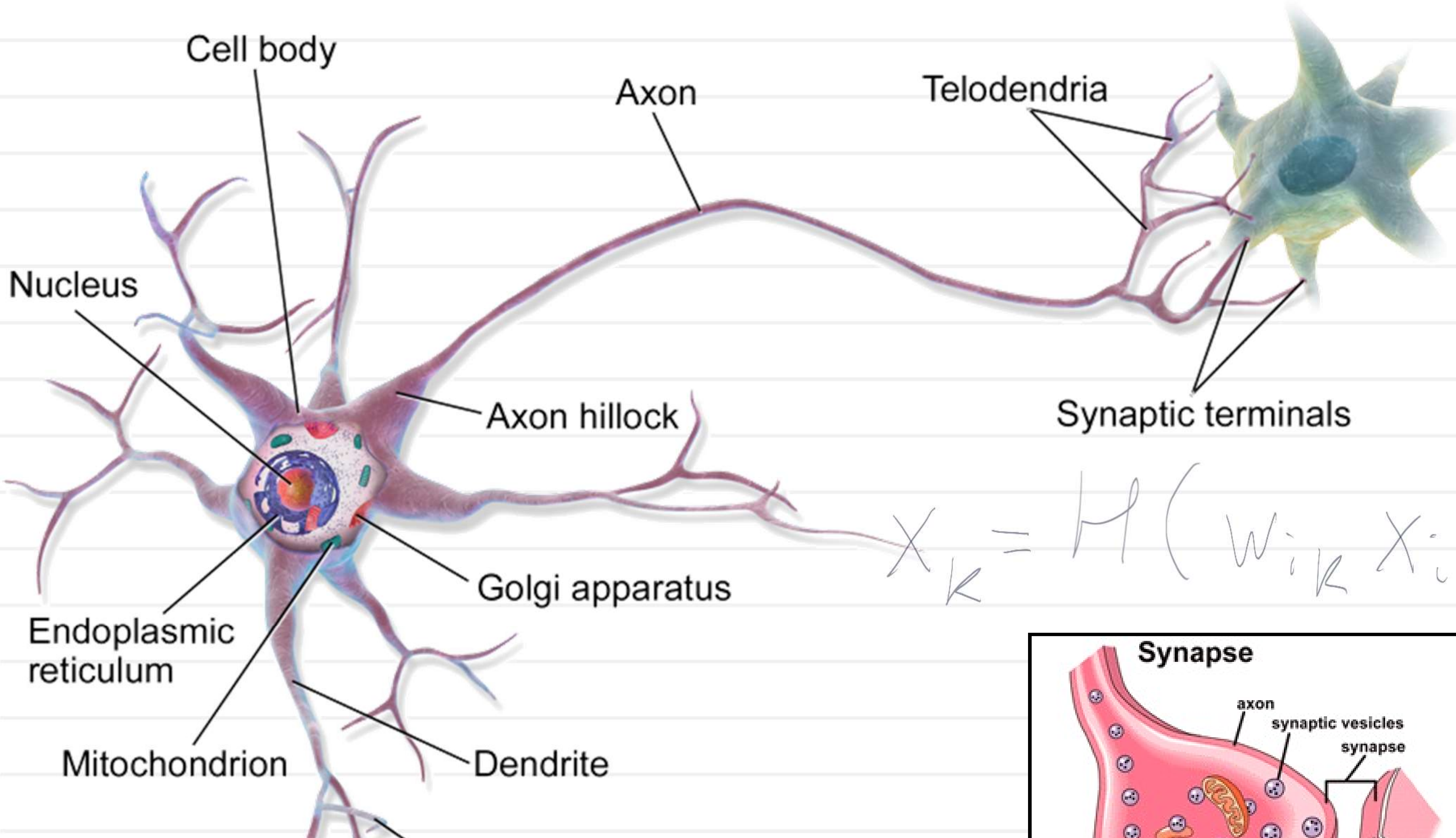
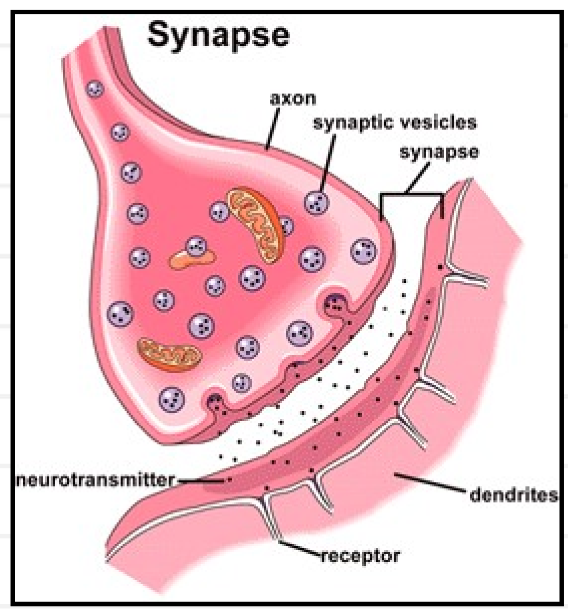
Lecture 3: Deep feed-forward neural networks

Neuron model



$$x_k = H(w_{ik} x_i - \tau)$$



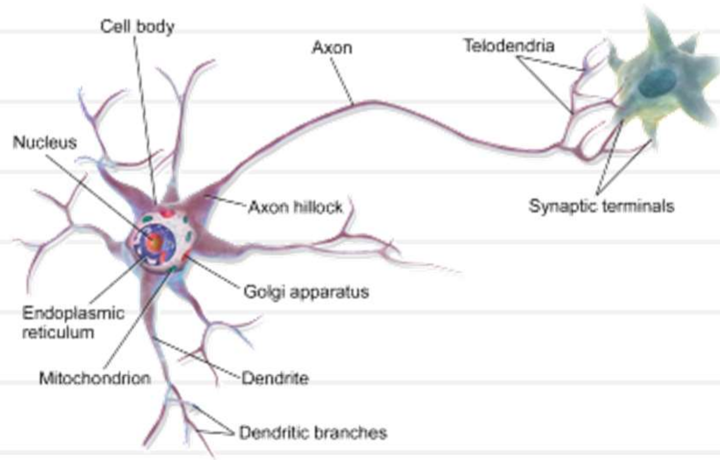
Brain statistics

Human brain:

- 100 billion neurons
- average neuron is connected to 1000-10000 other neurons
- 100 trillion synapses
- 10-25% is in visual cortex

Perceptron

[Rosenblatt 1957]: an "artificial neuron"



$y = H(w^T x)$

loop over examples

$y = H(w^T x_i);$

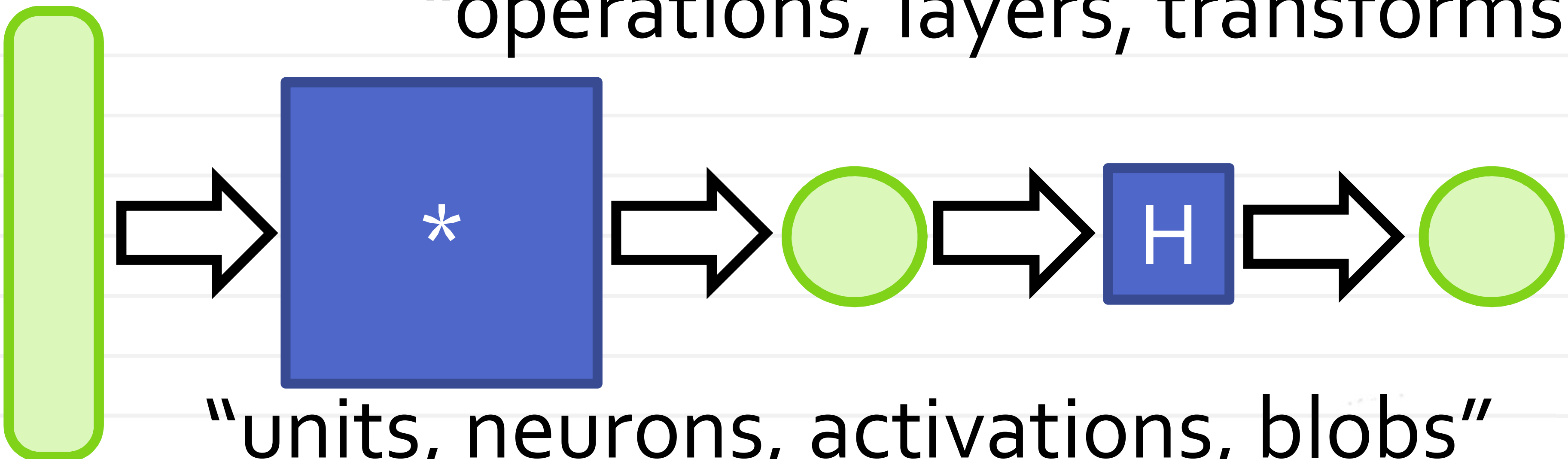
$w = w + 1/2\ x_i * (y_i - y);$

end

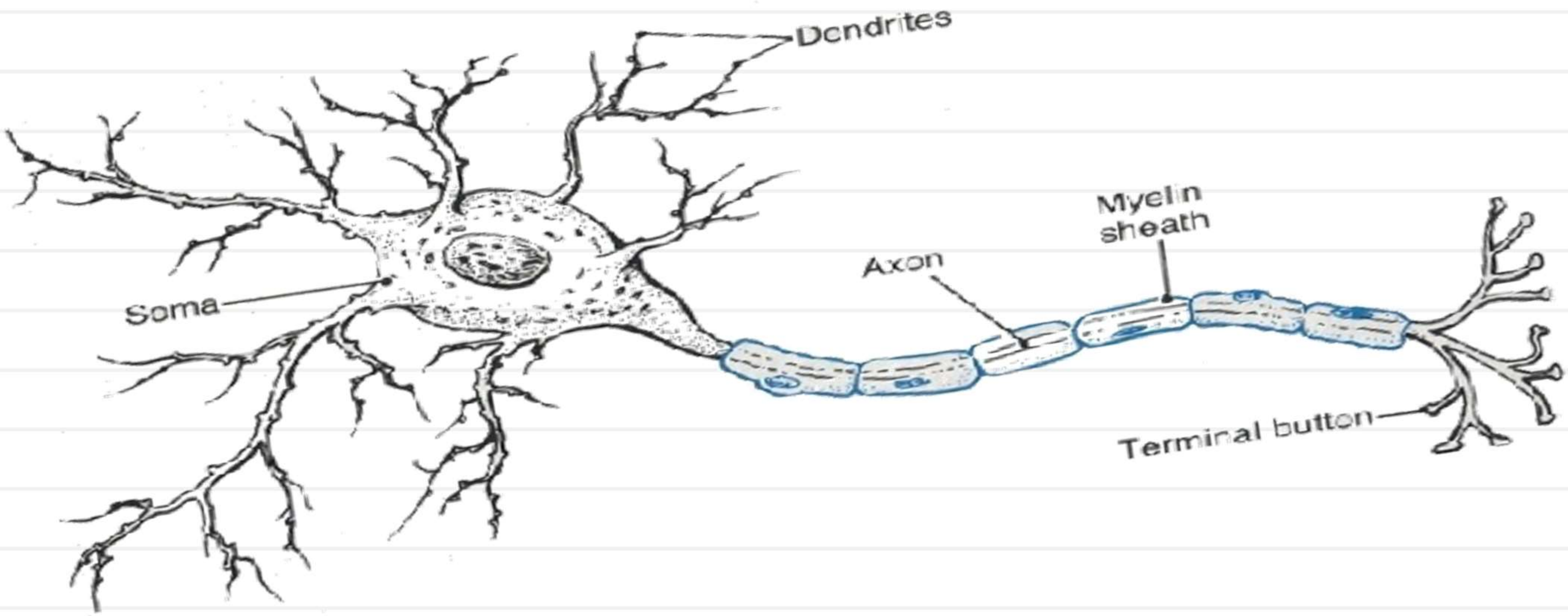
Converges to linear separator of the training data if it exists.

