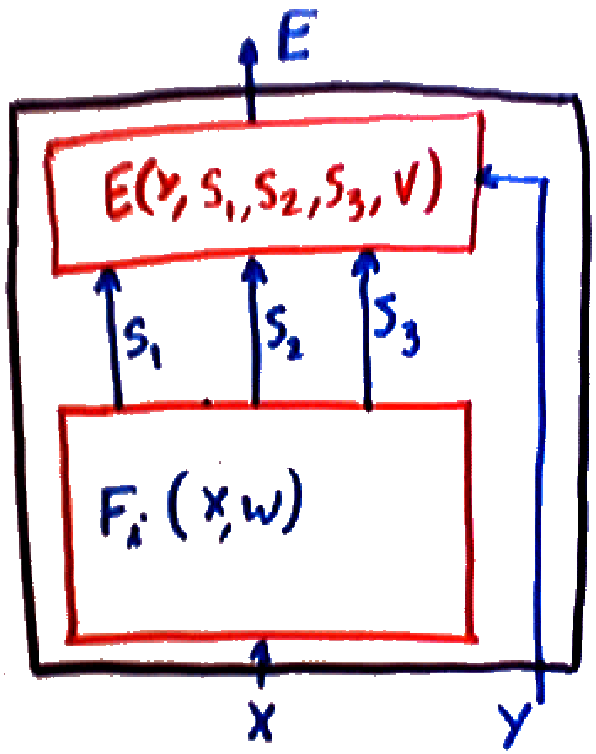
Parameter Sharing between Replicas



- We have seen this before: a parameter controls several replicas of a machine.
- $$E(Y_1, Y_2, X, W) = E_1(Y_1, X, W) + E_1(Y_2, X, W)$$
- gradient: $\frac{\partial E(Y_1, Y_2, X, W)}{\partial W} = \frac{\partial E_1(Y_1, X, W)}{\partial W} + \frac{\partial E_1(Y_2, X, W)}{\partial W}$
- W is shared between two (or more) instances of the machine: just sum up the gradient contributions from each instance.

Path Summation (Path Integral)

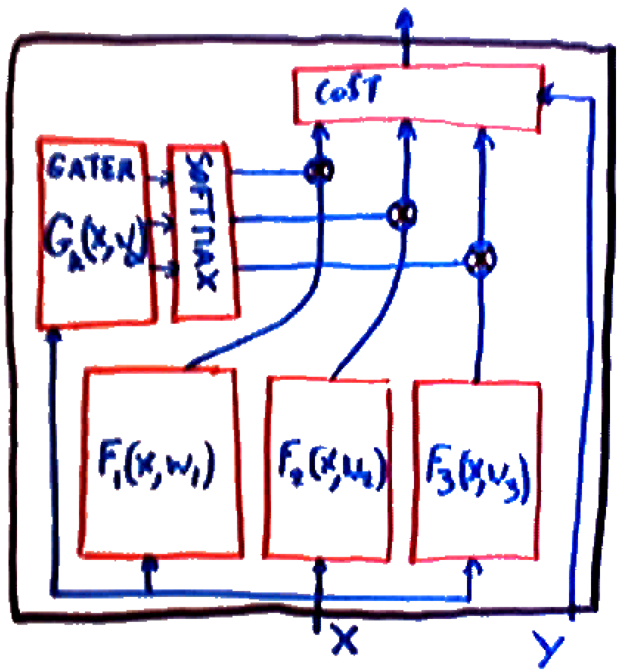
One variable influences the output through several others



- $E(Y, X, W) =$
$E(Y, F_1(X, W), F_2(X, W), F_3(X, W), V)$
- gradient: $\frac{\partial E(Y,X,W)}{\partial X} = \sum_i \frac{\partial E_i(Y,S_i,V)}{\partial S_i} \frac{\partial F_i(X,W)}{\partial X}$
- gradient: $\frac{\partial E(Y,X,W)}{\partial W} = \sum_i \frac{\partial E_i(Y,S_i,V)}{\partial S_i} \frac{\partial F_i(X,W)}{\partial W}$
- there is no need to implement these rules explicitely. They come out naturally of the object-oriented implementation.

