Multi-Layer Architectures Gradient Back-Propagation

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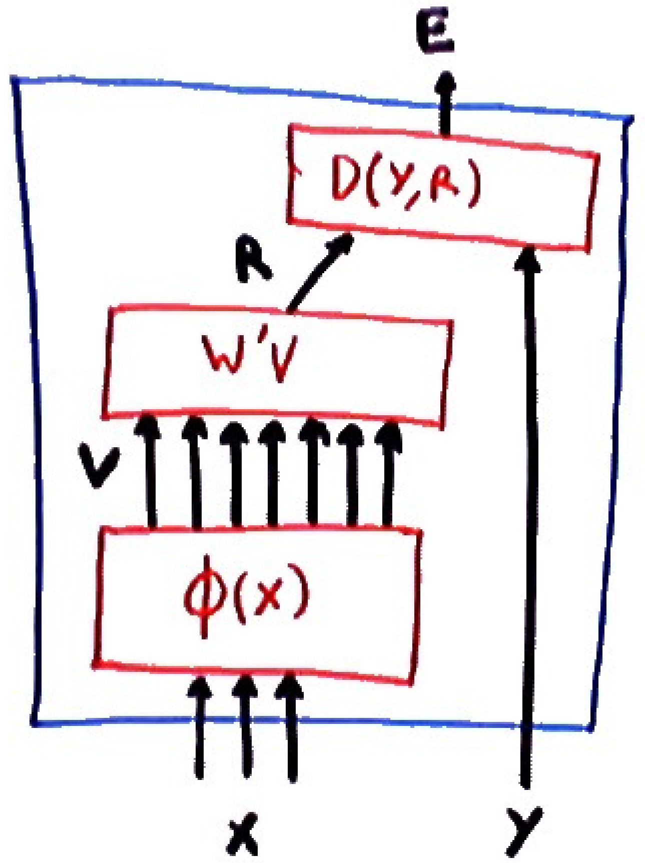
Non-Linear Models

- **We can always add “features”, “kernels”, or “basis function” in front of a linear model to make it non-linear.**
  - This is how non-linear SVMs are built.
- **Question: so, why would we need anything else?**
- **Answer: the complexity of the real world is very difficult to capture in a kernel.**
- **How do we solve:**
  - The invariance problem in image recognition.
  - The structured output problem in sequence labeling (parts of speech tagging, speech recognition, biological sequence analysis....).

Fixed Preprocessing (features, kernels, basis functions)

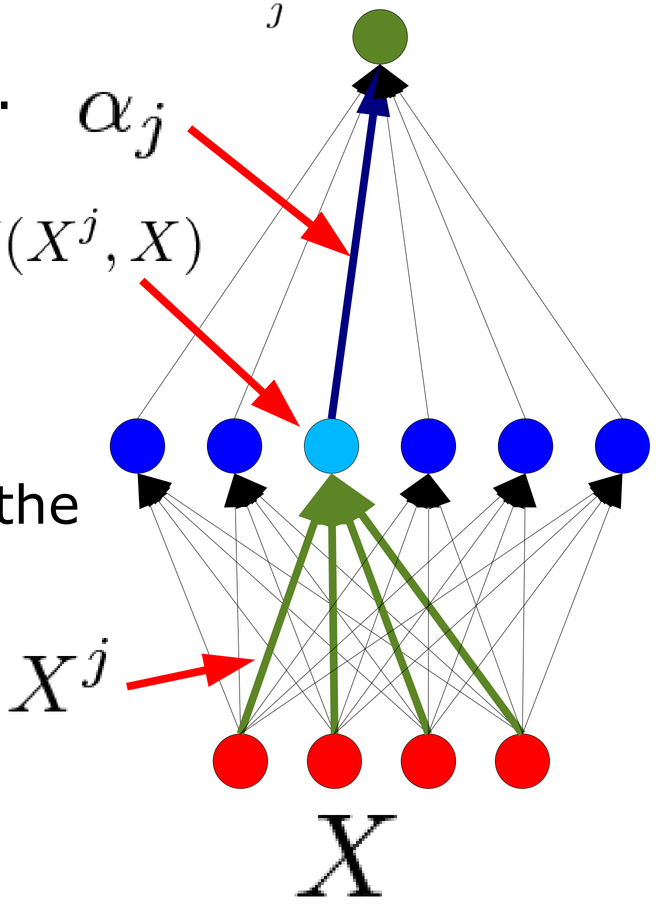


- Map the inputs into a (higher dimensional) "feature" space
  - With more dimensions, the task is more likely to be linearly separable.
- Problem: how should we pick the features so that the task becomes linearly separable in the feature space?
  - **Classical approach 1**: we use our prior knowledge about the problem to hand-craft an appropriate feature set.
  - **Classical Approach 2**: we use a "standard" set of basis functions (RBFs....)

Fixed Preprocessing: Kernels and SVMs

- **Simplest approach: The Kernel Method (thanks to Wahba's Representer Theorem)**
  - Make each basis function a "bump" function (a template matcher).
  - Place one bump around each training sample.
  - Compute a linear combination of the bumps.
  - In the "bump space", we get one separate dimension for each training sample, so if the bumps are narrow enough, we can learn any mapping on the training set.
  - To generalize on unseen samples, we adjust the bump widths and we regularize the weights.
  - We get a **Support Vector Machine.**
- **Problem: an SVM is a glorified template matcher which is only as good as its kernel.**

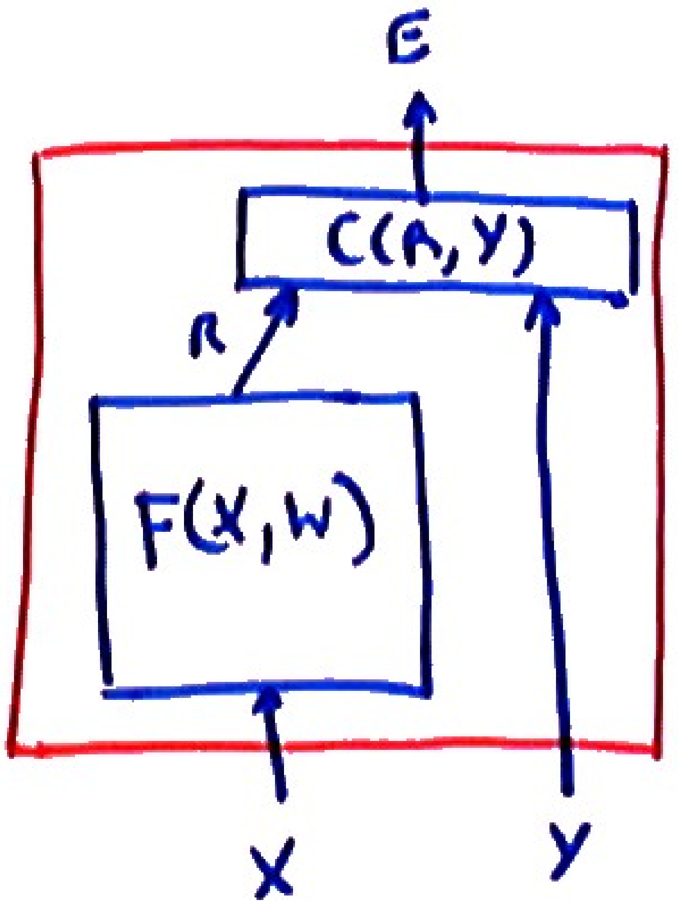
$$G(X,\alpha) = \sum_j \alpha_j K(X^j, X)$$