Terminology and graphical language

“operations, layers, transforms”



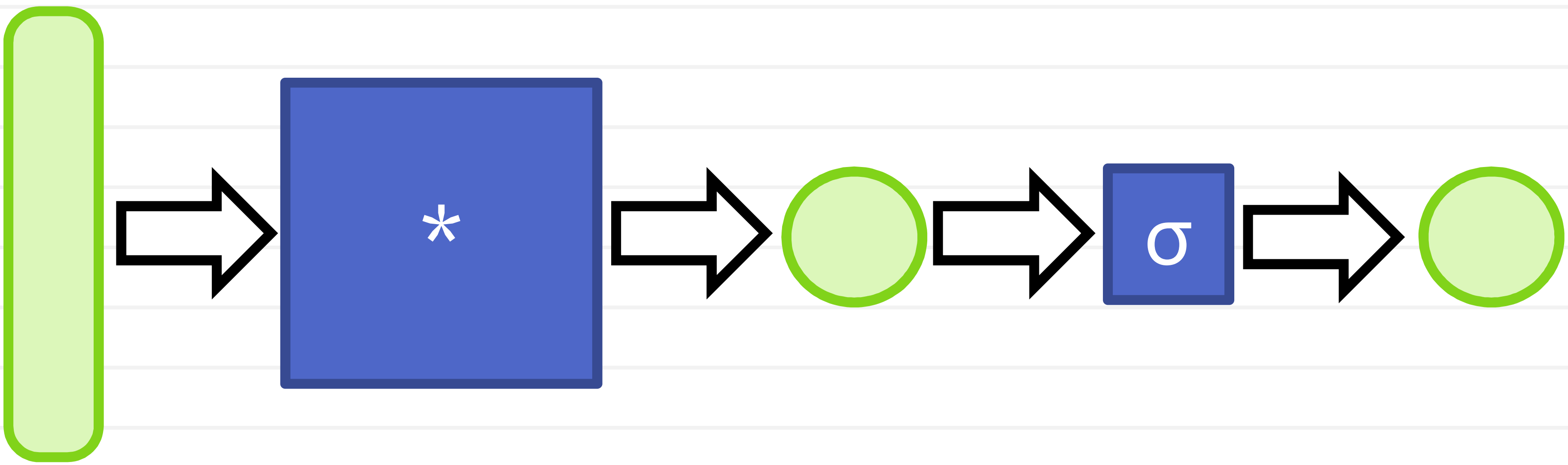
“units, neurons, activations, blobs”



Logistic regression

$$P(y(x)=y_i \mid w) = \frac{1}{1+e^{-y_i w^T x_i}} = \sigma(y_i w^T x_i)$$

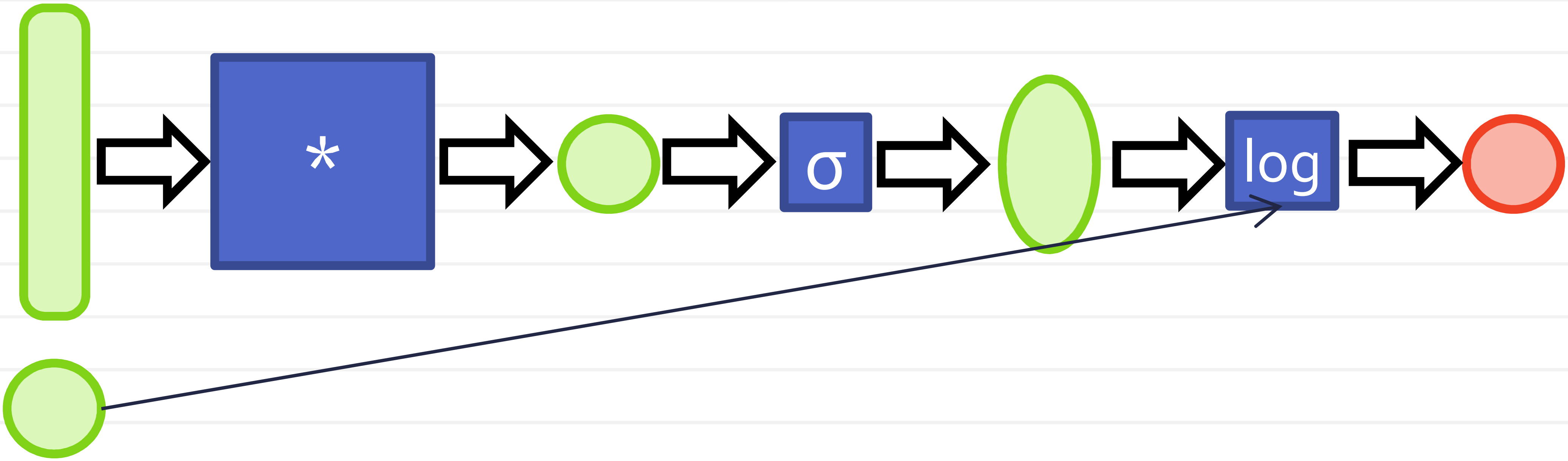
Same diagram/network:



Training logistic regression

$$E(\omega) = -\sum_{i=1}^{N} \log P(y(x)=y_i \mid \omega) =$$

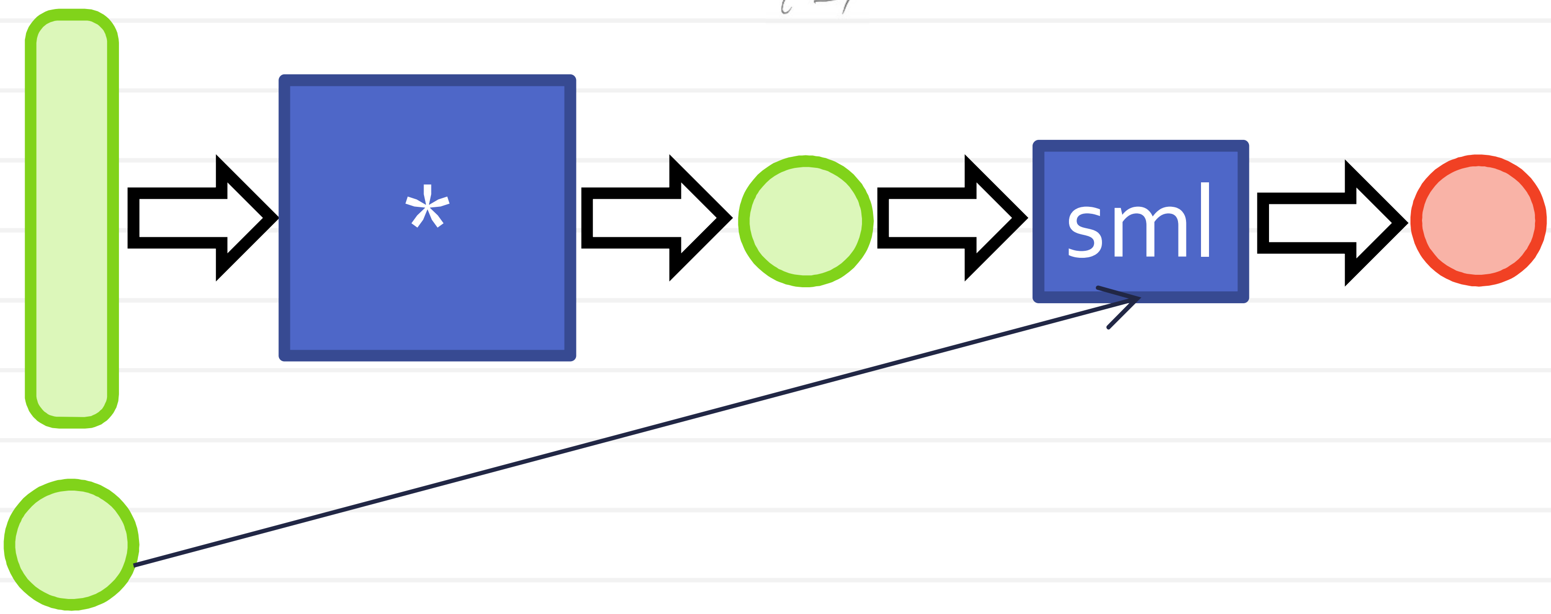
$$= \sum_{i=1}^{N} \log\left(1 + e^{-y_i \omega^T x_i}\right)$$



Logistic regression: simplifying training

$$E(\omega) = -\sum_{i=1}^{N} \log P(y(x)=y_i \mid \omega) =$$

$$= \sum_{i=1}^{N} \log\left(1 + e^{-y_i \omega^T x_i}\right)$$

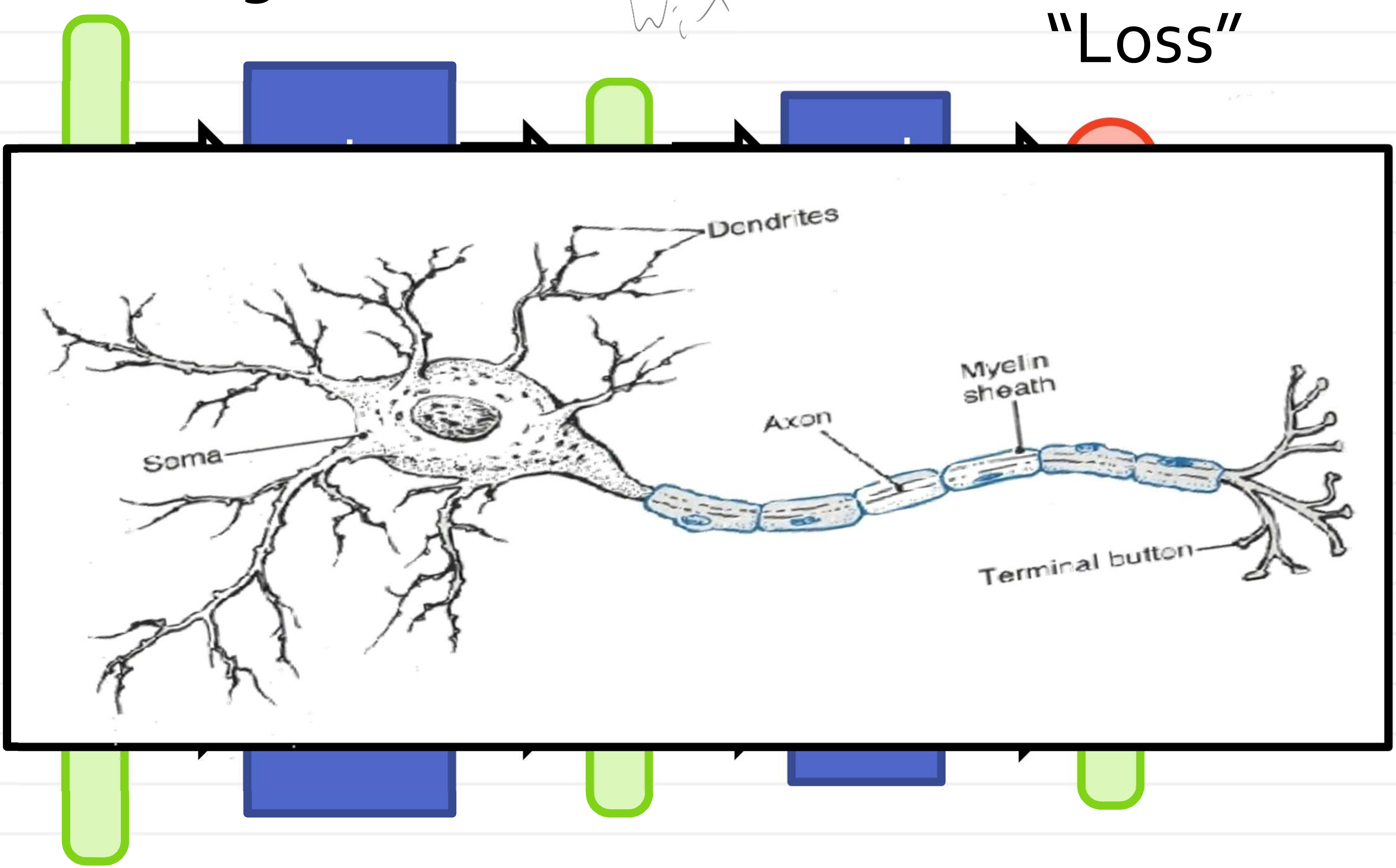


Softmax loss = log loss over softmax/logistic

Multinomial logistic regression

Training:

$W_i^T x$



Biological neuron layers

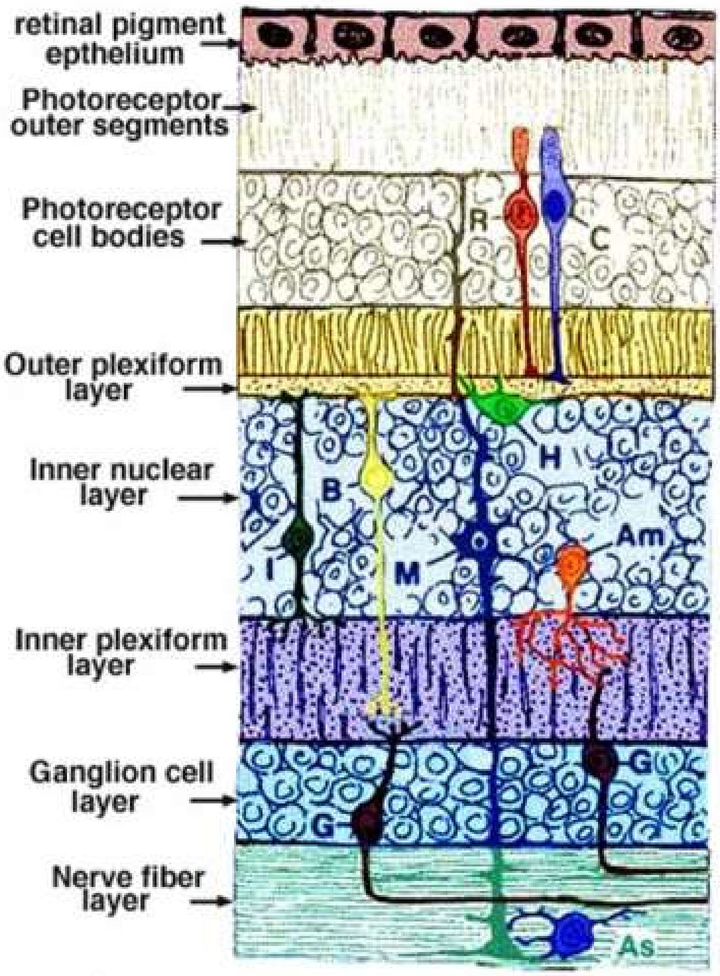


Fig. 5. Scheme of the layers of the developing retina around 5 months' gestation (Modified from Odgen, 1989).

