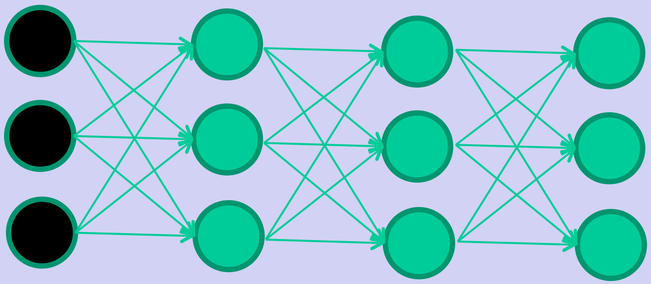
Introduction to Deep Learning

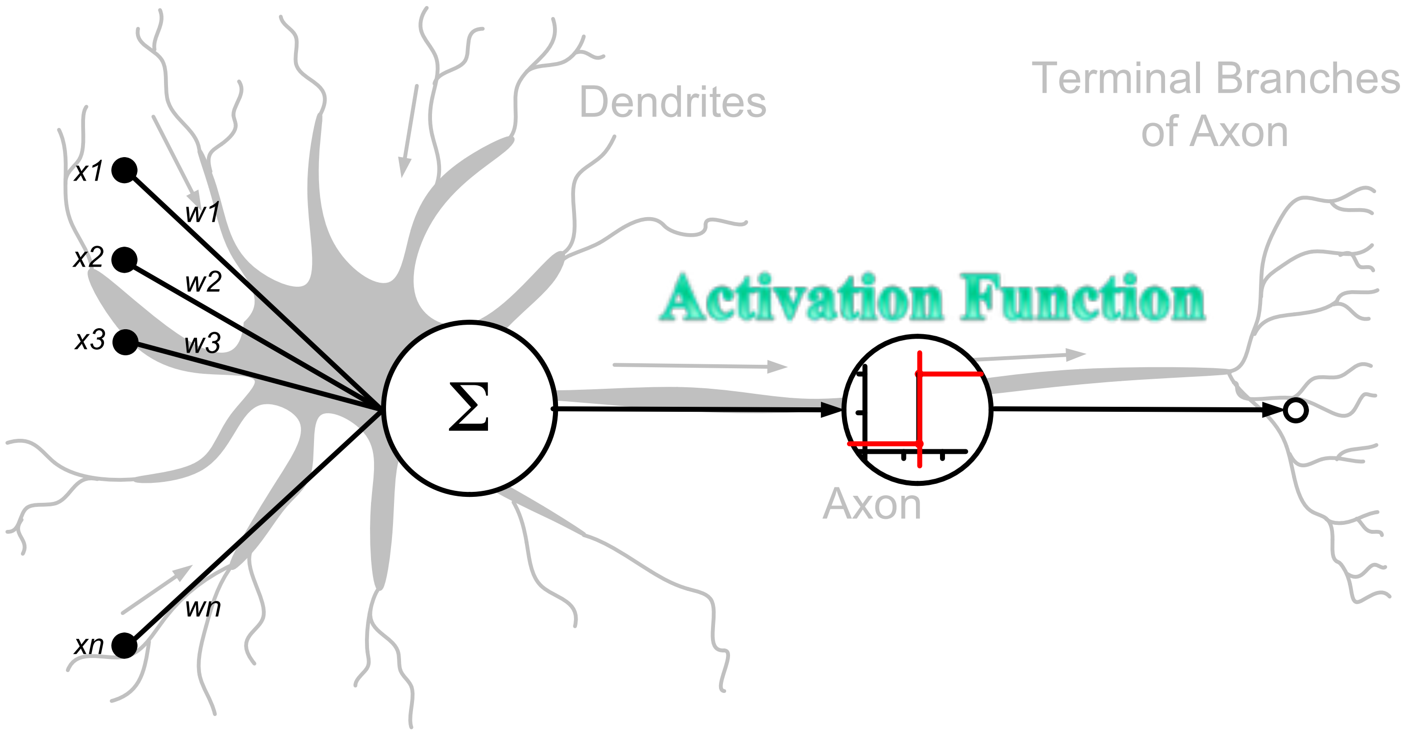
Some slides and images are taken from:

David Wolfe Corne https://www.macs.hw.ac.uk/~dwcorne/Teaching/introdl.ppt
Wikipedia
Geoffrey A. Hinton

Feedforward networks for function approximation and classification

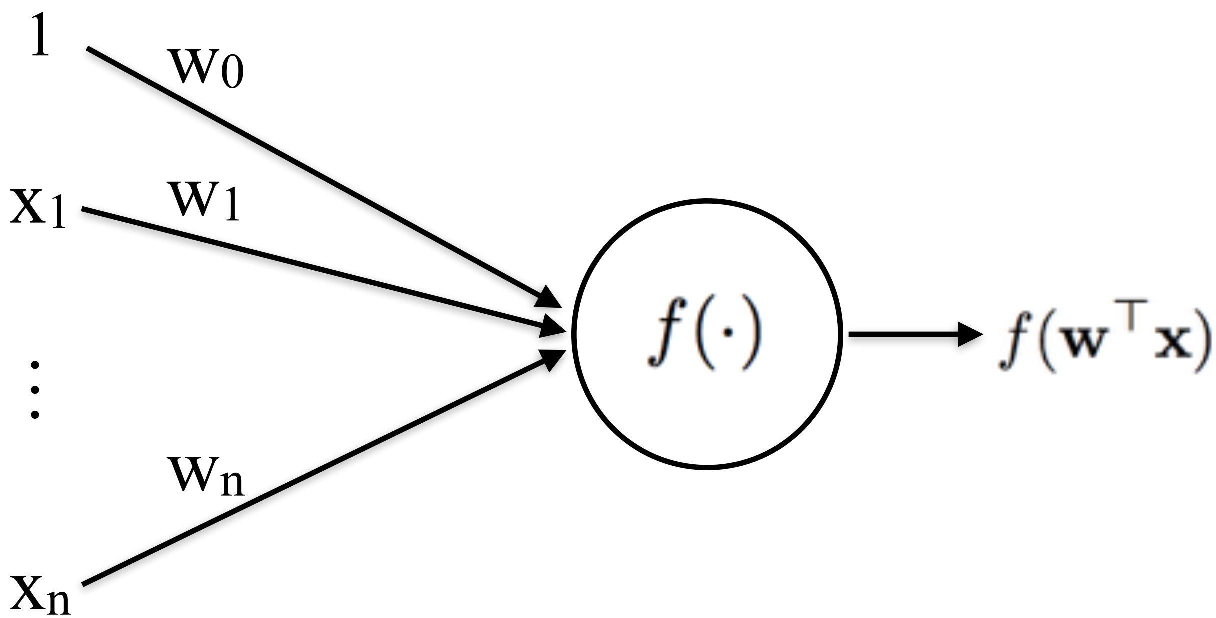


- Feedforward networks
- Deep tensor networks
- ConvNets

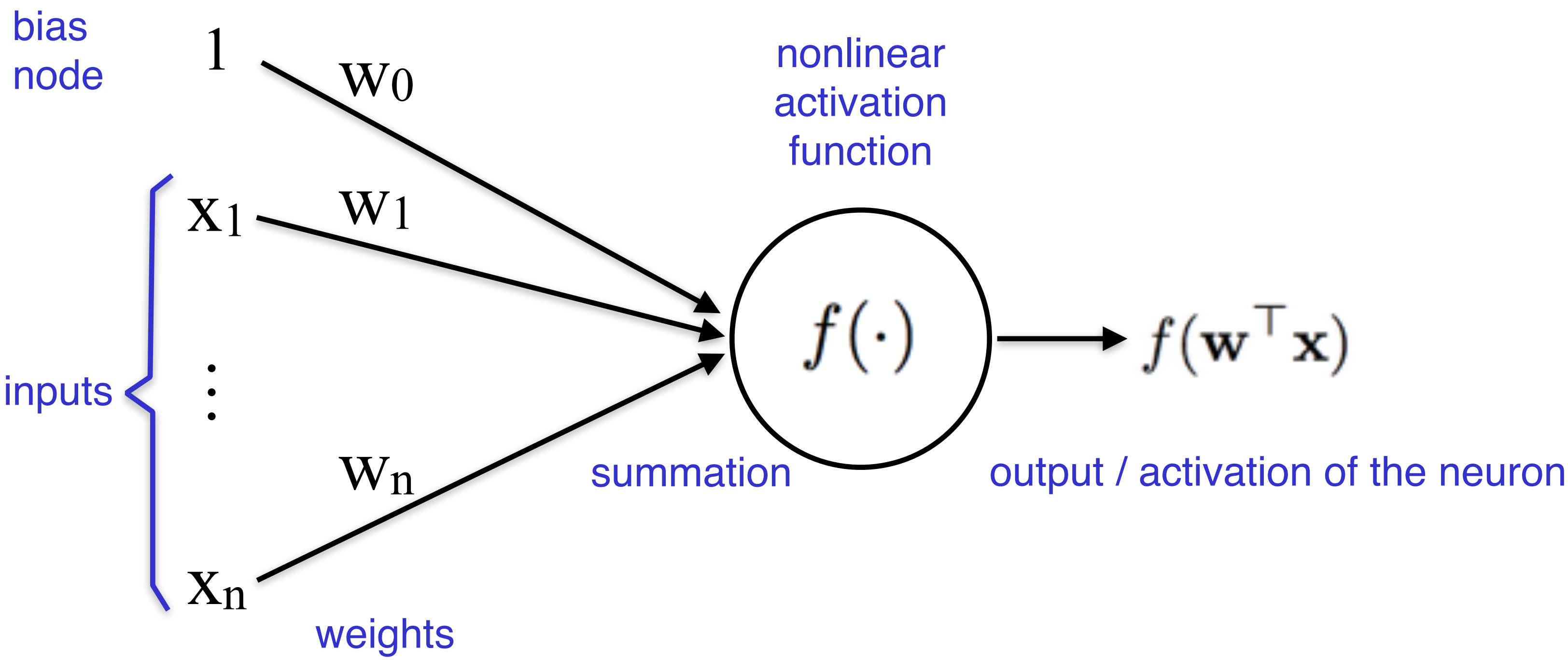


Dendrites
Terminal Branches of Axon
x1
x2
x3
xn
w1
w2
w3
wn
Σ
Activation Function
Axon

A single artificial neuron

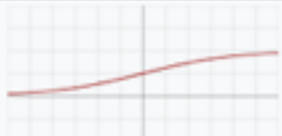
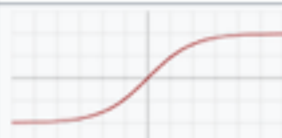
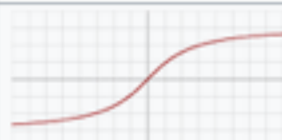
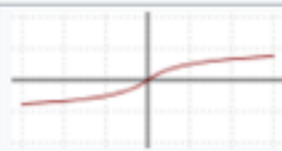