Trainable Front-End, Structured Architectures

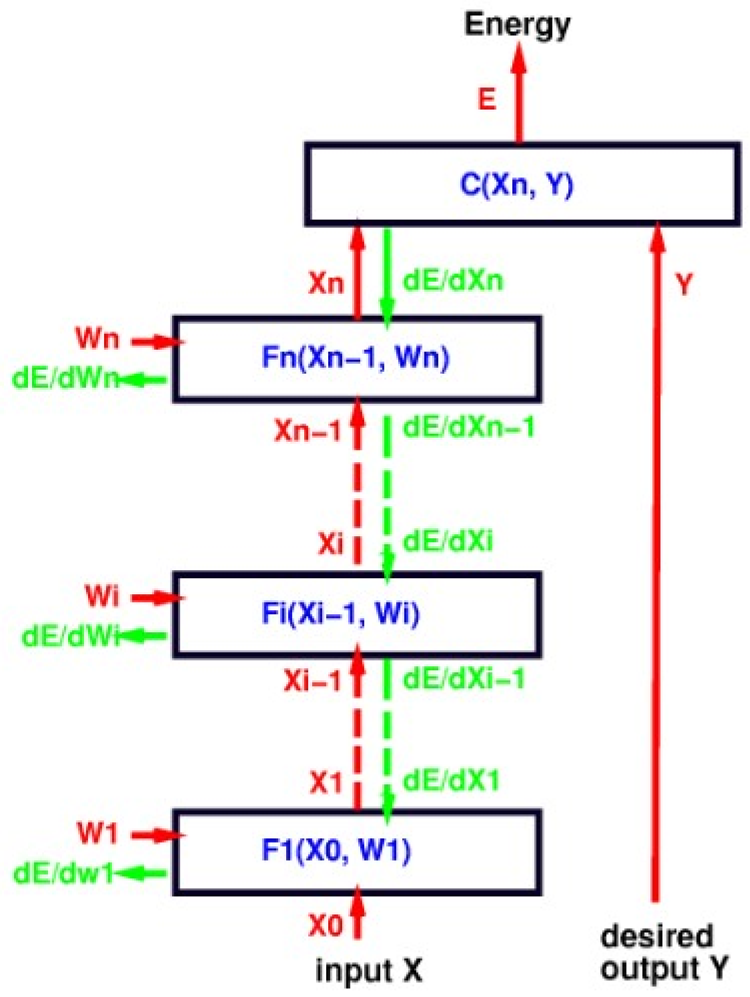
- **The Solutions:**
  - Invariance: Do not use a fixed front-end, **make it trainable**, so it can learn to extract invariant representations
  - Structure: Do not use simple linearly-parameterized classifiers, use architectures whose inference process involves multiple non-linear decisions, as well as search and “reasoning”.
- **We need total flexibility in the design of the architecture of the machine:**
  - So that we can tailor the architecture to the task
  - So that we can build our prior knowledge about the task into the architecture
- **Multi-Module Architectures.**

Multi-Module Architectures



- **For Supervised Learning**
  - We allow the function F(W,X) to be non-linearly parameterized in W.
  - This allows us to play with a large repertoire of functions with rich class boundaries.
  - We assume that F(W,X) is differentiable almost everywhere with respect to W.

Multi-Module Systems: Cascade

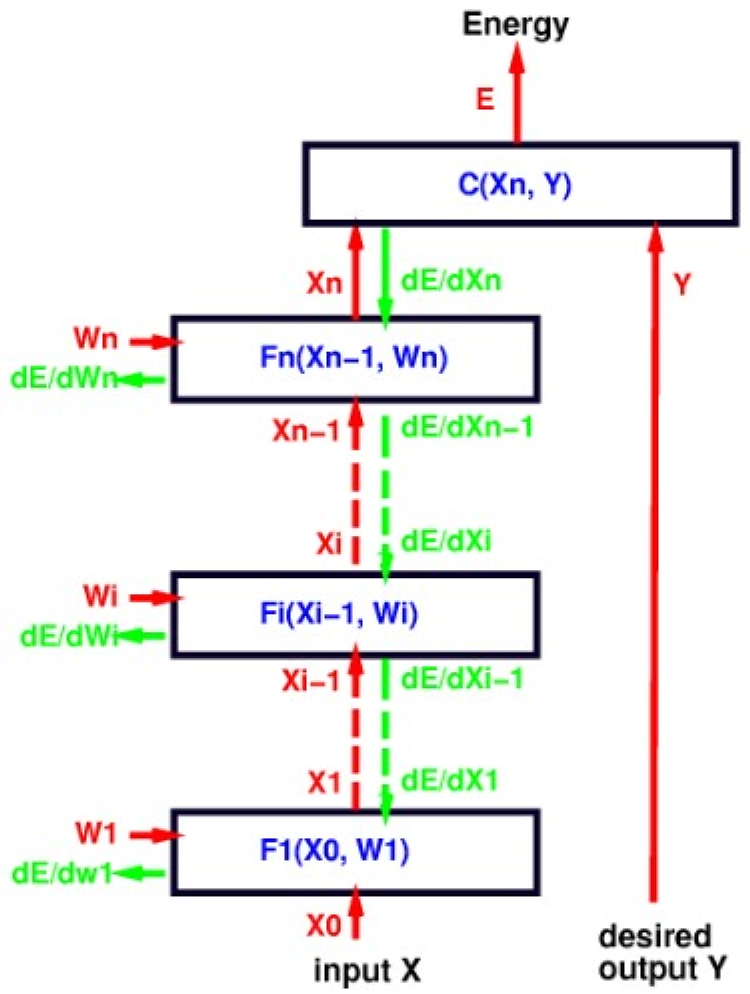


- Complex learning machines can be built by assembling Modules into networks.
- a simple example: layered, feed-forward architecture (cascade).
- computing the output from the input: forward propagation
- let $X = X_0$,

$$X_i = F_i(X_{i-1}, W_i) \quad \forall i \in [1, n]$$

$$E(Y, X, W) = C(X_n, Y)$$

Object-Oriented Implementation



- Each module is an object (instance of a class).
- Each class has an “fprop” (forward propagation) method that takes the input and output states as arguments and computes the output state from the input state.
- Lush:
  ```
  (==> module fprop input
  output)
  ```
- C++:
  ```
  module.fprop(input,output);
  ```

Gradient of the Loss, gradient of the Energy

- We assumed early on that the loss depends on W only through the terms $E(W, Y, X^i)$:

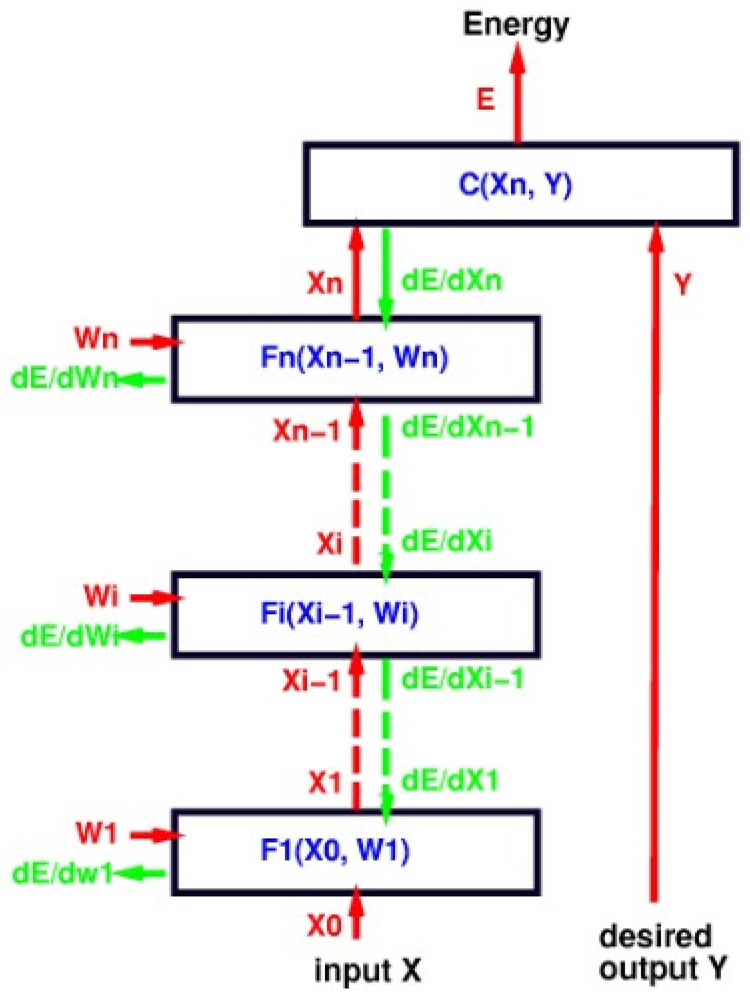
$$L(W, Y^i, X^i) = L(Y^i, E(W, 0, X^i), E(W, 1, X^i), \ldots, E(W, k-1, X^i))$$

- therefore:

$$\frac{\partial L(W, Y^i, X^i)}{\partial W} = \sum_Y \frac{\partial L(W, Y^i, X^i)}{\partial E(W, Y, X^i)} \frac{\partial E(W, Y, X^i)}{\partial W}]$$

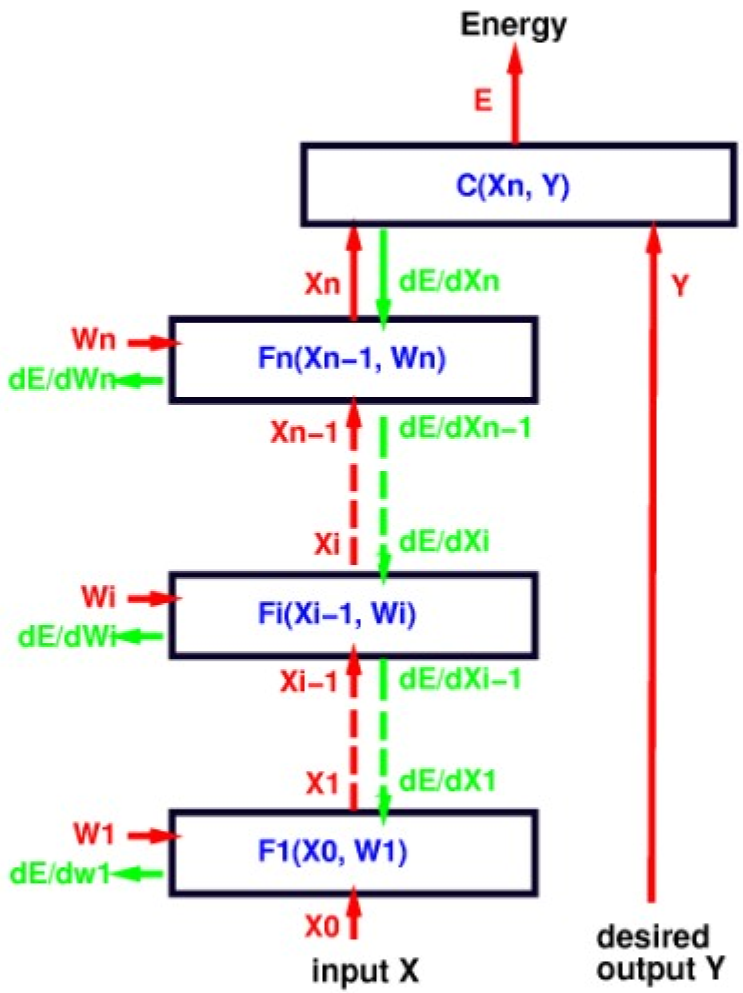
- We only need to compute the terms $\frac{\partial E(W,Y,X^i)}{\partial W}$
- Question: How do we compute those terms efficiently?

Computing the Gradients in Multi-Layer Systems



- To train a multi-module system, we must compute the gradient of E with respect to all the parameters in the system (all the W_i).
- Let's consider module i whose fprop method computes $X_i = F_i(X_{i-1}, W_i)$.
- Let's assume that we already know $\frac{\partial E}{\partial X_i}$, in other words, for each component of vector X_i we know how much E would wiggle if we wiggled that component of X_i.

Computing the Gradients in Multi-Layer Systems



- We can apply chain rule to compute $\frac{\partial E}{\partial W_i}$ (how much E would wiggle if we wiggled each component of W_i):

$$\frac{\partial E}{\partial W_i} = \frac{\partial E}{\partial X_i} \frac{\partial F_i(X_{i-1}, W_i)}{\partial W_i}$$

$$[1 \times N_w] = [1 \times N_x].[N_x \times N_w]$$

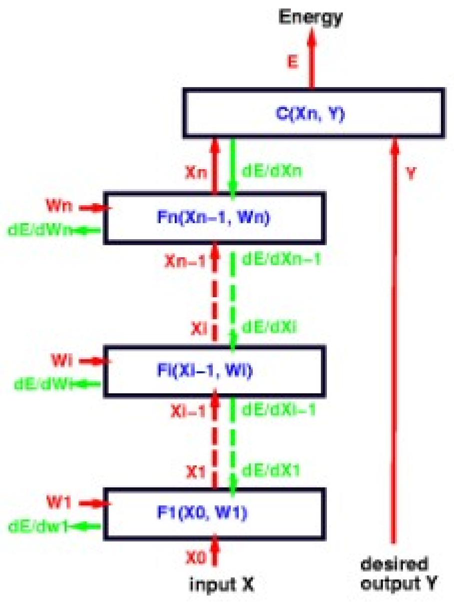
- $\frac{\partial F_i(X_{i-1}, W_i)}{\partial W_i}$ is the *Jacobian matrix* of F_i with respect to W_i.

$$\left[\frac{\partial F_i(X_{i-1}, W_i)}{\partial W_i}\right]_{kl} = \frac{\partial \left[F_i(X_{i-1}, W_i)\right]_k}{\partial [W_i]_l}$$

- Element (k, l) of the Jacobian indicates how much the k-th output wiggles when we wiggle the l-th weight.