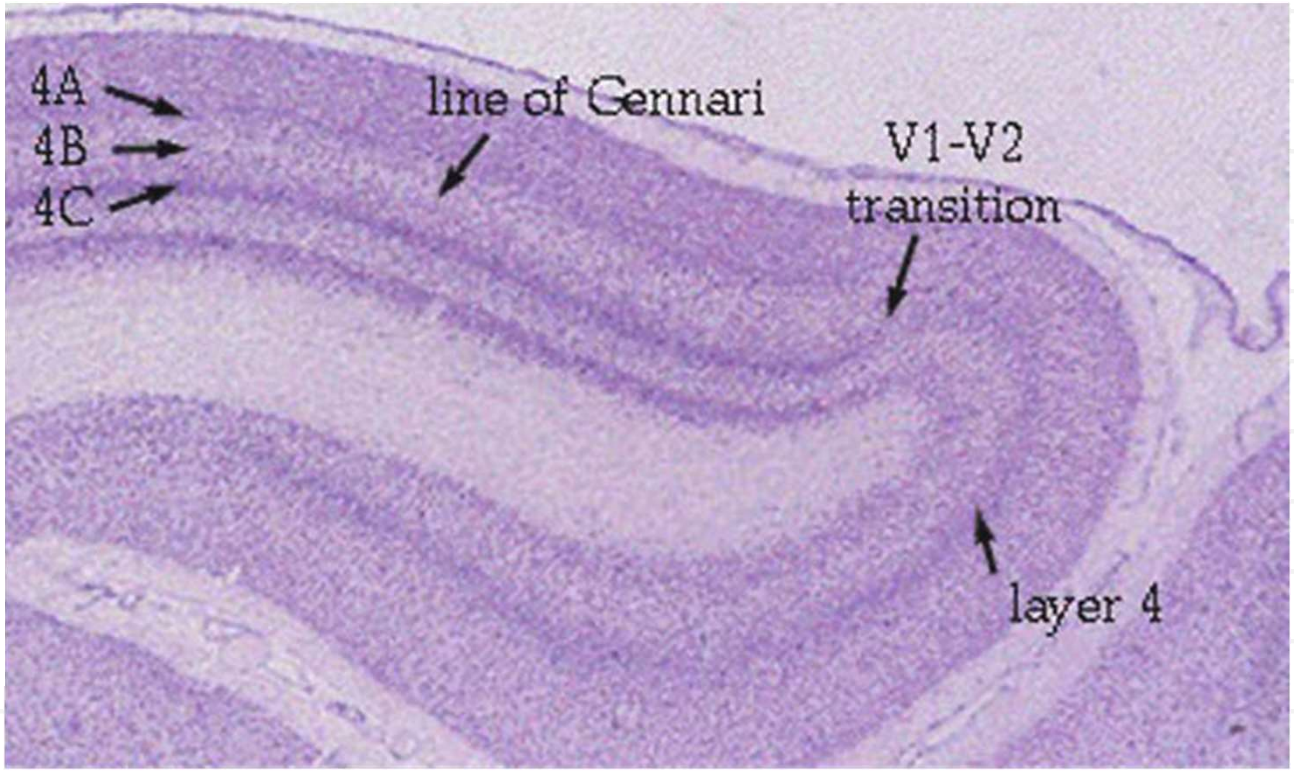
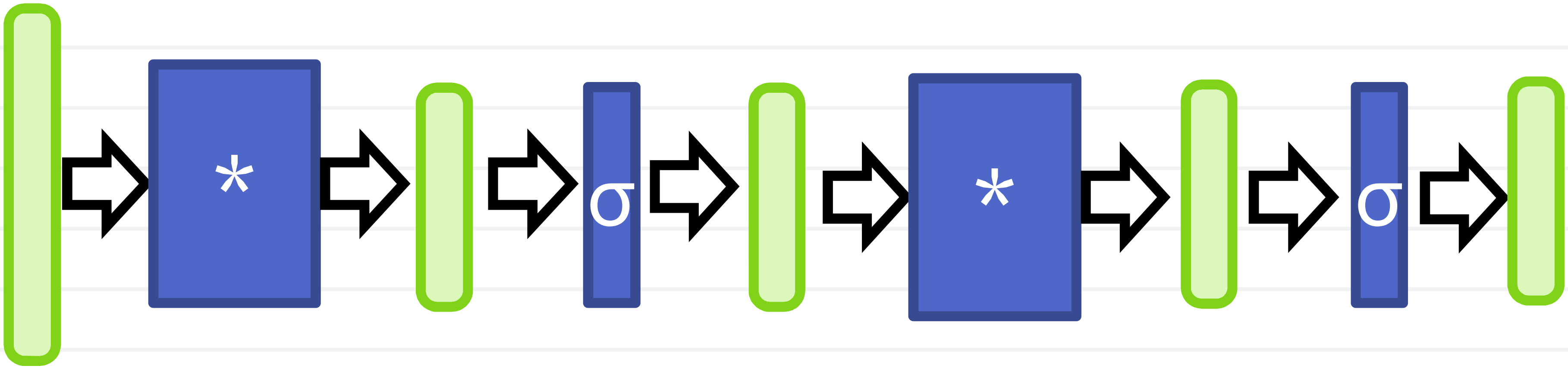


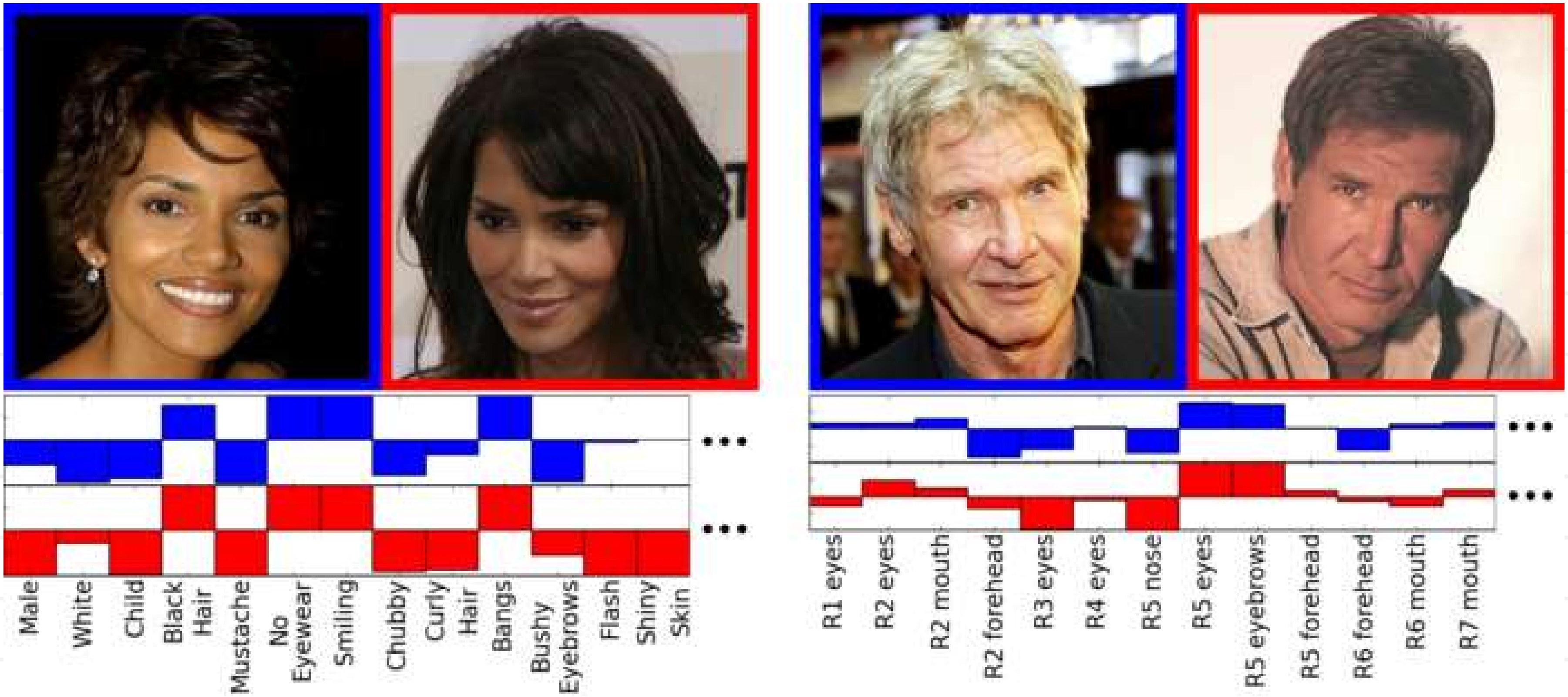
Figure 9. Nissl stained section of the visual cortex to show the border between area 17 (V1) and area 18 (V2).

Multi-layer perceptron idea



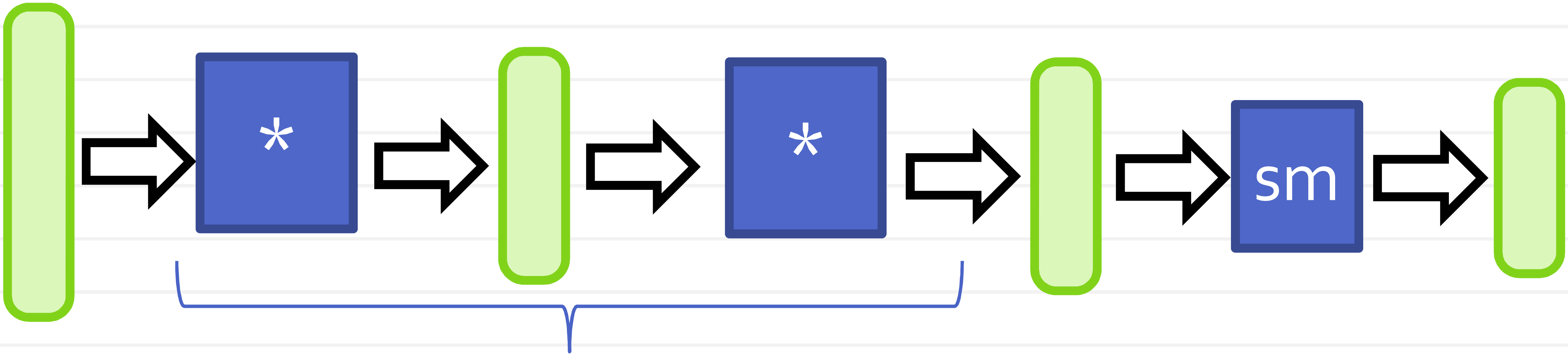
- First layer: parallel logistic regression
- Each predicts presence of some feature in the input
- Second layer is a logistic regression that "weighs" the input of the first layer

Classifier output as features



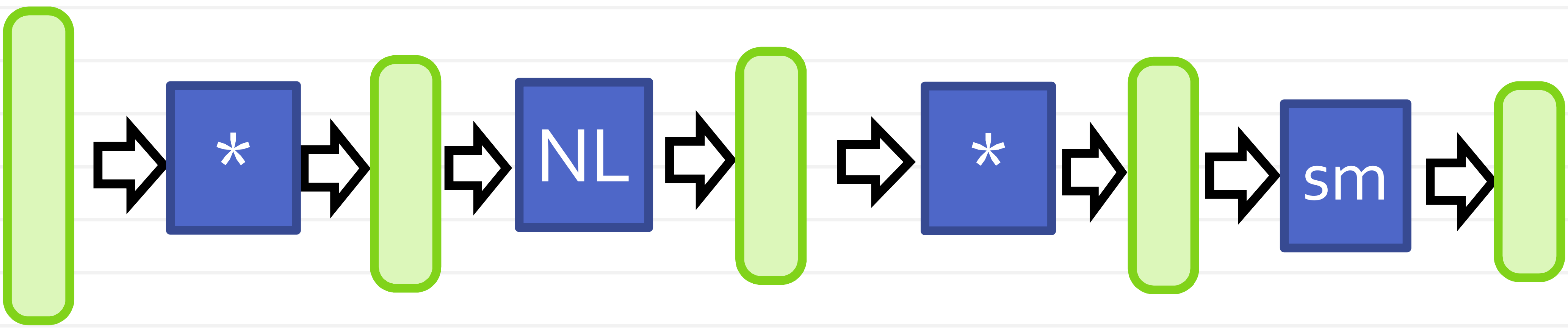
[Kumar et al. **Attribute and Simile Classifiers for Face Verification. ICCV 2009**]