A single artificial neuron



Activation functions

https://en.wikipedia.org/wiki/Activation_function

Identity		$f(x) = x$
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Logistic (a.k.a. Soft step)		$f(x) = \dfrac{1}{1 + e^{-x}}$
TanH		$f(x) = \tanh(x) = \dfrac{2}{1 + e^{-2x}} - 1$
ArcTan		$f(x) = \tan^{-1}(x)$
Softsign [7][8]		$f(x) = \dfrac{x}{1 + \lvert x \rvert}$
Rectified linear unit (ReLU)[9]		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$

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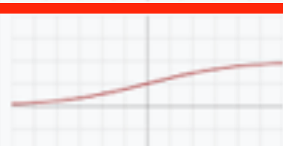
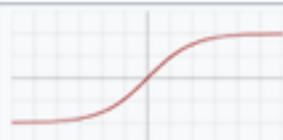
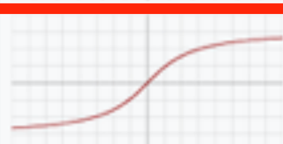
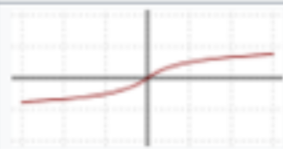
Logistic (a.k.a. Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$
TanH		$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$
ArcTan		$f(x) = \tan^{-1}(x)$
Softsign [7][8]		$f(x) = \frac{x}{1 + \lvert x \rvert}$
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Traditionally used

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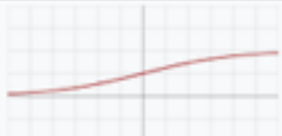
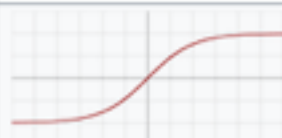
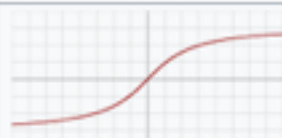
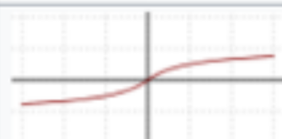
Logistic (a.k.a. Soft step)		$f(x) = \frac{1}{1+e^{-x}}$
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$
ArcTan		$f(x) = \tan^{-1}(x)$
Softsign [7][8]		$f(x) = \frac{x}{1+\lvert x \rvert}$
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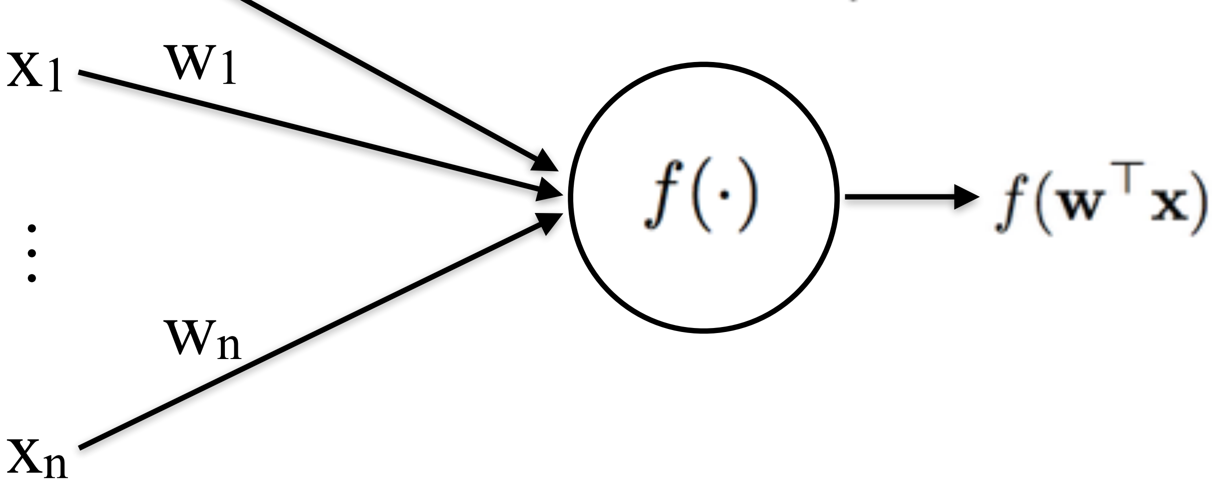
Currently most widely used. Empirically easier to train and results in sparse networks.

Nair and Hinton: Rectified linear units improve restricted Boltzmann machines ICLM'10, 807-814 (2010)
Glorot, Bordes and Bengio: Deep sparse rectifier neural networks. PMLR 15:315-323 (2011)

Perceptron (Rosenblatt 1957)

Used as a binary classifier - equivalent to support vector machine (SVM)

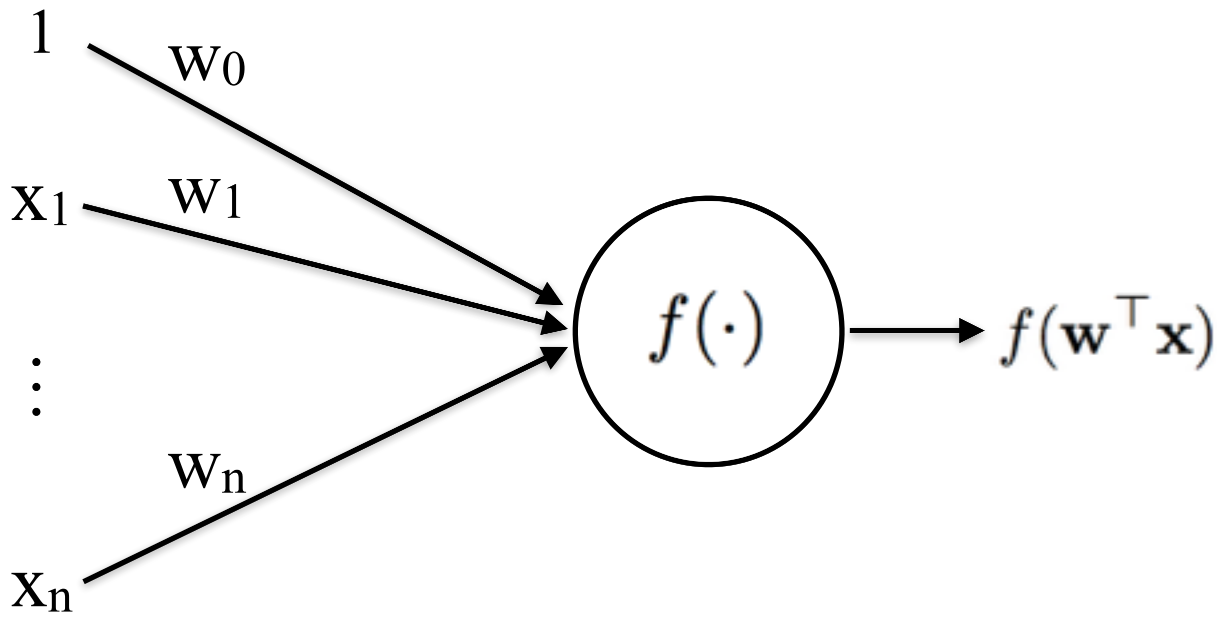
$$f(x) = \begin{cases} 1 & \text{if } w \cdot x > 0 \\ 0 & \text{otherwise} \end{cases}$$

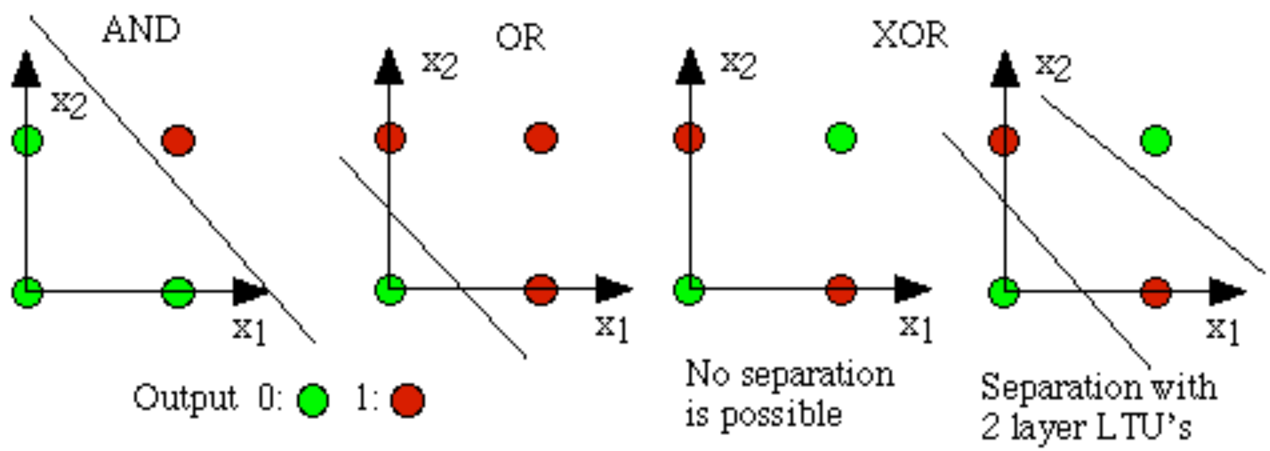


Train weights using examples $D = \{(\mathbf{x}_1, d_1), ..., (\mathbf{x}_S, d_S)\}$:

1. Initialize $\mathbf{w}$ with random values
2. For each example $(\mathbf{x}_j, d_j)$:
   (a) Calculate output: $y_j = f(\mathbf{w}^\top \mathbf{x}_j)$
   (b) Update weights: $\mathbf{w} \leftarrow \mathbf{w} + (d_j - y_j)\mathbf{x}_j$
3. Repeat 2 until convergence.