Computing the Gradients in Multi-Layer Systems

Using the same trick, we can compute $\frac{\partial E}{\partial X_{i-1}}$. Let's assume again that we already know $\frac{\partial E}{\partial X_i}$, in other words, for each component of vector X_i we know how much E would wiggle if we wiggled that component of X_i.



- We can apply chain rule to compute $\frac{\partial E}{\partial X_{i-1}}$ (how much E would wiggle if we wiggled each component of X_{i-1}):

$$\frac{\partial E}{\partial X_{i-1}} = \frac{\partial E}{\partial X_i}\frac{\partial F_i(X_{i-1}, W_i)}{\partial X_{i-1}}$$

- $\frac{\partial F_i(X_{i-1}, W_i)}{\partial X_{i-1}}$ is the *Jacobian matrix* of F_i with respect to X_{i-1}.
- F_i has two Jacobian matrices, because it has to arguments.
- Element (k, l) of this Jacobian indicates how much the k-th output wiggles when we wiggle the l-th input.
- **The equation above is a recurrence equation!**

Jacobians and Dimensions

- derivatives with respect to a column vector are line vectors (dimensions: $[1 \times N_{i-1}] = [1 \times N_i] * [N_i \times N_{i-1}]$)

$$\frac{\partial E}{\partial X_{i-1}} = \frac{\partial E}{\partial X_i} \frac{\partial F_i(X_{i-1}, W_i)}{\partial X_{i-1}}$$

- (dimensions: $[1 \times N_{wi}] = [1 \times N_i] * [N_i \times N_{wi}]$):

$$\frac{\partial E}{\partial W_i} = \frac{\partial E}{\partial X_i} \frac{\partial F_i(X_{i-1}, W_i)}{\partial W}$$

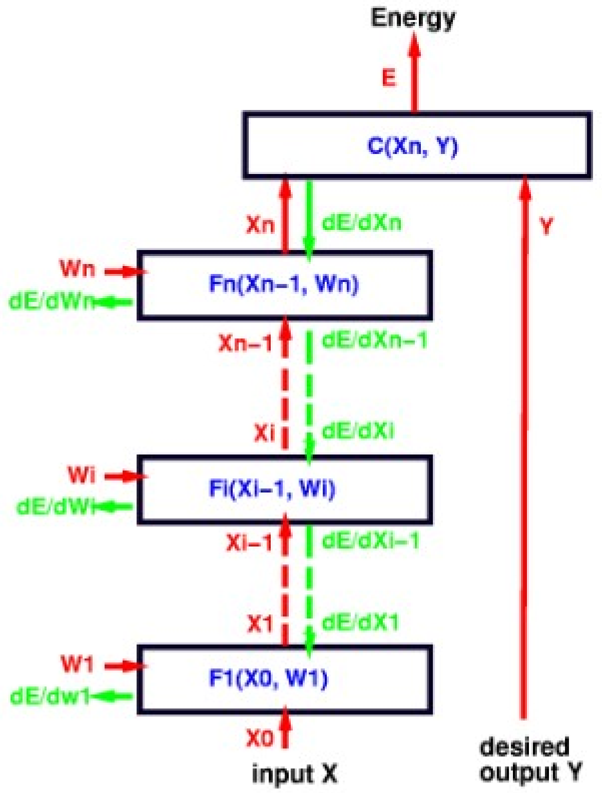
- we may prefer to write those equation with column vectors:

$$\frac{\partial E}{\partial X_{i-1}}' = \frac{\partial F_i(X_{i-1}, W_i)}{\partial X_{i-1}}' \frac{\partial E}{\partial X_i}'$$

$$\frac{\partial E}{\partial W_i}' = \frac{\partial F_i(X_{i-1}, W_i)}{\partial W}' \frac{\partial E}{\partial X_i}'$$

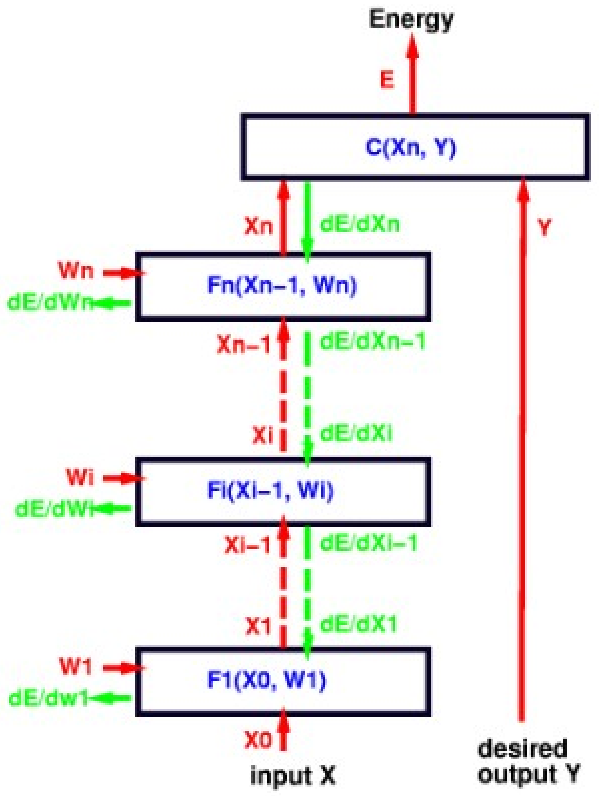
Back-propagation

To compute all the derivatives, we use a backward sweep called the **back-propagation algorithm** that uses the recurrence equation for $\frac{\partial E}{\partial X_i}$



- $\frac{\partial E}{\partial X_n} = \frac{\partial C(X_n, Y)}{\partial X_n}$
- $\frac{\partial E}{\partial X_{n-1}} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial X_{n-1}}$
- $\frac{\partial E}{\partial W_n} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial W_n}$
- $\frac{\partial E}{\partial X_{n-2}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial X_{n-2}}$
- $\frac{\partial E}{\partial W_{n-1}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial W_{n-1}}$
- ....etc, until we reach the first module.
- we now have all the $\frac{\partial E}{\partial W_i}$ for $i \in [1, n]$.