Artificial multilayer networks



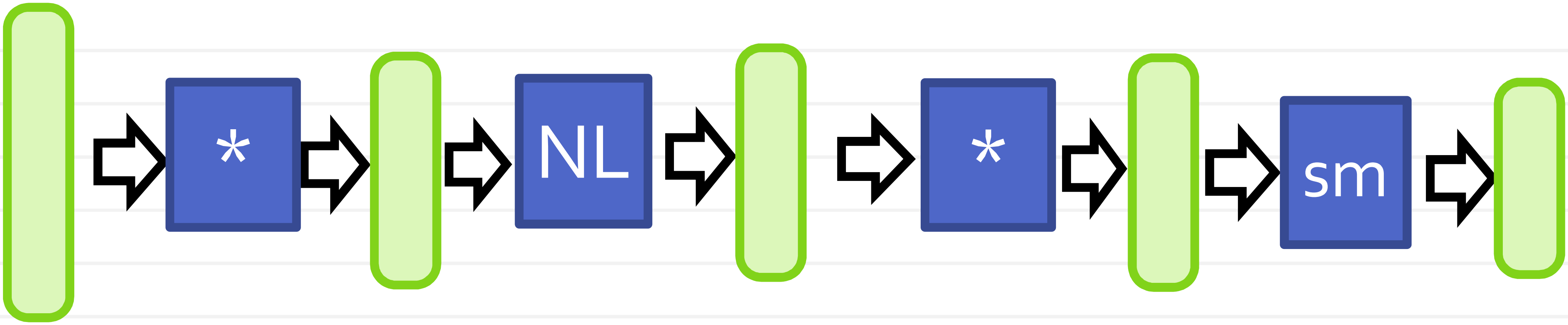
still single matrix multiplication

To get more powerful model need non-linearity:



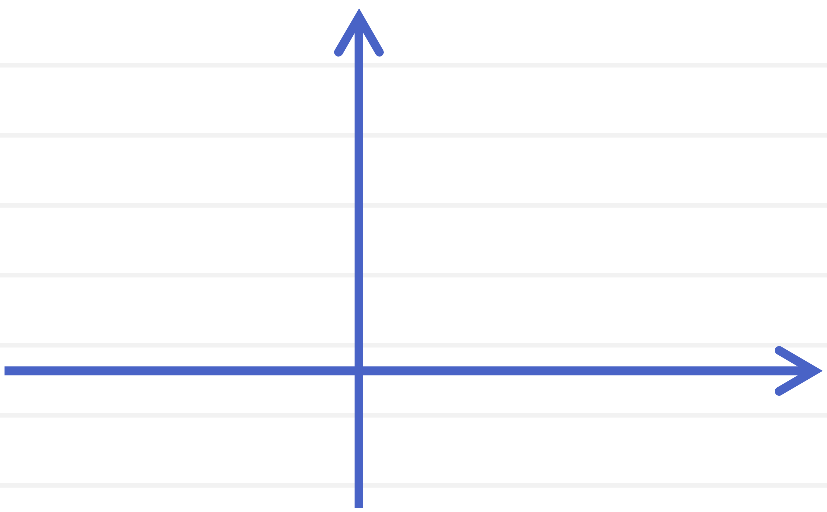
Adding non-linearities

To get more powerful model need non-linearity:



Possible *elementwise* non-linearities:

- Heaviside
- Sigmoid(logistic)/tanh
- More recently:
  ReLu(x) = max(0,x)



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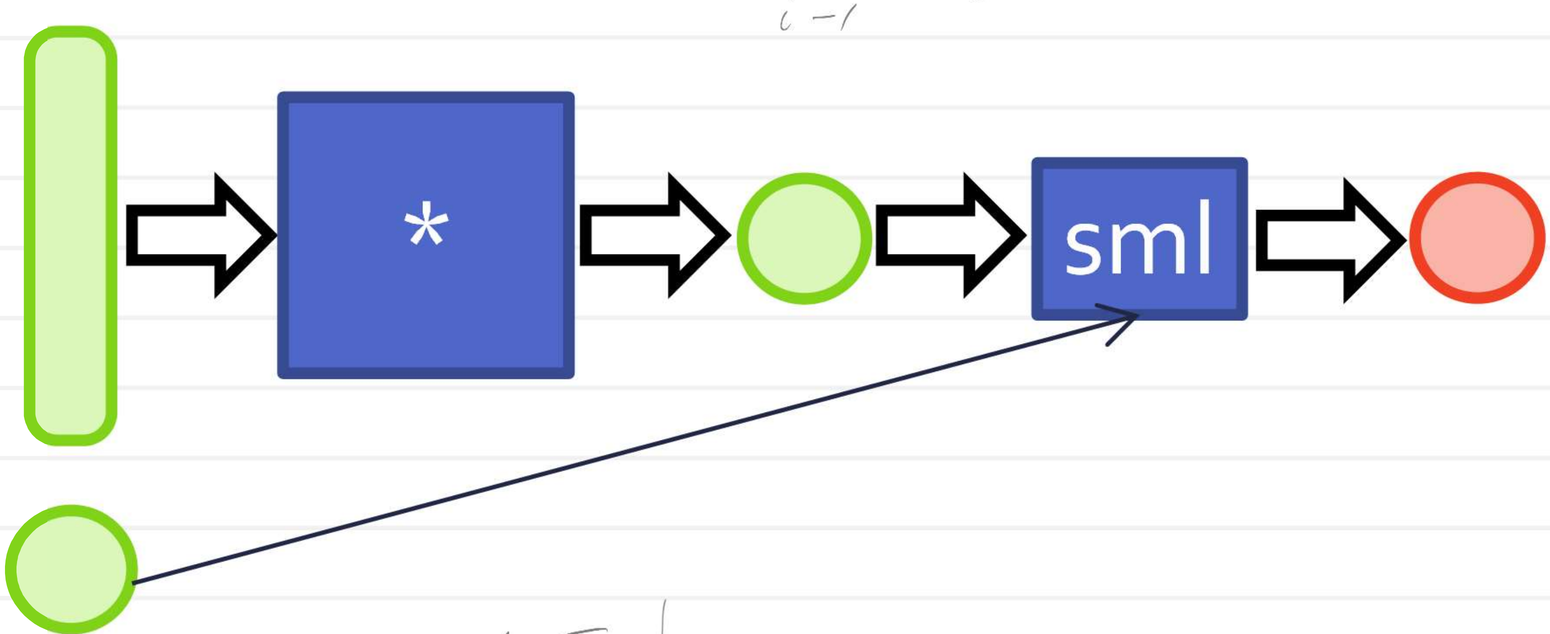
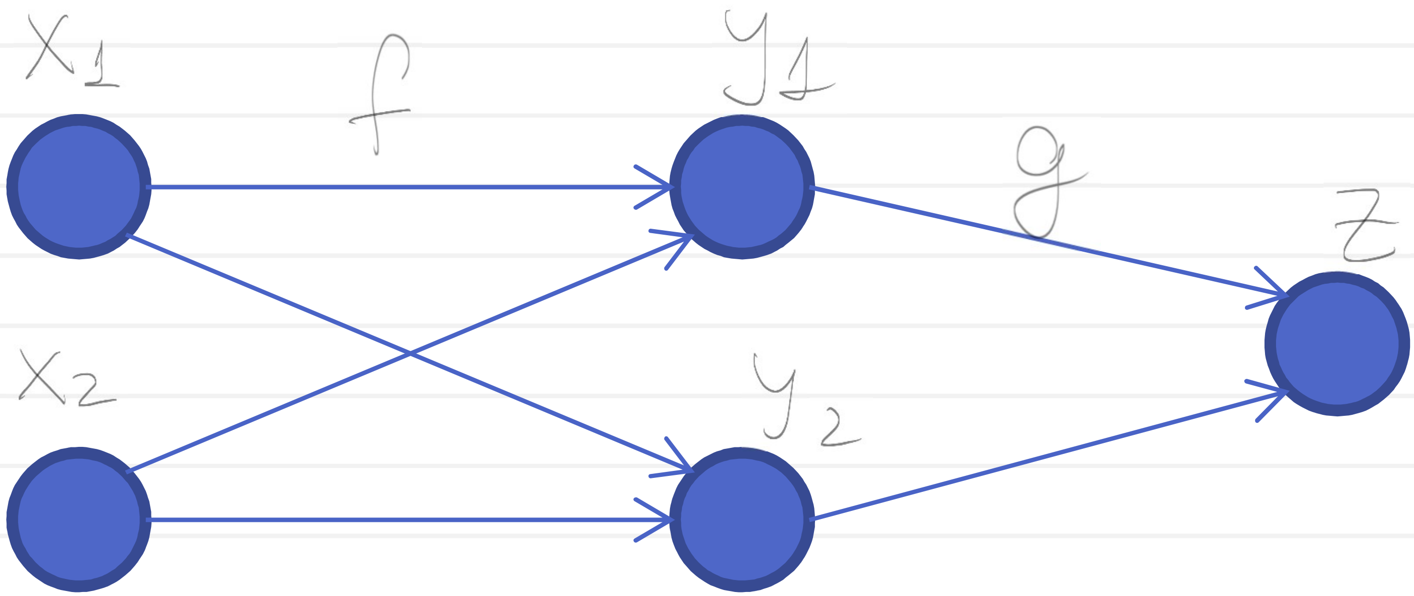
$$= -\sum_{i=1}^{N} \log\left(1 + e^{-y_i w^T x_i}\right)$$



$$\left.\frac{dE}{dw}\right|_{x_i} = \left(\sigma(y_i w^T x_i) - 1\right) y_i x_i$$

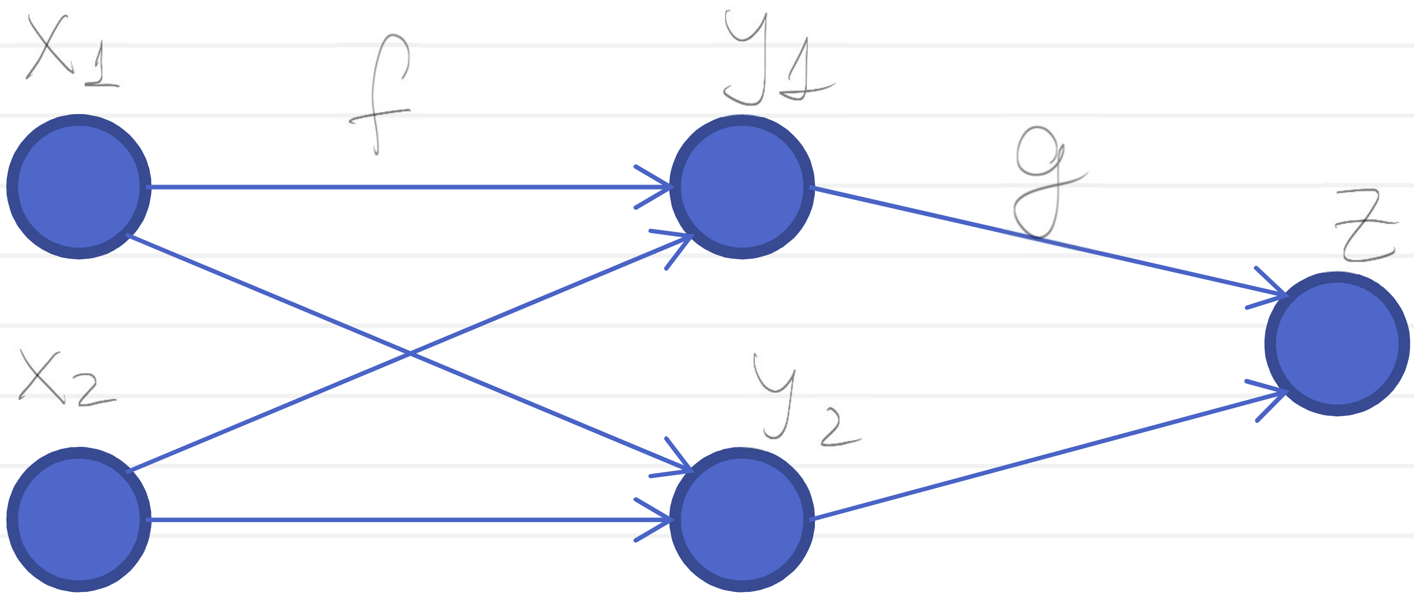
Recap: chainrule



$$\frac{\partial z}{\partial x_1} = \frac{\partial z}{\partial y_1} \cdot \frac{\partial y_1}{\partial x_1} + \frac{\partial z}{\partial y_2} \cdot \frac{\partial y_2}{\partial x_1}$$

$$\frac{dz}{dy} = \begin{bmatrix} \frac{\partial g}{\partial y_1}(y_1, y_2) \\ \frac{\partial g}{\partial y_2}(y_1, y_2) \end{bmatrix}$$