Mixtures of Experts

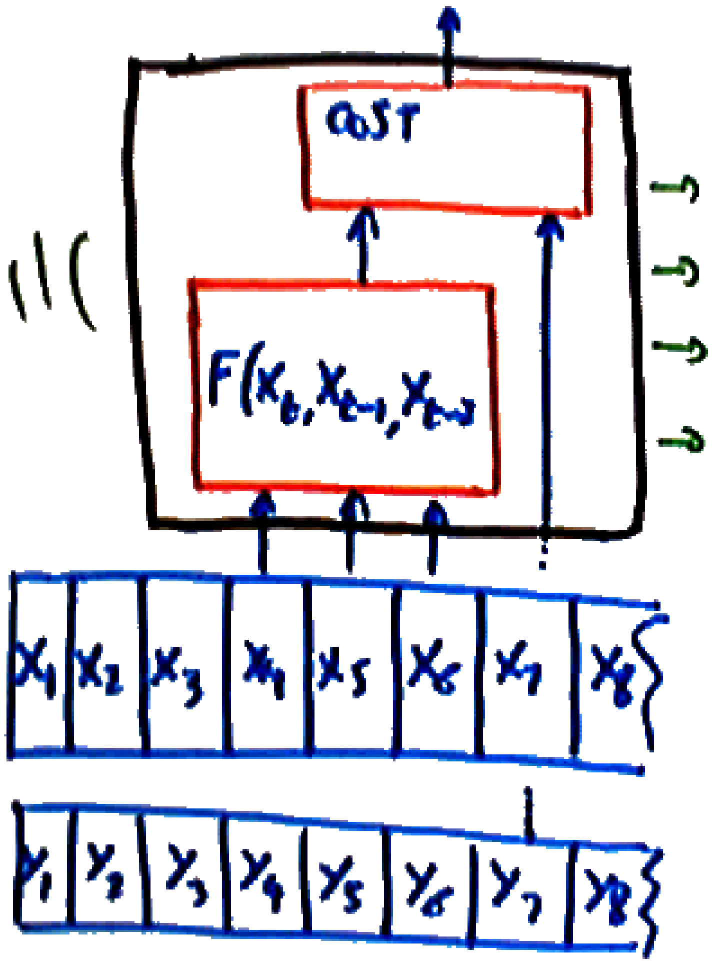
Sometimes, the function to be learned is consistent in restricted domains of the input space, but globally inconsistent. Example: piecewise linearly separable function.



- Solution: a machine composed of several "experts" that are specialized on subdomains of the input space.
- The output is a weighted combination of the outputs of each expert. The weights are produced by a "gater" network that identifies which subdomain the input vector is in.
- $F(X, W) = \sum_k u_k F^k(X, W^k)$ with
  $u_k = \frac{\exp(-\beta G_k(X, W^0))}{\sum_k \exp(-\beta G_k(X, W^0))}$
- the expert weights u_k are obtained by softmax-ing the outputs of the gater.
- example: the two experts are linear regressors, the gater is a logistic regressor.

Sequence Processing: Time-Delayed Inputs

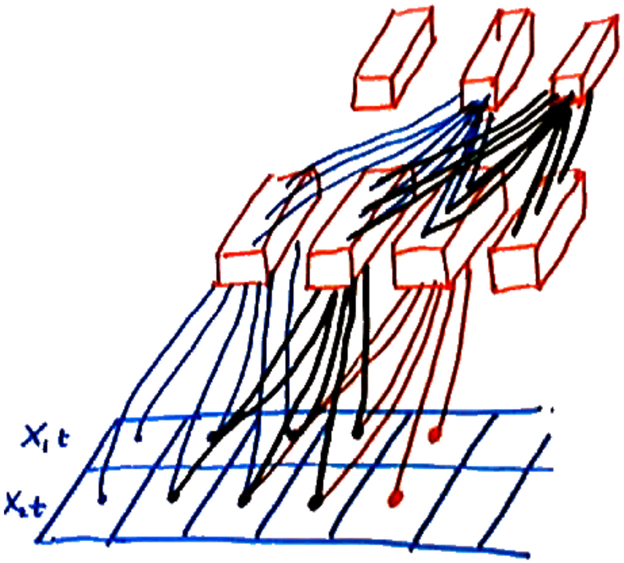
The input is a sequence of vectors X_t.