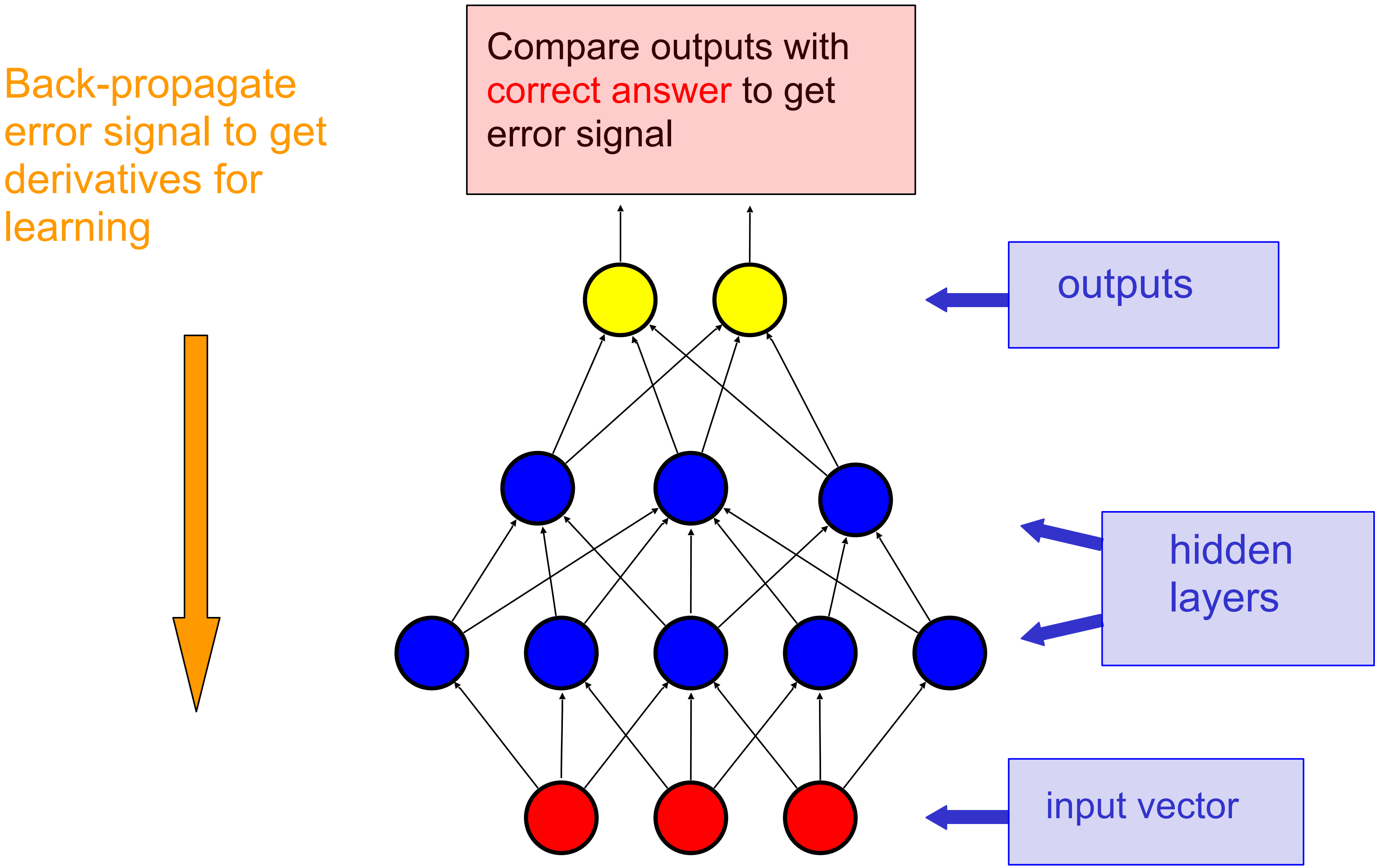
Perceptron (Rosenblatt 1957)





Second-generation neural networks (~1985)

Slide credit : Geoffrey Hinton



Second-generation neural networks (~1985)

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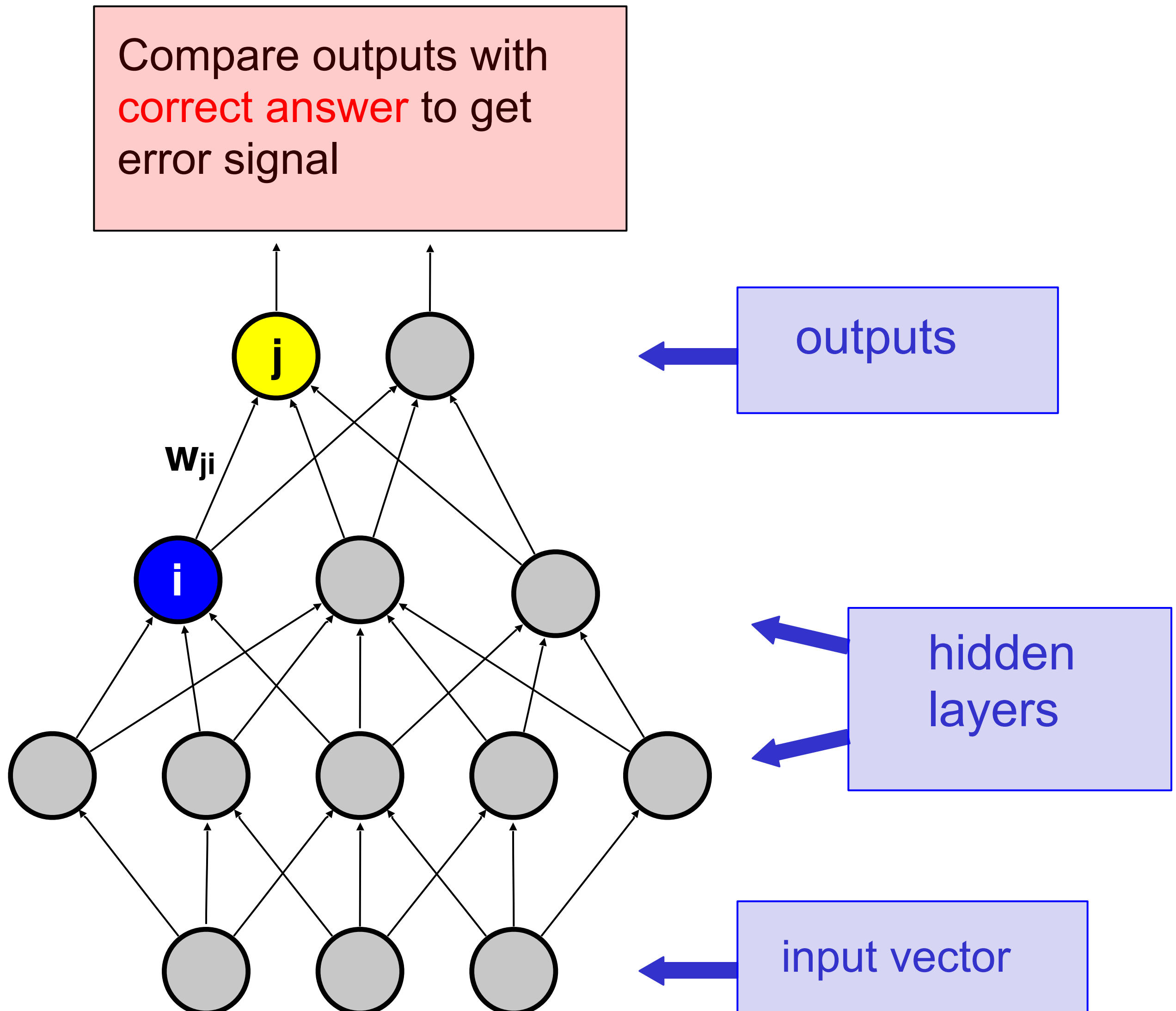
Error at output for a given example:

$$E = \frac{1}{2}\sum_j (y_j - d_j)^2$$



Second-generation neural networks (~1985)

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Error at output for a given example:

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Error sensitivity at output neuron j:

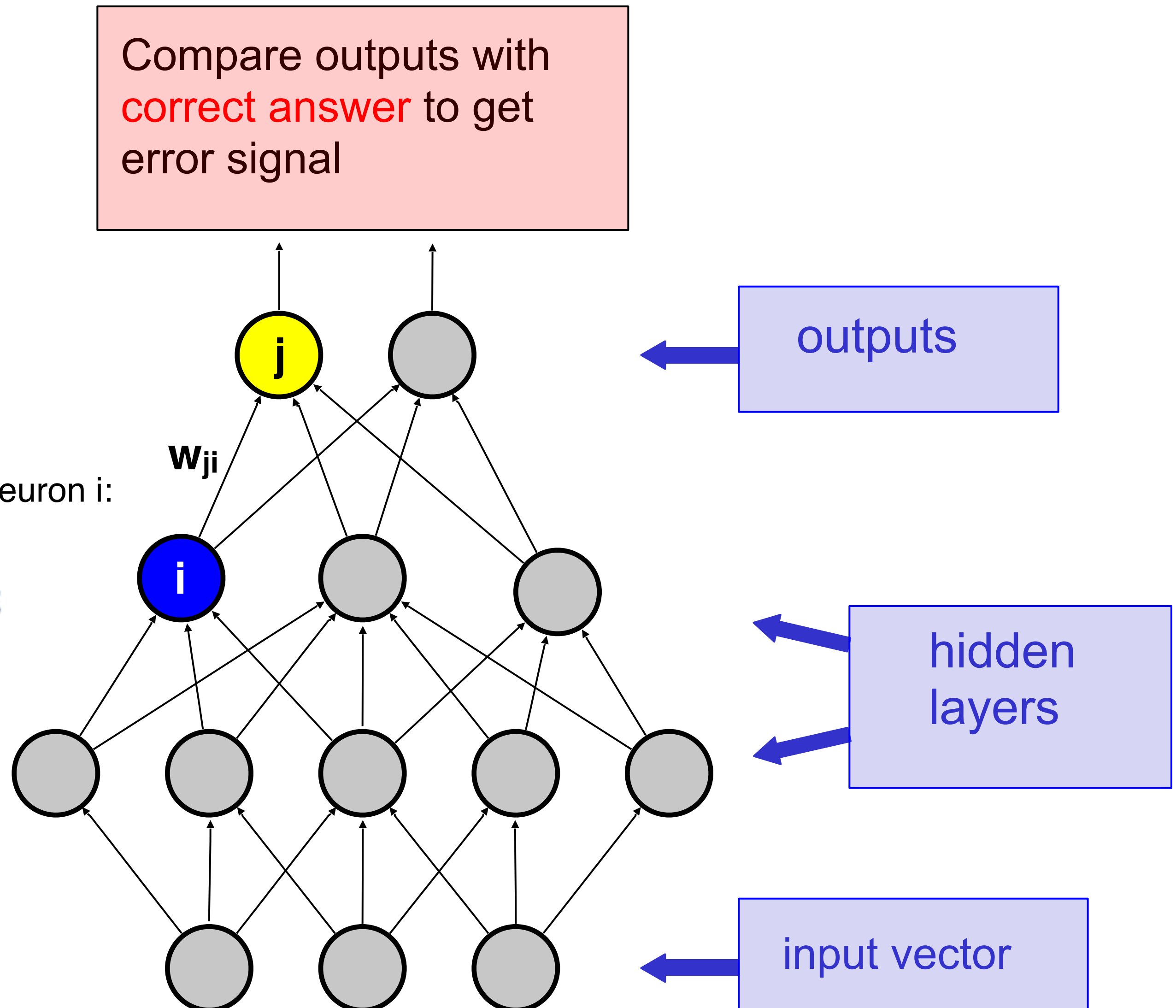
$$\frac{\partial E}{\partial y_j} = y_j - d_j$$