Recap: chainrule



$$\frac{\partial z}{\partial x_1} = \frac{\partial z}{\partial y_1} \cdot \frac{\partial y_1}{\partial x_1} + \frac{\partial z}{\partial y_2} \cdot \frac{\partial y_2}{\partial x_1}$$

$$\frac{\partial z}{\partial x_2} = \frac{\partial z}{\partial y_1} \cdot \frac{\partial y_1}{\partial x_2} + \frac{\partial z}{\partial y_2} \cdot \frac{\partial y_2}{\partial x_2}$$

Recap: chainrule

$$\frac{\partial z}{\partial x_1} = \frac{\partial z}{\partial y_1} \cdot \frac{\partial y_1}{\partial x_1} + \frac{\partial z}{\partial y_2} \cdot \frac{\partial y_2}{\partial x_1}$$

$$\frac{\partial z}{\partial x_2} = \frac{\partial z}{\partial y_1} \cdot \frac{\partial y_1}{\partial x_2} + \frac{\partial z}{\partial y_2} \cdot \frac{\partial y_2}{\partial x_2}$$

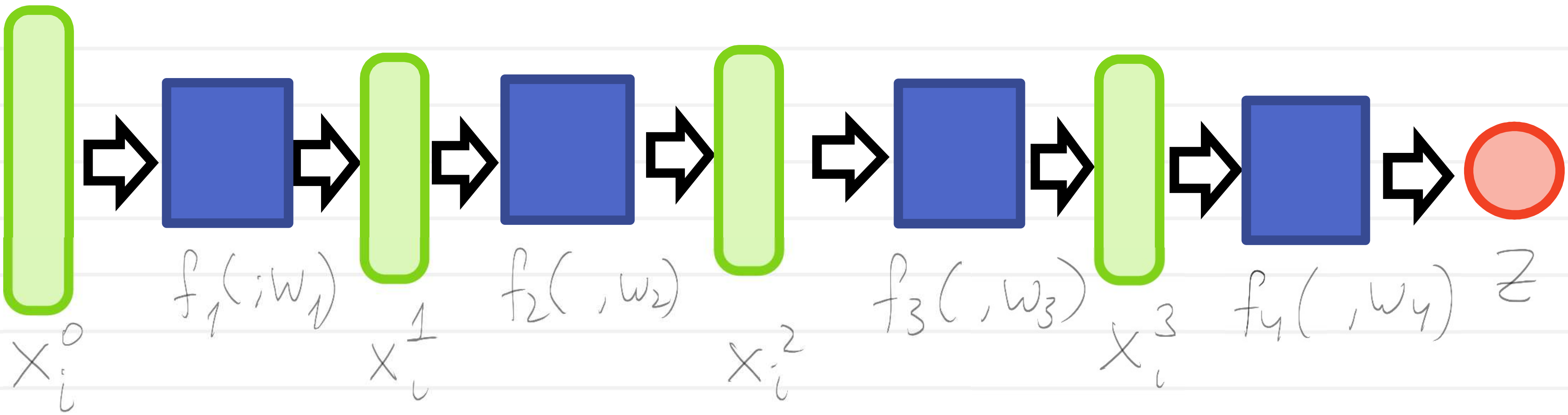
$$\frac{dz}{dx} = \begin{bmatrix} \frac{\partial z}{\partial x_1} \\ \frac{\partial z}{\partial x_2} \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial z}{\partial y_1} \\ \frac{\partial z}{\partial y_2} \end{bmatrix}$$

Recap: chainrule

$$\frac{dz}{dx} = \begin{bmatrix} \frac{\partial z}{\partial x_1} \\ \frac{\partial z}{\partial x_2} \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial z}{\partial y_1} \\ \frac{\partial z}{\partial y_2} \end{bmatrix}$$

$$\frac{dz}{dx} = \left(\frac{dy}{dx} \right)^T \frac{dz}{dy}$$

Computing deeper derivatives



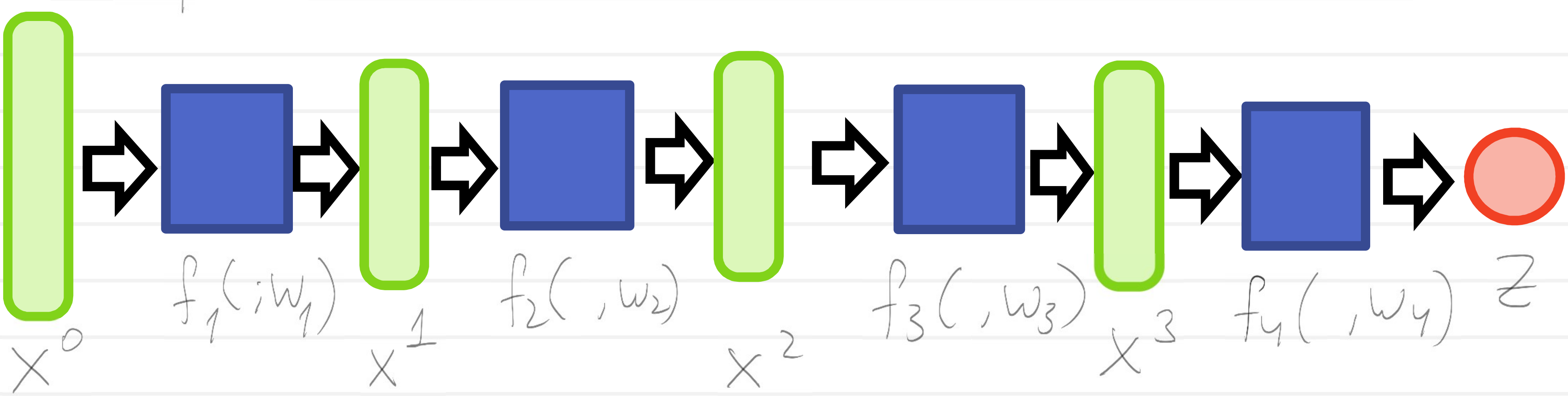
$$z = f_4(f_3(f_2(f_1(x;w_1);w_2);w_3);w_4)$$

Sequential computation: *backpropagation*

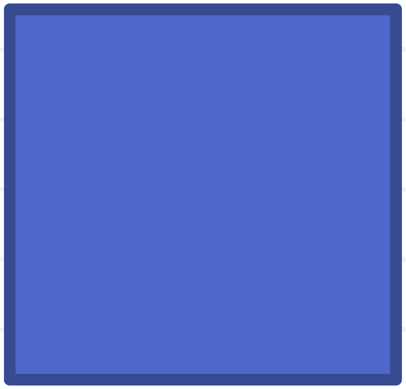
$$\frac{dz}{dW_3} = \frac{dx^3}{dW_3}^T \cdot \frac{dz}{dx^3} \qquad \frac{dz}{dx^2} = \frac{dx^3}{dx^2}^T \frac{dz}{dx^3}$$

$$\frac{dz}{dW_2} = \frac{dx^2}{dW_2}^T \cdot \frac{dz}{dx_2} \qquad \frac{dz}{dx^1} = \frac{dx^2}{dx^1}^T \frac{dz}{dx^2}$$

$$\frac{dz}{dW_1} = \frac{dx^1}{dW_1}^T \cdot \frac{dz}{dx_1} \qquad \frac{dz}{dx^0} = \frac{dx^1}{dx^0}^T \frac{dz}{dx^1}$$



Layer abstraction



Each layer is defined by:

- forward performance: $y = f(x)$
- backward performance:

$$z(x) = z(f(x;w)) \qquad y = f(x;w)$$

$$\frac{dz}{dx} = \frac{dy}{dx}^T \cdot \frac{dz}{dy} \qquad \frac{dz}{dw} = \frac{dy}{dw}^T \cdot \frac{dz}{dy}$$

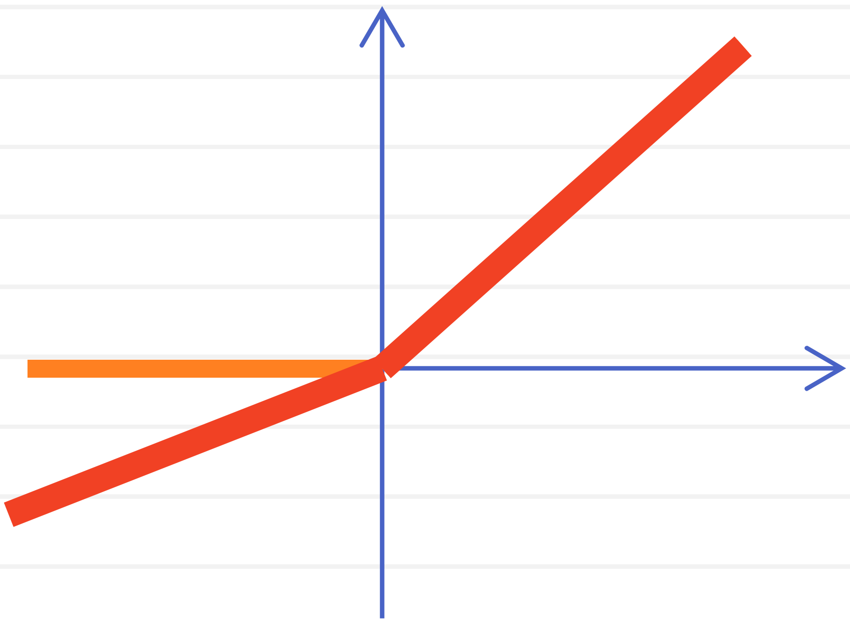
OOP pseudocode of deep learning

```
abstract class Layer {
        params w,dzdw;
        virtual y = forward(x);
        virtual dzdx = backward(dzdy,x,y);
        // should compute dzdw as well

        void update (tau) {
                w = w+tau*dzdw;
        }
};
```

Efficient implementations have to use vector/matrix instructions and work efficiently for minibatches!

Example: “leaky ReLu”



$$f(x;\alpha) = \max(x, \alpha x)$$

$$\frac{dz}{d\alpha} = [\alpha x > x]\, x^T \cdot \frac{dz}{dy}$$

Cornell University Library

arXiv.org > cs > arXiv:1502.01852

Computer Science > Computer Vision and Pattern Recognition

Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification

Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun

(Submitted on 6 Feb 2015)

Computing the partial derivatives

$$\frac{dz}{dx} = \frac{dy}{dx}^T \cdot \frac{dz}{dy} \qquad \frac{dz}{dw} = \frac{dy}{dw}^T \cdot \frac{dz}{dy}$$

Options for partial derivatives:

- Finite differences (bad idea)
- Derive gradients analytically (good idea)

Debugging is hard

Gradient checking is a good idea!

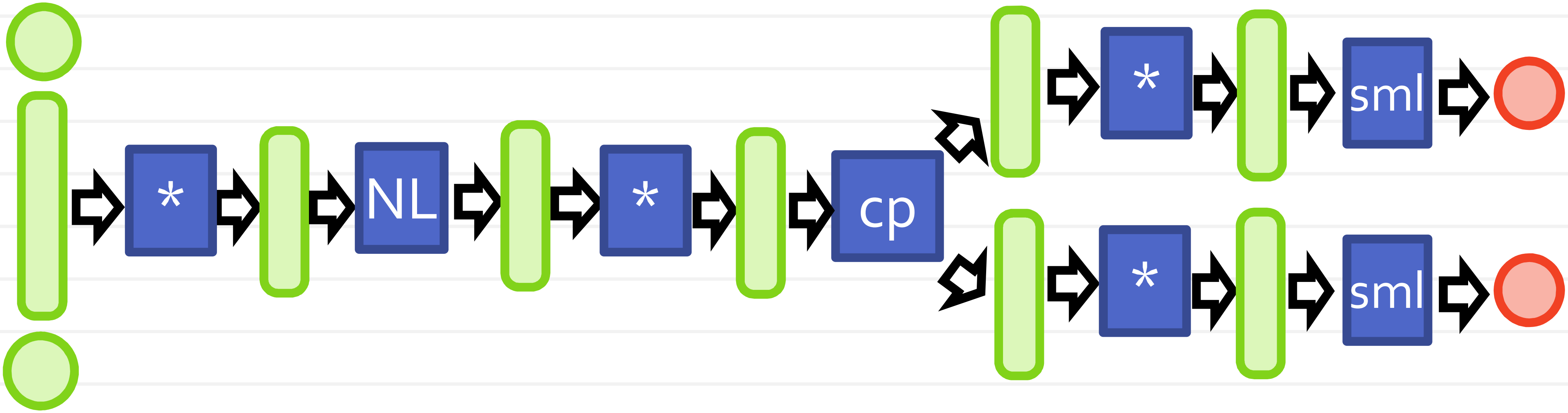
Recap

Deep learning:

- Define each layer
- Assemble a chain of layers
- Loop over minibatches
- For each minibatch find the stochastic gradient and update the parameters (use momentum, etc.)

