MACHINE LEARNING AND PATTERN RECOGNITION Spring 2004, Lecture 5a Architectures

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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:

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

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

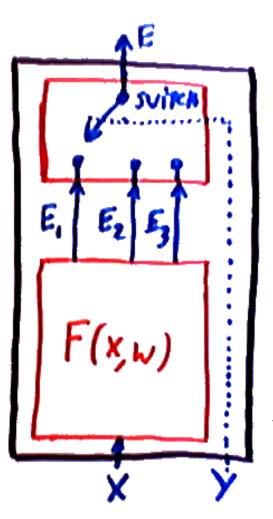
$$L(W) = \frac{1}{P} \sum_{i=1}^{P} \frac{1}{\beta} \sum_{k} D_{k}(y^{i}) \log \frac{D_{k}(y^{i})}{P(k|X^{i}, W)}$$

- 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.

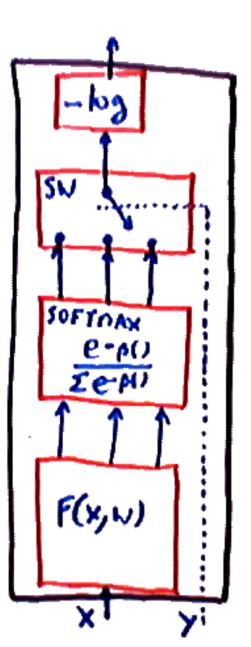
Multiclass Classification and KL-Divergence



- 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.

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

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).

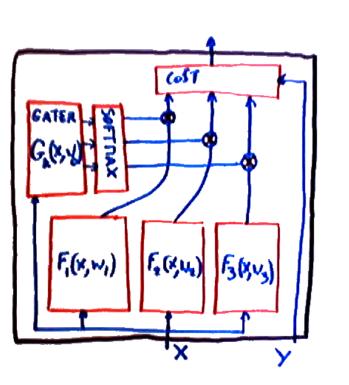
Machines can be transformed into various equivalent forms to factorize the computation in advantageous ways.

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.

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.



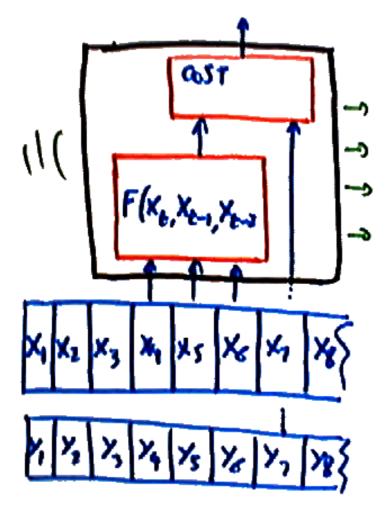
- Solution: a machine composed of several "experts" that are specialized on subdomains of the input space.
- The output is a weighted combination of the outputs of each expert. The weights are produced by a "gater" network that identifies which subdomain the input vector is in.

$$F(X, W) = \sum_{k} u_k F^k(X, W^k) \text{ with}$$
$$u_k = \frac{\exp(-\beta G_k(X, W^0))}{\sum_{k} \exp(-\beta G_k(X, W^0))}$$

- 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 .



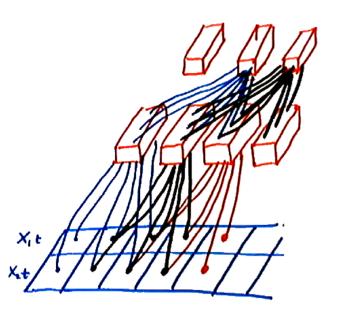
simple idea: the machine takes a time window as input

$$R = F(X_t, X_{t-1}, X_{t-2}, W)$$

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

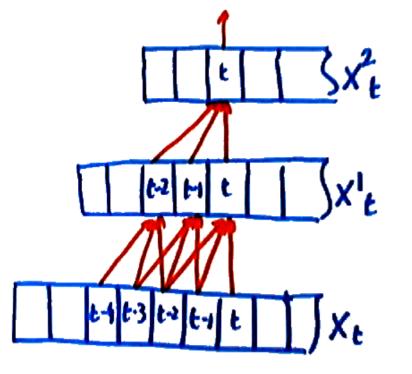
One layer produces a sequence for the next layer: stacked time-delayed layers.



- 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.



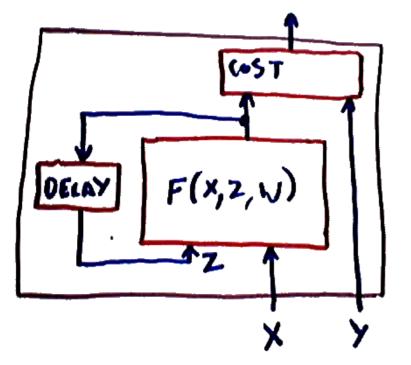
- in our example, this is influenced by 5 time steps on the input.
- train this network in isolation, taking those5 time steps as the input.
- Surprise: we have three identical replicas of the first layer units that share the same weights.
- We know how to deal with that.
- do the regular backprop, and 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.

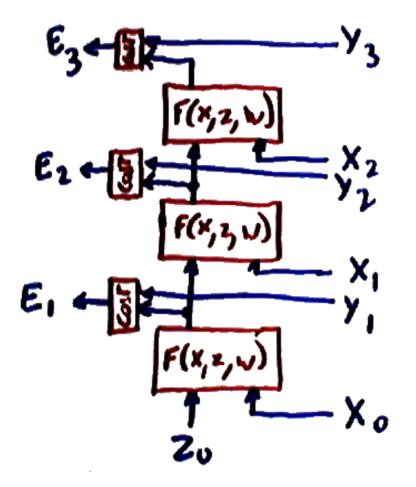
Simple Recurrent Machines

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...