Neural Networks

Lecture 2

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Overview

- Individual neuron
- Non-linearities (RELU, tanh, sigmoid)
- Single layer model
- Multiple layer models
- Theoretical discussion: representational power
- Examples shown decision surface for 1,2,3-layer nets
- Training models
- Backprop
- Example modules
- Special layers
- Practical training tips
- Setting learning rate
- Debugging training
- Regularization

Additional Readings

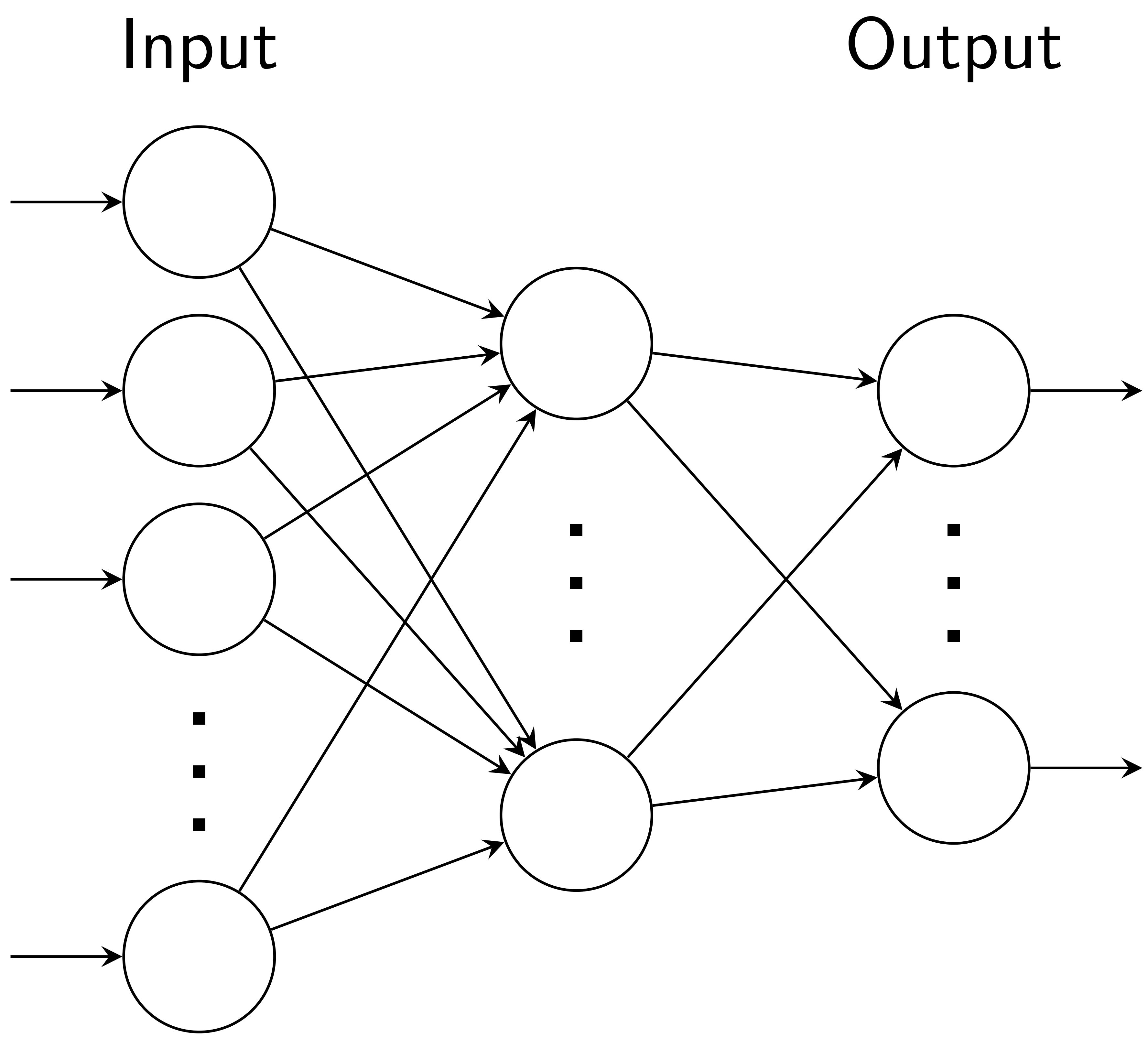
Useful books and articles

- Neural Networks for Pattern Reconition, Christopher M. Bishop, Oxford University Press 1995.
  - Red/Green cover, NOT newer book with yellow/beige cover.
- Andrej Karpathy's CS231n Stanford Course on Neural Nets
  `http://cs231n.github.io/`
- Yann LeCun's NYU Deep Learning course
  `http://cilvr.cs.nyu.edu/doku.php?id=courses:deeplearning2015:start`

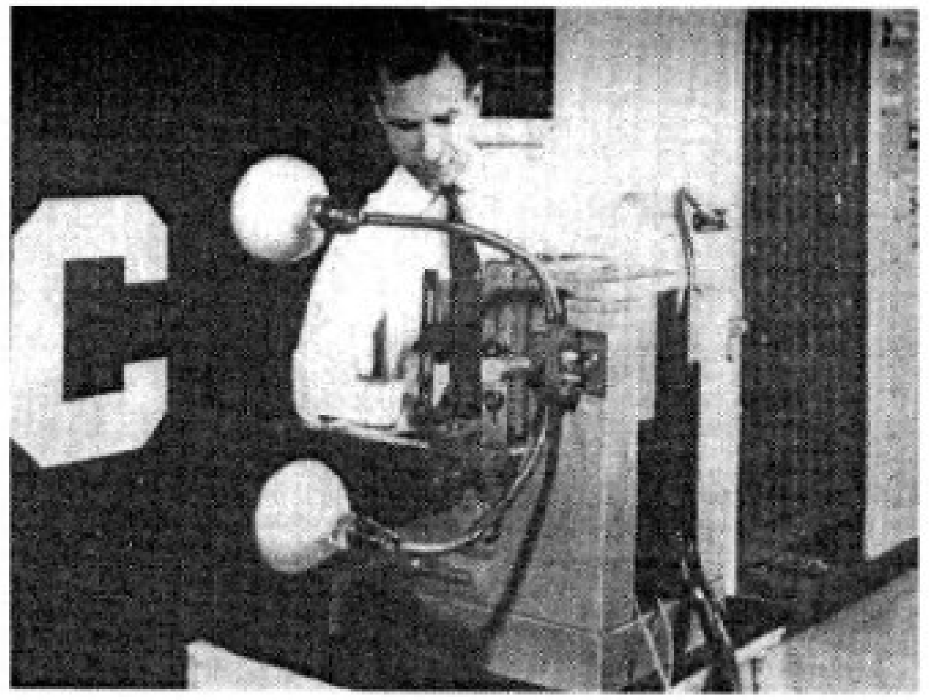
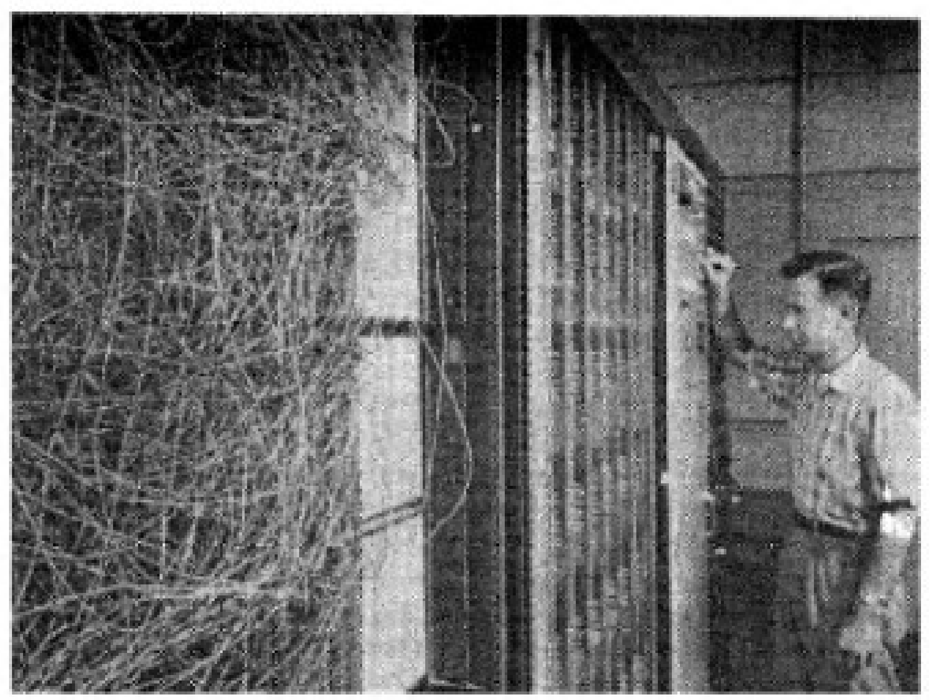
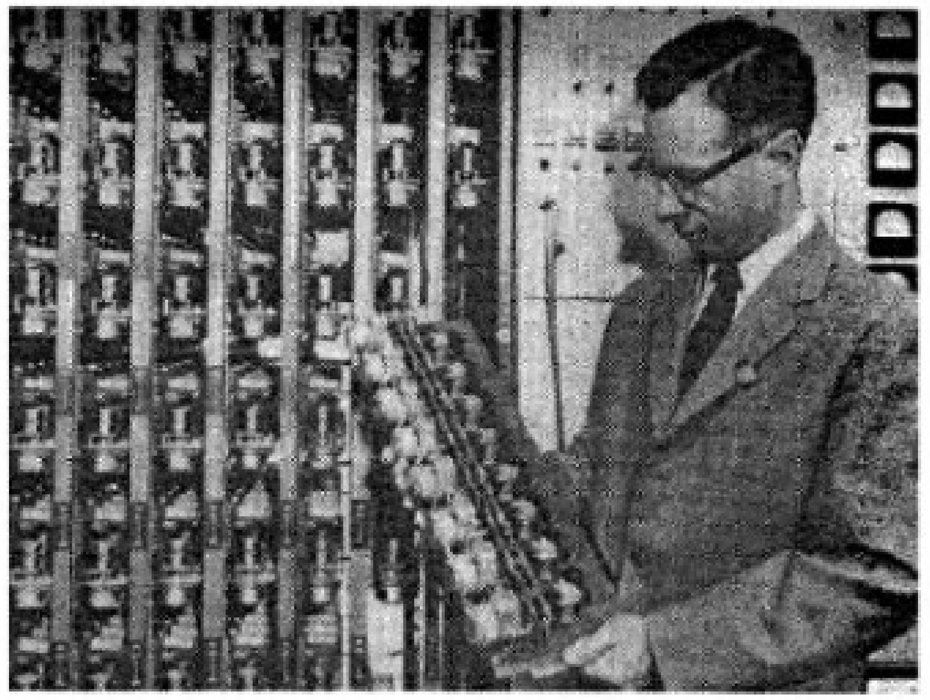
Neural Networks Overview

A bit more information about this

- Neural nets composed of layers of artificial *neurons*.
- Each layer computes some function of layer beneath.
- Inputs mapped in *feed-forward* fashion to output.
- Consider only feed-forward neural models at the moment, i.e. no cycles



- Neural nets are an example of *connectionism*. Connectionism [Hebb 1940s] argues that complex behaviors arise from interconnected networks of simple units. As opposed to formal operations on symbols (computationalism).
- Early work in 1940's and 1950's by Hebb, McCulloch and Pitts on artificial neurons.
- Perceptrons [Rosenblatt 1950's]. Single layer networks with simple learning rule.

- Perceptron book [Minsky and Pappert 1969]. Showed limitations of single layer models (e.g. cannot solve XOR).

Historical Overview

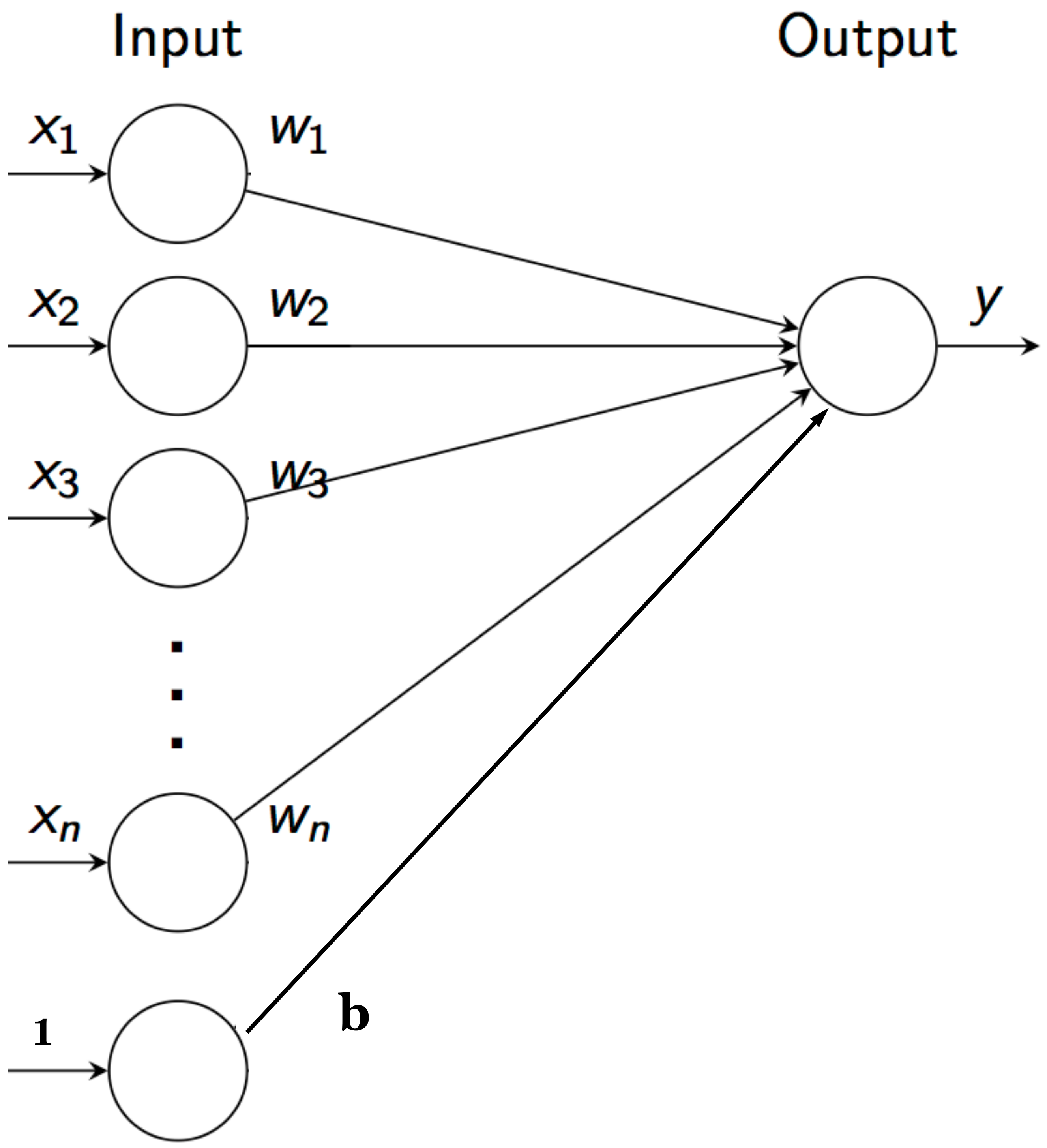
More recent history

- Back-propagation algorithm [Rumelhart, Hinton, Williams 1986]. Practical way to train networks.
- Neocognitron [Fukushima 1980]. Proto-ConvNet, inspired by [Hubel & Weisel 1959].
- Convolutional Networks [LeCun & others 1989].
- Bigger datasets, e.g. [ImageNet 2009]
- Neural Nets applied to speech [Hinton's group 2011].
- ConvNets applied to ImageNet Challenge 2012 [Krizhevsky, Sutskever & Hinton NIPS 2012]
- Last few years, improved ConvNet architectures. Closing on human performance.

An Individual Neuron

Also known as a unit

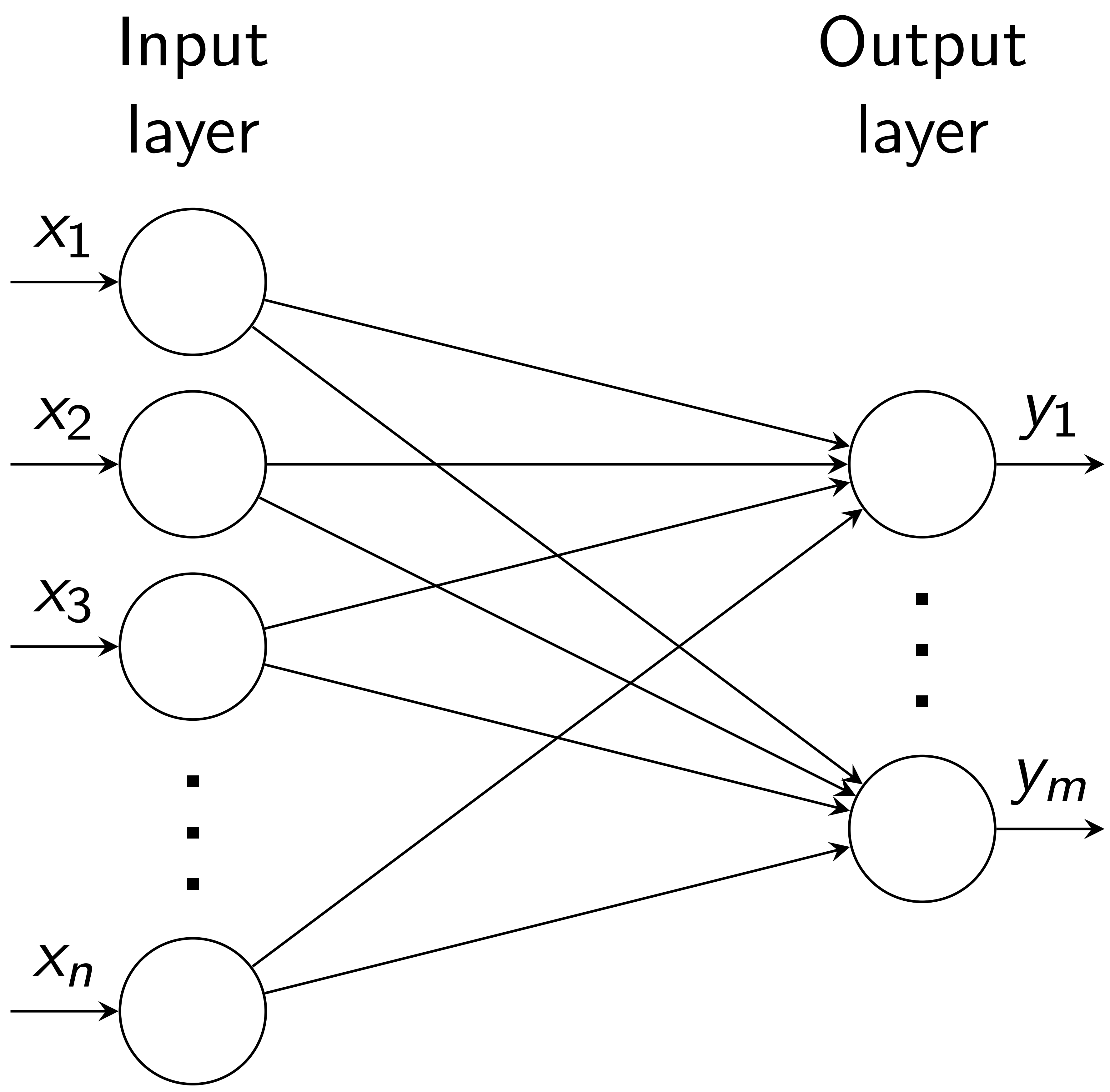
- Input: x ($n \times 1$ vector)
- Parameters: weights w ($n \times 1$ vector), bias b (scalar)
- Activation: $a = \sum_{i=1}^{n} x_i w_i + b$. Note a is a scalar. Multiplicative interaction between weights and input.
- Point-wise non-linear function: $\sigma(.)$, e.g. $\sigma(.) = tanh(.)$.
- Output: $y = f(a) = \sigma(\sum_{i=1}^{n} x_i w_i + b)$
- Can think of bias as weight w_0, connected to constant input 1: $y = f(\tilde{w}^T[1, x])$.