In fact, chain can easily be replaced with DAG

Example: multitask learning



Typical usecase:

- Two related tasks
- Limited labeled data for the main task
- Lots of labeled data for auxiliary task

Zoo of layers

Multiplicative layer
Convolutional layer

Copy layer
Split layer
Cat layer
Merge layer

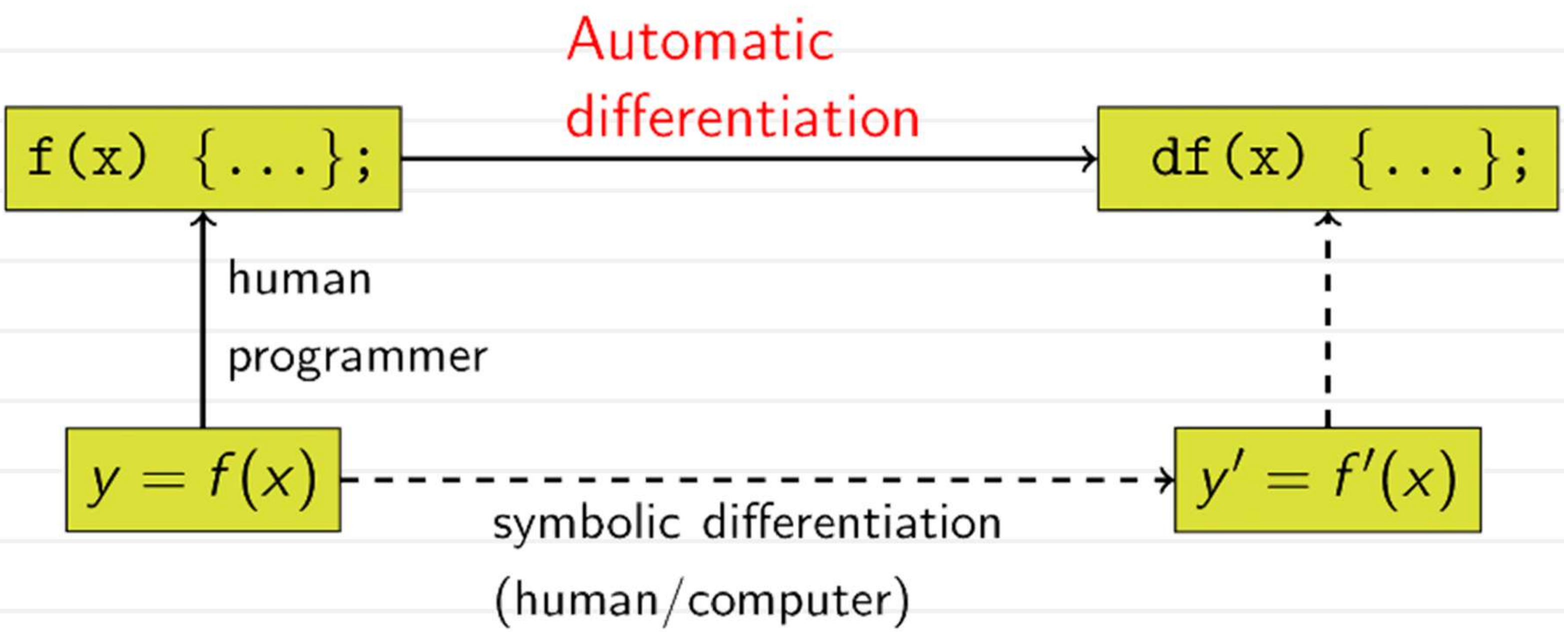
ReLu layer
Sigmoid layer
Softmax layer
Normalization layer
Max-pooling layer

Log-loss layer
Softmax loss layer
Hinge loss layer
L2-loss layer
Contrastive loss layer

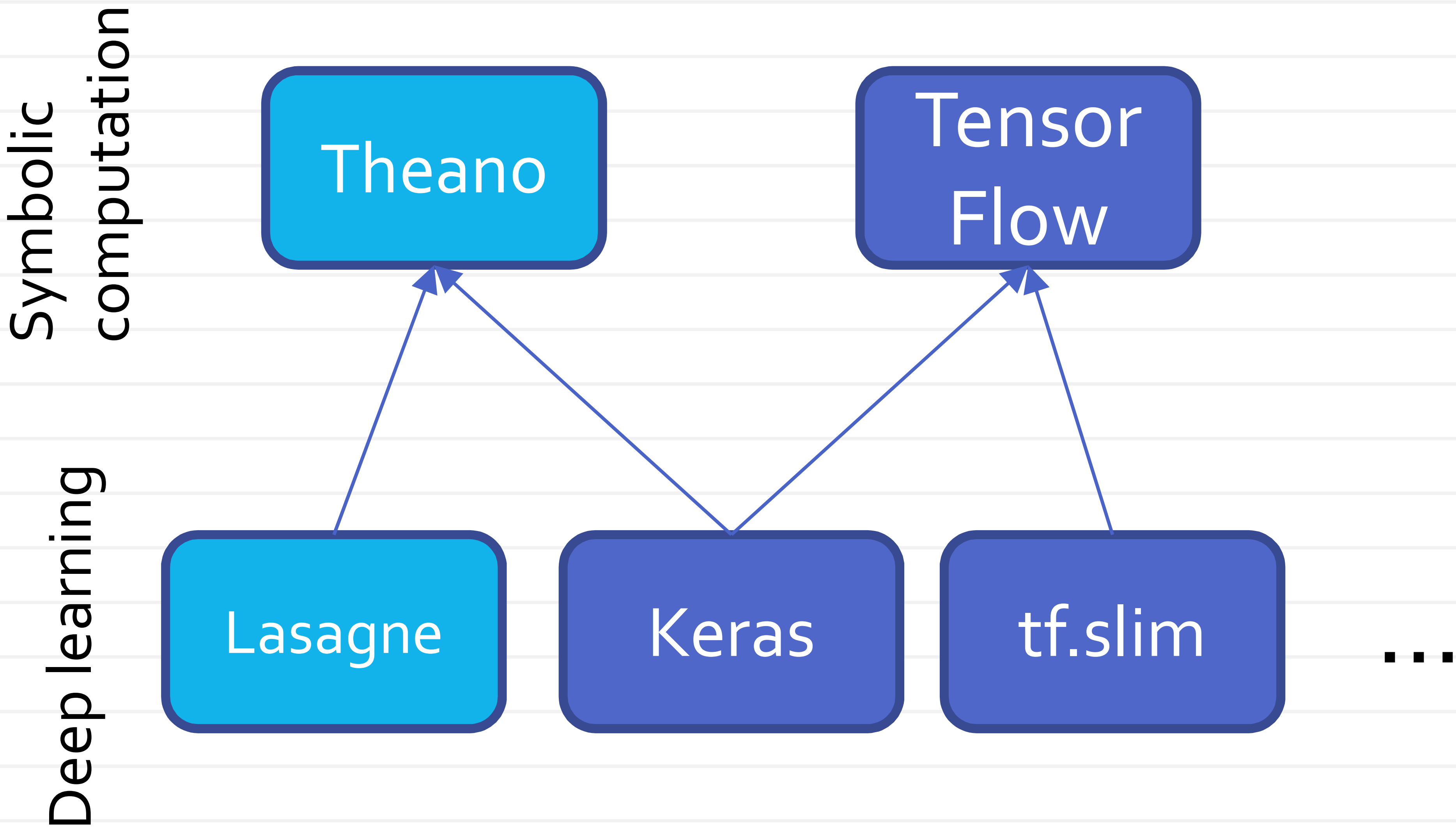
Data providers

Deep learning/symbolic comp. packages

- All packages facilitate stacking layers and defining new layers
- Differ on languages/levels of granularity
- Some allow **symbolic differentiation**
- Some allow **automatic differentiation**



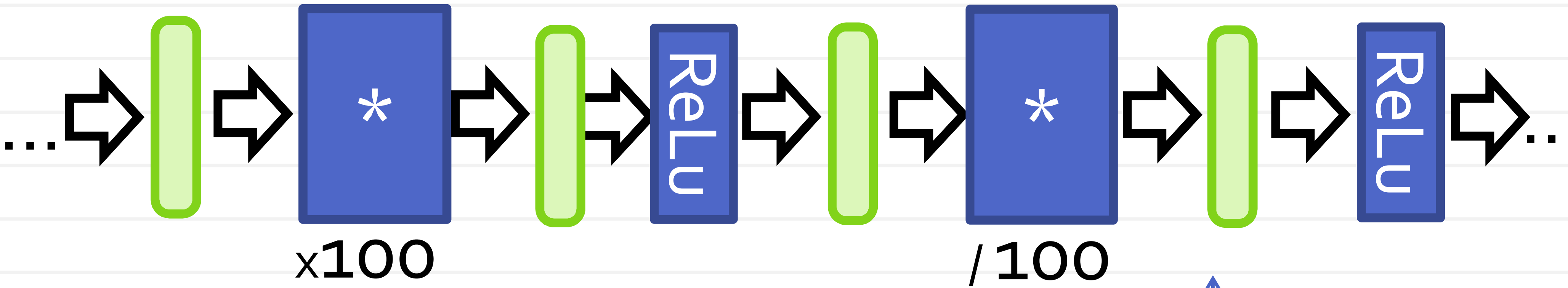
Theano and TensorFlow "ecosystems"



Other DL packages

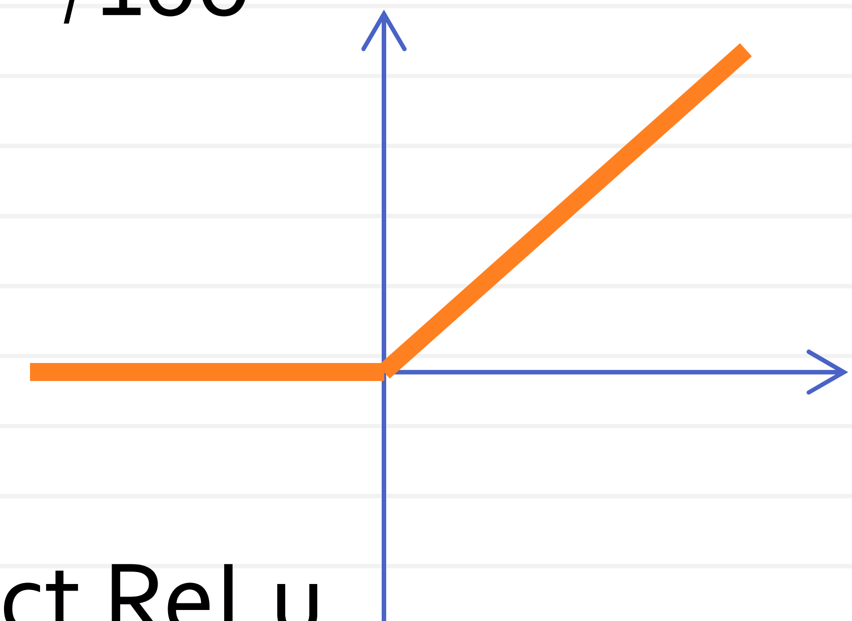
- Torch (Lua/C++), +autograd
- PyTorch, Chainer (Python, autodiff included)
- Caffe (C++ lmdb, Python/Matlab intefaces)
- MxNet (C++, Python, Julia, R, JavaScript)
- MatConvNet (MATLAB)
- ….