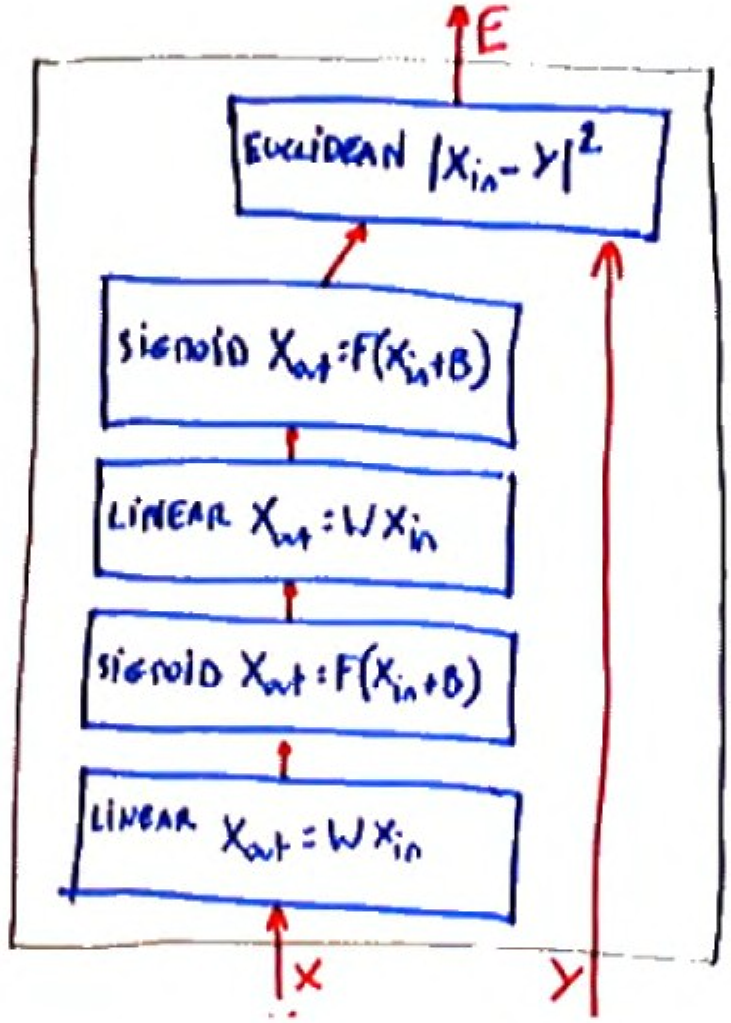
Object-Oriented Implementation



- Each module is an object (instance of a class).
- Each class has a "bprop" (backward propagation) method that takes the input and output states as arguments and computes the derivative of the energy with respect to the input from the derivative with respect to the output:
- Lush: `(==> module bprop input output)`
- C++: `module.bprop(input,output);`
- the objects `input` and `output` contain two slots: one vector for the forward state, and one vector for the backward derivatives.
- the method `bprop` computes the backward derivative slot of `input`, by multiplying the backward derivative slot of `output` by the Jacobian of the module at the forward state of `input`.

Modules in a Multi-layer Neural Net

A fully-connected, feed-forward, multi-layer neural nets can be implemented by stacking three types of modules.

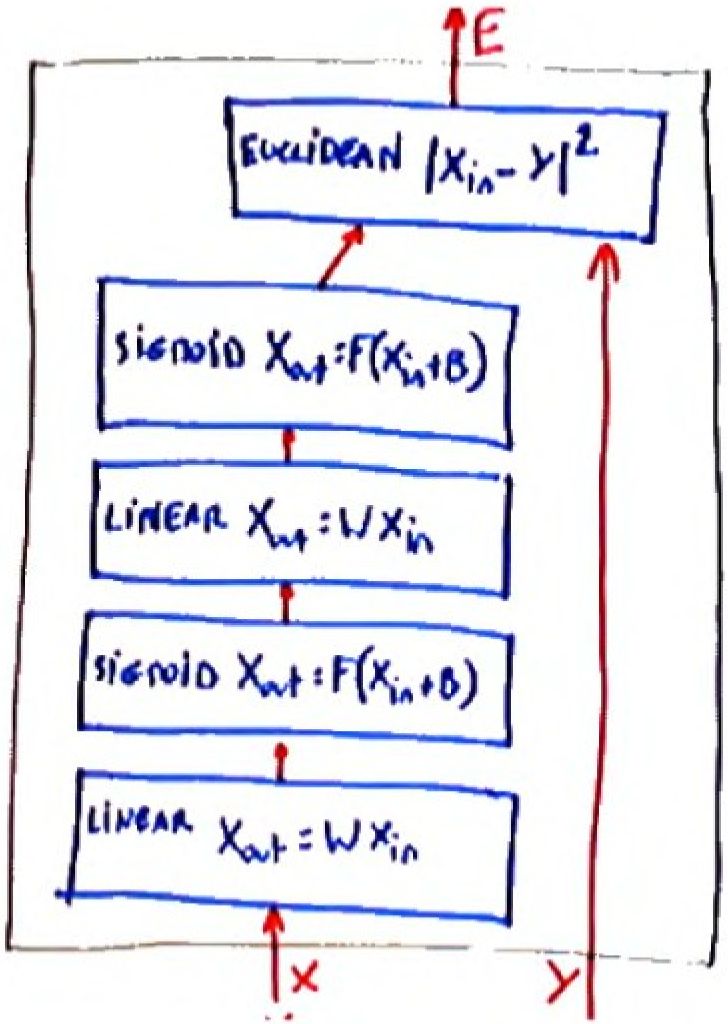

E
EUCLIDEAN $|X_{in} - Y|^2$
SIGMOID $X_{out} = F(X_{in}+B)$
LINEAR $X_{out} = W X_{in}$
SIGMOID $X_{out} = F(X_{in}+B)$
LINEAR $X_{out} = W X_{in}$
X
Y

- Linear modules: X_{in} and X_{out} are vectors, and W is a weight matrix.

$$X_{\text{out}} = W X_{\text{in}}$$

- Sigmoid modules: $(X_{\text{out}})_i = \sigma((X_{\text{in}})_i + B_i)$ where B is a vector of trainable "biases", and σ is a sigmoid function such as tanh or the logistic function.
- a Euclidean Distance module $E = \frac{1}{2}||Y - X_{\text{in}}||^2$. With this energy function, we will use the neural network as a regressor rather than a classifier.

Loss Function


E
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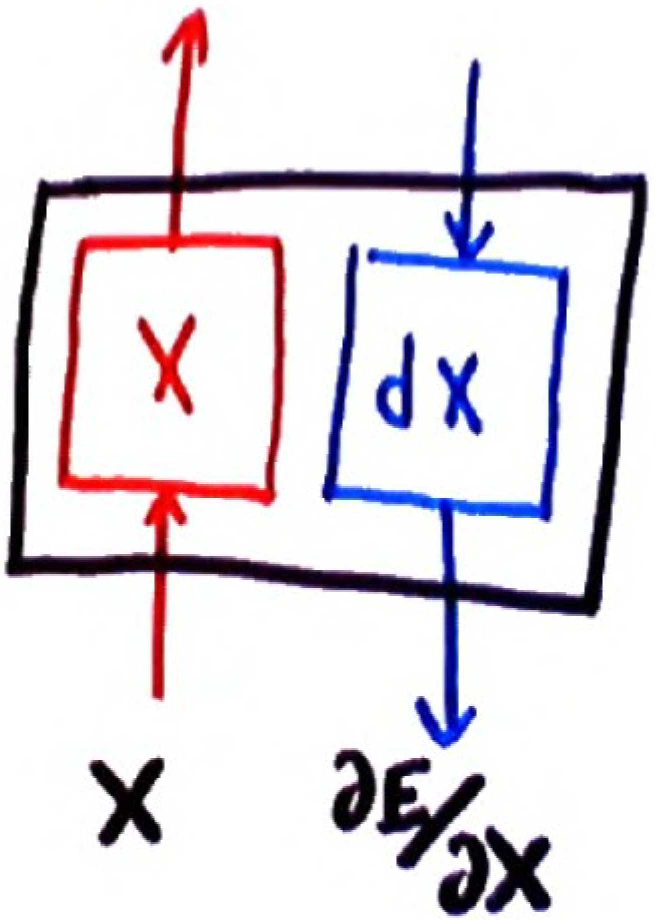
LINEAR $X_{out} = W X_{in}$
X
Y