Single Layer Network

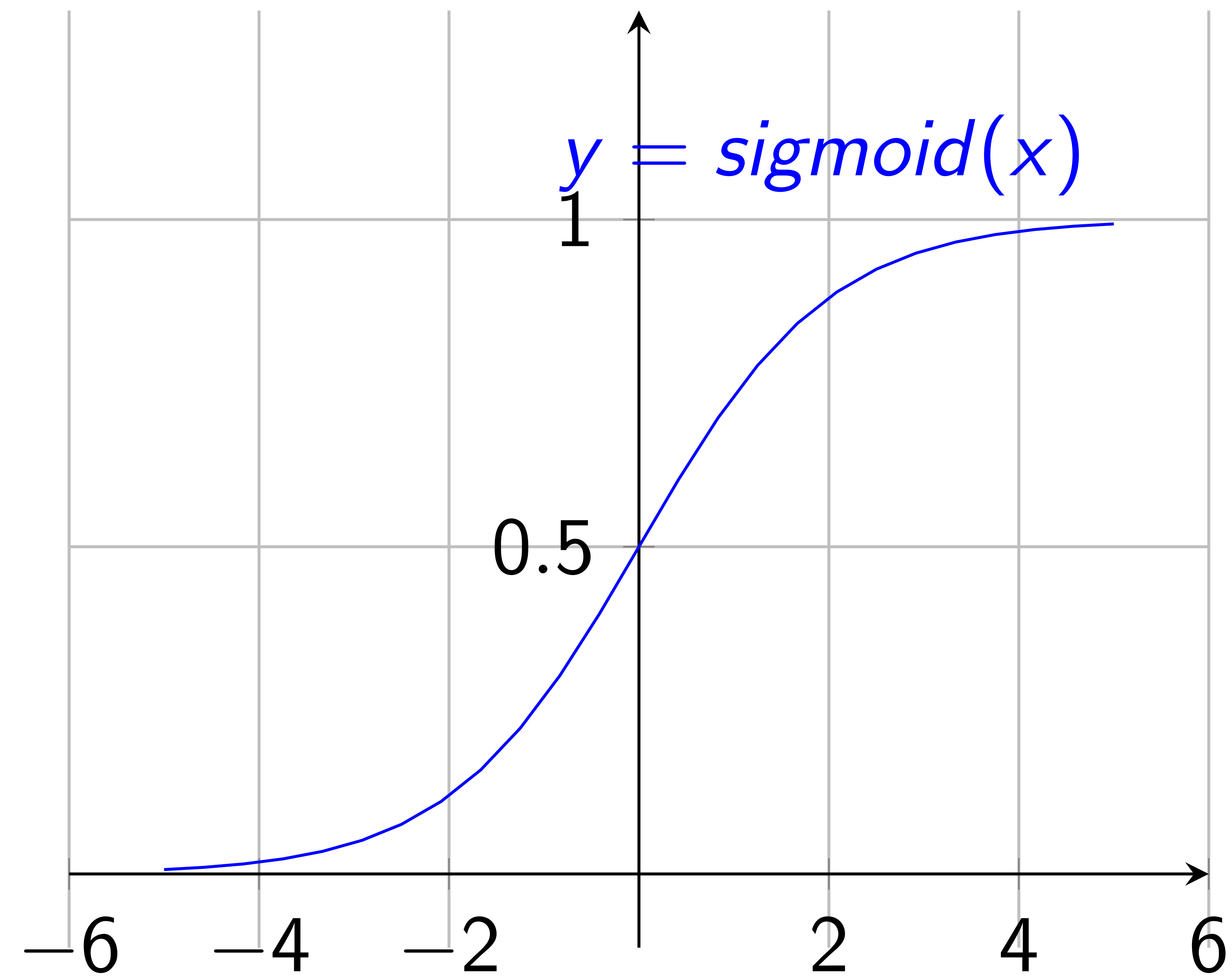
Multiple outputs

- Input: x ($n \times 1$ vector)
- m neurons
- Parameters:
  - weight matrix W ($n \times m$)
  - bias vector b ($m \times 1$)
- Non-linear function $\sigma(.)$
- Output: $y = \sigma(Wx + b)$ ($m \times 1$)



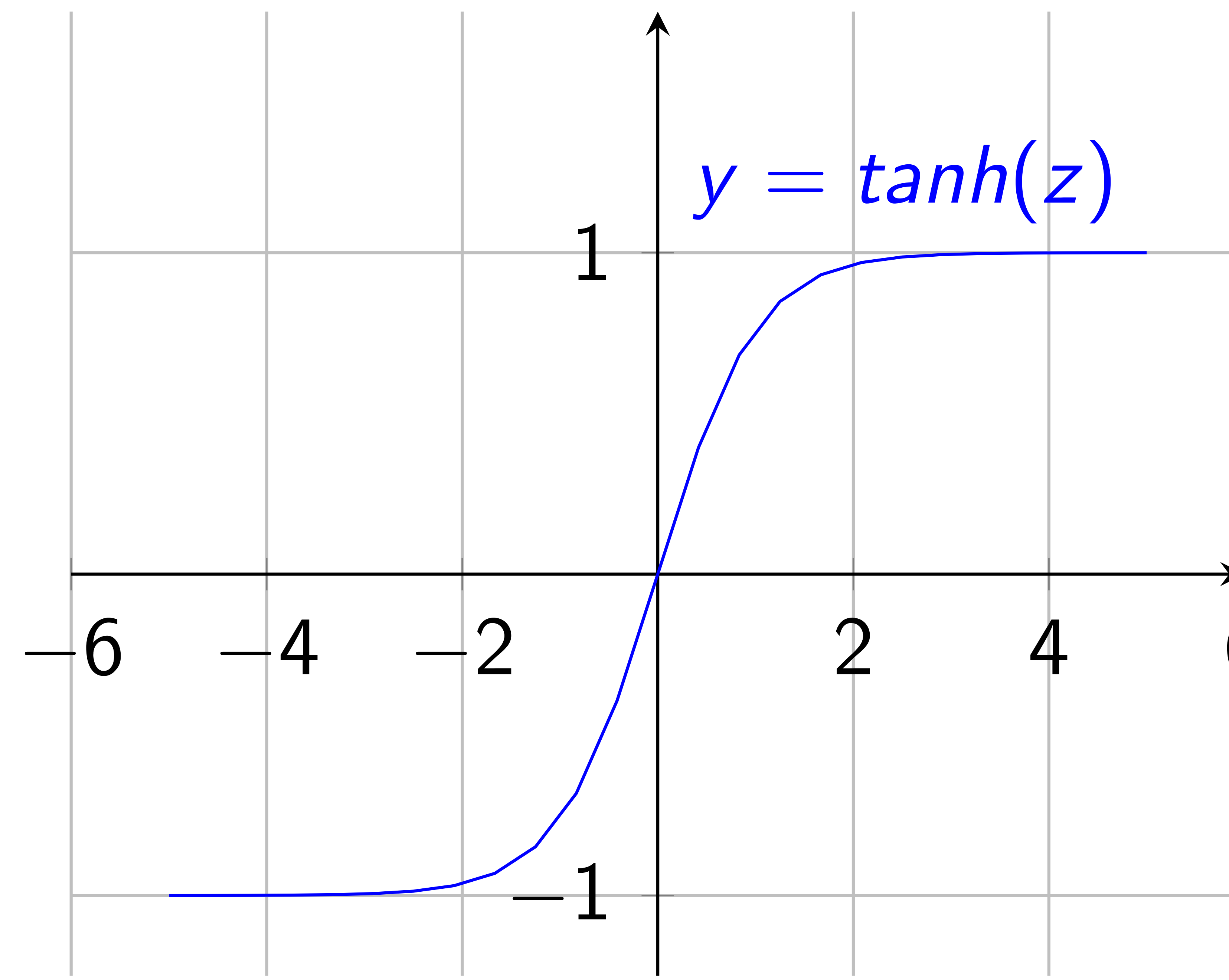
Non-linearities: Sigmoid

- $\sigma(z) = \frac{1}{1+e^{-z}}$
- Interpretation as firing rate of neuron
- Bounded between [0,1]
- Saturation for large +ve,-ve inputs
- Gradients go to zero
- Outputs centered at 0.5 (poor conditioning)
- Not used in practice



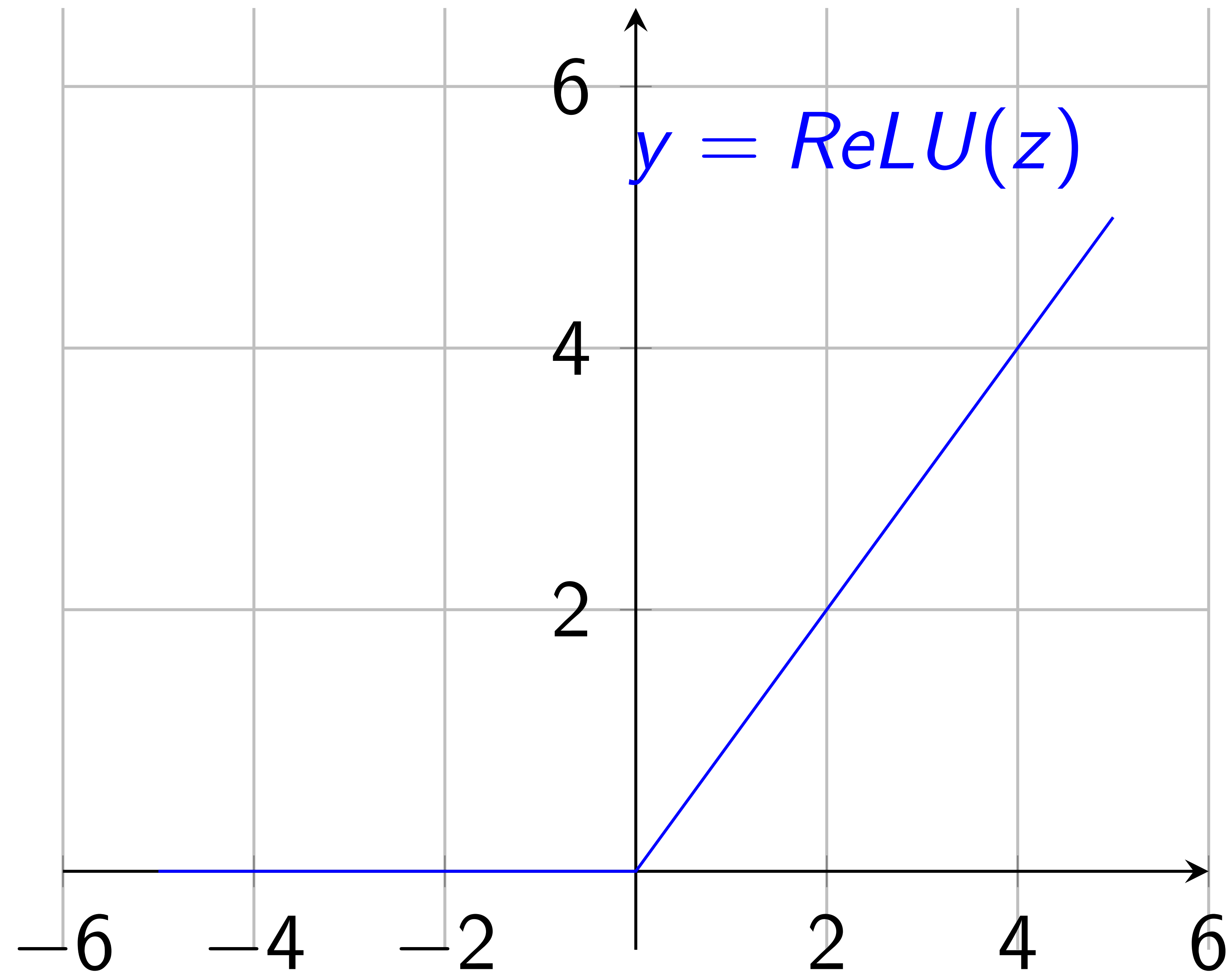
Non-linearities: Tanh

- $\sigma(z) = \tanh(z)$
- Bounded in [+1,-1] range
- Saturation for large +ve, -ve inputs
- Outputs centered at zero
- Preferable to sigmoid

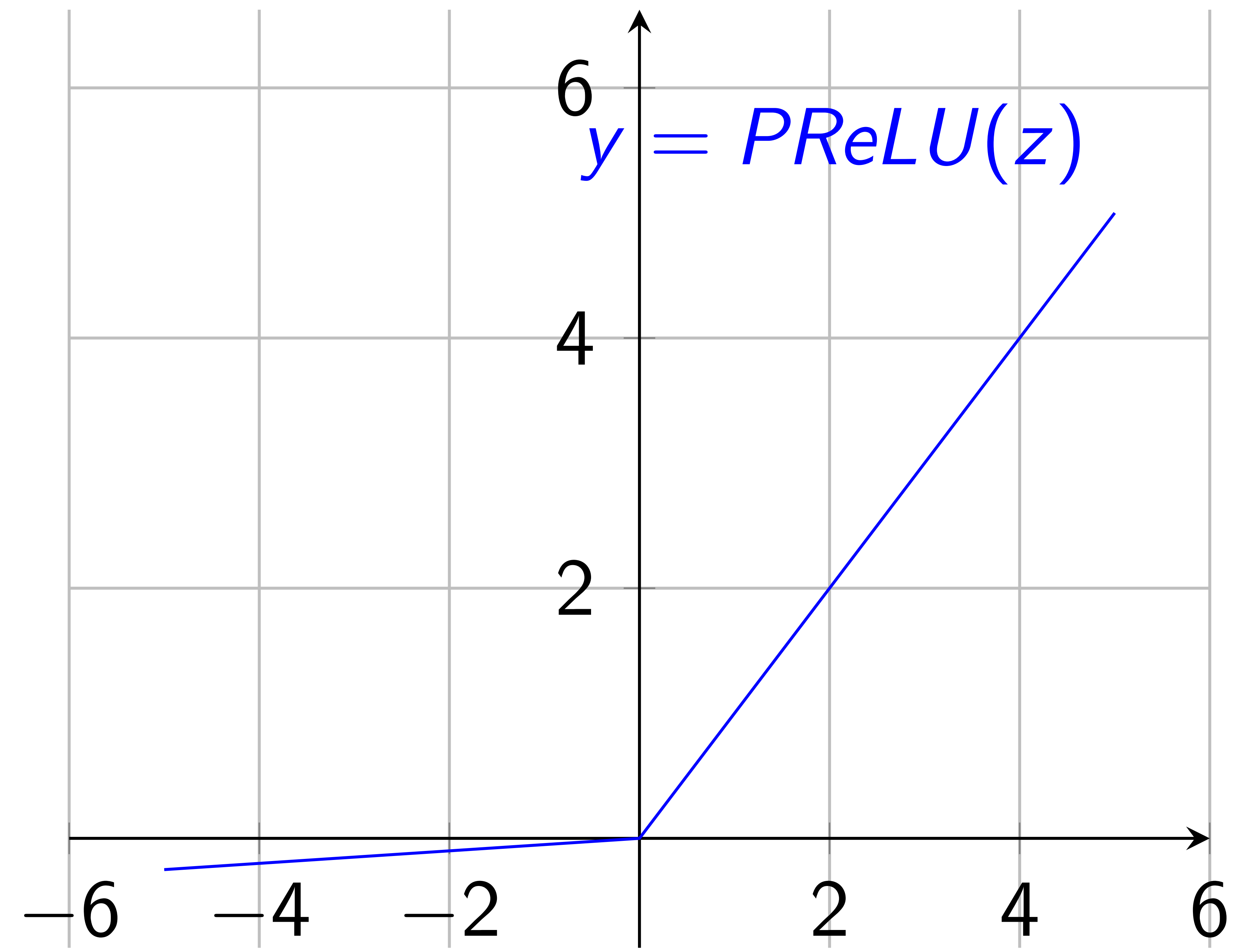


Non-linearities: Rectified Linear (ReLU)

- $\sigma(z) = max(z, 0)$
- Unbounded output (on positive side)
- Efficient to implement: $\frac{d\sigma(z)}{dz} = \{0, 1\}$.
- Also seems to help convergence (see 6x speedup vs tanh in Krizhevsky et al.)
- Drawback: if strongly in negative region, unit is dead forever (no gradient).
- Default choice: widely used in current models.



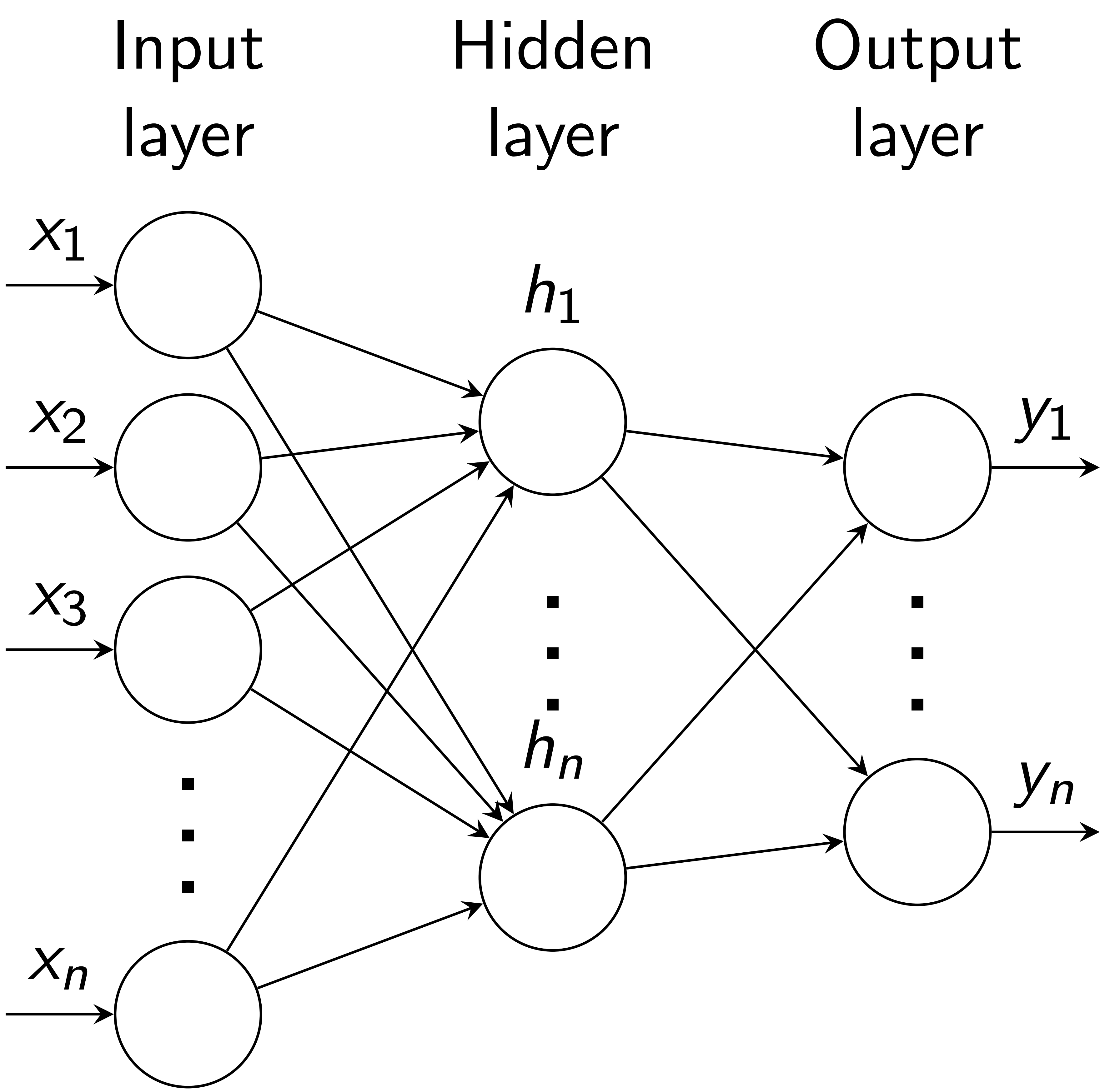
- Leaky Rectified Linear $\sigma(z) = 1[z > 0]max(0, x) + 1[z < 0]max(0, \alpha z)$
- where α is small, e.g. 0.02
- Also known as probabilistic ReLU (PReLU)
- Has non-zero gradients everywhere (unlike ReLU)
- α can also be learned (see Kaiming He et al. 2015).



Multiple Layers

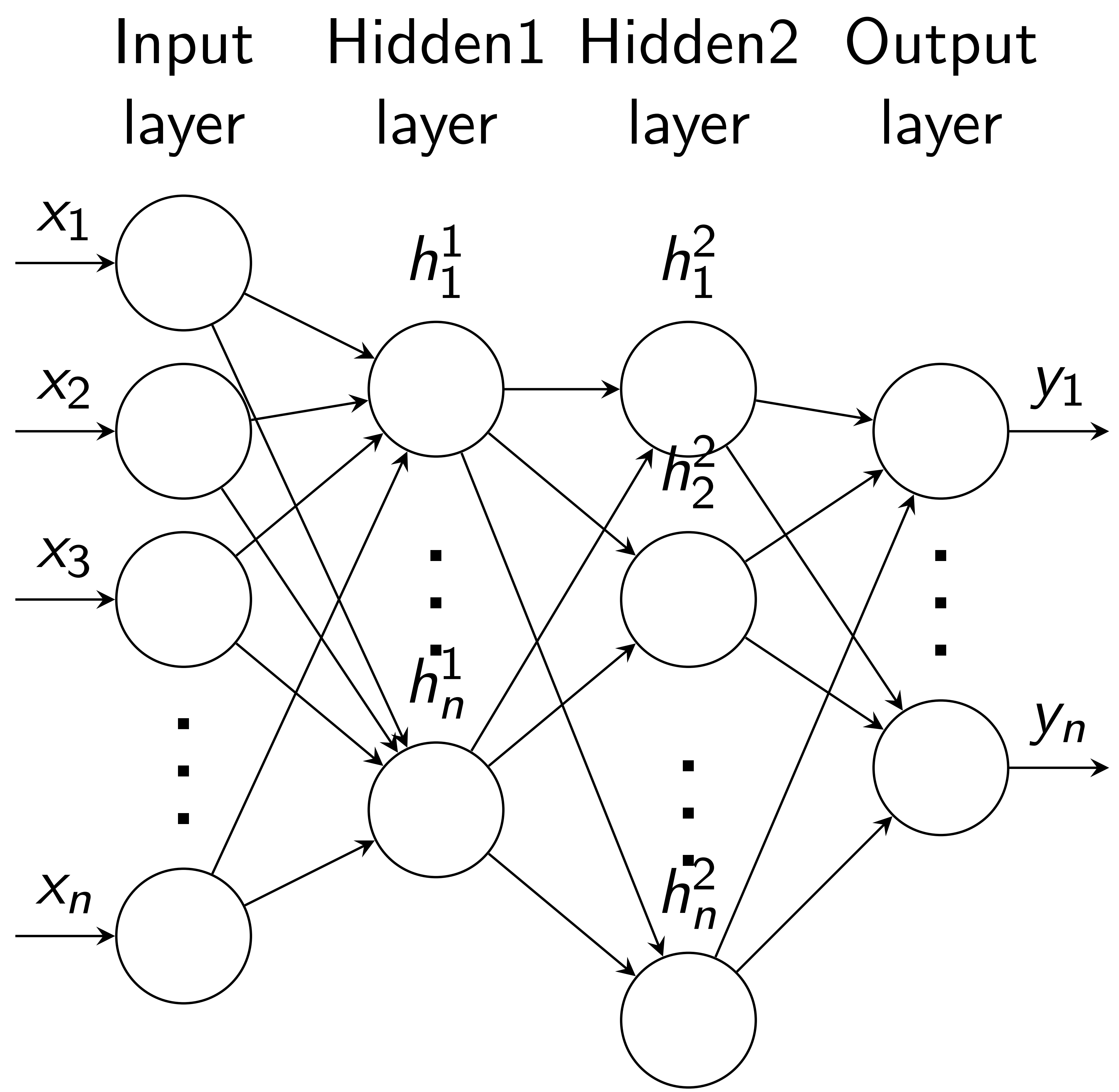
A bit more information about this

- Neural networks is composed of multiple layers of neurons.
- Acyclic structure. Basic model assumes full connections between layers.
- Layers between input and output are called *hidden*.
- Various names used:
  - Artificial Neural Nets (ANN)
  - Multi-layer Perceptron (MLP)
  - Fully-connected network
- Neurons typically called *units*.