Reparameterization in ReLu Networks



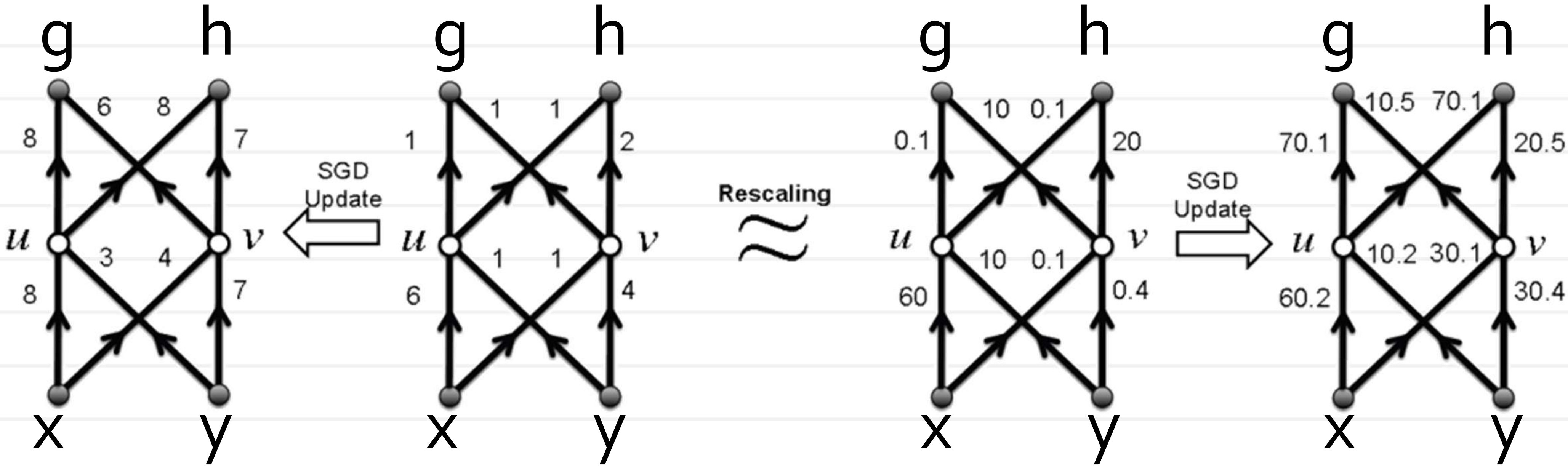
$\alpha > 0$

$1/\alpha \, \mathrm{ReLu}(\alpha\, x) = \mathrm{ReLu}\,(x)$

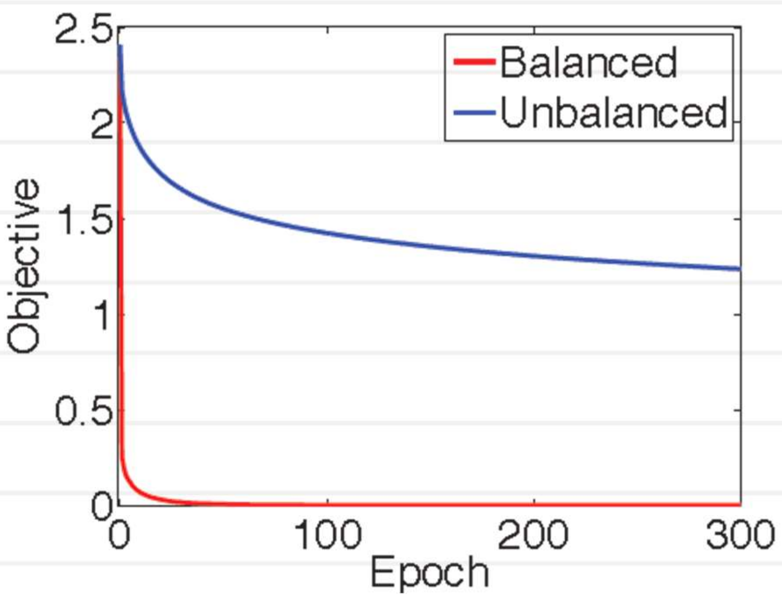


Thus: we can easily construct ReLu networks with **different** weights implementing the **same** function

Gauge freedom and SGD

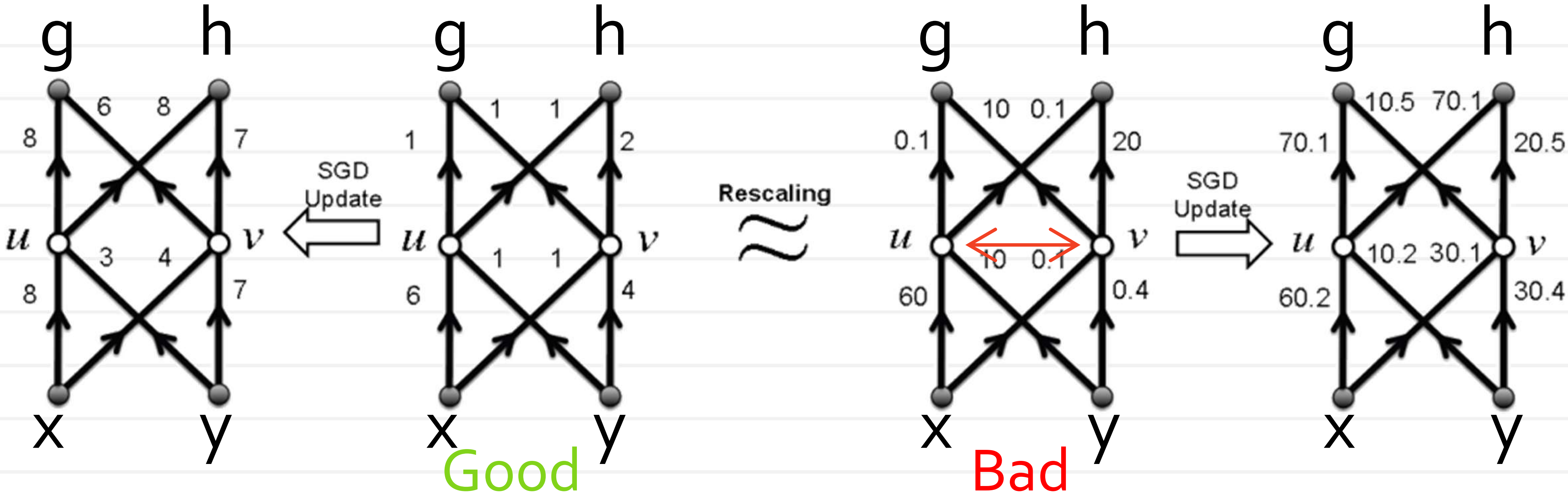


1 SGD step for (x,y = 1,1) and L = g+h



[Neyshabur, Salakhutdinov, Srebro, Path-SGD: Path-Normalized Optimization in Deep Neural Networks, NIPS2015]

Initialization schemes



- **Basic idea 1:** units should have comparable total input weights
- **Basic idea 2:** use layers which keep magnitude
- E.g. [Glorot&Bengio 2010] aka "Xavier-initialization":

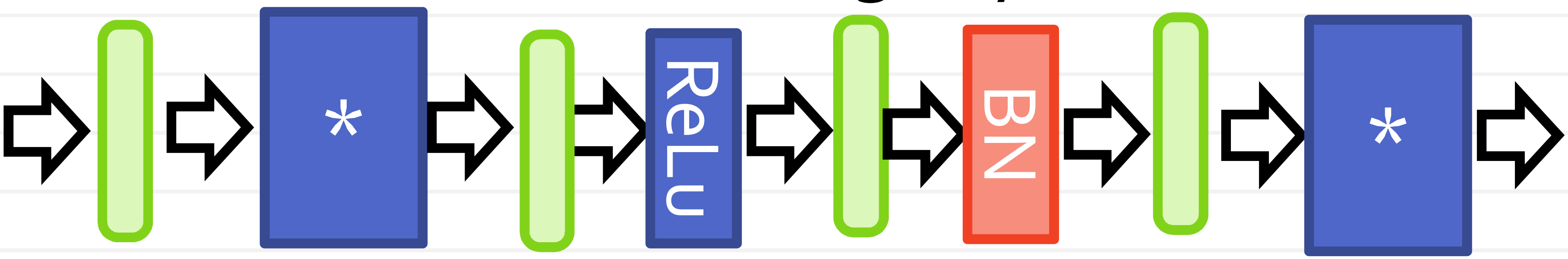
$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}, \frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}\right]$$

- E.g. [He et al, Arxiv15] for ReLu networks:

$$W \sim \mathcal{N}(0, \sqrt{2/n_i})$$

Batch normalization

[Szegedy and Ioffe 2015]

...


...

- Makes the training process invariant to some re-parameterizations
- Use mini-batch statistics at training time
- Use population statistics at test time
- At test time can be "incorporated" into adjacent multiplicative layer

Batch normalization layer

covariant to reparameterization

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

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

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

learnable by SGD

[Szegedy and Ioffe 2015]

"All you need is a good init"

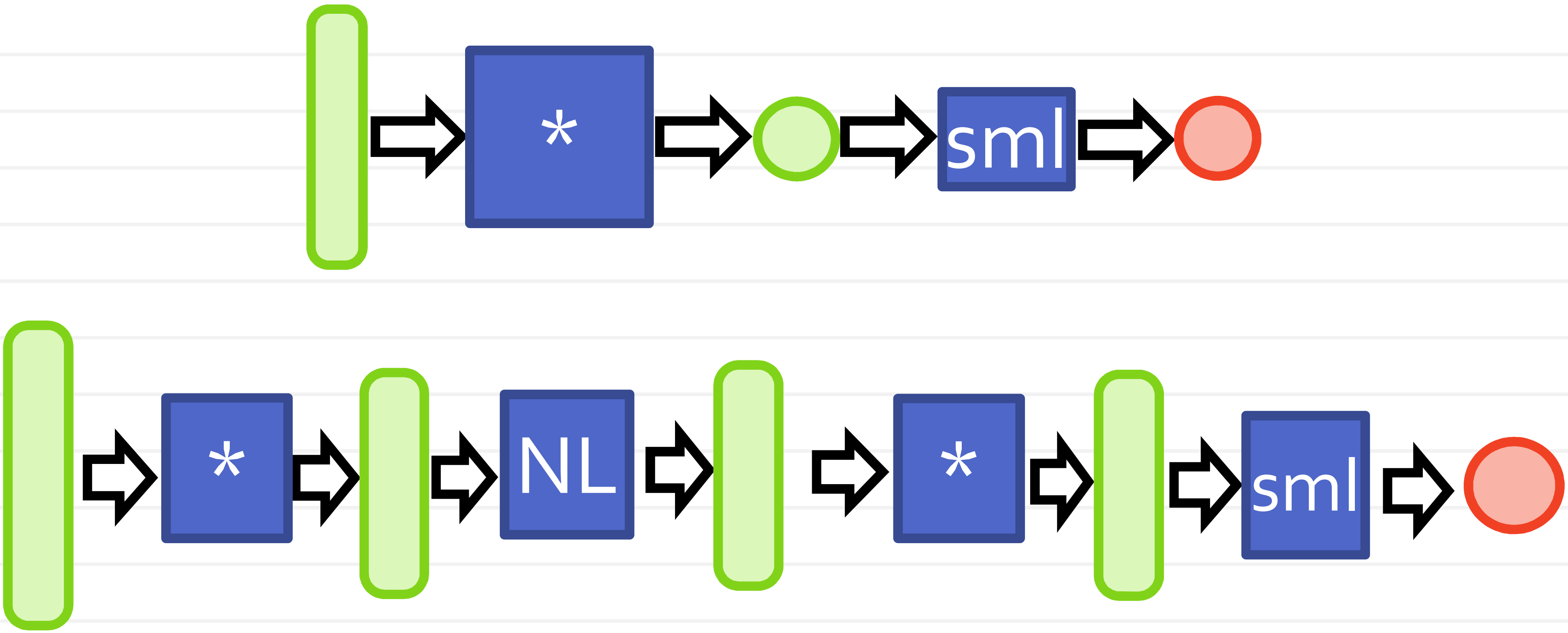
Algorithm 1 Layer-sequential unit-variance orthogonal initialization. L – convolution or full-connected layer, W_L - its weights, B_L - its output blob., Tol_{var} - variance tolerance, T_i – current trial, T_{max} – max number of trials.