Backpropagate error sensitivity to neuron i:

$$\frac{\partial E}{\partial y_i} = \sum_j \frac{\partial E}{\partial y_j} f'(x_j) w_{ji}$$

Sensitivity on weight w_{ji}:

$$\frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial x_j} y_i$$



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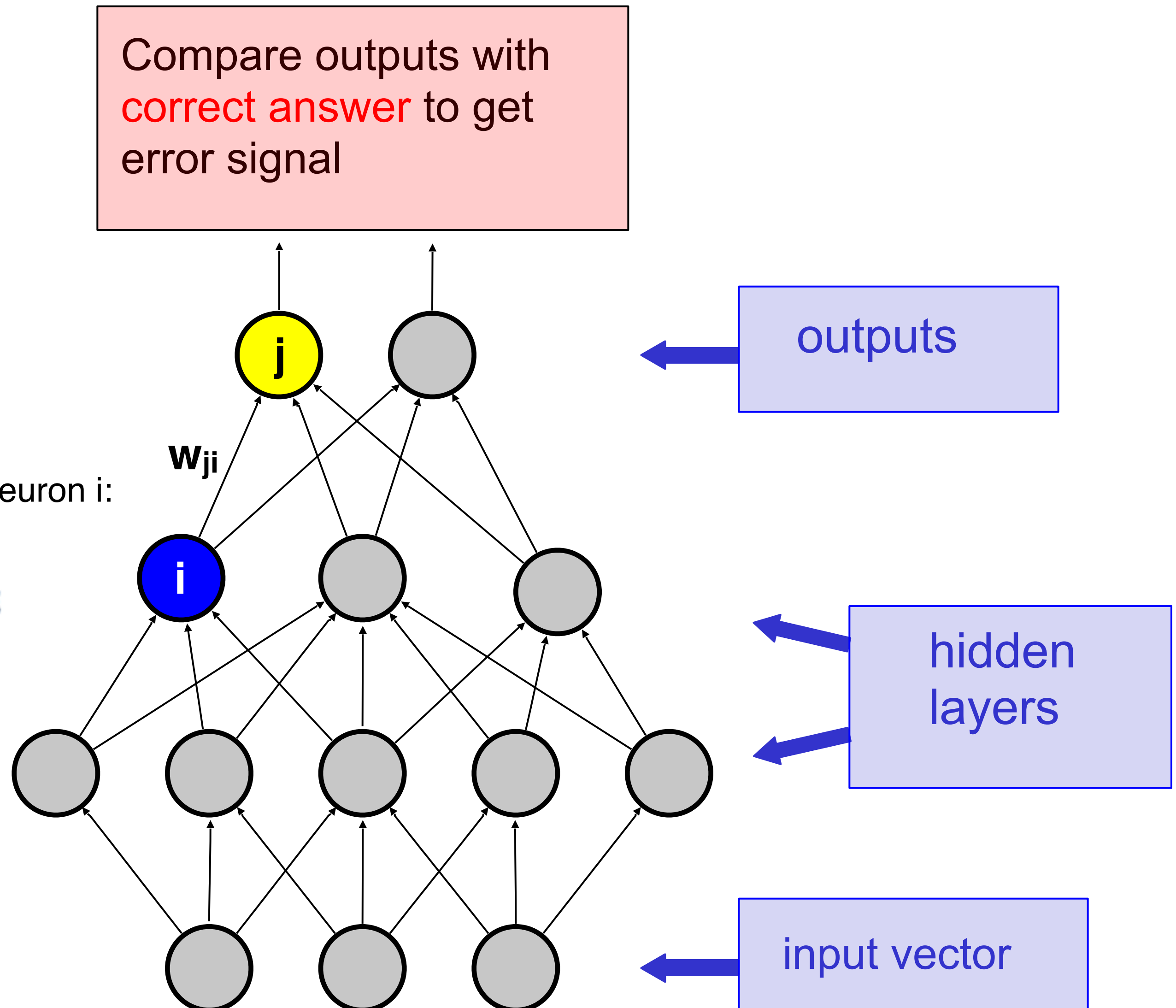
$$\frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial x_j} y_i$$

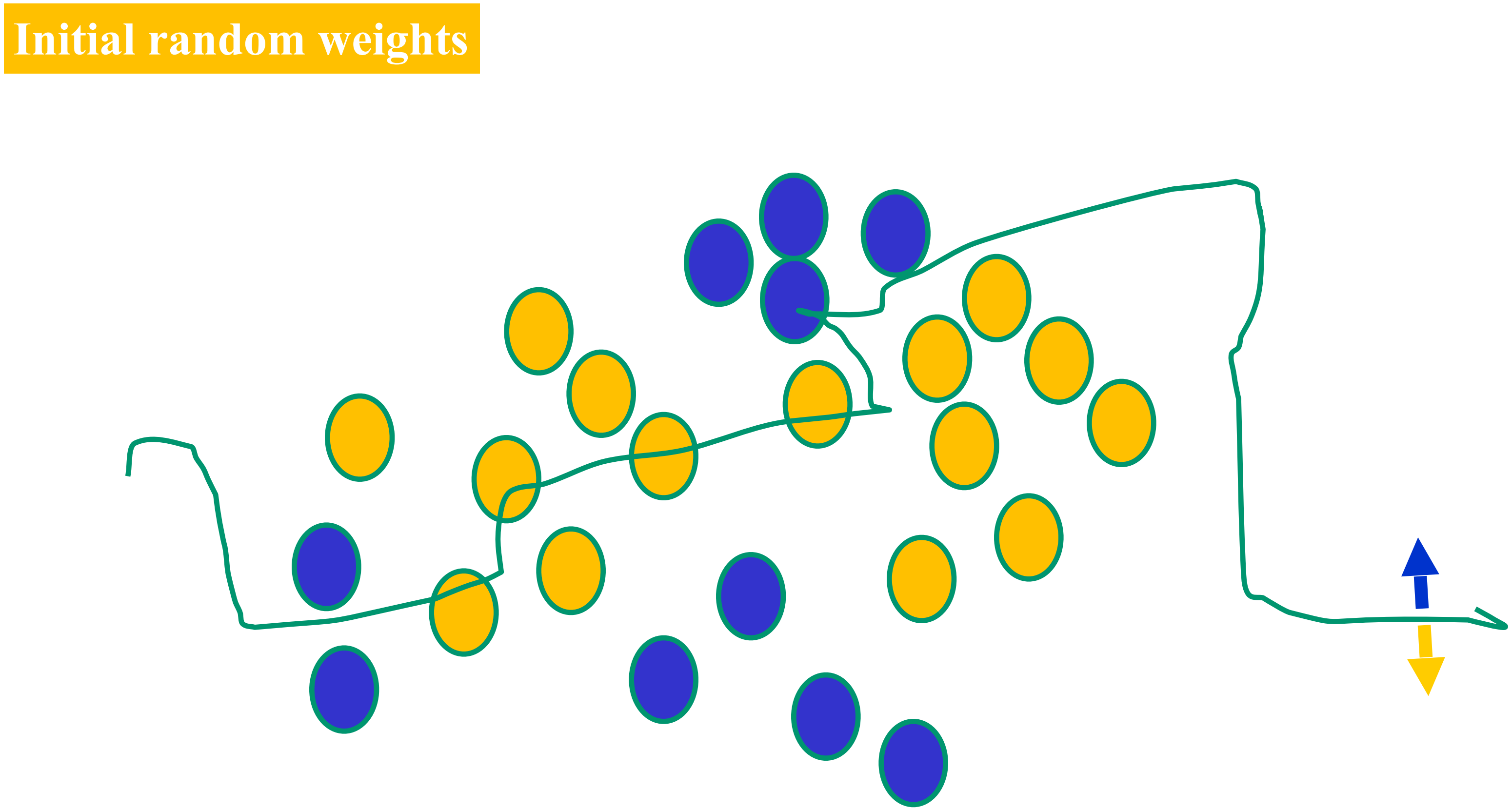
Update weight w_{ji}:

$$\Delta w_{ji} = -\epsilon \frac{\partial E}{\partial w_{ji}}$$

learning rate

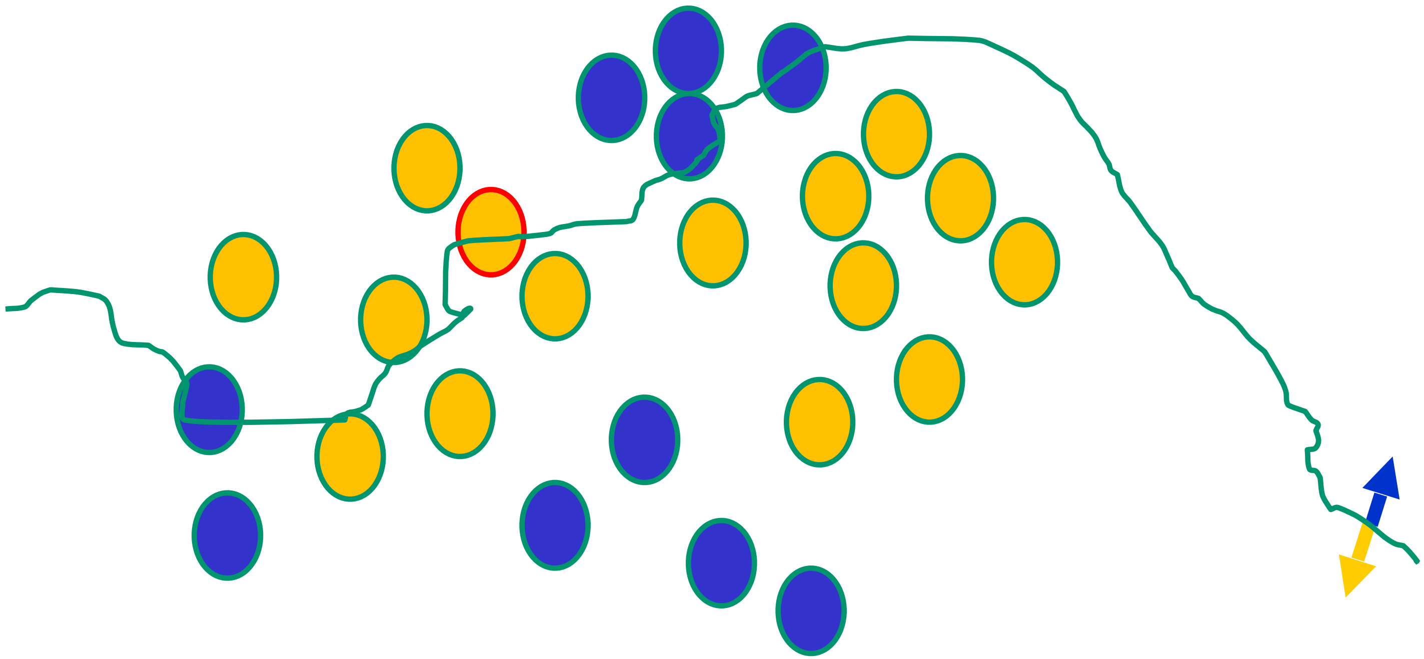


A decision boundary perspective on learning



A decision boundary perspective on learning

Present a training instance / adjust the weights



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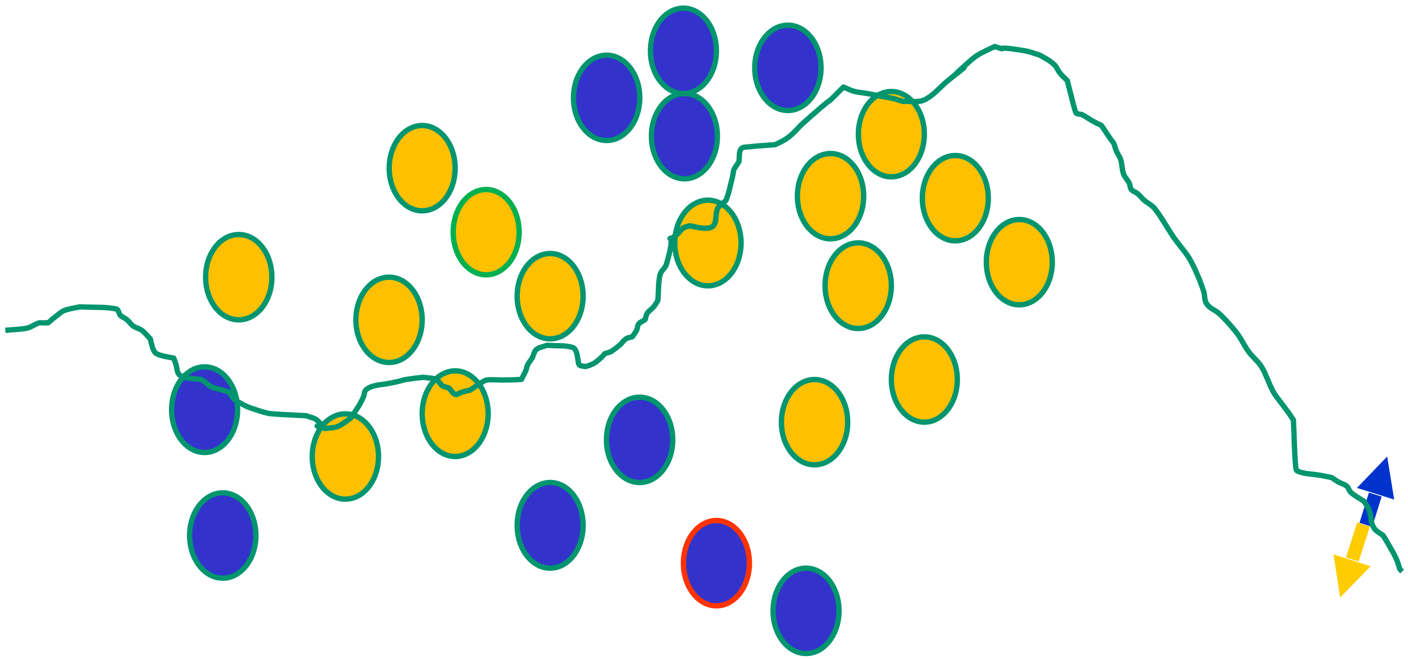

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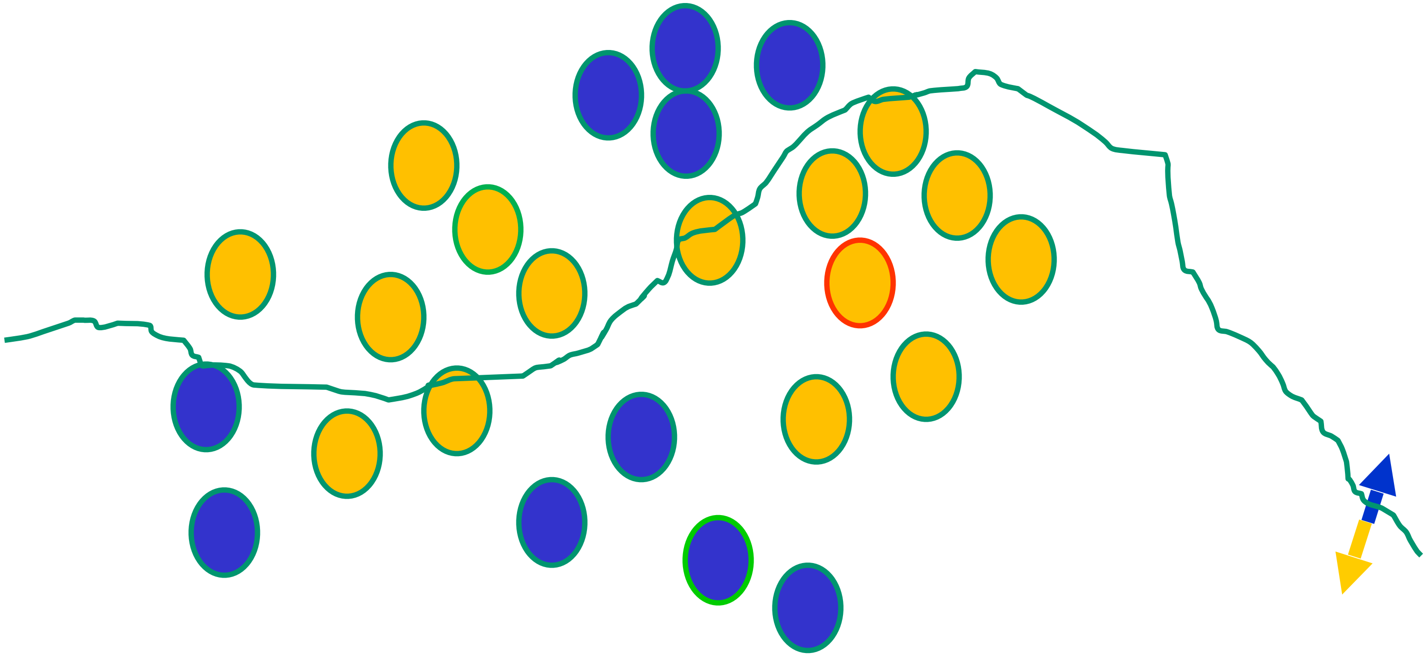

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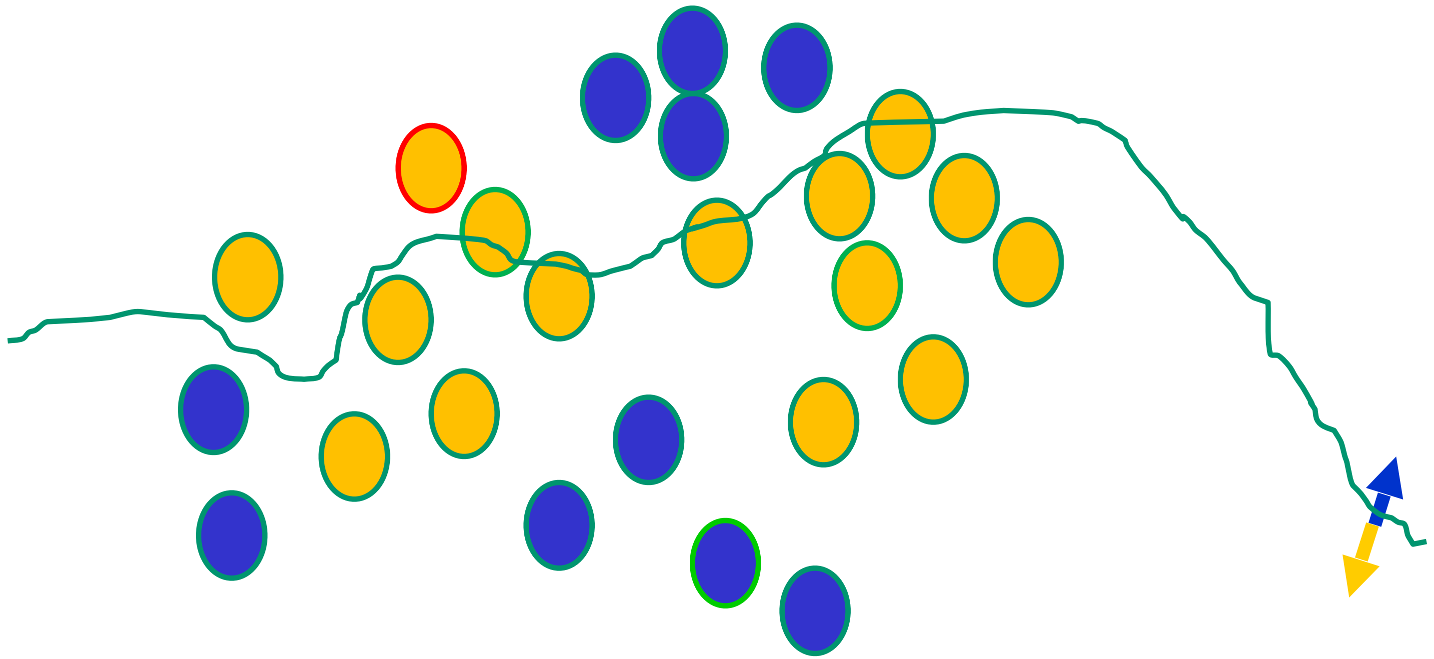
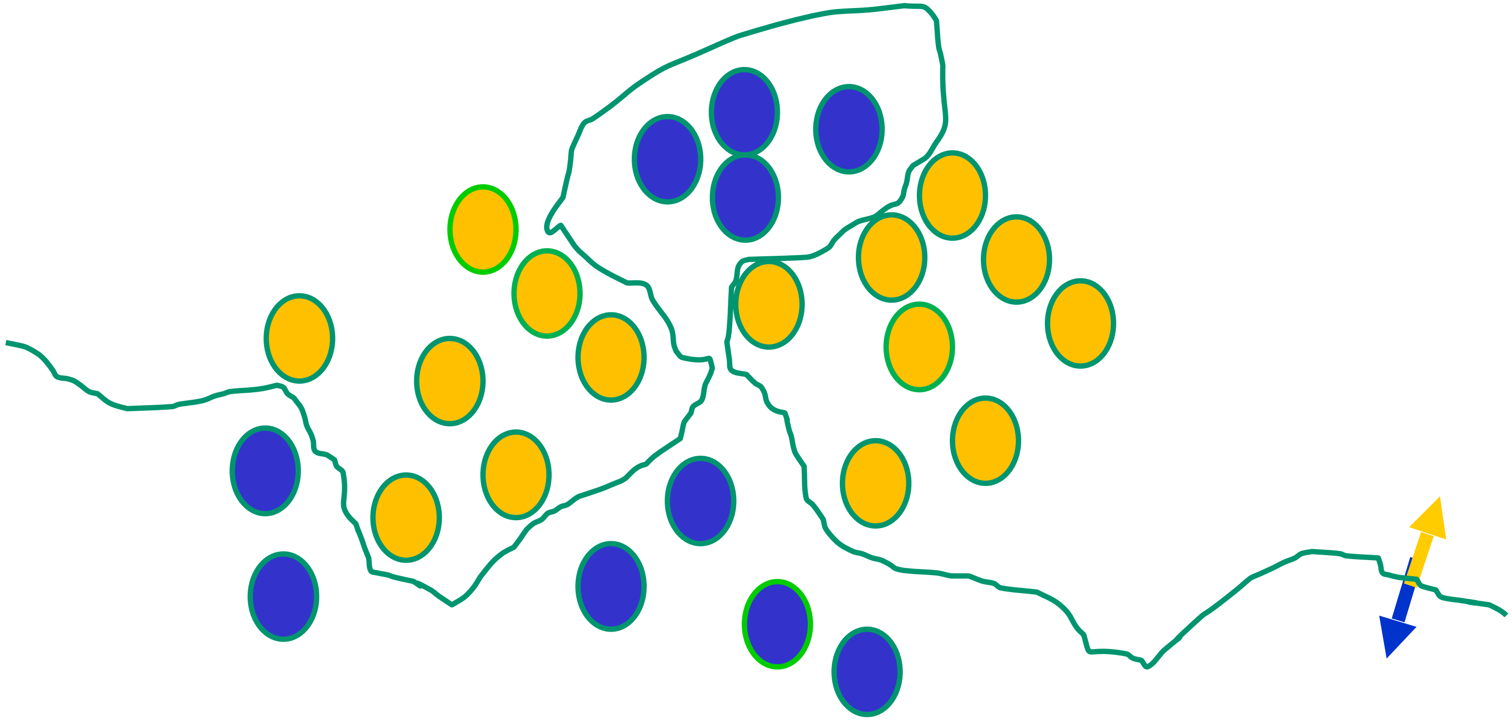