- simple idea: the machine takes a time window as input
- $R = F(X_t, X_{t-1}, X_{t-2}, W)$
- Examples of use:
  - predict the next sample in a time series (e.g. stock market, water consumption)
  - predict the next character or word in a text
  - classify an intron/exon transition in a DNA sequence

Sequence Processing: Time-Delay Networks

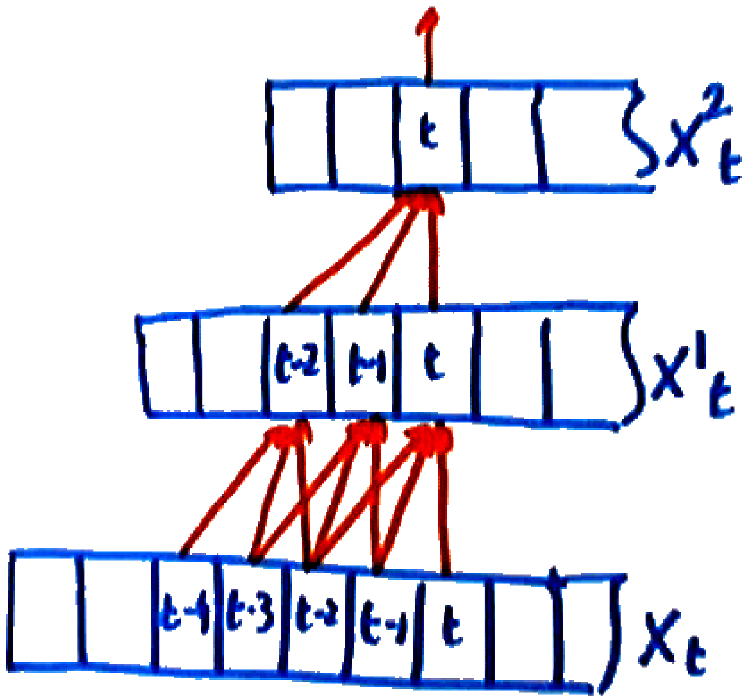
One layer produces a sequence for the next layer: stacked time-delayed layers.



- layer1 $X_t^1 = F^1(X_t, X_{t-1}, X_{t-2}, W^1)$
  layer2 $X_t^2 = F^1(X_t^1, X_{t-1}^1, X_{t-2}^1, W^2)$
  cost $E_t = C(X_t^1, Y_t)$
- Examples:
  - predict the next sample in a time series with long-term memory (e.g. stock market, water consumption)
  - recognize spoken words
  - recognize gestures and handwritten characters on a pen computer.
- How do we train?

Training a TDNN

Idea: isolate the minimal network that influences the energy at one particular time step t.

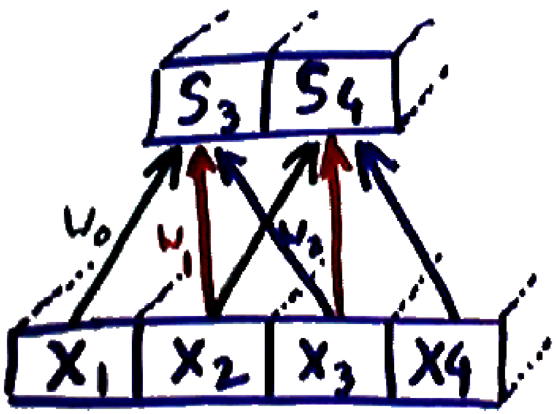


- in our example, this is influenced by 5 time steps on the input.
- train this network in isolation, taking those 5 time steps as the input.
- Surprise: we have three identical replicas of the first layer units that share the same weights.
- We know how to deal with that.
- do the regular backprop, and add up the contributions to the gradient from the 3 replicas

Convolutional Module

If the first layer is a set of linear units with sigmoids, we can view it as performing a sort of *multiple discrete convolutions* of the input sequence.

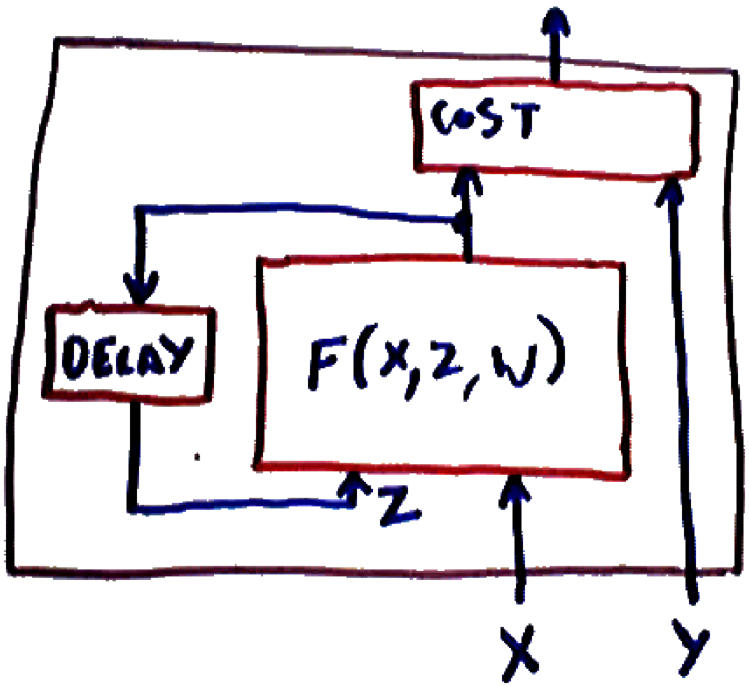
$$\frac{\partial E}{\partial W_0} = \frac{\partial E}{\partial S_3} \cdot X_1 + \frac{\partial E}{\partial S_4} \cdot X_2 + \cdots$$