3 layer MLP

- By convention, number of layers is hidden + output (i.e. does not include input).
- So 3-layer model has 2 hidden layers.
- Parameters: weight matrices W^1, W^2, W^3 and bias vectors b^1, b^2, b^3.

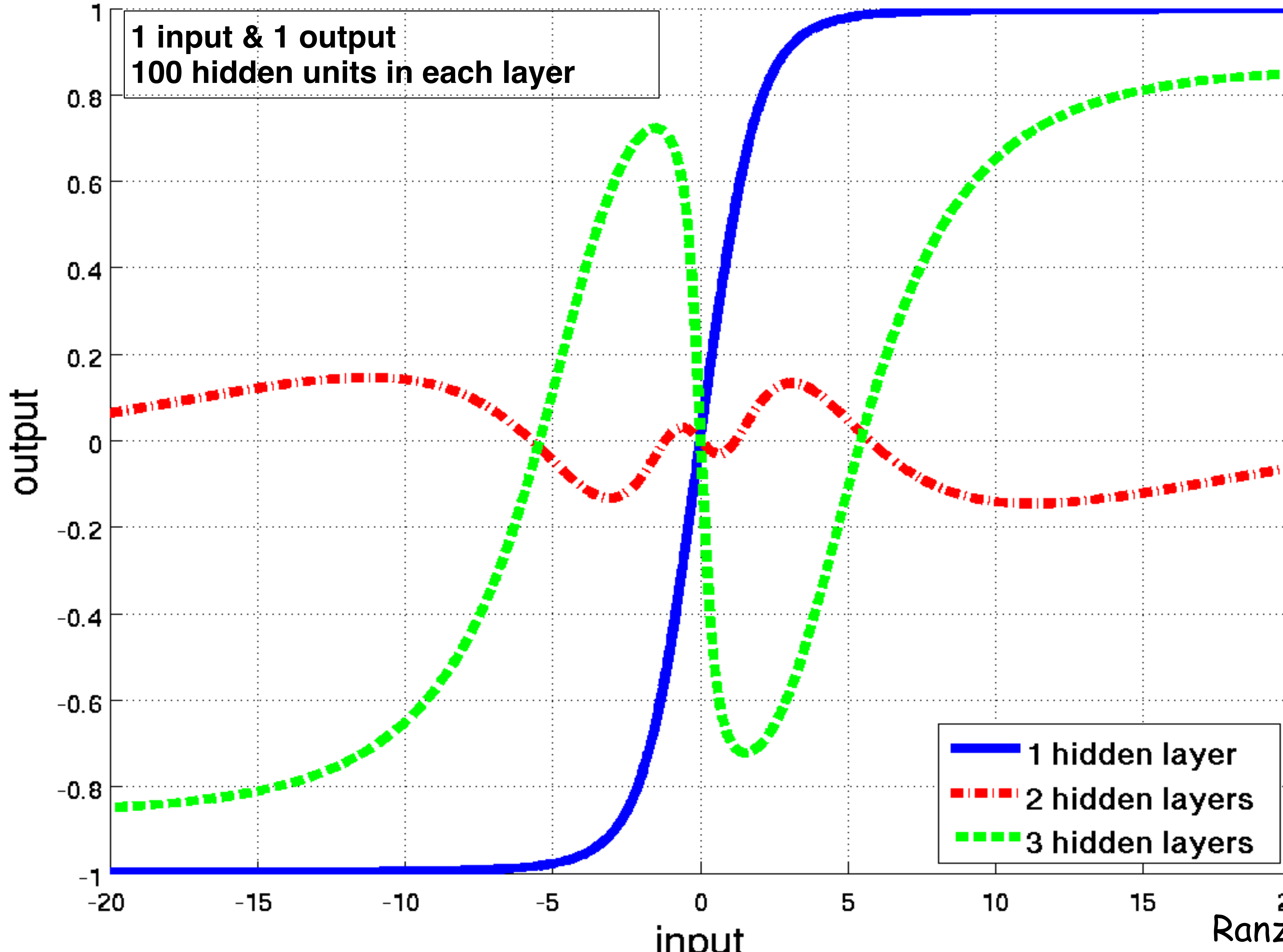


Architecture Selection for MLPs

How to pick number of layers and units/layer

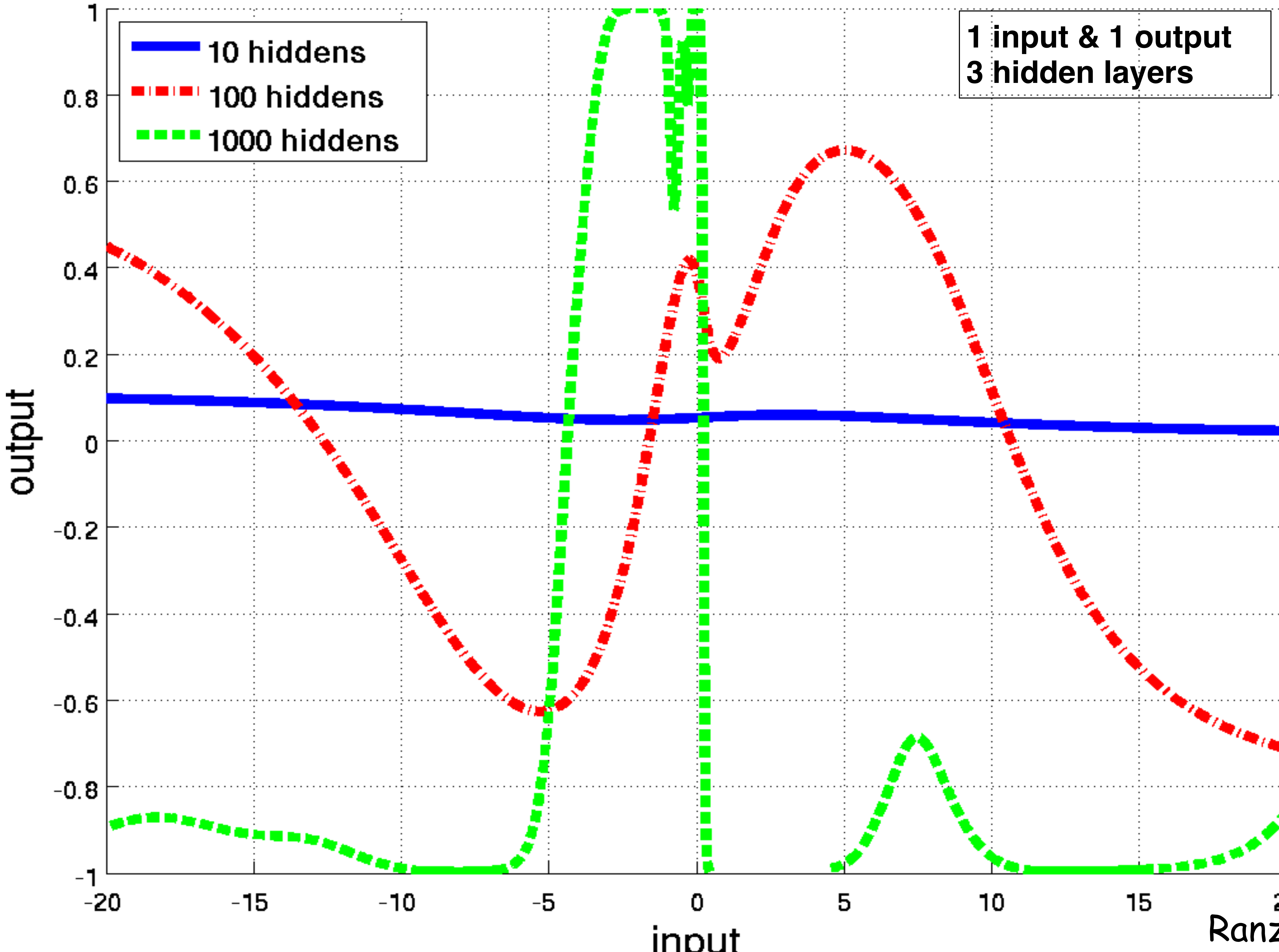
- No good answer:
  - Problem has now shifted from picking good features to picking good architectures.
  - (Non-answer) Pick using validation set.
  - Hyper-parameter optimization [e.g. Snoek 2012 `https://arxiv.org/pdf/1206.2944`].
  - Active area of research.
- For fully connected models, 2 or 3 layers seems the most that can be effectively trained (more later).
- Regarding number of units/layer:
  - Parameters grows with (units/layer)^2.
  - With large units/layer, can easily overfit.
  - For classificaion, helps to expand towards output.

TOY EXAMPLE: SYNTHETIC DATA



Ranzato

TOY EXAMPLE: SYNTHETIC DATA



Representational Power

What functions can you represent with an MLP?

- 1 layer? Linear decision surface.
- 2+ layers? In theory, can represent *any* function. Assuming non-trivial non-linearity.
  - Bengio 2009, `http://www.iro.umontreal.ca/~bengioy/papers/ftml.pdf`
  - Bengio, Courville, Goodfellow book `http://www.deeplearningbook.org/contents/mlp.html`
  - Simple proof by M. Neilsen `http://neuralnetworksanddeeplearning.com/chap4.html`
  - D. Mackay book `http://www.inference.phy.cam.ac.uk/mackay/itprnn/ps/482.491.pdf`
- But issue is efficiency: very wide two layers vs narrow deep model?
- In practice, more layers helps.
- But beyond 3, 4 layers no improvement for fully connected layers.

Training a model: Overview

How to set the parameters

- Given dataset $\{x, y\}$, pick appropriate cost function C.
- Forward-pass (f-prop) examples through the model to get predictions.
- Get error using cost function C to compare prediction to targets y.
- Use back-propagation (b-prop) to pass error back through model, adjusting parameters to minimize loss/energy E.
- Back-propagation is essentially chain rule of derivatives back through the model.
- Each layer is differentiable w.r.t. to parameters and input.
- Once gradients obtained, use Stochastic Gradient Descent (SGD) to update weights.

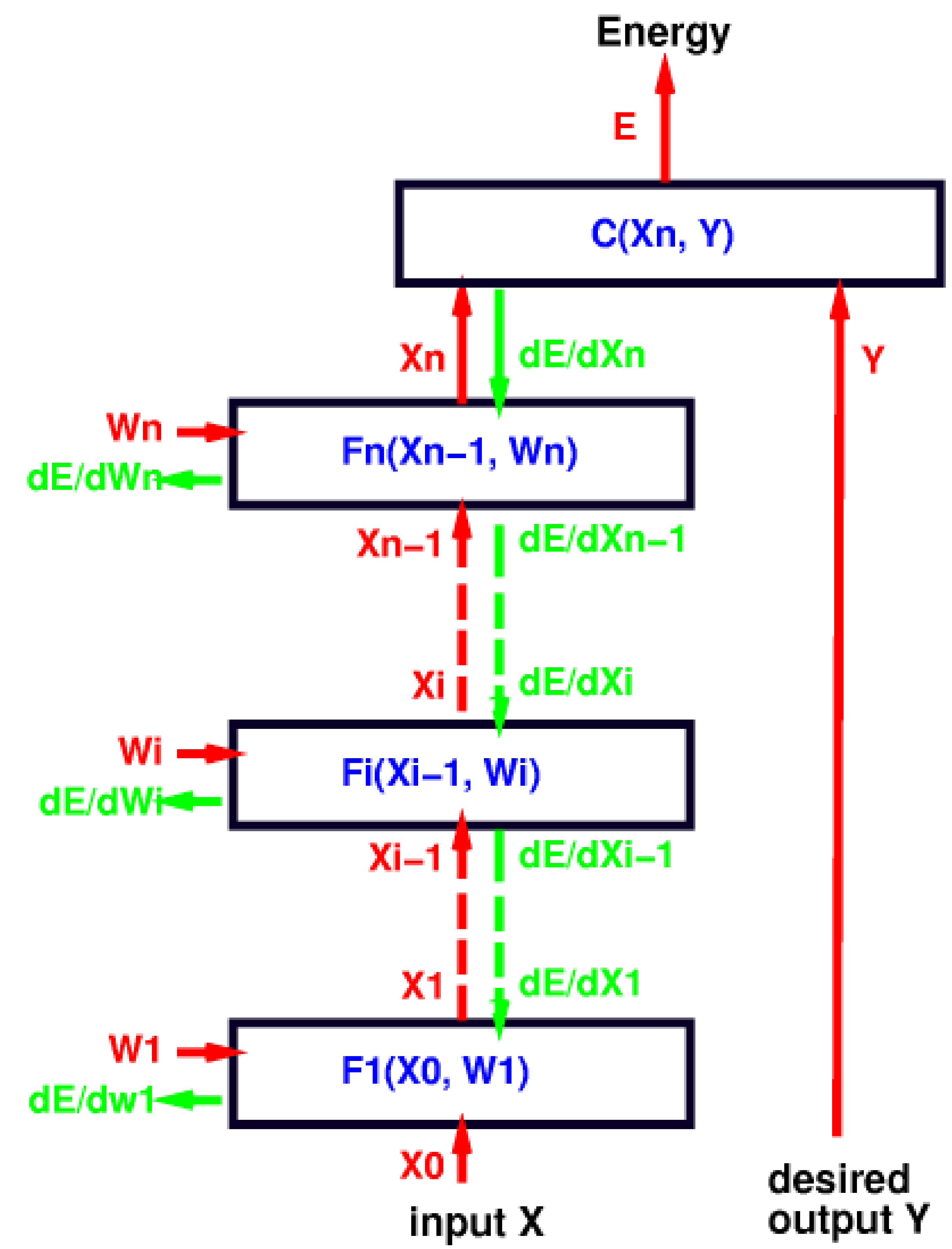
Stochastic Gradient Descent

- Want to minimize overall loss function E.
- Loss is sum of individual losses over each example.
- In gradient descent, we start with some initial set of parameters θ^0
- Update parameters: $\theta^{k+1} \leftarrow \theta^k + \eta \nabla \theta$.
- k is iteration index, η is learning rate (scalar; set semi-manually).
- Gradients $\nabla \theta = \frac{\partial E}{\partial \theta}$ computed by b-prop.
- In *Stochastic* gradient descent, compute gradient on sub-set (batch) of data.
- If batchsize=1 then θ is updated after each example.
- Gradient direction is noisy, relative to average over all examples (standard gradient descent).

Computing Gradients in a multi-stage architecture

Forward Pass

- Consider model with N layers. Layer i has *vector* of weights W_i.
- F-Prop (in red) takes input x and passes it through each layer F_i: $x_i = F_i(x_{i-1}, W_i)$
- Output of each layer x_i; prediction x_n is output of top layer.
- Cost function C compares x_n to y.
- Overall energy $E = \sum_{m=1}^{M} C(x_n^m, y^m)$, i.e sum over all examples of $C(x_n, y)$.

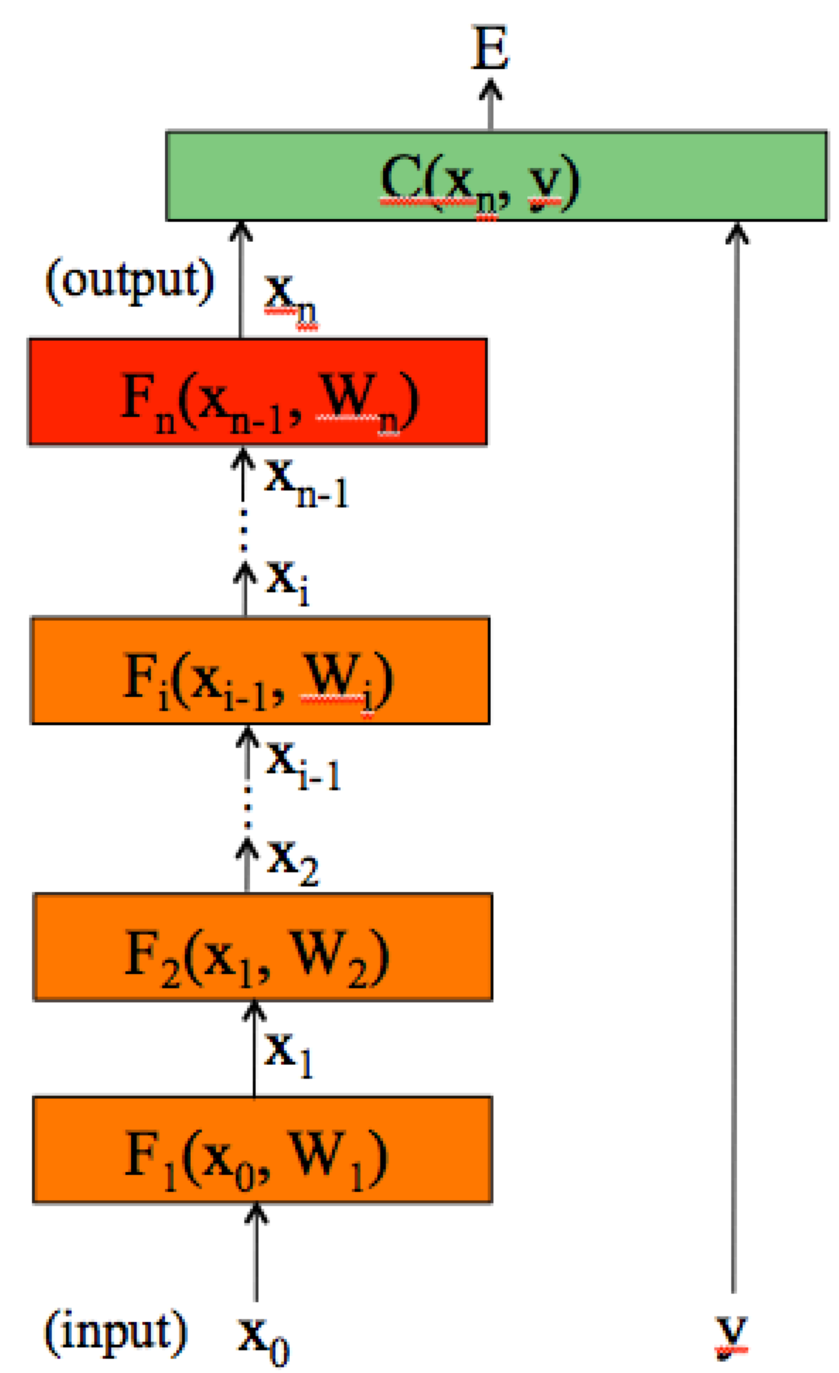


[Figure: Y. LeCun and M. Ranzato]

Computing gradients

To compute the gradients, we could start by wring the full energy E as a function of the network parameters.

$$E(\theta) = \sum_{m=1}^{M} C\left(F_n\left(F_{n-1}\left(F_2\left(F_1\left(x_0^m, w_1\right), w_2\right), w_{n-1}\right), w_n\right), y^m\right)$$



And then compute the partial derivatives… instead, we can use the chain rule to derive a compact algorithm: **back-propagation**

Matrix calculus

- x column vector of size [n×1]

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- We now define a function on vector x: y = F(x)
- If y is a scalar, then

$$\partial y / \partial x = \begin{bmatrix} \partial y / \partial x_1 & \partial y / \partial x_2 & \cdots & \partial y / \partial x_n \end{bmatrix}$$

The derivative of y is a row vector of size [1×n]

- If y is a vector [m×1], then (*Jacobian formulation*):

$$\partial y / \partial x = \begin{bmatrix} \partial y_1 / \partial x_1 & \partial y_1 / \partial x_2 & \cdots & \partial y_1 / \partial x_n \\ \vdots & \vdots & \cdots & \vdots \\ \partial y_m / \partial x_1 & \partial y_m / \partial x_2 & \cdots & \partial y_m / \partial x_n \end{bmatrix}$$

The derivative of y is a matrix of size [m×n]

(m rows and n columns)

Matrix calculus

- If y is a scalar and x is a matrix of size [n×m], then

$$\partial y / \partial X = \begin{bmatrix} \partial y / \partial x_{11} & \partial y / \partial x_{21} & \cdots & \partial y / \partial x_{n1} \\ \vdots & \vdots & \cdots & \vdots \\ \partial y / \partial x_{1m} & \partial y / \partial x_{12} & \cdots & \partial y / \partial x_{nm} \end{bmatrix}$$

$\cdots$

The output is a matrix of size [m×n]

Matrix calculus

- Chain rule:

For the function: z = h(x) = f (g(x))

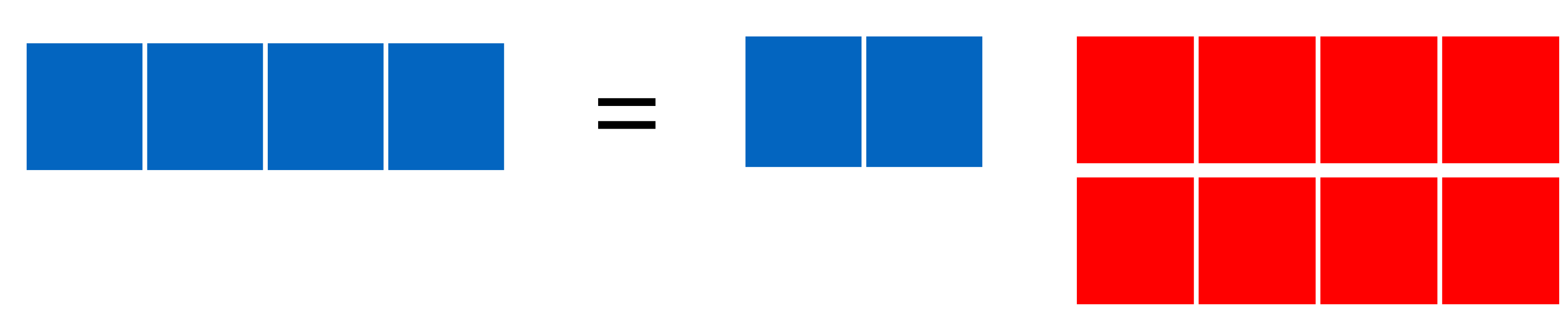
Its derivative is: h'(x) = f' (g(x)) g'(x)

and writing z=f(u), and u=g(x):

$$\underbrace{\left.\frac{dz}{dx}\right|_{x=a}}_{[m\times n]} = \underbrace{\left.\frac{dz}{du}\right|_{u=g(a)}}_{[m\times p]} \cdot \underbrace{\left.\frac{du}{dx}\right|_{x=a}}_{[p\times n]}$$

with p = length vector u = |u|, m = |z|, and n = |x|

Example, if |z|=1, |u| = 2, |x|=4

h'(x) = 

Matrix calculus

- Chain rule:

For the function: $h(x) = f_n(f_{n-1}(\ldots(f_1(x))\ ))$

With $u_1 = f_1(x)$
$u_i = f_i(u_{i-1})$
$z = u_n = f_n(u_{n-1})$

The derivative becomes a product of matrices:

$$\left.\frac{dz}{dx}\right|_{x=a} = \left.\frac{dz}{du_{n-1}}\right|_{u_{n-1}=f_{n-1}(u_{n-2})} \cdot \left.\frac{du_{n-1}}{du_{n-2}}\right|_{u_{n-2}=f_{n-2}(u_{n-3})} \cdot \ldots \cdot \left.\frac{du_2}{du_1}\right|_{u_1=f_1(a)} \cdot \left.\frac{du_1}{dx}\right|_{x=a}$$

(exercise: check that all the matrix dimensions work fine)

Computing gradients

The energy E is the sum of the costs associated to each training example x^m, y^m

$$E(\theta) = \sum_{m=1}^{M} C\left(x_n^m, y^m; \theta\right)$$

Its gradient with respect to the networks parameters is:

$$\frac{\partial E}{\partial \theta_i} = \sum_{m=1}^{M} \frac{C\left(x_n^m, y^m; \theta\right)}{\partial \theta_i}$$

is how much E varies when the parameter θ_i is varied.