Here, we will us the simple Energy Loss function L_{energy}:

$$L_{\text{energy}}(W, Y^i, X^i) = E(W, Y^i, X^i)$$

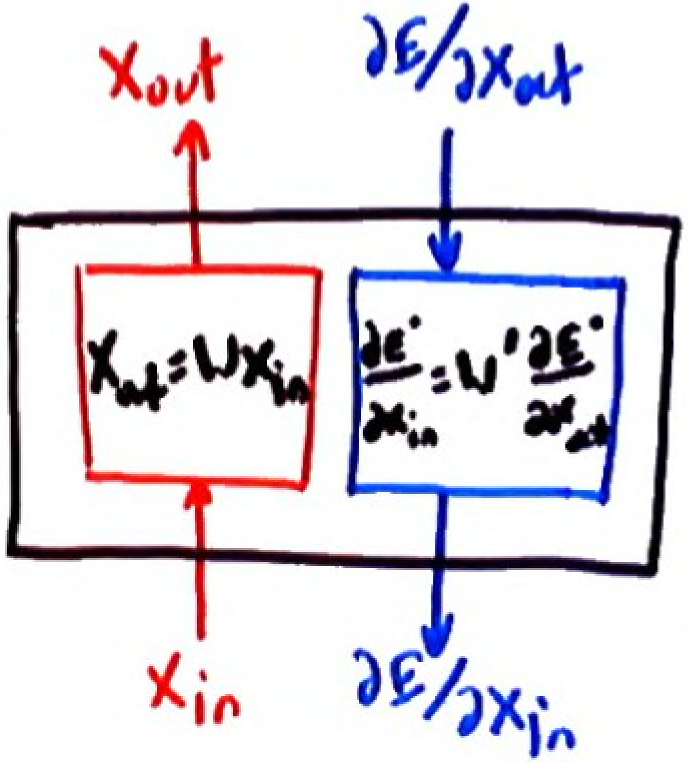
OO Implementation: the `state1` Class



the internal state of the network will be kept in a “state” class that contains two scalars, vectors, or matrices: (1) the state proper, (2) the derivative of the energy with respect to that state.

Linear Module

The input vector is multiplied by the weight matrix.



X_{out}
$\partial E/\partial X_{out}$
$X_{out} = W X_{in}$
$\frac{\partial E}{\partial X_{in}}' = W' \frac{\partial E}{\partial X_{out}}'$
X_{in}
$\partial E/\partial X_{in}$

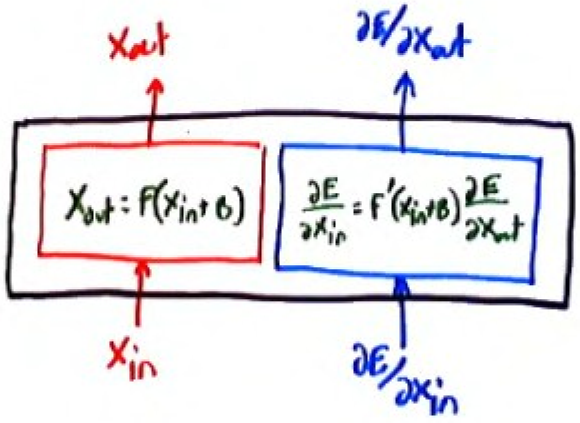
- fprop: $X_{\text{out}} = W X_{\text{in}}$
- bprop to input:
$$\frac{\partial E}{\partial X_{\text{in}}} = \frac{\partial E}{\partial X_{\text{out}}} \frac{\partial X_{\text{out}}}{\partial X_{\text{in}}} = \frac{\partial E}{\partial X_{\text{out}}} W$$
- by transposing, we get column vectors:
$$\frac{\partial E}{\partial X_{\text{in}}}' = W' \frac{\partial E}{\partial X_{\text{out}}}'$$
- bprop to weights:
$$\frac{\partial E}{\partial W_{ij}} = \frac{\partial E}{\partial X_{\text{out}i}} \frac{\partial X_{\text{out}i}}{\partial W_{ij}} = X_{\text{in}j} \frac{\partial E}{\partial X_{\text{out}i}}$$
- We can write this as an outer-product:
$$\frac{\partial E}{\partial W}' = \frac{\partial E}{\partial X_{\text{out}}}' X'_{in}$$

Linear Module

Lush implementation:

```
(defclass linear-module object w)
(defmethod linear-module linear-module (ninputs noutputs)
  (setq w (matrix noutputs ninputs)))
(defmethod linear-module fprop (input output)
  (==> output resize (idx-dim :w:x 0))
  (idx-m2dotm1 :w:x :input:x :output:x) ())
(defmethod linear-module bprop (input output)
  (idx-m2dotm1 (transpose :w:x) :output:dx :input:dx)
  (idx-m1extm1 :output:dx :input:x :w:dx) ())
```

Sigmoid Module (tanh: hyperbolic tangent)

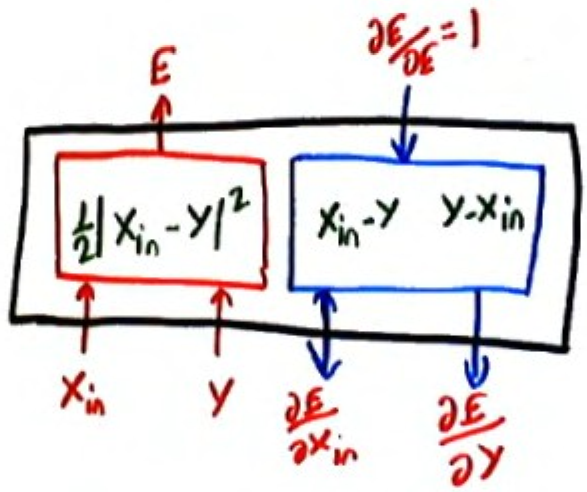


X_{out}
$\partial E/\partial X_{out}$
$X_{out} = F(X_{in}+B)$
$\frac{\partial E}{\partial X_{in}} = F'(X_{in}+B)\frac{\partial E}{\partial X_{out}}$
X_{in}
$\partial E/\partial X_{in}$