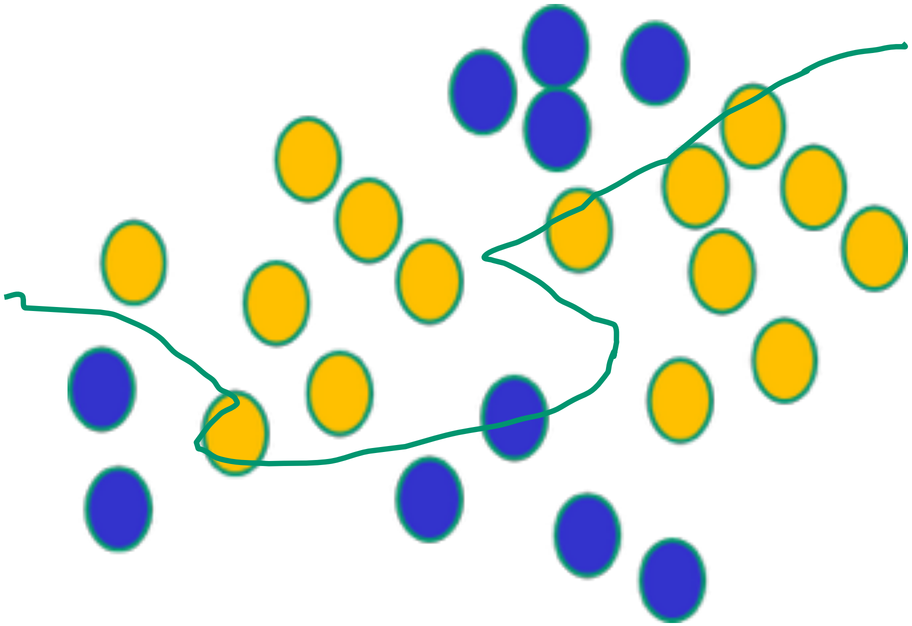
A decision boundary perspective on learning

Eventually ....

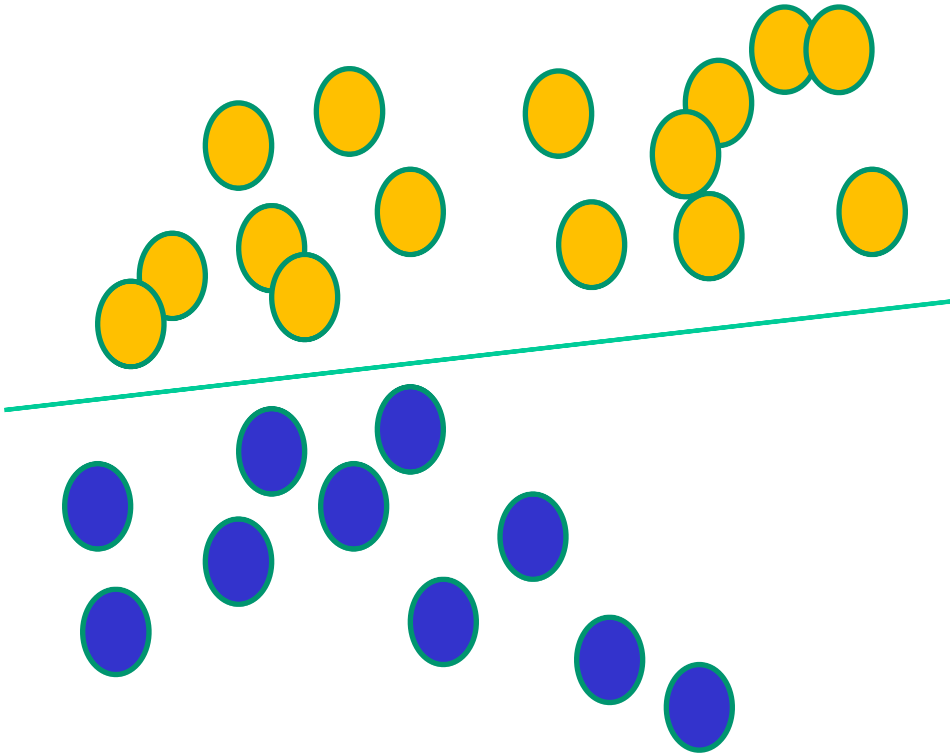


Nonlinear versus linear models

NNs use nonlinear *f*(x) so they can draw complex boundaries, but keep the data unchanged



Kernel methods only draw straight lines, but transform the data first in a way that makes it linearly separable

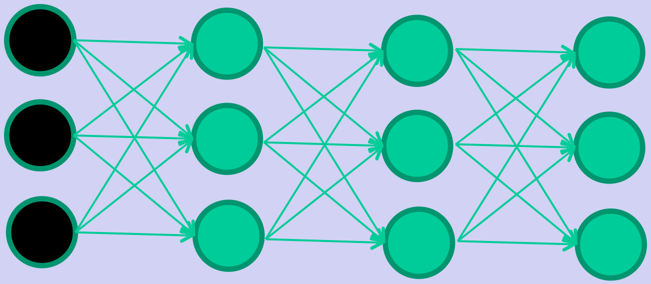


Universal Representation Theorem

- Networks with a **single** hidden layer can represent **any** function F(x) with arbitrary precision in the large hidden layer size limit

- However, that doesn‘t mean, networks with single hidden layers are efficient in representing arbitrary functions. For many datasets, deep networks can represent the function F(x) even with narrow layers.

What does a neural network learn?