Computing gradients

We could write the cost function to get the gradients:

$$C(x_n, y; \theta) = C(F_n(x_{n-1}, w_n), y)$$

with $\theta = [w_1, w_2, \cdots, w_n]$

If we compute the gradient with respect to the parameters of the last layer (output layer) w_n, using the chain rule:

$$\frac{\partial C}{\partial w_n} = \frac{\partial C}{\partial x_n} \cdot \frac{\partial x_n}{\partial w_n} = \frac{\partial C}{\partial x_n} \cdot \frac{\partial F_n(x_{n-1}, w_n)}{\partial w_n}$$

(how much the cost changes when we change w_n: is the product between how much the cost changes when we change the output of the last layer and how much the output changes when we change the layer parameters.)

Computing gradients: cost layer

If we compute the gradient with respect to the parameters of the last layer (output layer) w_n, using the chain rule:

$$\frac{\partial C}{\partial w_n} = \frac{\partial C}{\partial x_n} \cdot \frac{\partial x_n}{\partial w_n} = \frac{\partial C}{\partial x_n} \cdot \frac{\partial F_n\left(x_{n-1}, w_n\right)}{\partial w_n}$$

Will depend on the layer structure and non-linearity.

For example, for an Euclidean loss:

$$C(x_n, y) = \frac{1}{2}\left\| x_n - y \right\|^2$$

The gradient is:

$$\frac{\partial C}{\partial x_n} = x_n - y$$

Computing gradients: layer i

We could write the full cost function to get the gradients:

$$C(x_n, y; \theta) = C\Big(F_n\Big(F_{n-1}\Big(F_2\big(F_1(x_0, w_1), w_2\big), w_{n-1}\Big), w_n\Big), y\Big)$$

If we compute the gradient with respect to w_i, using the chain rule:

$$\frac{\partial C}{\partial w_i} = \underbrace{\frac{\partial C}{\partial x_n} \cdot \frac{\partial x_n}{\partial x_{n-1}} \cdot \frac{\partial x_{n-1}}{\partial x_{n-2}} \cdot \ \cdots \ \frac{\partial x_{i+1}}{\partial x_i}}_{\frac{\partial C}{\partial x_i}} \cdot \frac{\partial x_i}{\partial w_i}$$

And this can be computed iteratively!

$$\frac{\partial F_i(x_{i-1}, w_i)}{\partial w_i}$$

This is easy.

Backpropagation

$$\frac{\partial C}{\partial w_i} = \underbrace{\frac{\partial C}{\partial x_n} \cdot \frac{\partial x_n}{\partial x_{n-1}} \cdot \frac{\partial x_{n-1}}{\partial x_{n-2}} \cdot \ldots \cdot \frac{\partial x_{i+1}}{\partial x_i}}_{\frac{\partial C}{\partial x_i}} \cdot \frac{\partial x_i}{\partial w_i}$$

$$\frac{\partial F_i(x_{i-1}, w_i)}{\partial w_i}$$

If we have the value of $\frac{\partial C}{\partial x_i}$ we can compute the gradient at the layer bellow as:

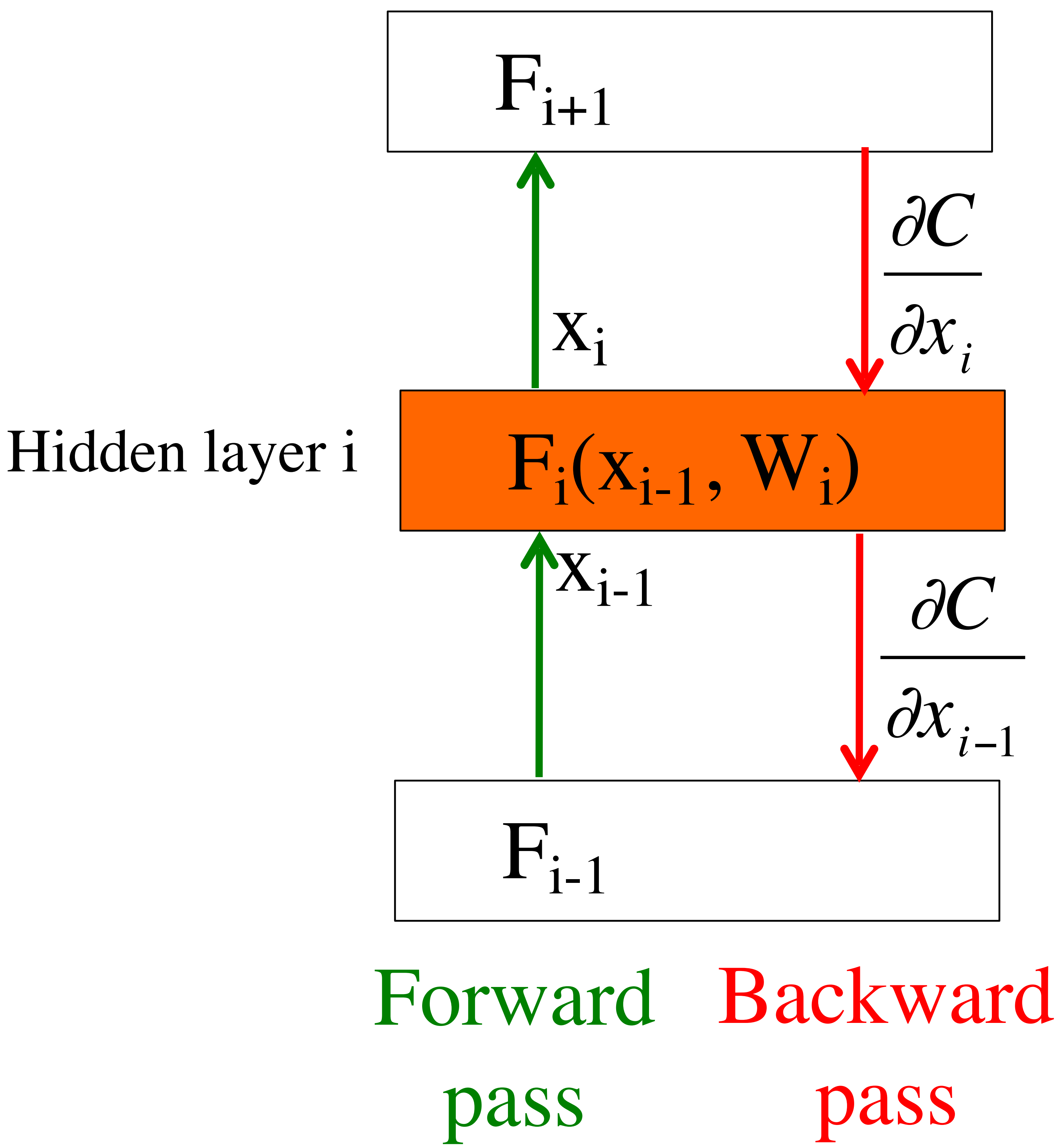
$$\frac{\partial C}{\partial x_{i-1}} = \frac{\partial C}{\partial x_i} \cdot \frac{\partial x_i}{\partial x_{i-1}}$$

Gradient layer i-1

Gradient layer i

$$\frac{\partial F_i(x_{i-1}, w_i)}{\partial x_{i-1}}$$

Backpropagation: layer i



- Layer i has two inputs (during training)

$$x_{i-1} \qquad \frac{\partial C}{\partial x_i}$$

- For layer i, we need the derivatives:

$$\frac{\partial F_i(x_{i-1}, w_i)}{\partial x_{i-1}} \qquad \frac{\partial F_i(x_{i-1}, w_i)}{\partial w_i}$$

- We compute the outputs

$$x_i = F_i(x_{i-1}, w_i)$$

$$\frac{\partial C}{\partial x_{i-1}} = \frac{\partial C}{\partial x_i} \cdot \frac{\partial F_i(x_{i-1}, w_i)}{\partial x_{i-1}}$$

- The weight update equation is:

$$\frac{\partial C}{\partial w_i} = \frac{\partial C}{\partial x_i} \cdot \frac{\partial F_i(x_{i-1}, w_i)}{\partial w_i}$$

$$w_i^{k+1} \leftarrow w_i^k + \eta_t \frac{\partial E}{\partial w_i}$$

(sum over all training examples to get E)

Backpropagation: summary

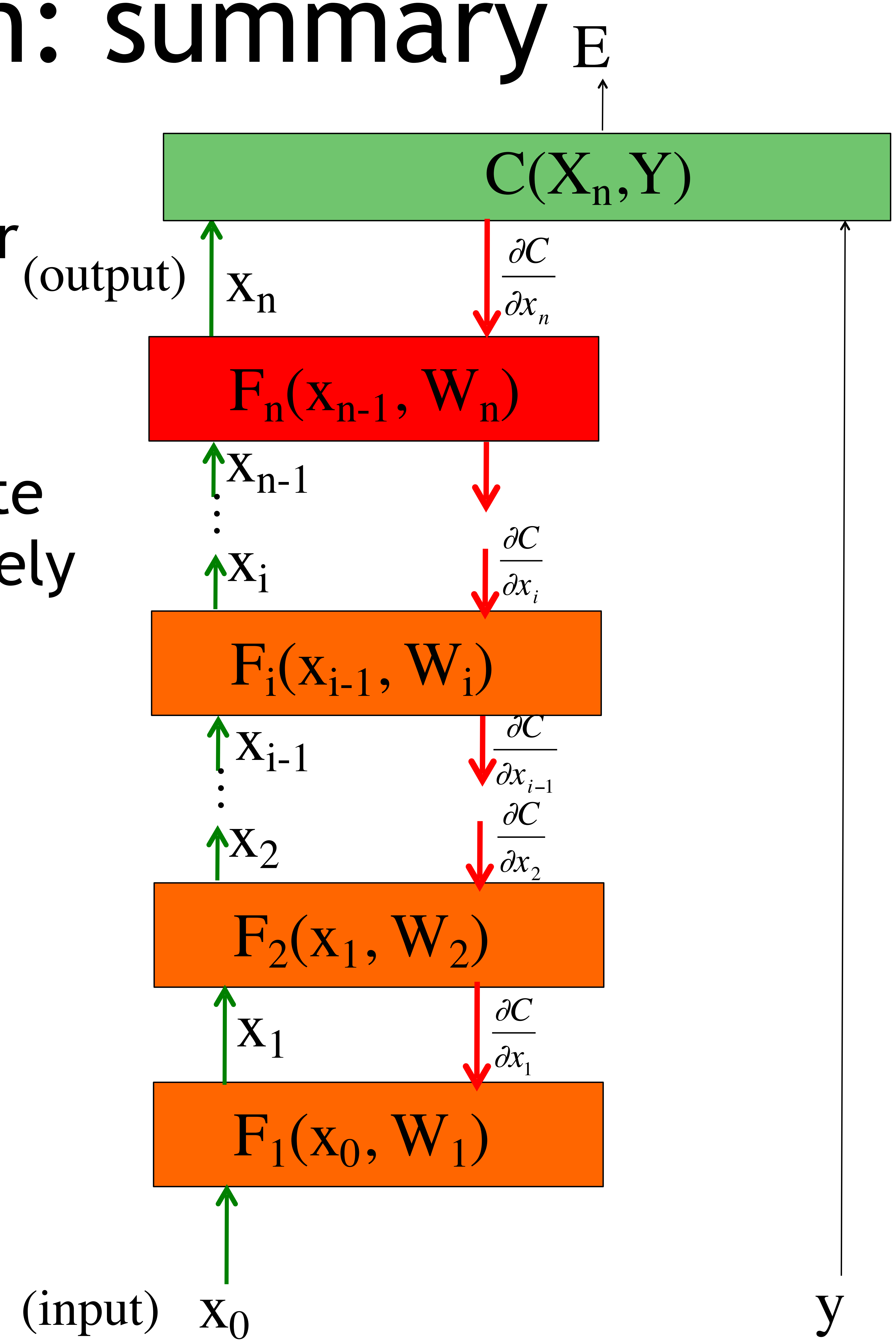
- Forward pass: for each training example. Compute the outputs for all layers

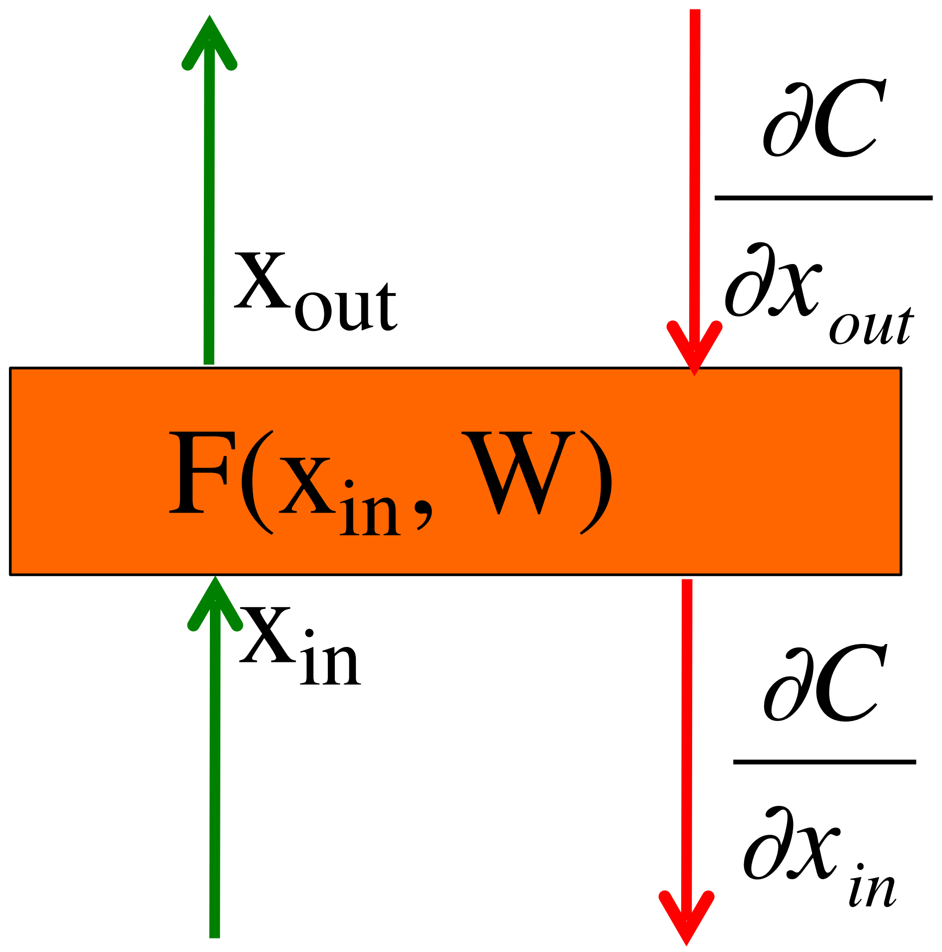
$$x_i = F_i(x_{i-1}, w_i)$$

- Backwards pass: compute cost derivatives iteratively from top to bottom:

$$\frac{\partial C}{\partial x_{i-1}} = \frac{\partial C}{\partial x_i} \cdot \frac{\partial F_i(x_{i-1}, w_i)}{\partial x_{i-1}}$$

- Compute gradients and update weights.





Linear Module

- Forward propagation: $x_{out} = F(x_{in}, W) = W x_{in}$

With W being a matrix of size $|x_{out}| \times |x_{in}|$

- Backprop to input:

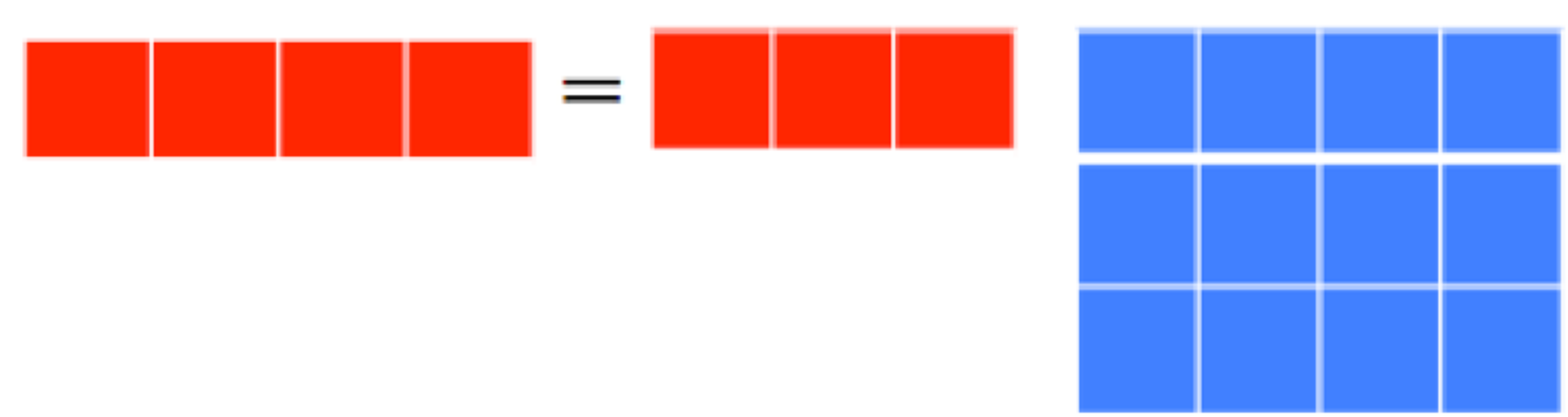
$$\frac{\partial C}{\partial x_{in}} = \frac{\partial C}{\partial x_{out}} \cdot \frac{\partial F(x_{in}, W)}{\partial x_{in}} = \frac{\partial C}{\partial x_{out}} \cdot \frac{\partial x_{out}}{\partial x_{in}}$$

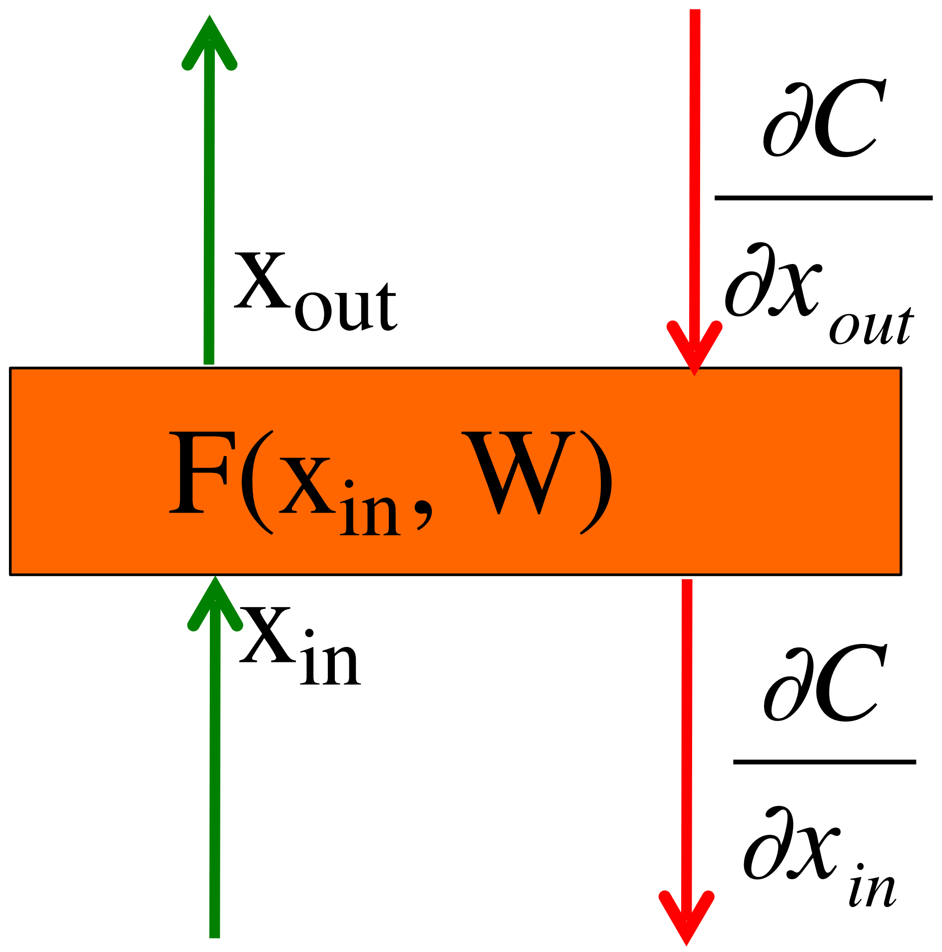
If we look at the j component of output x_{out}, with respect to the i component of the input, x_{in}:

$$\frac{\partial x_{out_i}}{\partial x_{in_j}} = W_{ij} \longrightarrow \frac{\partial F(x_{in}, W)}{\partial x_{in}} = W$$