- fprop: $(X_{\text{out}})_i = \tanh((X_{\text{in}})_i + B_i)$
- bprop to input:
  $(\frac{\partial E}{\partial X_{\text{in}}})_i = (\frac{\partial E}{\partial X_{\text{out}}})_i \tanh'((X_{\text{in}})_i + B_i)$
- bprop to bias:
  $\frac{\partial E}{\partial B_i} = (\frac{\partial E}{\partial X_{\text{out}}})_i \tanh'((X_{\text{in}})_i + B_i)$
- $\tanh(x) = \frac{2}{1+\exp -x} - 1 = \frac{1-\exp(-x)}{1+\exp(-x)}$

```
(defclass tanh-module object bias)
(defmethod tanh-module tanh-module l
  (setq bias (apply matrix l)))
(defmethod tanh-module fprop (input output)
  (==> output resize (idx-dim :bias:x 0))
  (idx-add :input:x :bias:x :output:x)
  (idx-tanh :output:x :output:x))
(defmethod tanh-module bprop (input output)
  (idx-dtanh (idx-add :input:x :bias:x) :input:dx)
  (idx-mul :input:dx :output:dx :input:dx)
  (idx-copy :input:dx :bias:dx) ())
```

Euclidean Module



E
$\partial E / \partial E = 1$
$\frac{1}{2}||X_{in} - Y||^2$
$X_{in} - Y$
$Y - X_{in}$
X_{in}
Y
$\frac{\partial E}{\partial X_{in}}$
$\frac{\partial E}{\partial Y}$

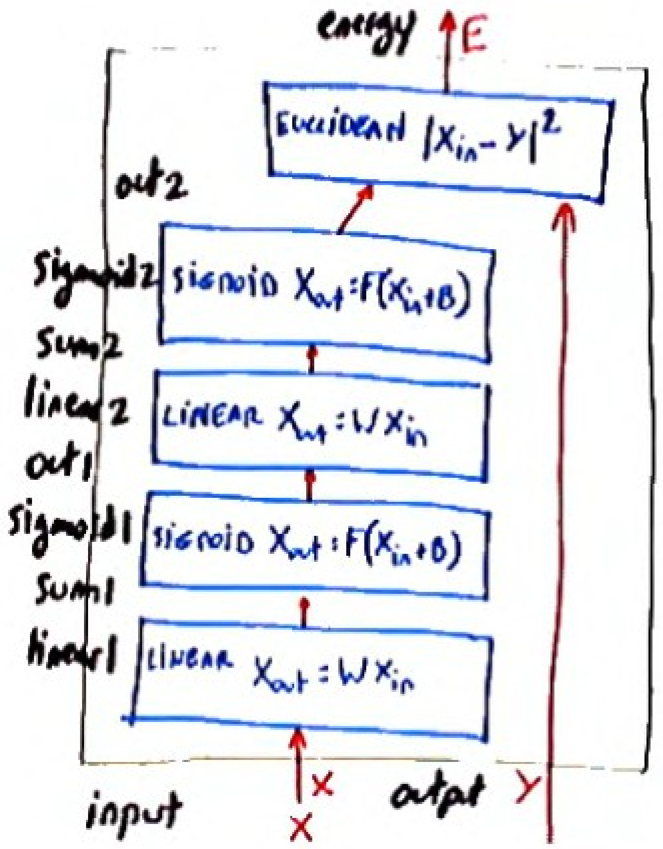
- fprop: $X_{\text{out}} = \frac{1}{2}||X_{\text{in}} - Y||^2$
- bprop to X input: $\frac{\partial E}{\partial X_{\text{in}}} = X_{\text{in}} - Y$
- bprop to Y input: $\frac{\partial E}{\partial Y} = Y - X_{\text{in}}$

```
(defclass euclidean-module object)
(defmethod euclidean-module run (input1 input2 output)
  (idx-copy :input1:x :input2:x)
  (:output:x 0) ())
(defmethod euclidean-module fprop (input1 input2 output)
  (idx-sqrdist :input1:x :input2:x :output:x)
  (:output:x (* 0.5 (:output:x))) ())
(defmethod euclidean-module bprop (input1 input2 output)
  (idx-sub :input1:x :input2:x :input1:dx)
  (idx-dotm0 :input1:dx :output:dx :input1:dx)
  (idx-minus :input1:dx :input2:dx))
```

Assembling the Network: A single layer

```
;; One layer of a neural net
(defclass nn-layer object
  linear  ; linear module
  sum  ; weighted sums
  sigmoid ; tanh-module
  )
(defmethod nn-layer nn-layer (ninputs noutputs)
  (setq linear (new linear-module ninputs noutputs))
  (setq sum (new state noutputs))
  (setq sigmoid (new tanh-module noutputs)) ())
(defmethod nn-layer fprop (input output)
  (==> linear fprop input sum)
  (==> sigmoid fprop sum output) ())
(defmethod nn-layer bprop (input output)
  (==> sigmoid bprop sum output)
  (==> linear bprop input sum) ())
```

Assembling a 2-layer Net


energy
E
EUCLIDEAN $|X_{in} - Y|^2$
out2
sigmoid2
SIGMOID $X_{out} = F(X_{in}+B)$
sum2
linear2
LINEAR $X_{out} = W X_{in}$
out1
sigmoid1
SIGMOID $X_{out} = F(X_{in}+B)$
sum1
linear1
LINEAR $X_{out} = W X_{in}$
input
X
X
otpt
Y

- Class implementation for a 2 layer, feed forward neural net.

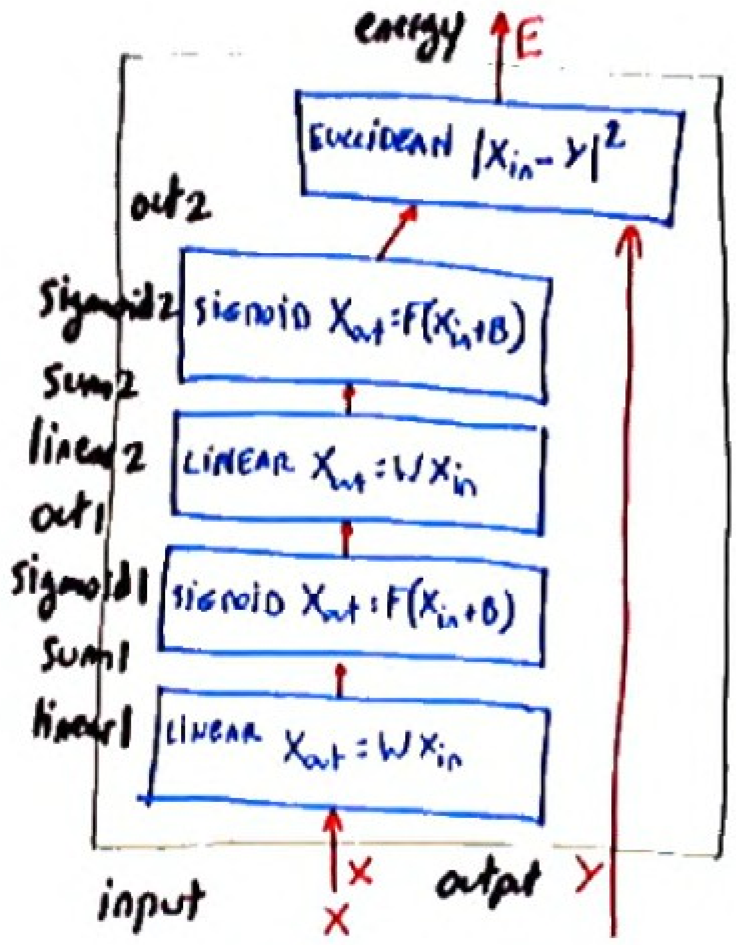
```
(defclass nn-2layer object
  layer1  ; first layer module
  hidden  ; hidden state
  layer2 ; second layer
  )
(defmethod nn-2layer nn-2layer (ninputs nhi
   (setq layer1 (new nn-layer ninputs nhidde
   (setq hidden (new state nhidden))
   (setq layer2 (new nn-layer nhidden noutpu
```

Assembling the Network: fprop and bprop

Implementation of a 2 layer, feed forward neural net.