Feature detectors

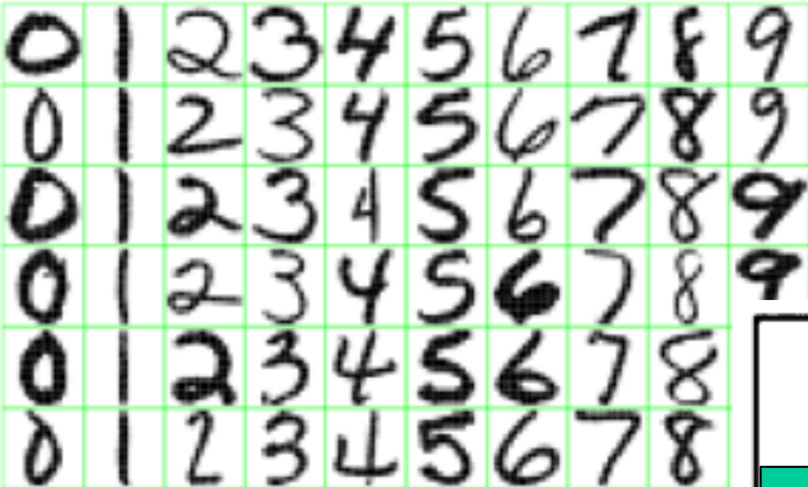
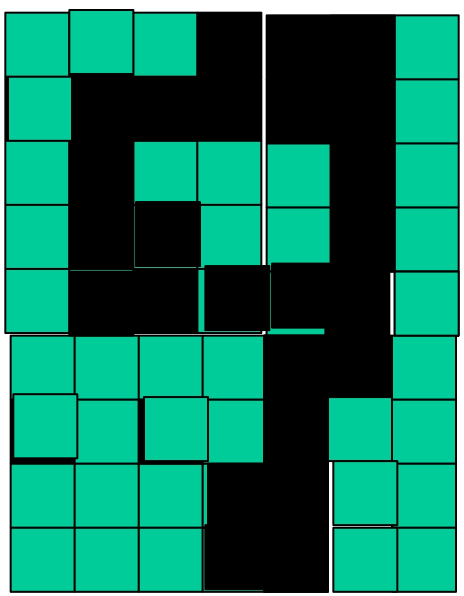
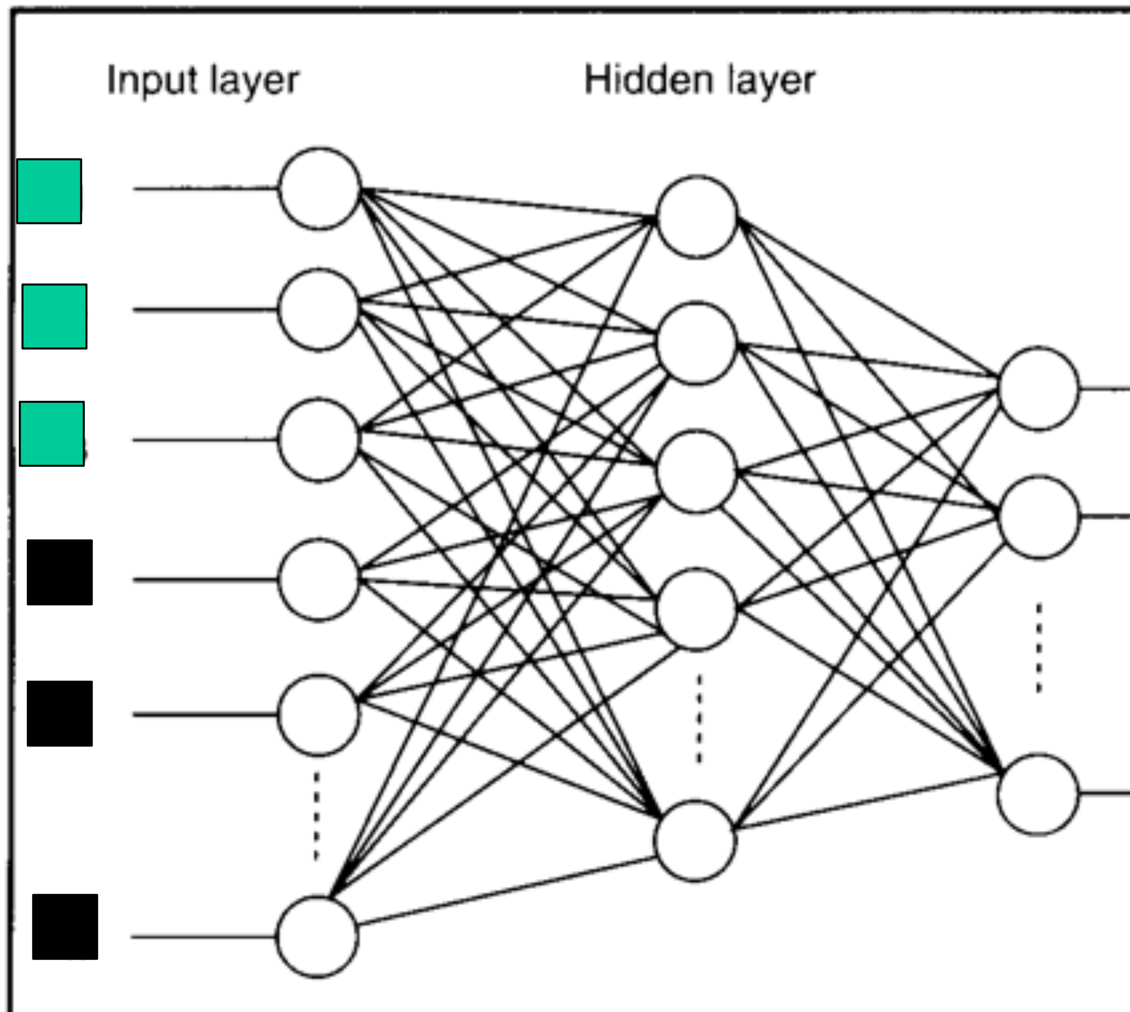
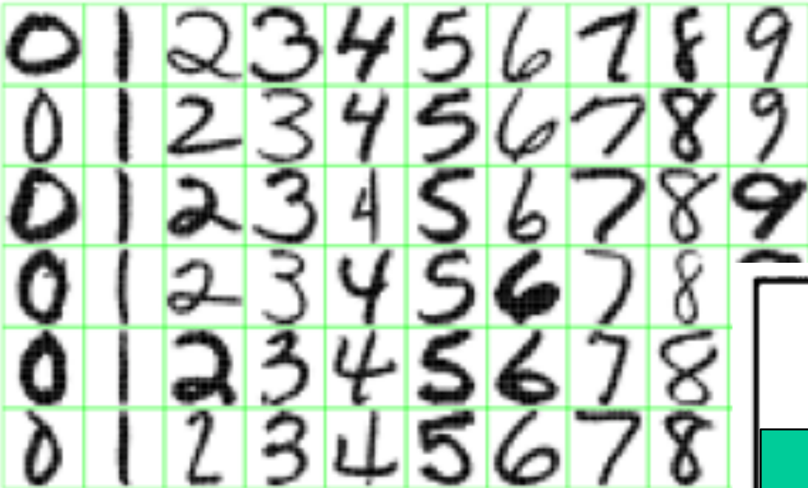


Figure 1.2: *Examples of handwritten digits from postal envelopes.*





What is this unit doing?