Therefore:

$$\boxed{\frac{\partial C}{\partial x_{in}} = \frac{\partial C}{\partial x_{out}} \cdot W}$$





Linear Module

- Forward propagation: $x_{out} = F(x_{in}, W) = W x_{in}$
- Backprop to weights:

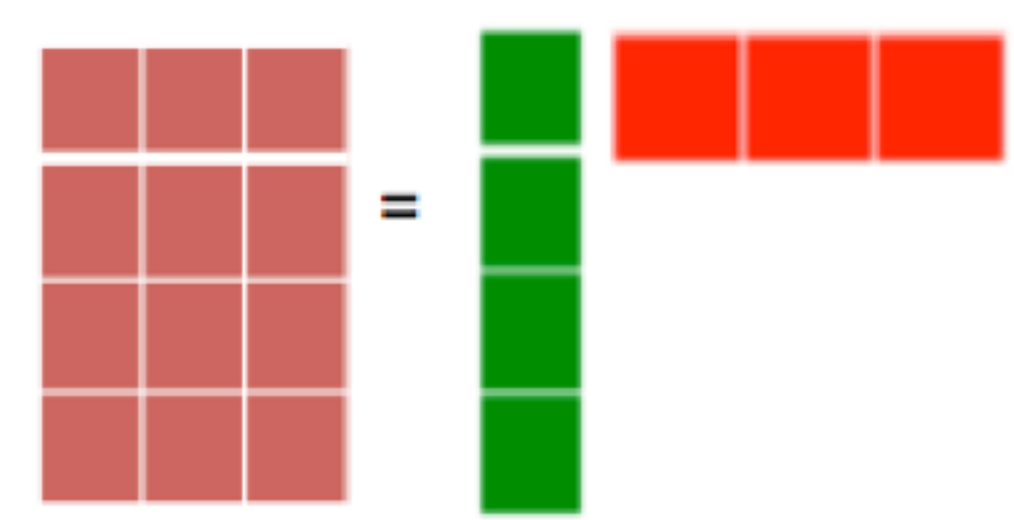
$$\frac{\partial C}{\partial W} = \frac{\partial C}{\partial x_{out}} \cdot \frac{\partial F(x_{in}, W)}{\partial W} = \frac{\partial C}{\partial x_{out}} \cdot \frac{\partial x_{out}}{\partial W}$$

If we look at how the parameter W_{ij} changes the cost, only the i component of the output
will change, therefore:

$$\frac{\partial C}{\partial W_{ij}} = \frac{\partial C}{\partial x_{out_i}} \cdot \frac{x_{out_i}}{\partial W_{ij}} = \frac{\partial C}{\partial x_{out_i}} \cdot x_{in_j}$$

$$\frac{\partial x_{out_i}}{\partial W_{ij}} = x_{in_j}$$

$$\boxed{\frac{\partial C}{\partial W} = x_{in} \cdot \frac{\partial C}{\partial x_{out}}}$$

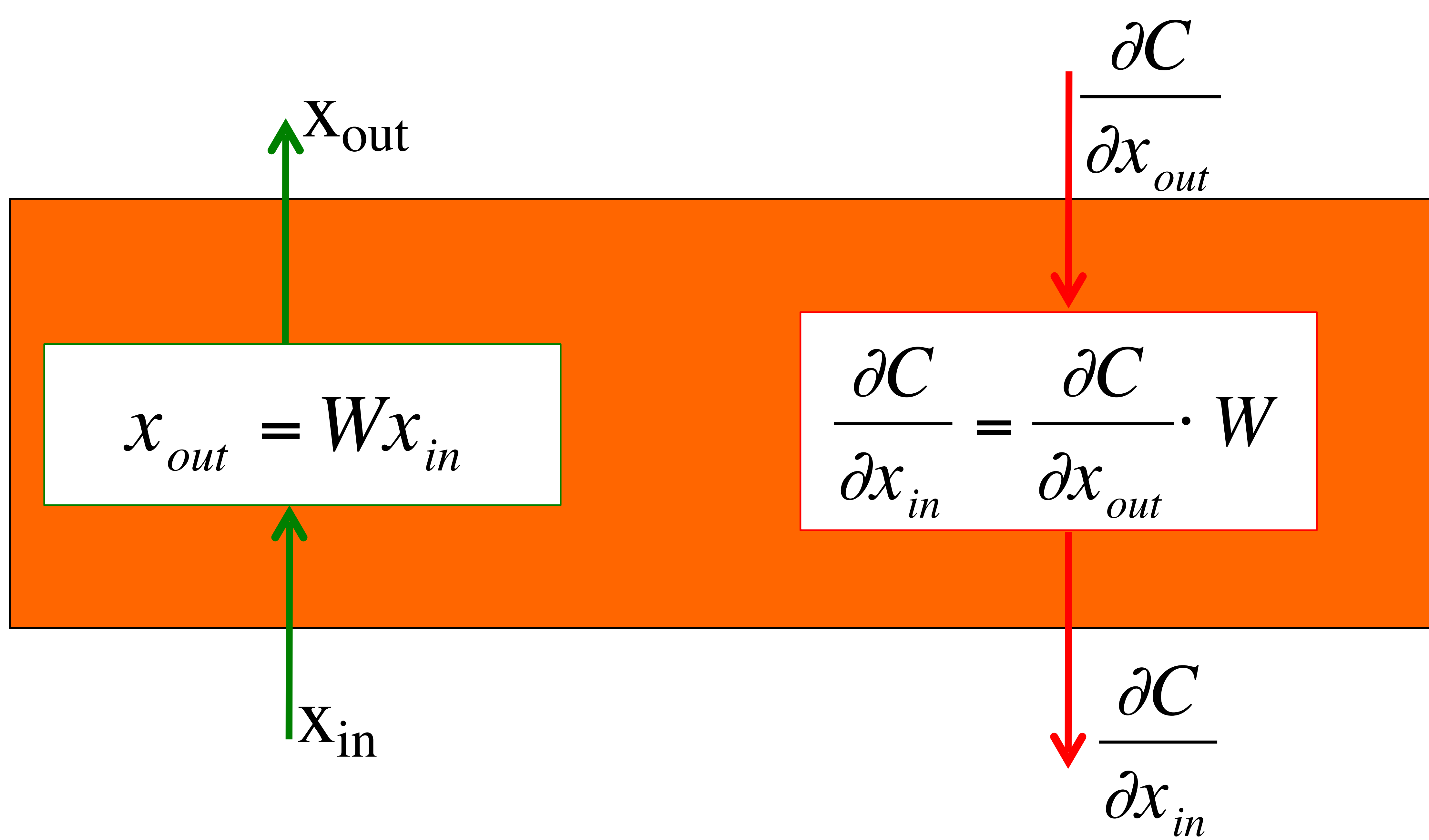


And now we can update the weights (by summing over all the training examples):

$$W_{ij}^{k+1} \leftarrow W_{ij}^{k} + \eta_t \frac{\partial E}{\partial W_{ij}}$$

(sum over all training examples to get E)

Linear Module

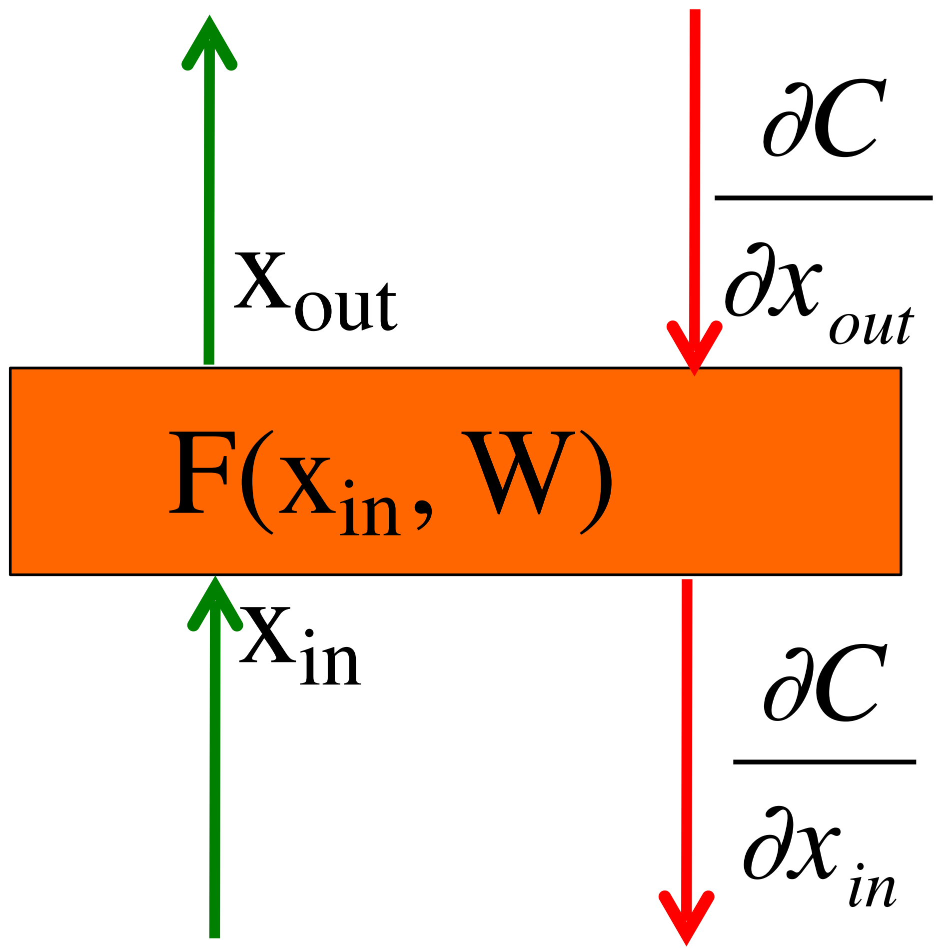


$$\boxed{\frac{\partial C}{\partial W} = x_{in} \cdot \frac{\partial C}{\partial x_{out}}}$$

Weight updates

$$W^{k+1} \leftarrow W^{k} + \eta_t \left(\frac{\partial E}{\partial W} \right)^T$$

Pointwise function



- Forward propagation:

$$x_{out_i} = h(x_{in_i} + b_i)$$

h = an arbitrary function, b_i is a bias term.

- Backprop to input: $\frac{\partial C}{\partial x_{in_i}} = \frac{\partial C}{\partial x_{out_i}} \cdot \frac{\partial x_{out_i}}{\partial x_{in_i}} = \frac{\partial C}{\partial x_{out_i}} \cdot h'(x_{in_i} + b_i)$

- Backprop to bias: $\frac{\partial C}{\partial b_i} = \frac{\partial C}{\partial x_{out_i}} \cdot \frac{\partial x_{out_i}}{\partial b_i} = \frac{\partial C}{\partial x_{out_i}} \cdot h'(x_{in_i} + b_i)$

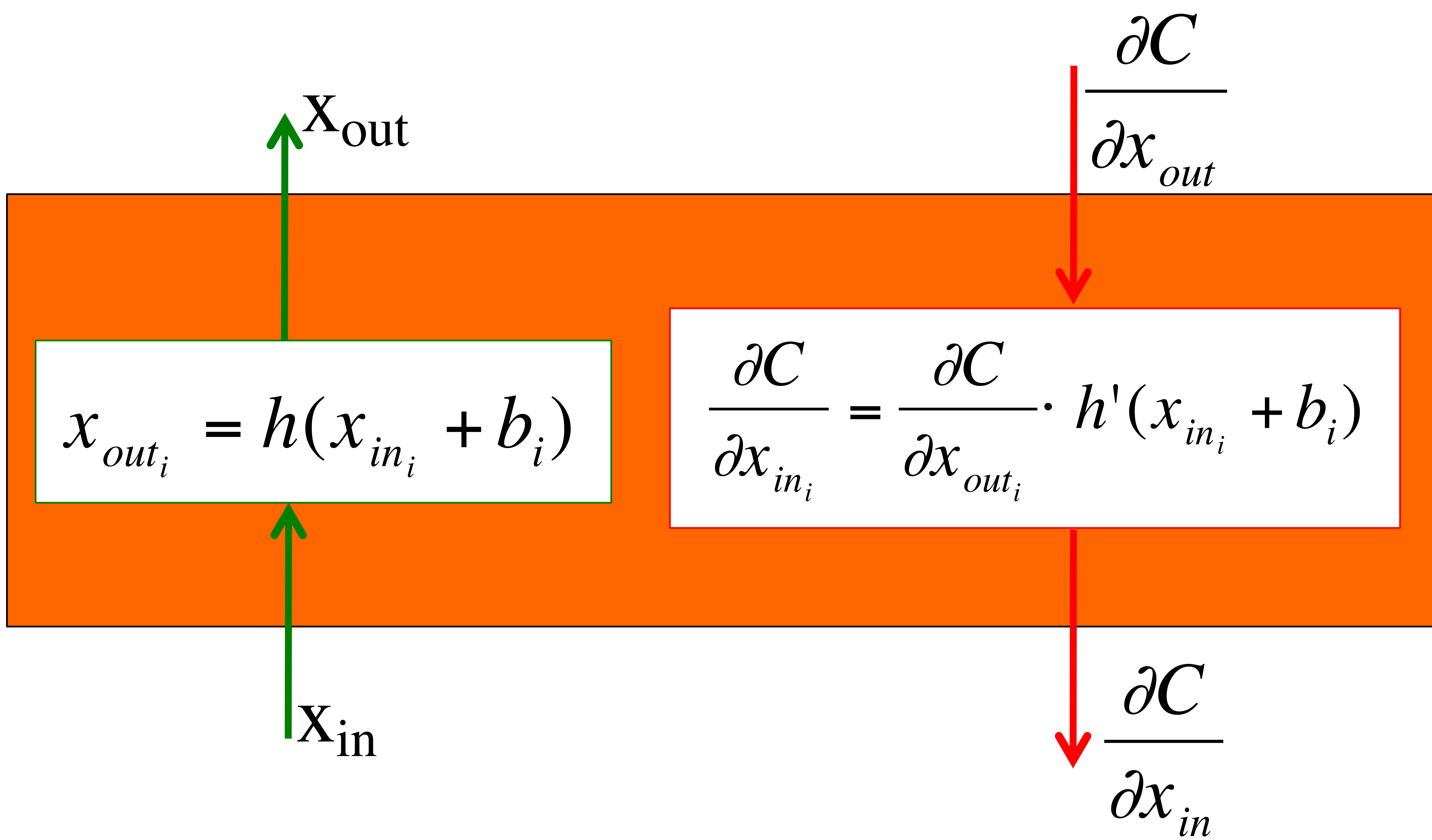
We use this last expression to update the bias.

Some useful derivatives:

For hyperbolic tangent: $\tanh'(x) = 1 - \tanh^2(x)$

For ReLU: h(x) = max(0,x) h'(x) = 1 [x>0]

Pointwise function

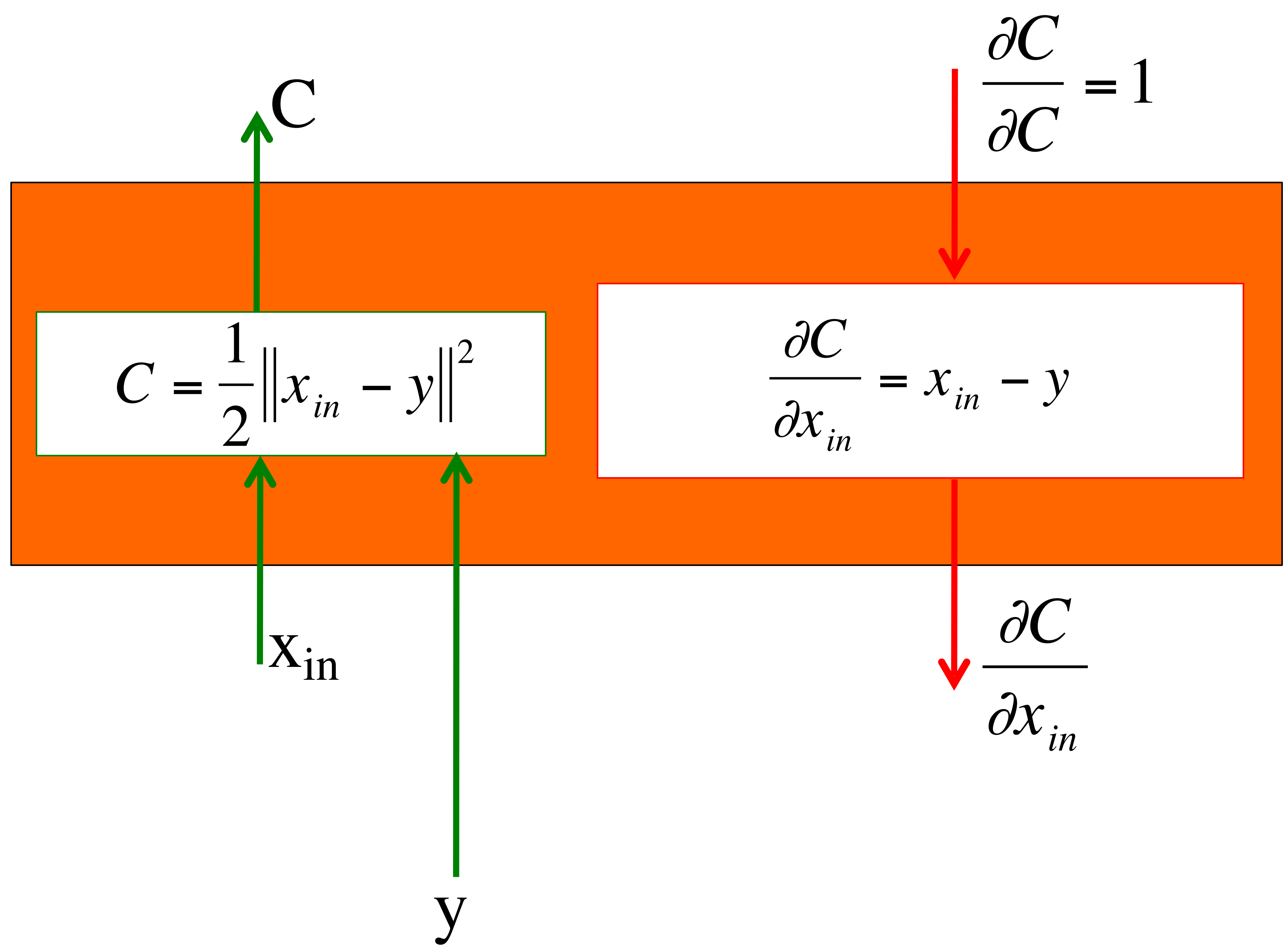


$$\frac{\partial C}{\partial b_i} = \frac{\partial C}{\partial x_{out_i}} \cdot h'(x_{in_i} + b_i)$$

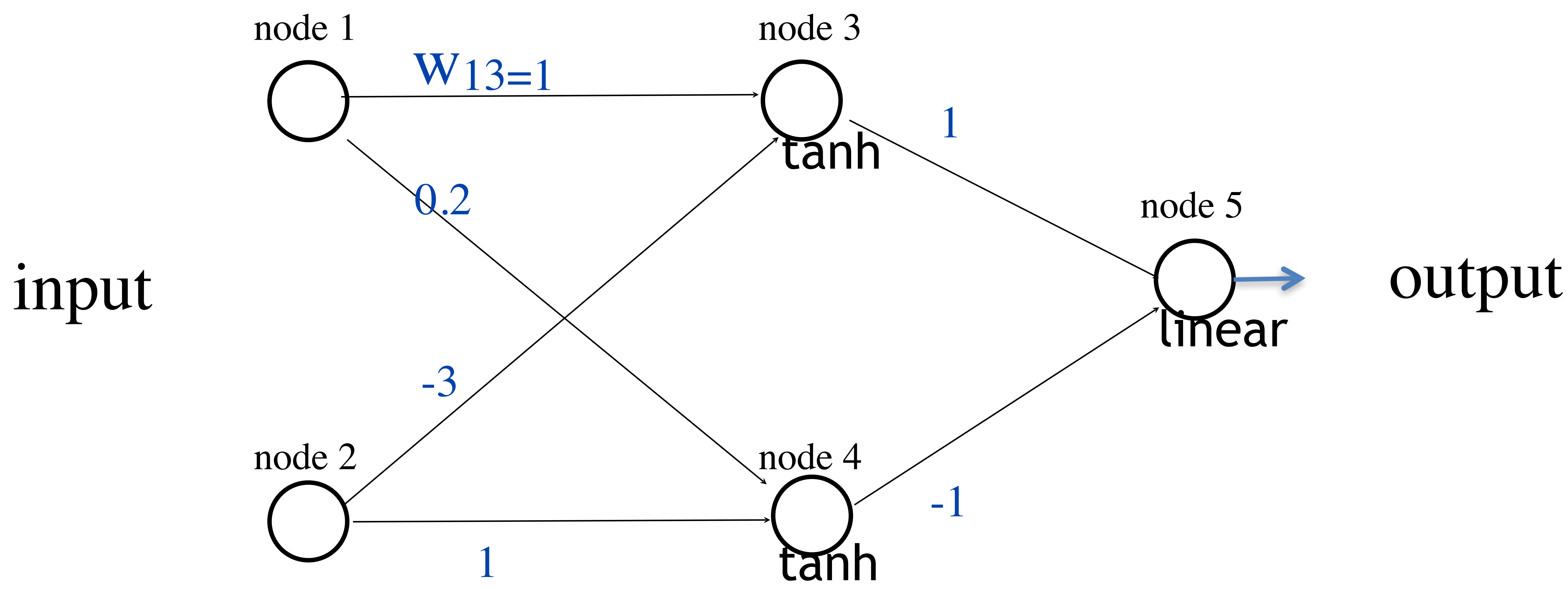
Weight updates

$$b_i^{k+1} \leftarrow b_i^k + \eta_t \frac{\partial E}{\partial b_i}$$

Euclidean cost module



Back propagation example



Learning rate = -0.2 (because we used positive increments)