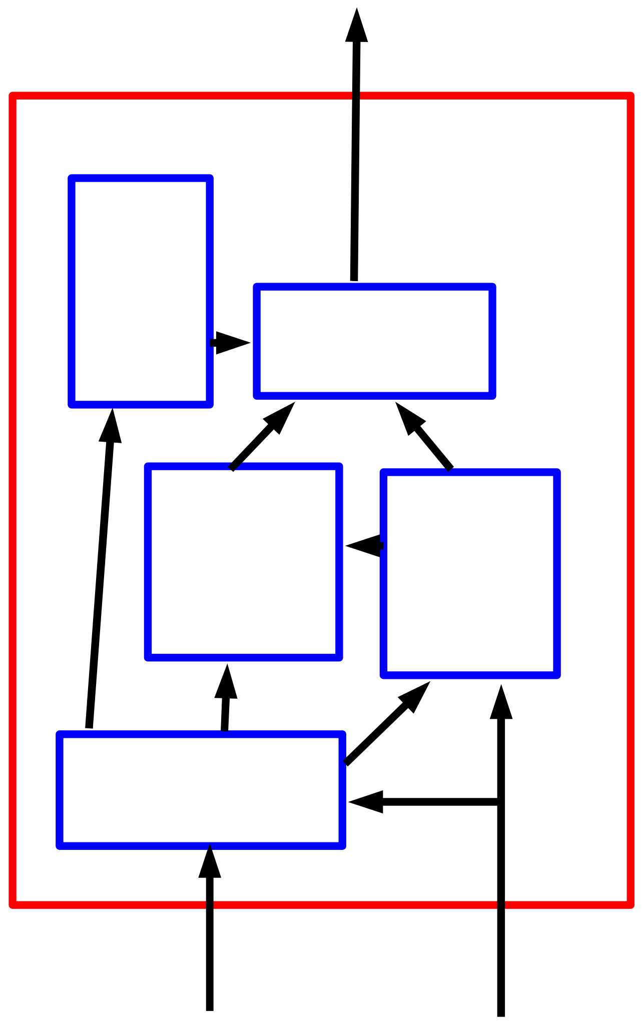
```
(defmethod nn-2layer fprop (input output)
  (==> layer1 fprop input hidden)
  (==> layer2 fprop hidden output) ())

(defmethod nn-2layer bprop (input output)
  (==> layer2 bprop hidden output)
  (==> layer1 bprop input hidden) ())
```

Assembling the Network: training



- A training cycle:
- pick a sample (X^i, Y^i) from the training set.
- call fprop with (X^i, Y^i) and record the error
- call bprop with (X^i, Y^i)
- update all the weights using the gradients obtained above.
- with the implementation above, we would have to go through each and every module to update all the weights. In the future, we will see how to "pool" all the weights and other free parameters in a single vector so they can all be updated at once.

Any Architecture works

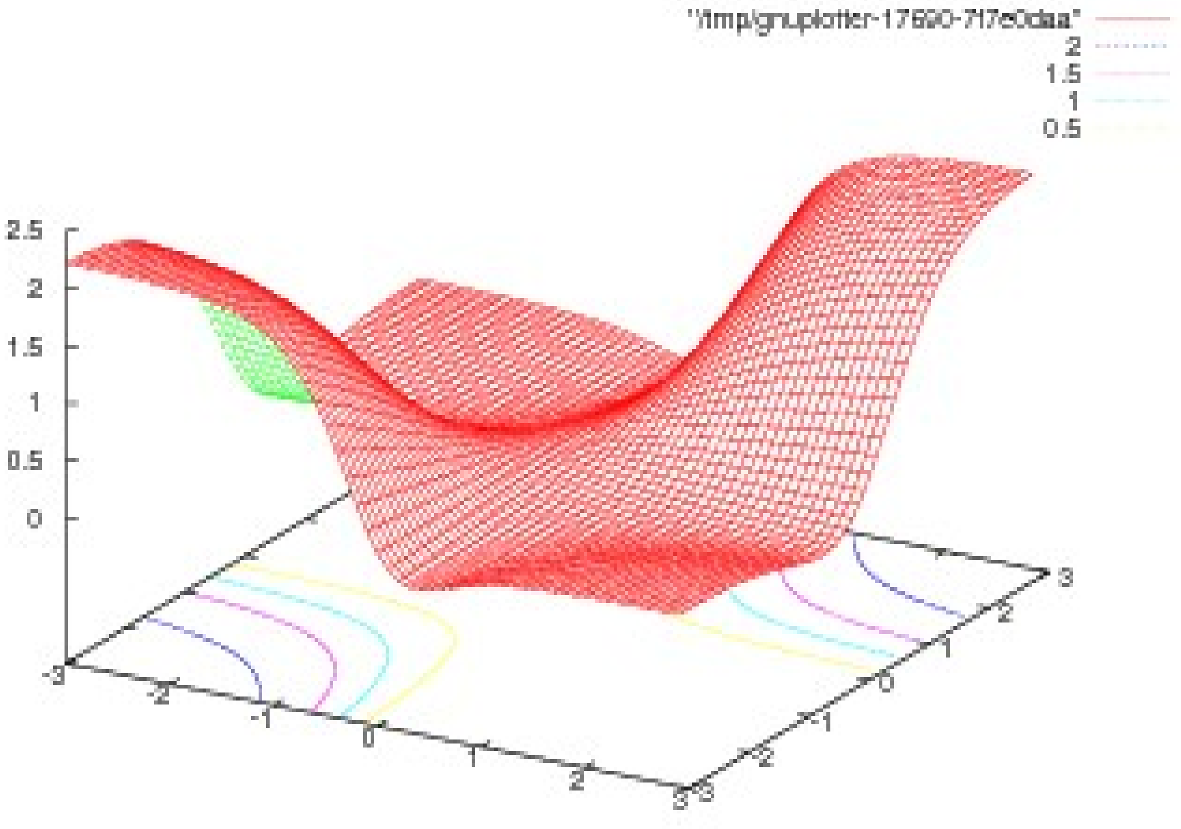


- **Any connection is permissible**
  - Networks with loops must be "unfolded in time".
- **Any module is permissible**
  - As long as it is continuous and differentiable almost everywhere with respect to the parameters, and with respect to non-terminal inputs.

Deep Supervised Learning is Hard

- **Example: what is the loss function for the simplest 2-layer neural net ever**
  - Function: 1-1-1 neural net. Map 0.5 to 0.5 and -0.5 to -0.5 (identity function) with quadratic cost:

$$y = \tanh(W_1 \tanh(W_0.x)) \quad L = (0.5 - \tanh(W_1 \tanh(W_0 0.5)^2$$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