Pre-initialize network with orthonormal matrices as in Saxe et al. (2014)
for each layer L **do**
  while $|Var(B_L) - 1.0| \geq Tol_{var}$ and $(T_i < T_{max})$ **do**
    do Forward pass with a mini-batch
    calculate $Var(B_L)$
    $W_L = W_L \ / \ \sqrt{Var(B_L)}$
  end while
end for

- Initialize with orthonormal matrices (using SVD) – orthogonal columns
- Re-normalize (as in batchnorm)

[Mishkin & Matas, ICLR16]

Back to regularization



- Overfitting is severe for deep models (why?)
- The progress on deep learning was "delayed" till huge amount of data

Recap: regularization

4 strategies to avoid overfitting (aka *regularize learning*):

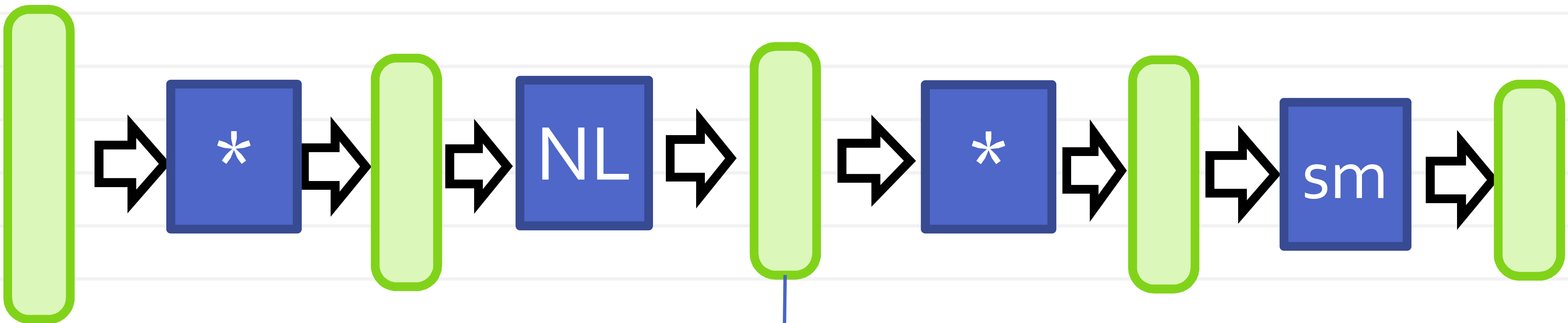
- Pick a “simpler” model (e.g. conv nets)
- Stop optimization early (always keep checking progress on)
- Impose smoothness (weight decay)
- Bag multiple models

Bagging multiple NN

- Different local minima help
- Diversifying architectures helps even more
- Unit weights are often prefered to tuned weights
- (Almost) all classification competitions are won by ensembles of deep models

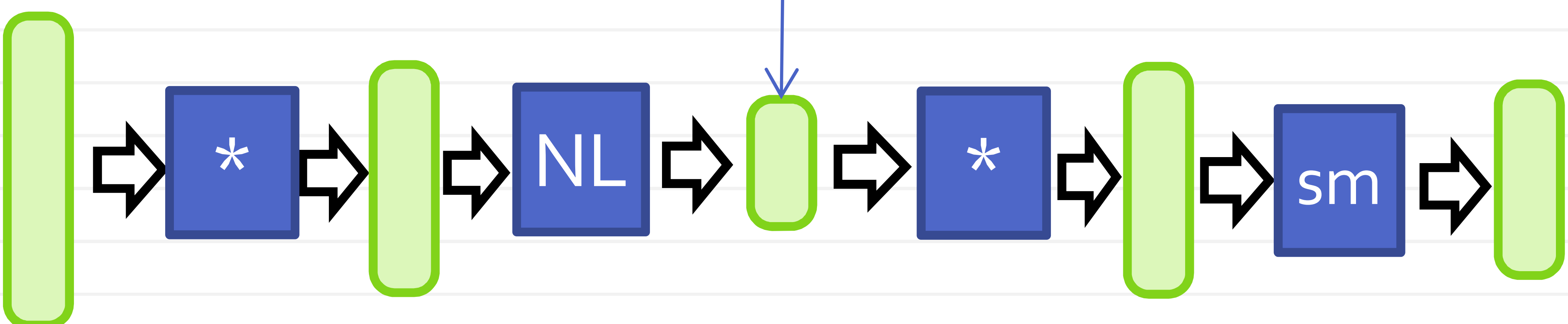
Dropout idea

Pseudo-ensemble training:



A derived model:

subsampling

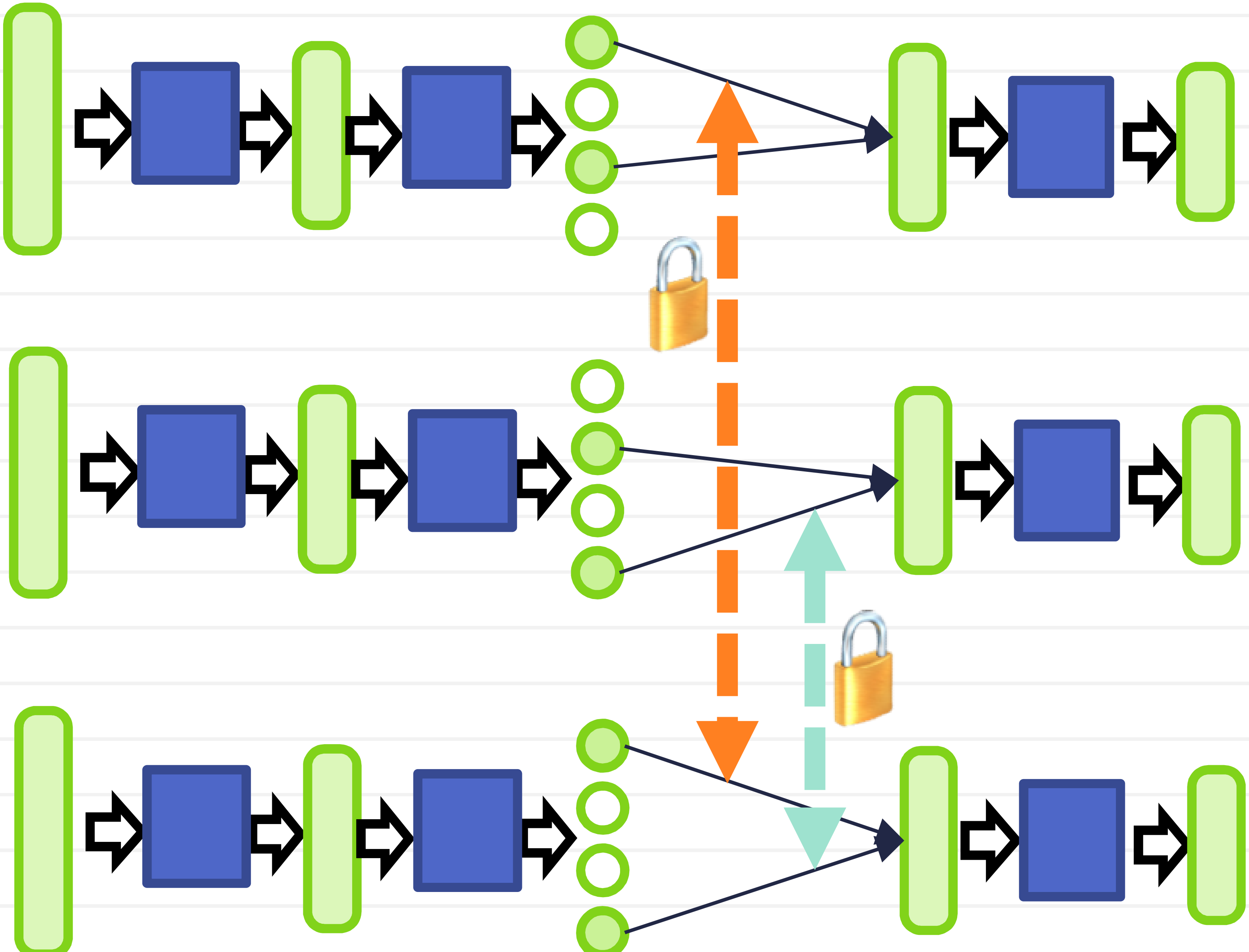


Goal: "train" an exponential number of such reduced models

[Srivastava et al. 2011]

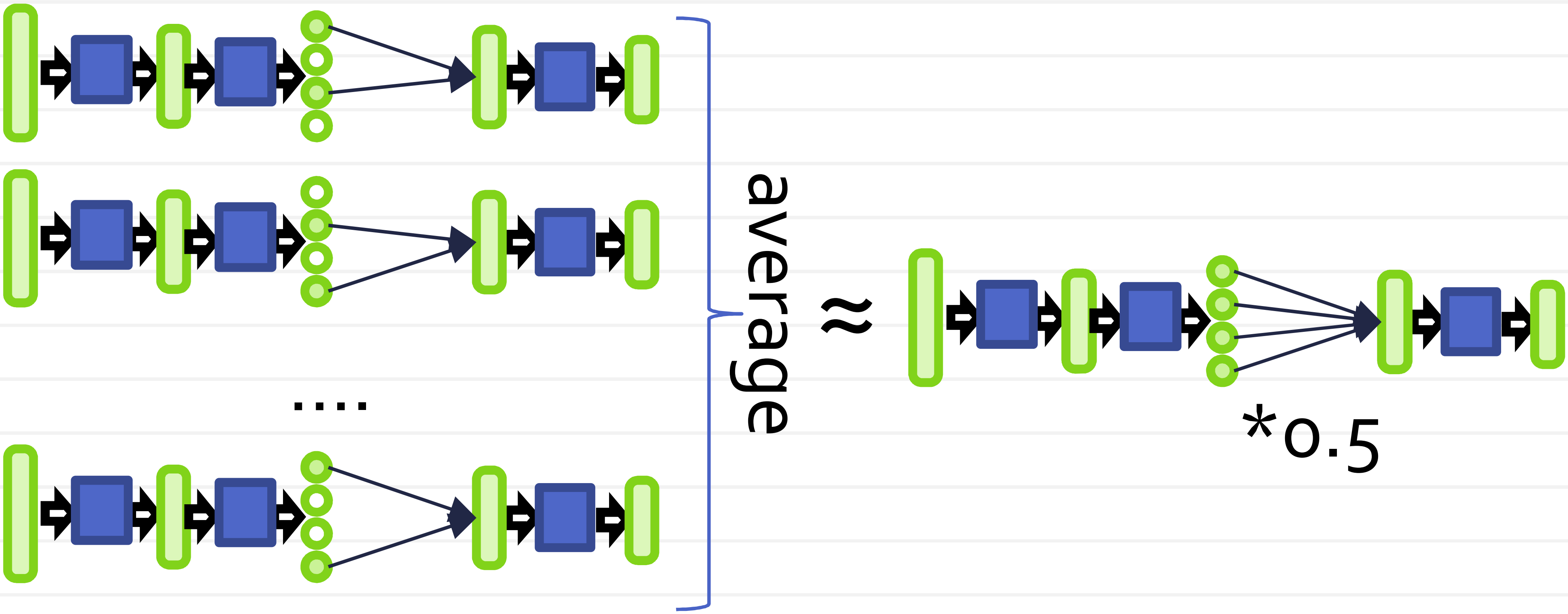
Dropout idea: train time

Training a very big ensemble of models:



[Srivastava et al. 2011]

Dropout idea: from train to test

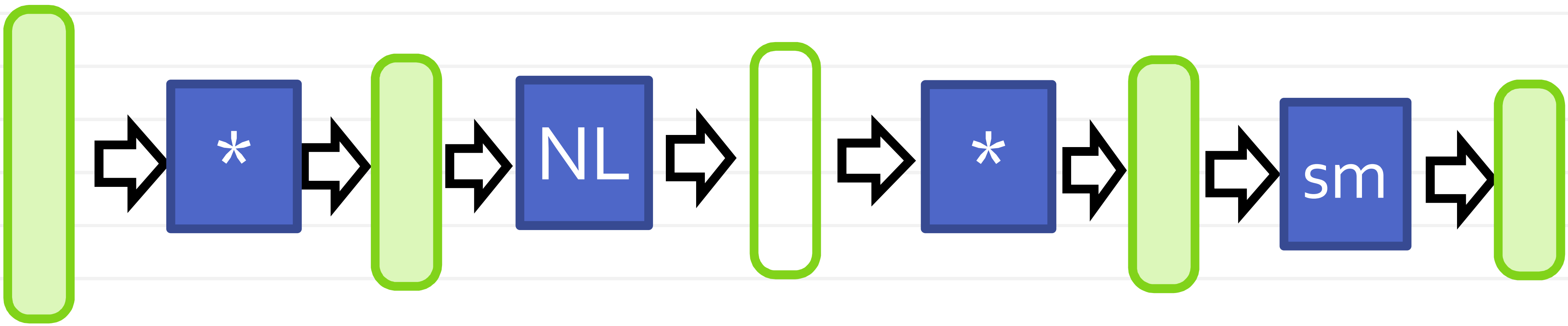


- Approximation is not exact for the last layer
- …but works well in practice

[Srivastava et al. 2011]

Dropout idea: recap

Pseudo-ensemble training:



- At training time, define which units are active at random (*mask*)
- At test time, let them all be active but multiply by dropout probability

[Srivastava et al. 2011]

How to implement dropout

Define it as a layer!

Forward propagation:

$$n \sim \text{Bernoulli}(p)$$

$$y = x \odot n$$

Backward propagation:

$$\frac{dz}{dx} = \frac{dz}{dy} \odot n$$

At test time: average all models with n=1/p

Recap

- Deep learning emerge naturally from shallow models (e.g. logistic regression)
- Loose connection to biological neural networks
- Modular paradigm is important
- Several very good packages for feed-forward models exist

Bibliography

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Attribute and simile classifiers for face verification. ICCV 2009: 365-372

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