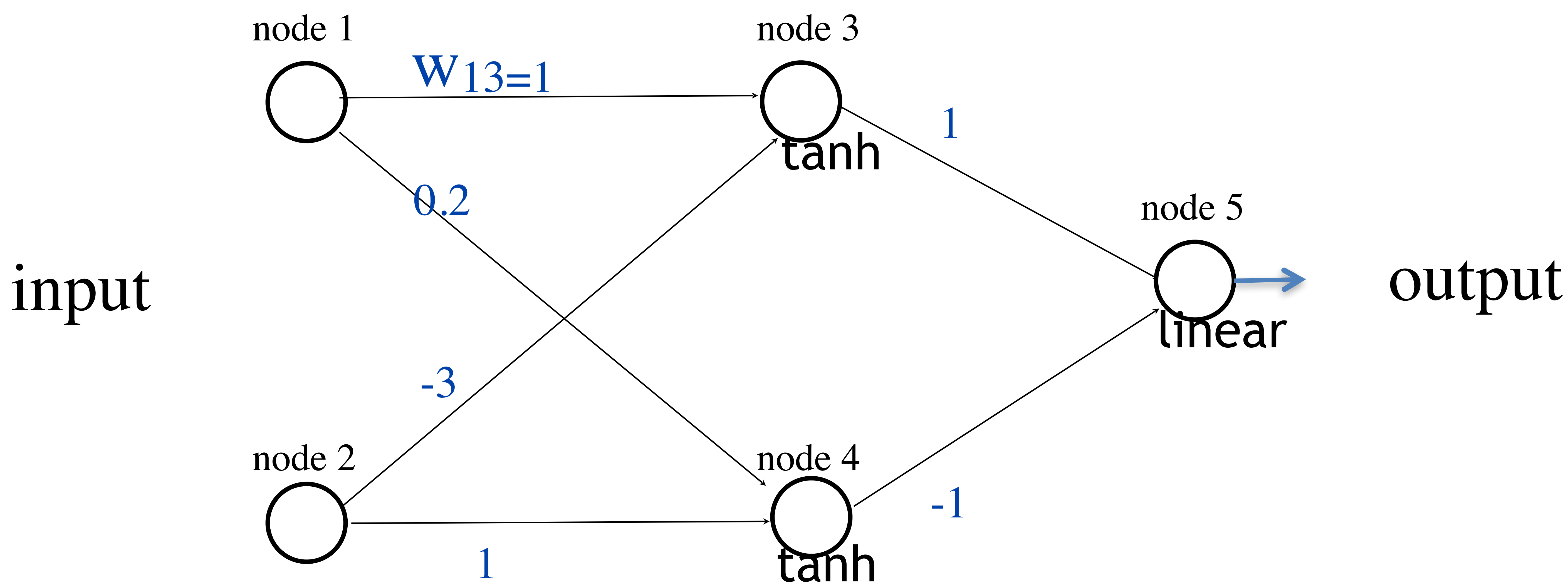
Euclidean loss

Training data:

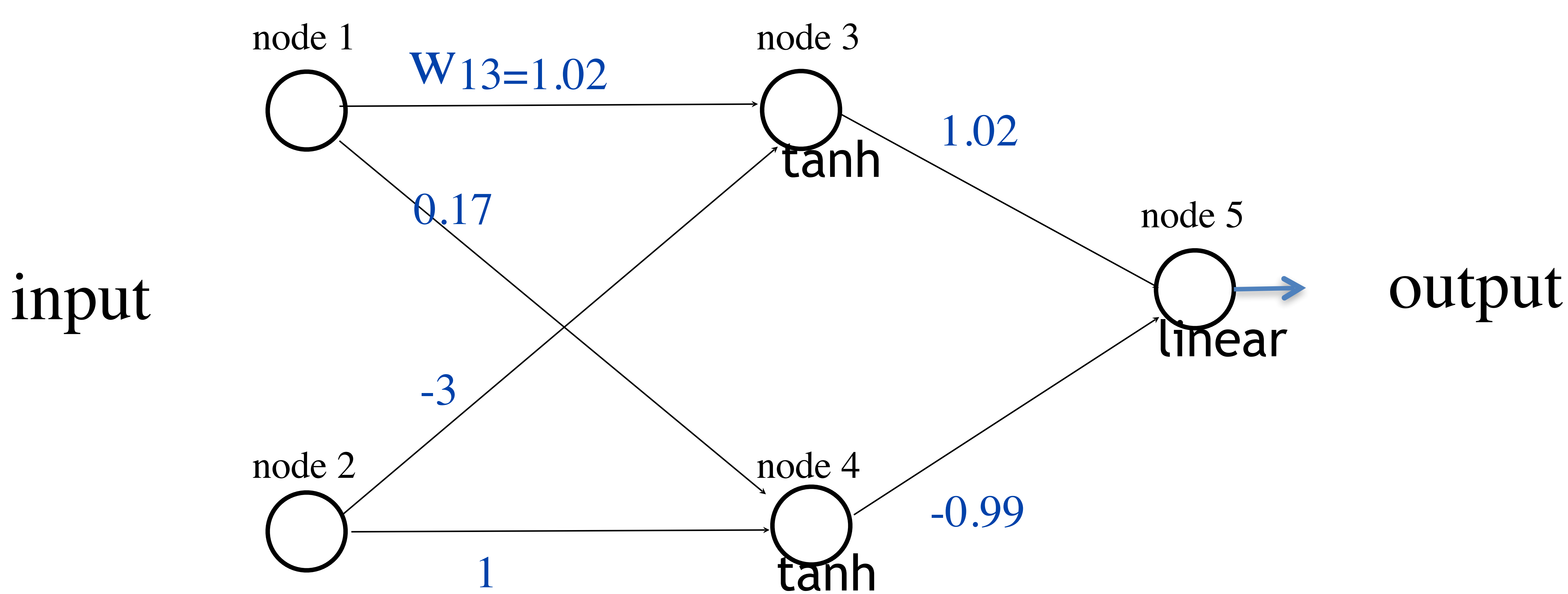
	input		desired output
	node 1	node 2	node 5
	1.0	0.1	0.5

Exercise: run one iteration of back propagation

Back propagation example



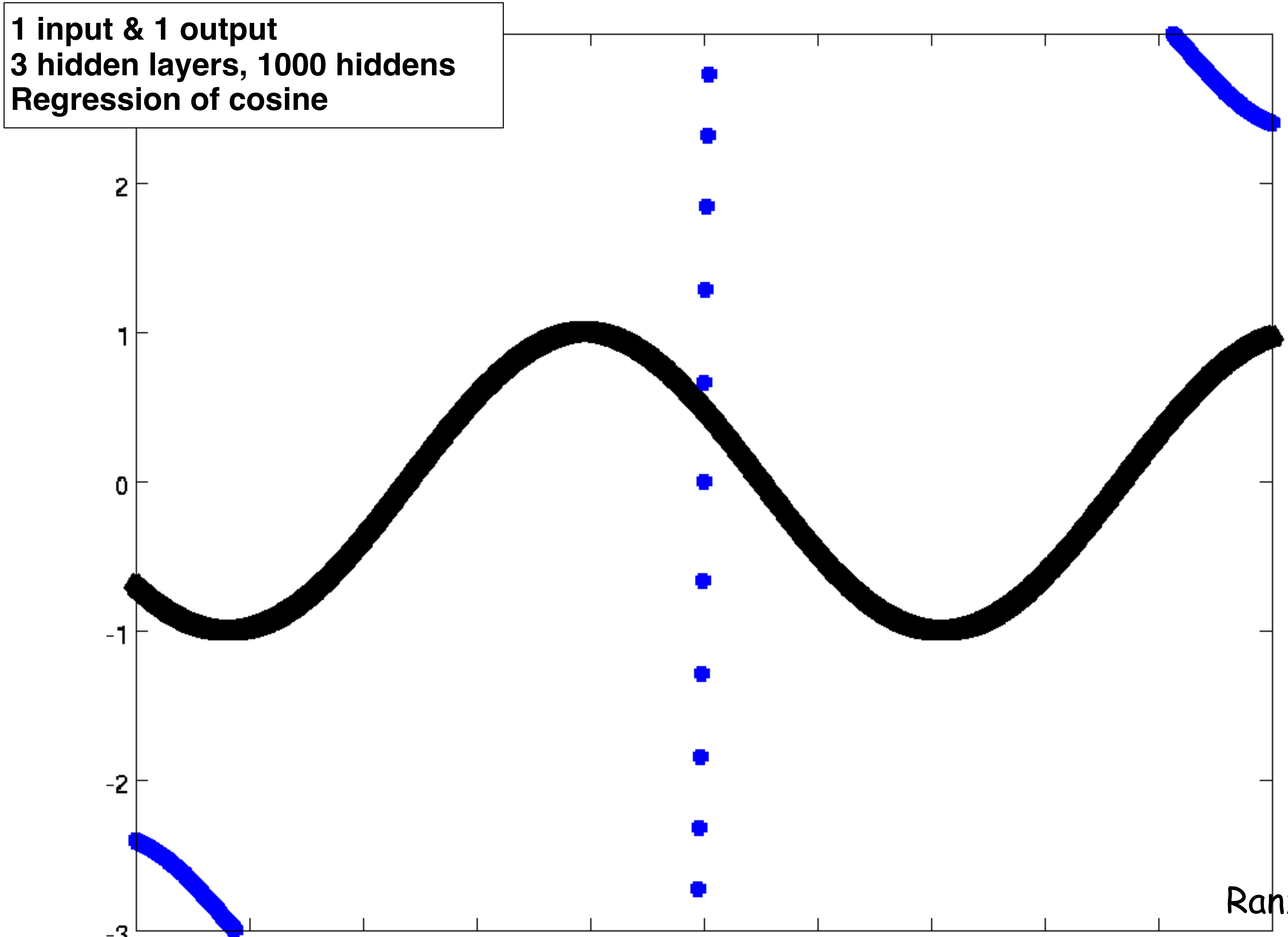
After one iteration (rounding to two digits):



Toy Code: Neural Net Trainer in MATLAB

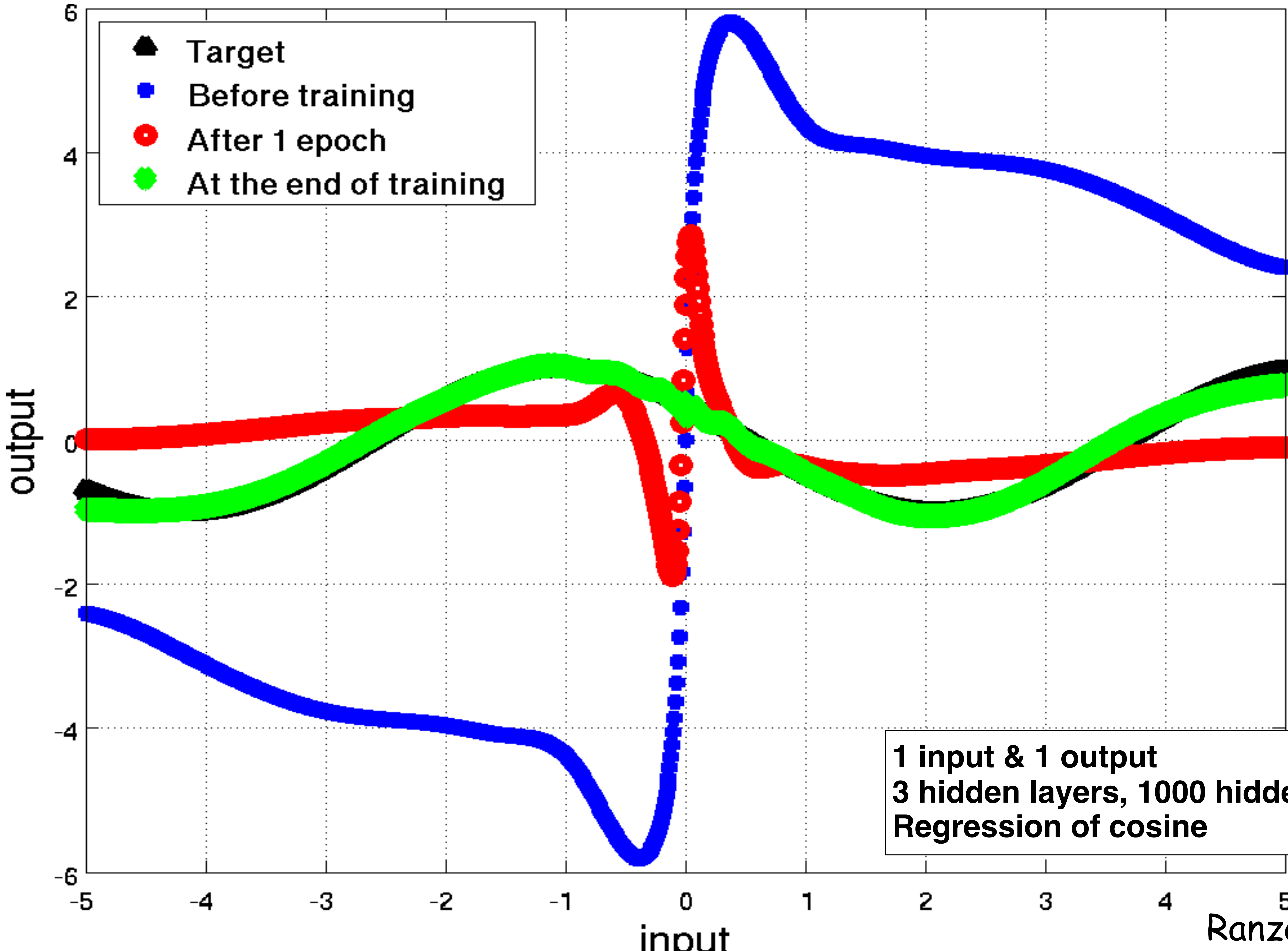
```
% F-PROP
for i = 1 : nr_layers - 1
  [h{i}  jac{i}]  =  logistic(W{i} * h{i-1} +  b{i});
end
h{nr_layers-1}  =  W{nr_layers-1} * h{nr_layers-2}  +   b{nr_layers-1};
prediction  =  softmax(h{l-1});

% CROSS ENTROPY LOSS
loss  =  -  sum(sum(log(prediction)  .*  target));

% B-PROP
dh{l-1}  =  prediction  -  target;
for i = nr_layers – 1 : -1 : 1
  Wgrad{i}  =  dh{i} * h{i-1}';
  bgrad{i}  =  sum(dh{i}, 2);
  dh{i-1}  =  (W{i}' * dh{i})  .*  jac{i-1};
end

% UPDATE
for i = 1 : nr_layers - 1
  W{i}  =  W{i}  –  (lr / batch_size)  *  Wgrad{i};
  b{i}  =  b{i}  –  (lr / batch_size)  *  bgrad{i};
end
```

TOY EXAMPLE: SYNTHETIC DATA



Ranzato

TOY EXAMPLE: SYNTHETIC DATA

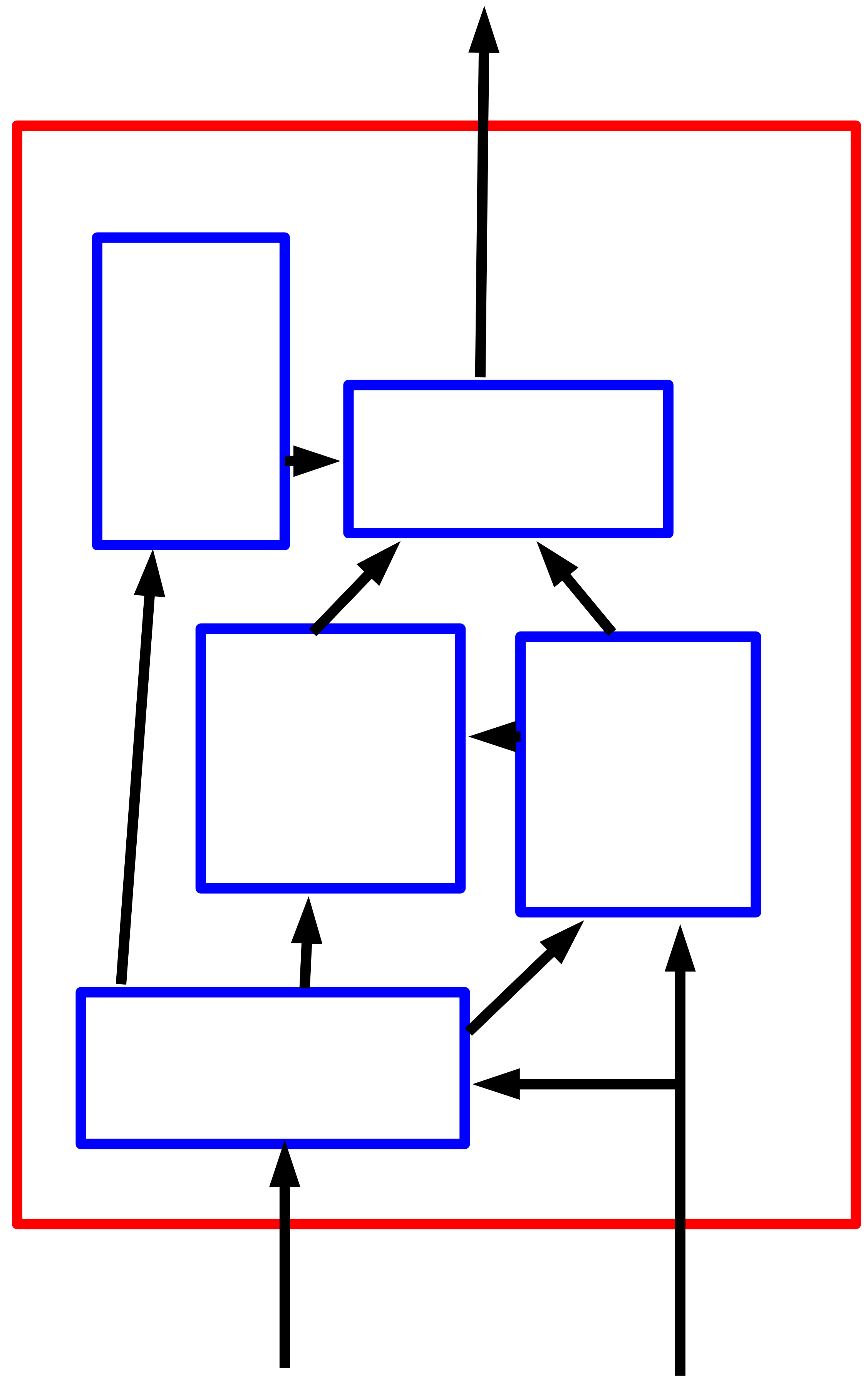


1 input & 1 output
3 hidden layers, 1000 hiddens
Regression of cosine

Ranzato

Alternate Topologies

- Models with complex graph structures can be trained by backprop.
- Each node in the graph must be differentiable w.r.t. parameters and inputs.
- If no cycles exist, then b-prop takes a single pass.
- If cycles exist, we have a *recurrent network* which will be discussed in subsequent lectures.