- 1D convolution operation: $S^1_t = \sum_{j=1}^{T} W^{1'}_j X_{t-j}$.
- $w_j k \;\; j \in [1, T]$ is a *convolution kernel*
- sigmoid $X^1_t = \tanh(S^1_t)$
- derivative: $\frac{\partial E}{\partial w^1_j k} = \sum_{t=1}^{3} \frac{\partial E}{\partial S^1_t} X_{t-j}$

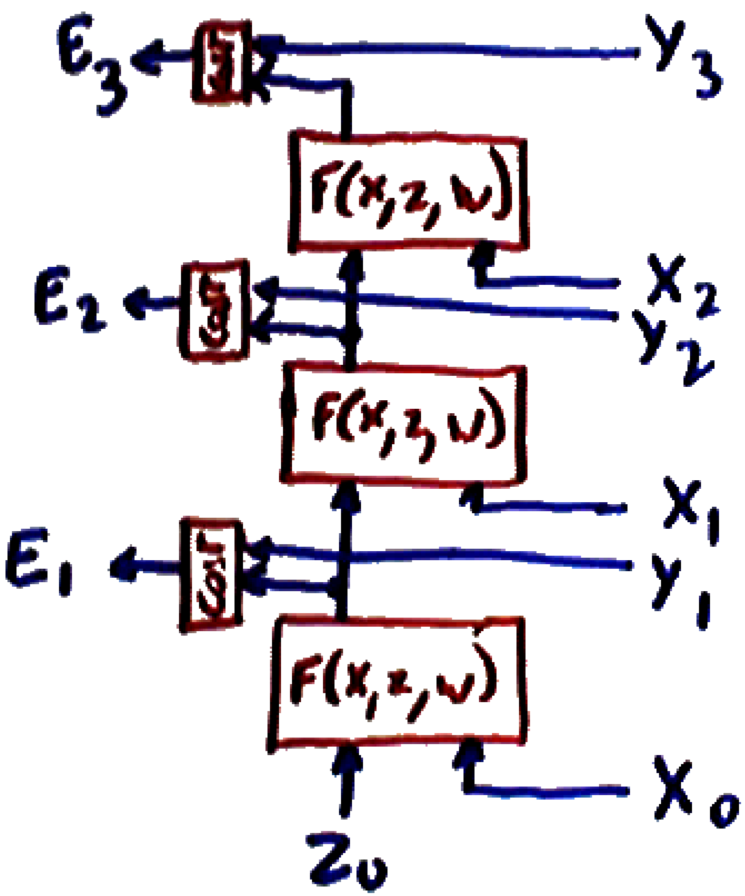
Simple Recurrent Machines

The output of a machine is fed back to some of its inputs Z. $Z_{t+1} = F(X_t, Z_t, W)$, where t is a time index. The input X is not just a vector but a sequence of vectors X_t.



- This machine is a *dynamical system* with an internal state Z_t.
- Hidden Markov Models are a special case of recurrent machines where F is linear.

Unfolded Recurrent Nets and Backprop through time



- To train a recurrent net: "unfold" it in time and turn it into a feed-forward net with as many layers as there are time steps in the input sequence.
- An unfolded recurrent net is a very "deep" machine where all the layers are identical and share the same weights.
- $\frac{\partial E}{\partial W} = \sum_t \frac{\partial E}{\partial Z_t} \frac{\partial F(X_t, Z_t, W)}{\partial W}$
- This method is called *back-propagation through time*.
- examples of use: process control (steel mill, chemical plant, pollution control....), robot control, dynamical system modelling...