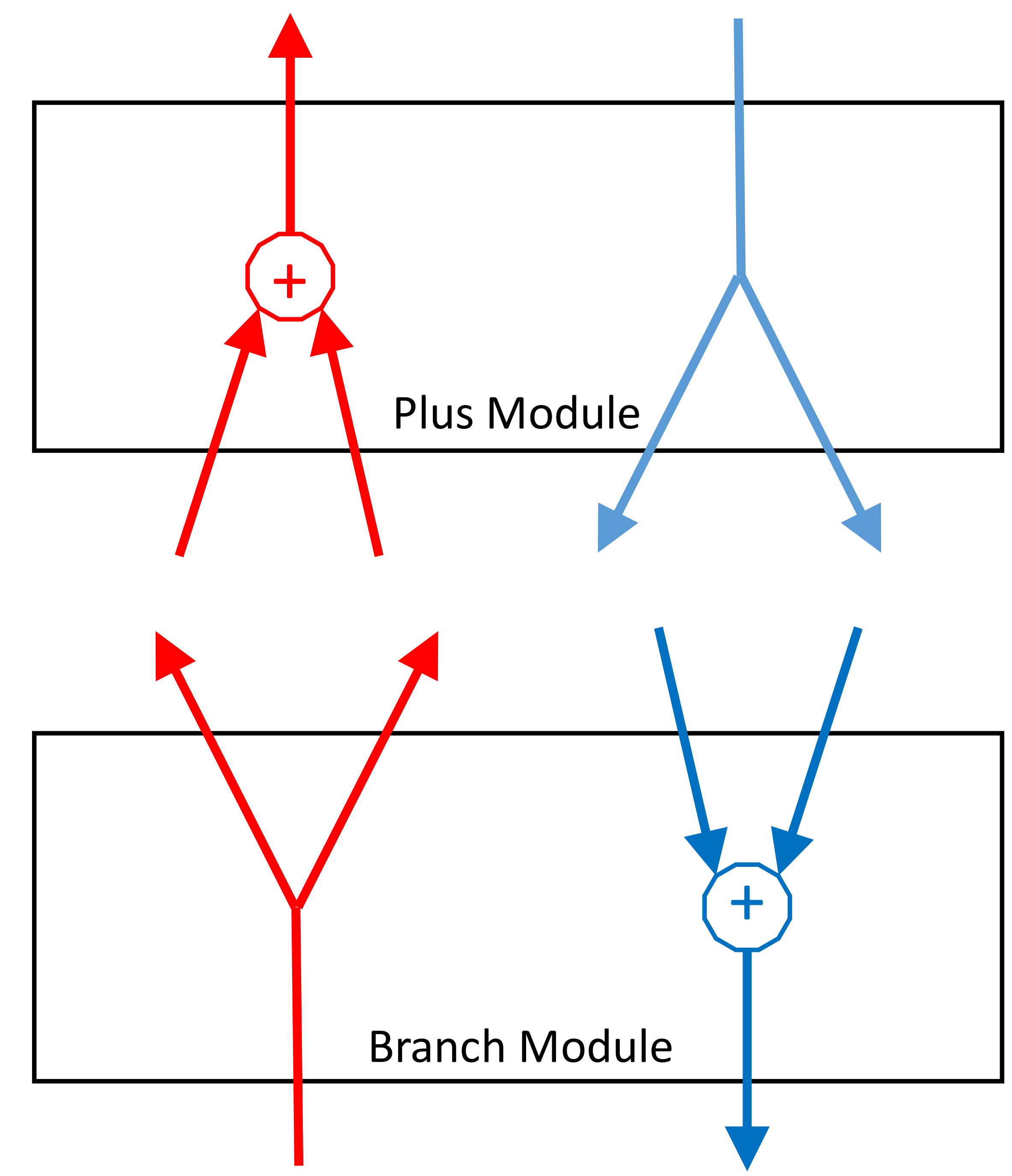


[Figure: Y. LeCun and M. Ranzato]

Branch / Plus Module

- Plus module has K inputs $x_1, \ldots, x_K$. Output is sum of inputs: $x_{out} = \sum_{k=1}^{K} x_k$
- Plus B-prop: $\frac{\partial E}{\partial x_k} = \frac{\partial E}{\partial x_{out}} \forall k$

- Branch module has a single input, but K outputs $x_1, \ldots, x_K$ that are just copies of input: $x_k = x_{in} \forall k$
- Branch B-prop: $\frac{\partial E}{\partial x_{in}} = \sum_{k=1}^{K} \frac{\partial E}{\partial x_k}$.



[Slide: Y. LeCun and M. Ranzato]

Softmax Module

- Single input x. Normalized output vector z, i.e. $\sum_i z_i = 1$.
- F-Prop: $z_i = \frac{\exp -\beta x_i}{\sum_k \exp -\beta x_k}$
- β is "temperature", usually set to 1.
- B-prop:
  If $i = j$, then $\frac{\partial z_i}{\partial x_j} = z_i(1 - z_i)$.
  If $i \neq j$, then $\frac{\partial z_i}{\partial x_j} = -z_i z_j$.
- Often combined with cross-entropy cost function:
  $E = -\sum_{c=1}^{C} y_i log(z_i)$.
- Conveniently, this yields b-prop: $\frac{\partial E}{\partial x_i} = x_i - y_i$.

Practical Tips for Backprop
[from M. Ranzato and Y. LeCun]

- Use ReLU non-linearities (tanh and logistic are falling out of favor).
- Use cross-entropy loss for classification.
- Use Stochastic Gradient Descent on minibatches.
- Shuffle the training samples.
- Normalize the input variables (zero mean, unit variance). More on this later.
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization on the weights (or a combination) But it's best to turn it on after a couple of epochs
- Use dropout for regularization (Hinton et al 2012 http://arxiv.org/abs/1207.0580)
- See also [LeCun et al. Efficient Backprop 1998]
- And also Neural Networks, Tricks of the Trade (2012 edition) edited by G. Montavon, G. B. Orr, and K-R Muller (Springer)

Training

- Many parameters: $O(10^6+)$
  - 2^{nd} order methods not practical (Hessian too big)
- Big datasets: $O(10^6)$
  - Expensive to compute full objective, i.e. loss on all examples

- Use 1^{st} order methods and update using subset of examples
  - Pick random batch at each iteration

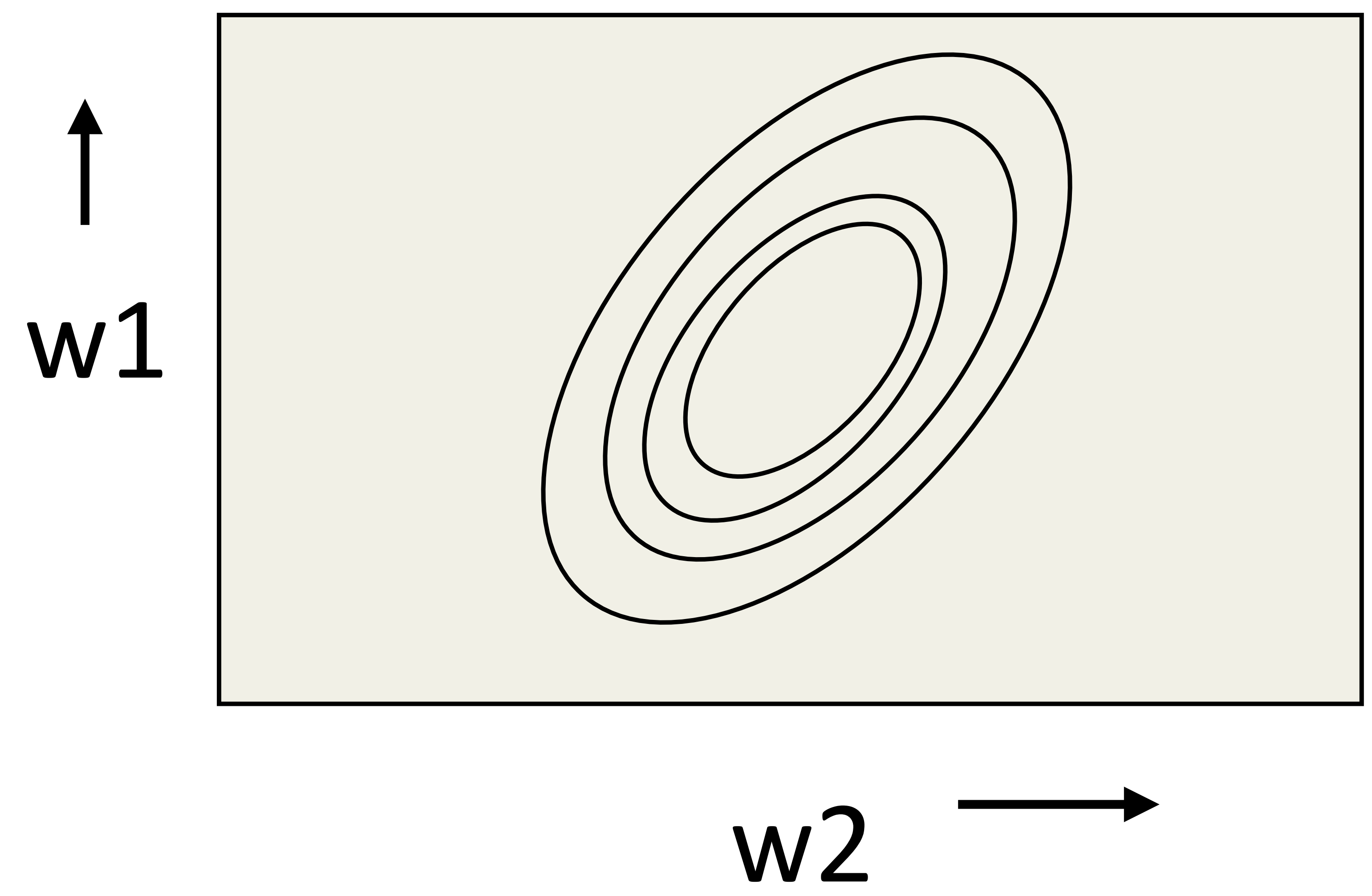
Stochastic Gradient Descent (SGD)

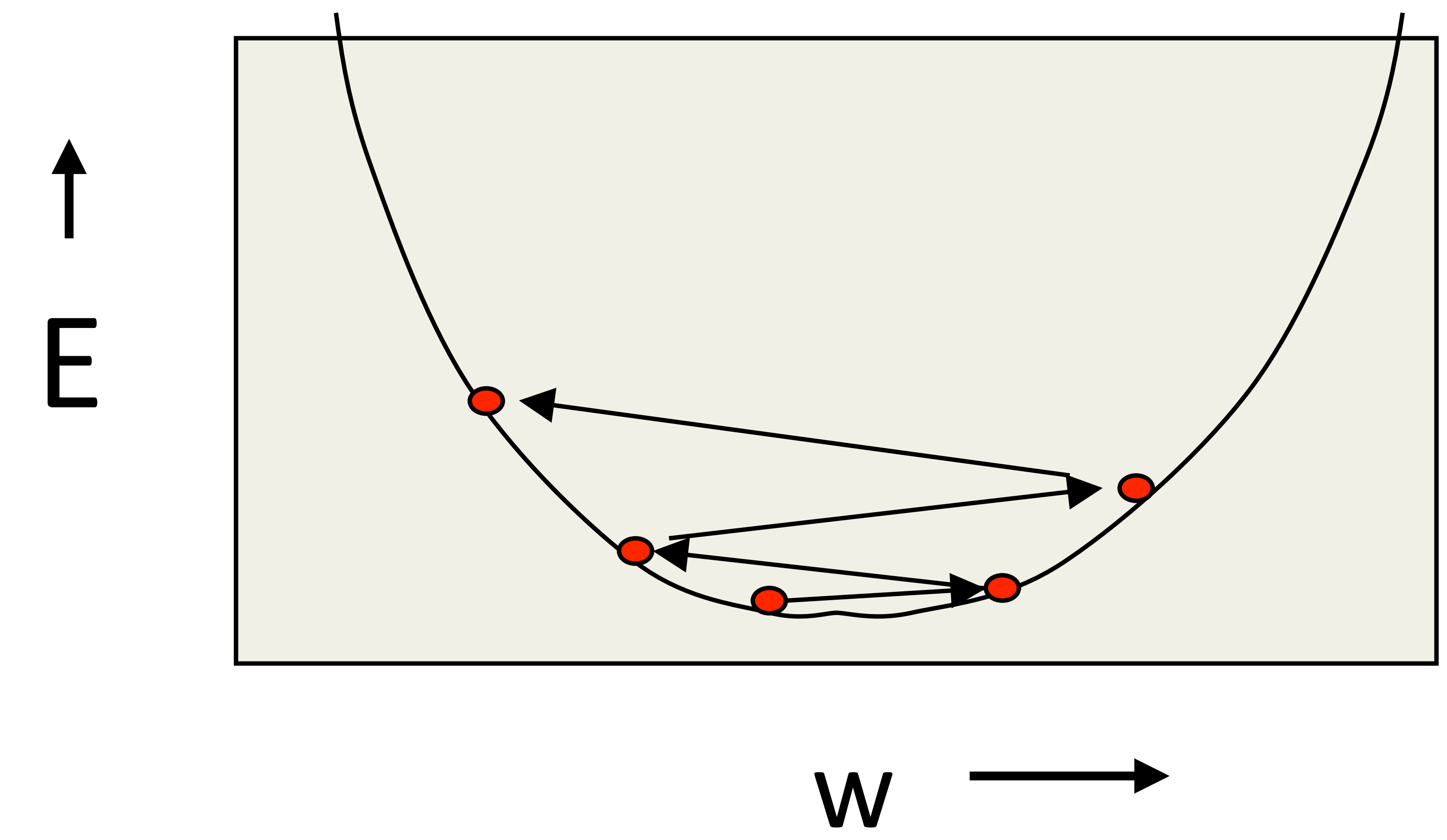
$$\Delta_t = \mu\Delta_{t-1} - \eta\nabla L_t(\theta_t)$$
$$\theta_{t+1} = \theta_t + \Delta_t$$

- Fixed learning rate η
  - Large as possible without being unstable, e.g. 0.01
- Momentum term μ
  - Typically ~0.9
  - Smooths updates → helps convergence
  - Also Nesterov version: apply momentum before gradient

Setting the Learning Rate

- Learning rate η has dramatic effect on resulting model.
- Pretend energy surface is quadratic bowl (in reality, much more complex).
- Gradient descent direction is just local, so if surface is highly elipitical then easy to have learning rate too large and oscillate.
- Difficult to have single learning rate that works for all dimensions.

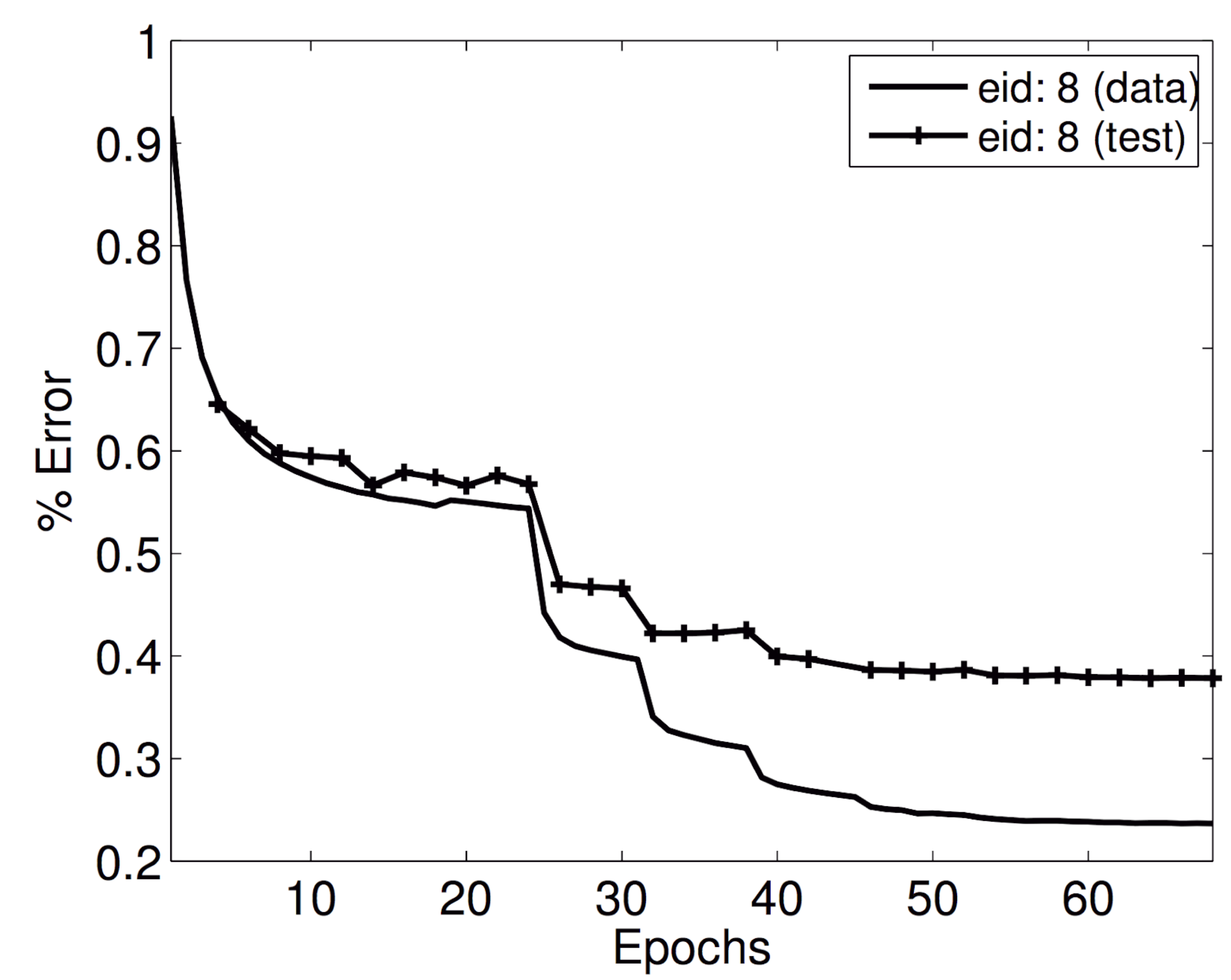




[Figures: G. Hinton]

Annealing of Learning Rate

- Constant learning rate η typically not optimal.
- Start with largest value that for which training loss decreases, e.g. 0.1.
- Then train until validation error flatens out.
- Divide η by, say, 0.3.
- Repeat.



AdaGrad

- Learning rate now scaled per-dimension
- Decreased for dimensions with high variance
- Issue: learning rate monotonically decreases
  - Stop making progress after while

$$\theta_{t+1} = \theta_t - \eta \frac{\nabla L_t(\theta_t)}{\sqrt{\sum_{t'=1}^{t} \nabla L_{t'}(\theta_{t'})^2}}$$

[Adaptive Subgradient Methods for Online Learning and Stochastic Optimization, Duchi et al., JMLR 2011]

RMSProp

- Similar to AdaGrad, but now with moving average
  - Small μ emphasizes recent gradients

$$\Delta_t = \mu \Delta_{t-1} + (1-\mu) \nabla L_t(\theta_t)^2$$

$$\theta_{t+1} = \theta_t - \eta \frac{\nabla L_t(\theta_t)}{\sqrt{\Delta_t}}$$

ADAM

- ADApative Moment Estimation
- Combines AdaGrad and RMSProp

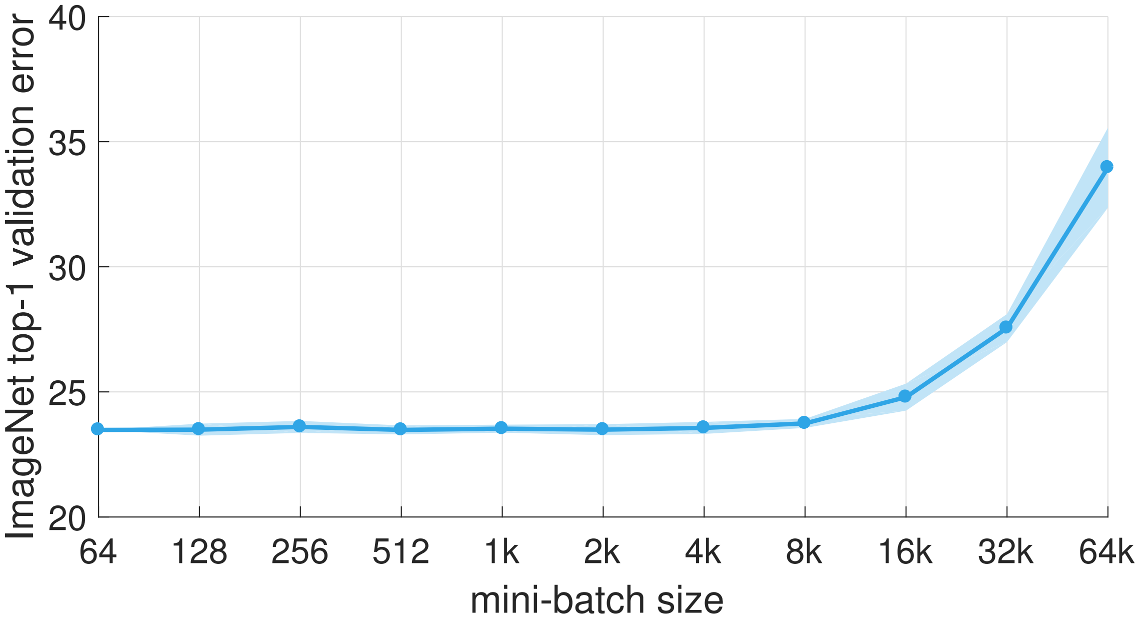
- Idea: maintain moving averages of gradient and gradient^2
- Update $\propto \dfrac{\text{Mean gradient}}{\sqrt{\text{Mean gradient}^2}}$

For more details, see: https://moodle2.cs.huji.ac.il/nu15/pluginfile.php/316969/mod_resource/content/1/adam_pres.pdf

[Adam: A Method for Stochastic Optimization, Kingma & Ba, arXiv:1412.6980]

Batch-size

- [Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour, Goyal et al., arXiv 1706.02677, 2017]
- Scale learning rate with batch-size
- Large-batch size efficiently implemented via synchronous parallel training



Momentum

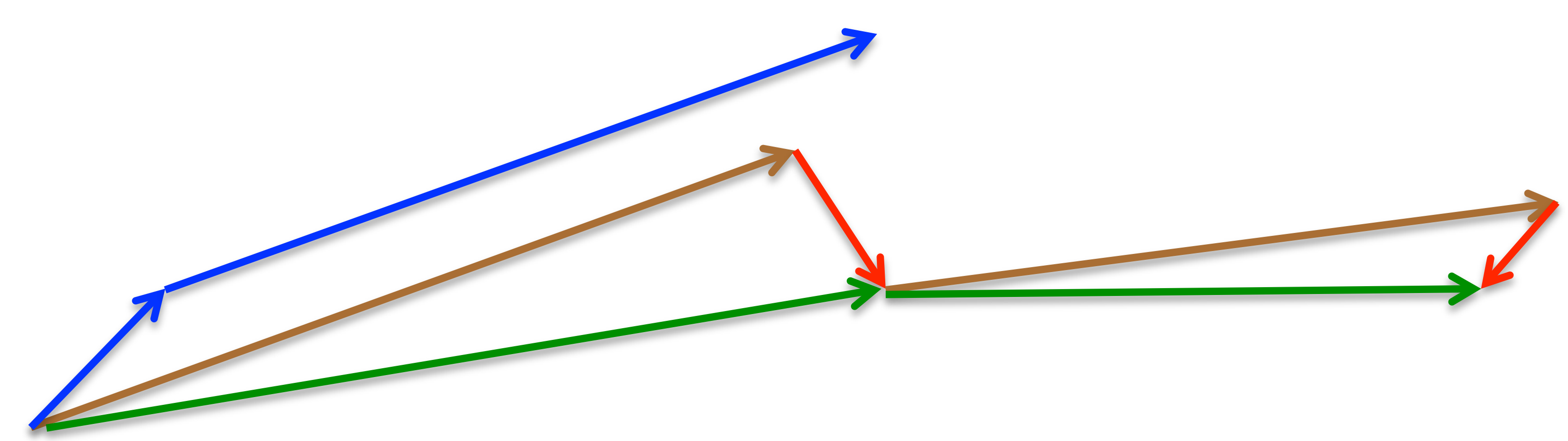
To speed convergence

- Add momentum term to the weight update.
- Encourages updates to keep following previous direction.
- Damps oscillations in directions of high curvature.
- Builds up speed in directions with gentle but consistent gradient.
- Usually helps speed up convergence.
- $\theta^{k+1} \leftarrow \theta^k + \alpha(\Delta\theta)^{k-1} - \eta\nabla\theta$
- α typically around 0.9.

[Slide: G. Hinton]

Nesterov Momentum

- Simple idea.
- Update weights with momentum vector.
- Then measure gradient and take step.
- This is opposite order to regular momentum.



[Figure: G. Hinton]

Batch Normalization

- Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift, Sergey Ioffe, Christian Szegedy, arXiv:1502.03167

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_\mathcal{B} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_\mathcal{B})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

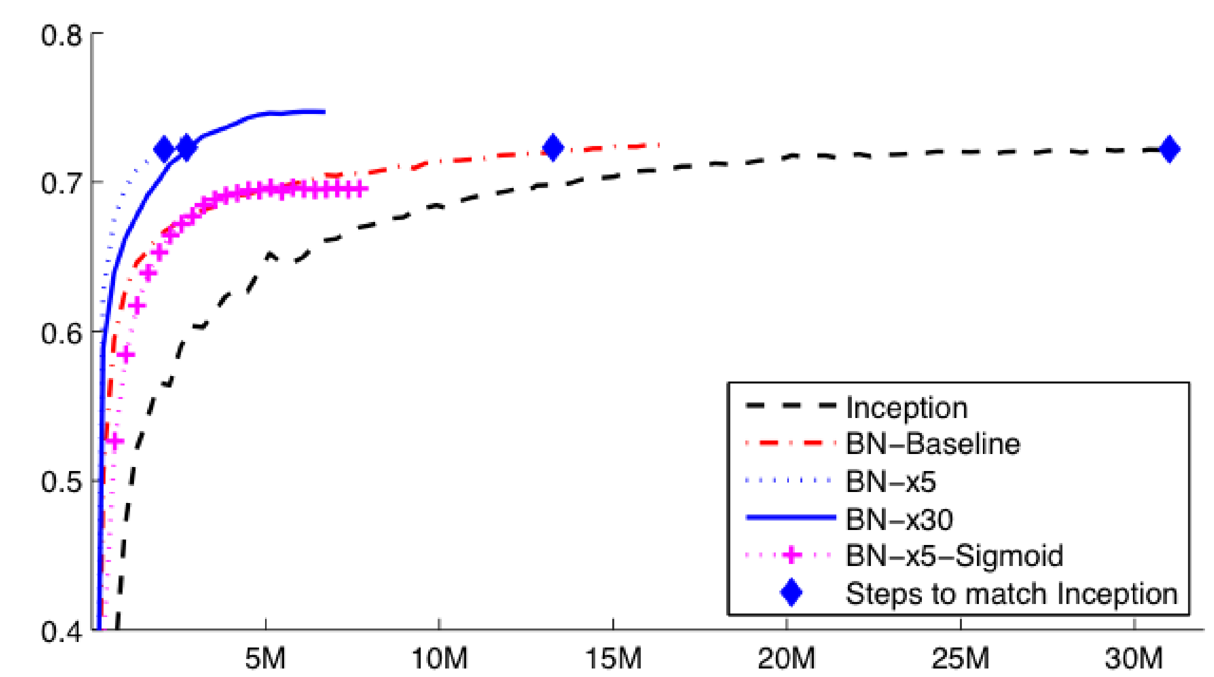
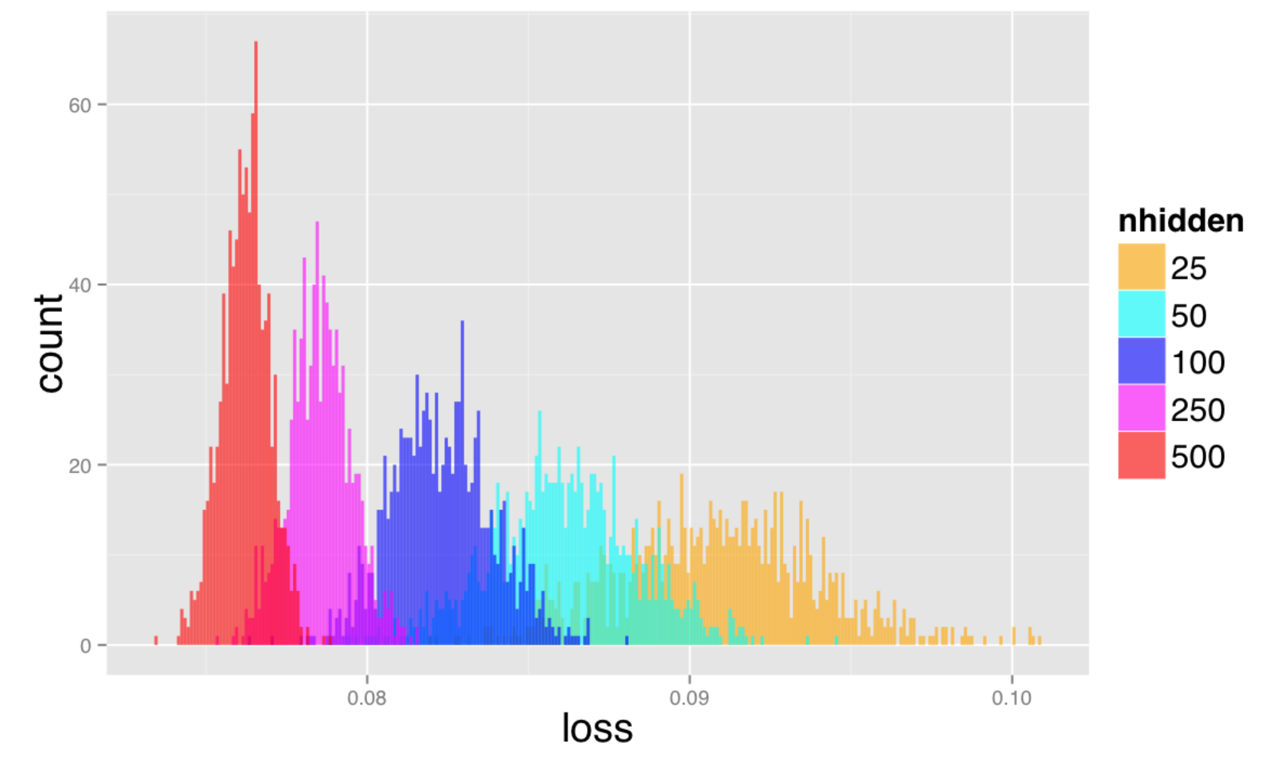


Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

Local Minima

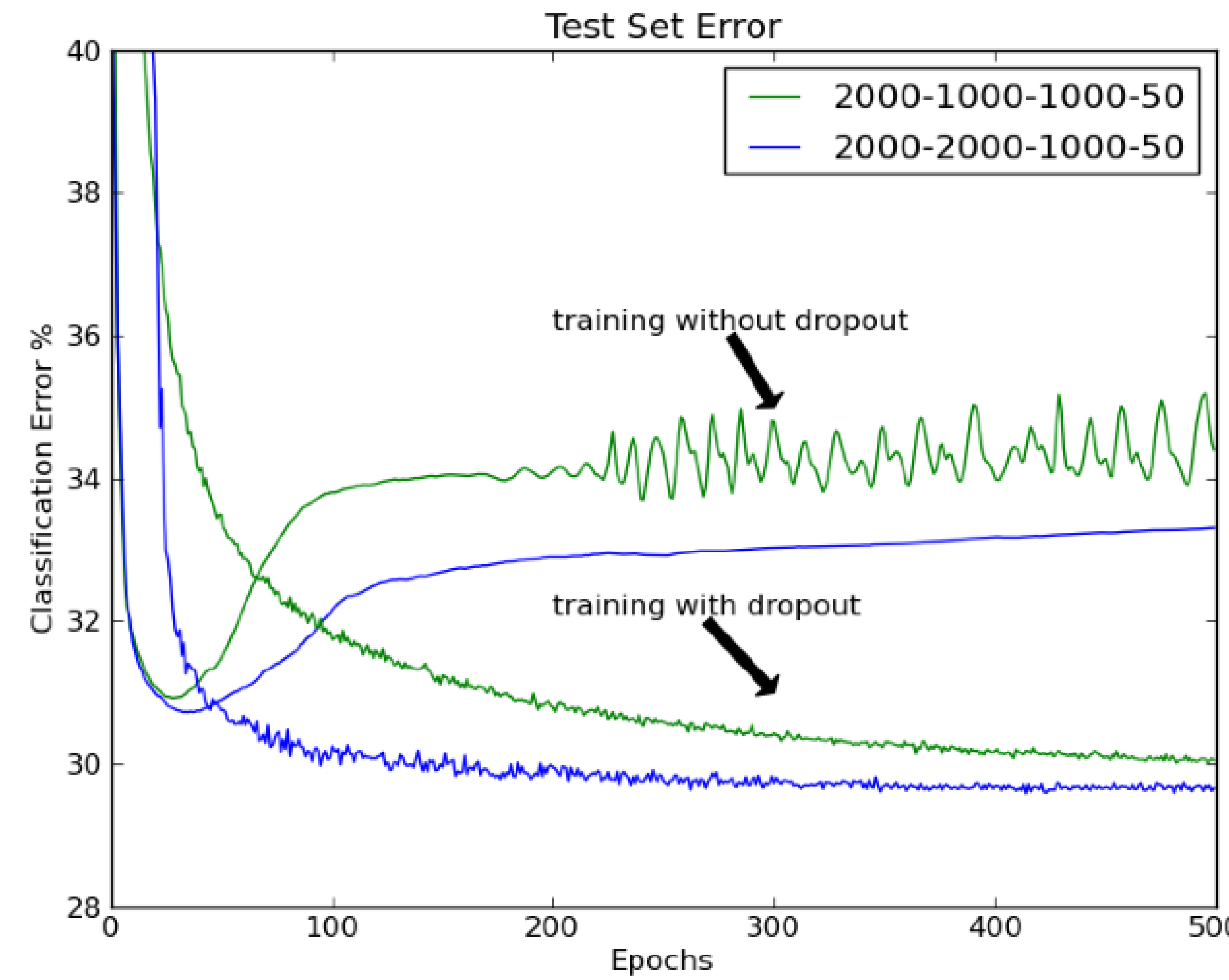
Non-convexity of energy surface

- Non-convexity means there are multiple minima.
- Gradient descent is local method: minima you fall into depends on your initial starting point.
- Maybe some mimima have much lower energy than others?
- The Loss Surfaces of Multilayer Networks Choromanska et al. `http://arxiv.org/pdf/1412.0233v3.pdf`



DropOut

- G. E. Hinton, N. Srivastava, A. Krizhevsky, I. Sutskever and R. R. Salakhutdinov, Improving neural networks by preventing co-adaptation of feature detectors, arXiv:1207.0580 2012
- Fully connected layers only.
- Randomly set activations in layer to zero
- Gives ensemble of models
- Similar to bagging [Breiman94], but differs in that parameters are shared



Debugging Training

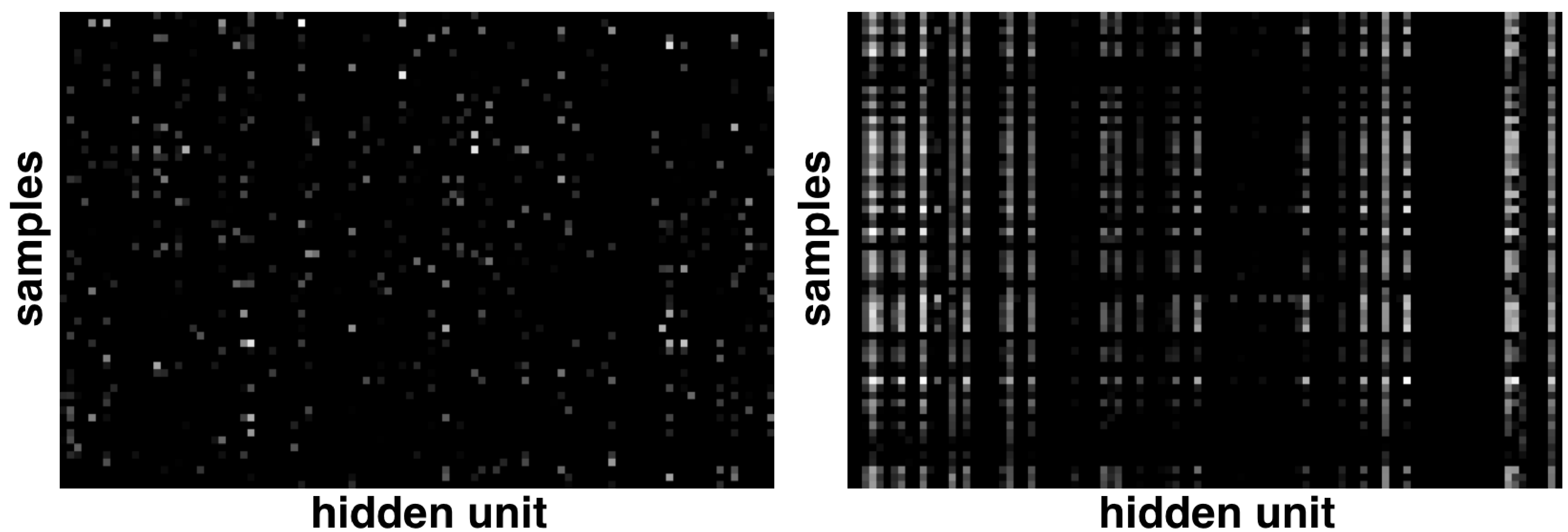
What to do when its not working

- Training diverges:
    - Learning rate may be too large decrease learning rate
    - BPROP is buggy numerical gradient checking
- Parameters collapse / loss is minimized but accuracy is low
    - Check loss function:
    - Is it appropriate for the task you want to solve?
    - Does it have degenerate solutions? Check pull-up term.
- Network is underperforming
    - Compute flops and nr. params. if too small, make net larger
    - Visualize hidden units/params fix optmization
- Network is too slow
    - Compute flops and nr. params. GPU,distrib. framework, make net smaller

Debugging Training (2)

What to do when its not working

- Inspect hidden units.
- Should be sparse across samples and features (left).
- In bad training, strong correlations are seen (right), and also units ignore input.

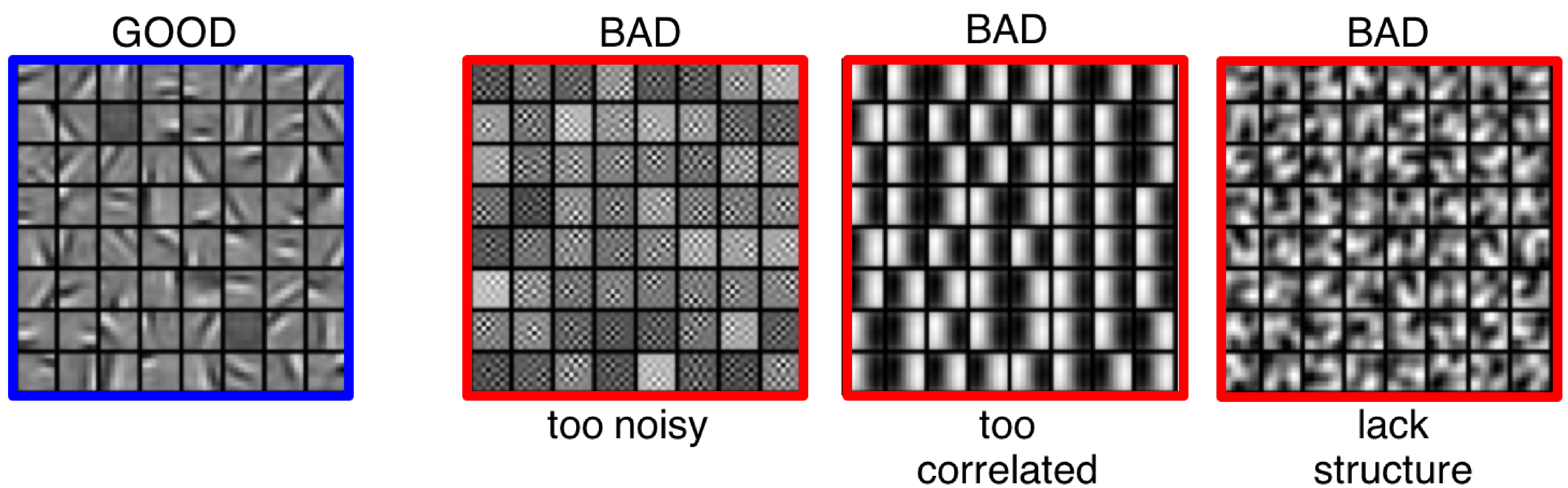


[Figures: M. Ranzato]

Debugging Training (3)

What to do when its not working

- Visualize weights

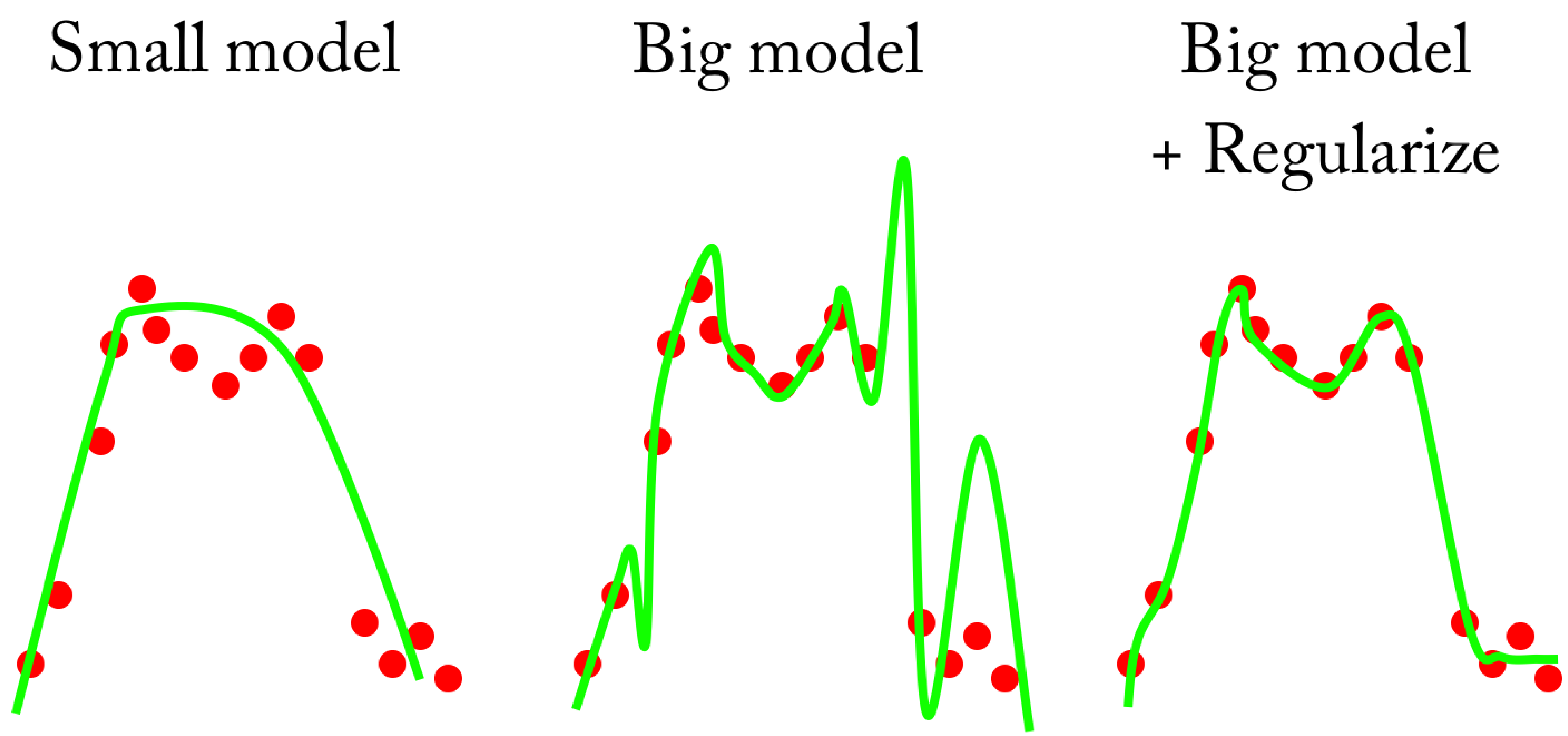


Good training: learned filters exhibit structure and are uncorrelated.

[Figure: M. Ranzato]

Regularization

The Intuition



- Better to have big model and regularize, than unfit with small model.

Regularizing the model

Help to prevent over-fitting

- Weight sharing (greatly reduce the number of parameters)
- Data augmentation (e.g., jittering, noise injection, etc.)
- Dropout.
- Weight decay (L2, L1).
- Sparsity in the hidden units.
- Multi-task learning.