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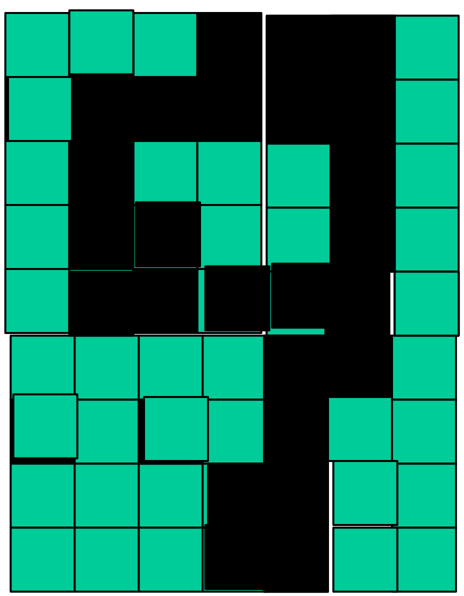
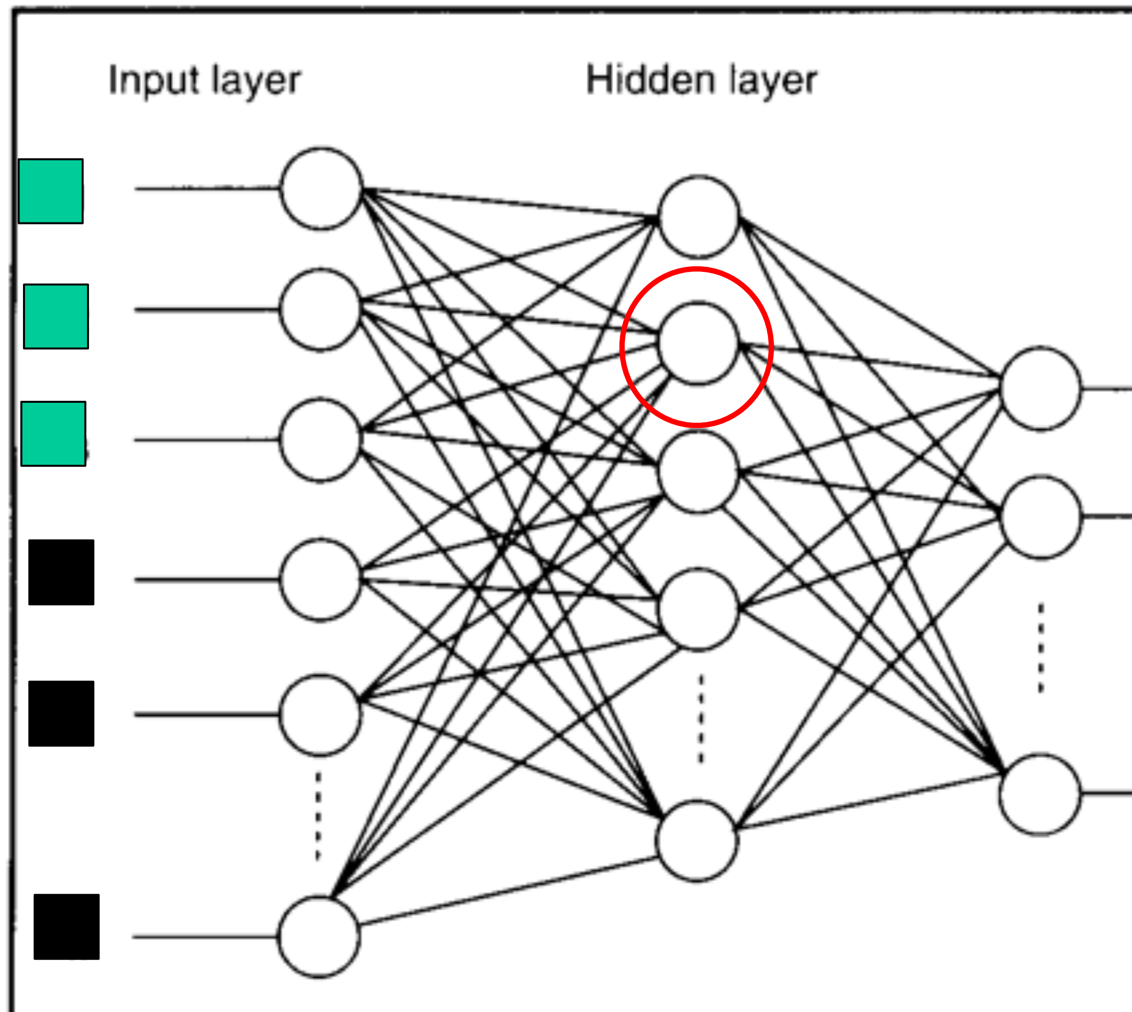
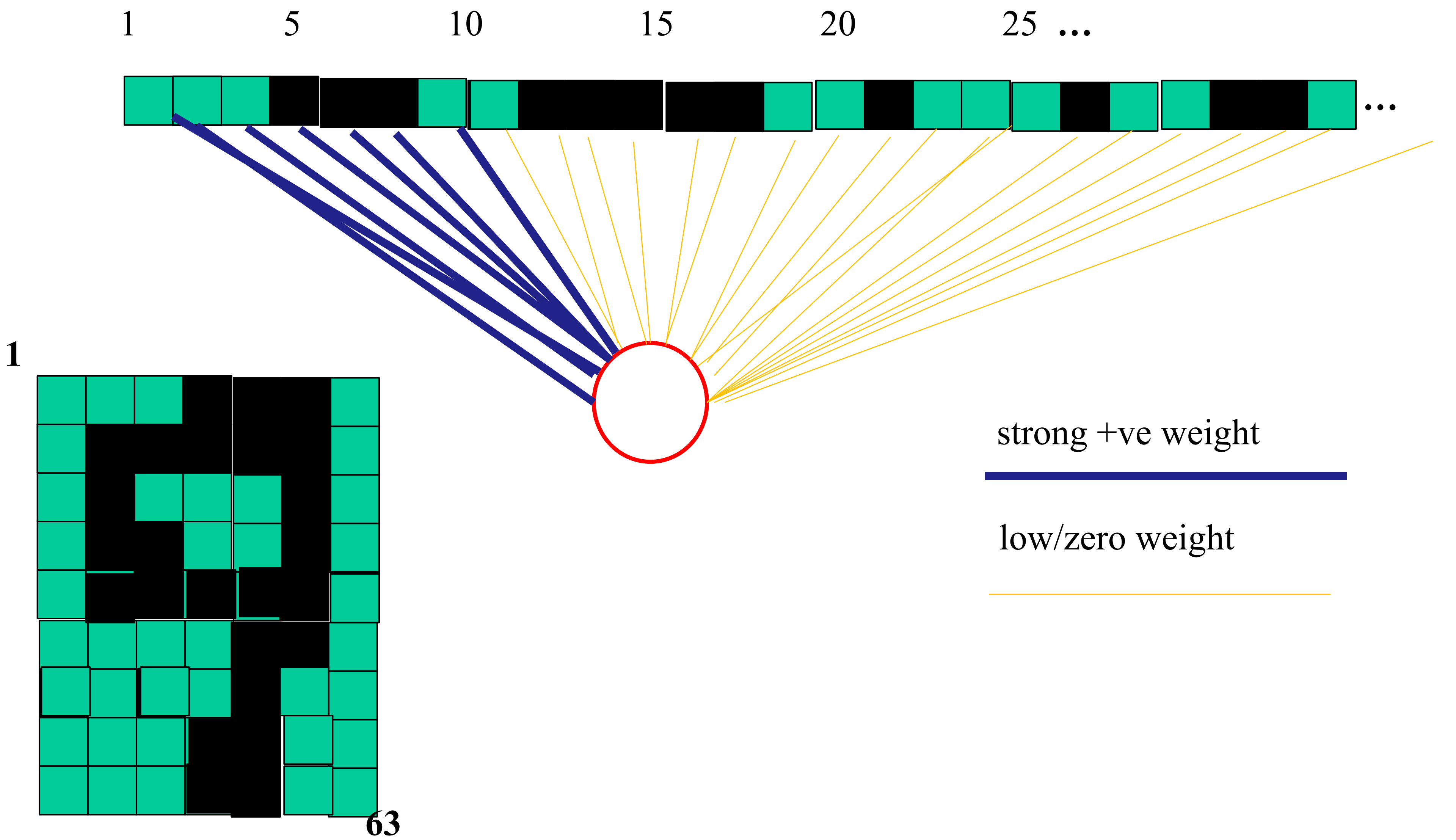
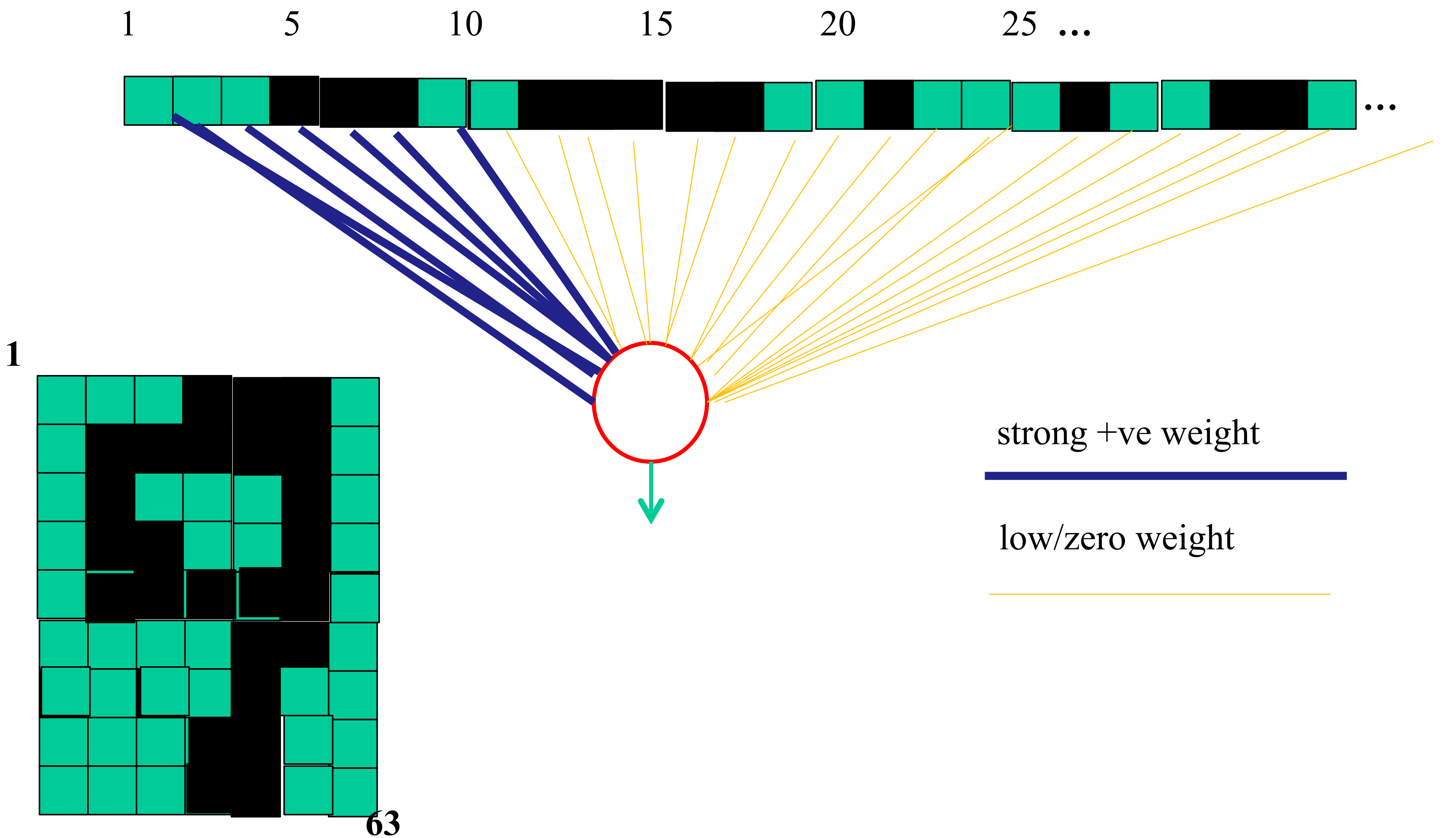




Hidden layer units become self-organized feature detectors



what does this unit detect?



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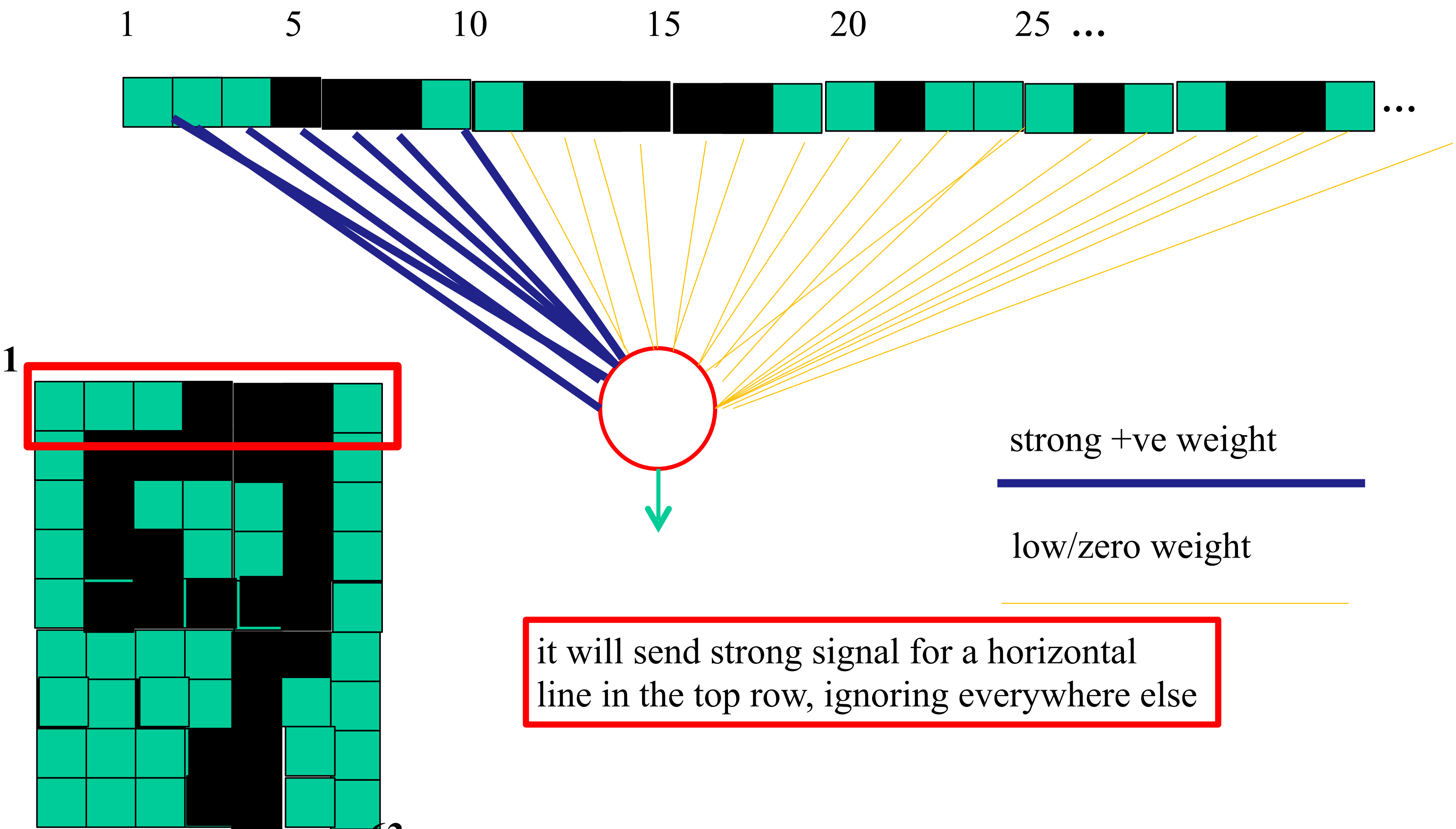
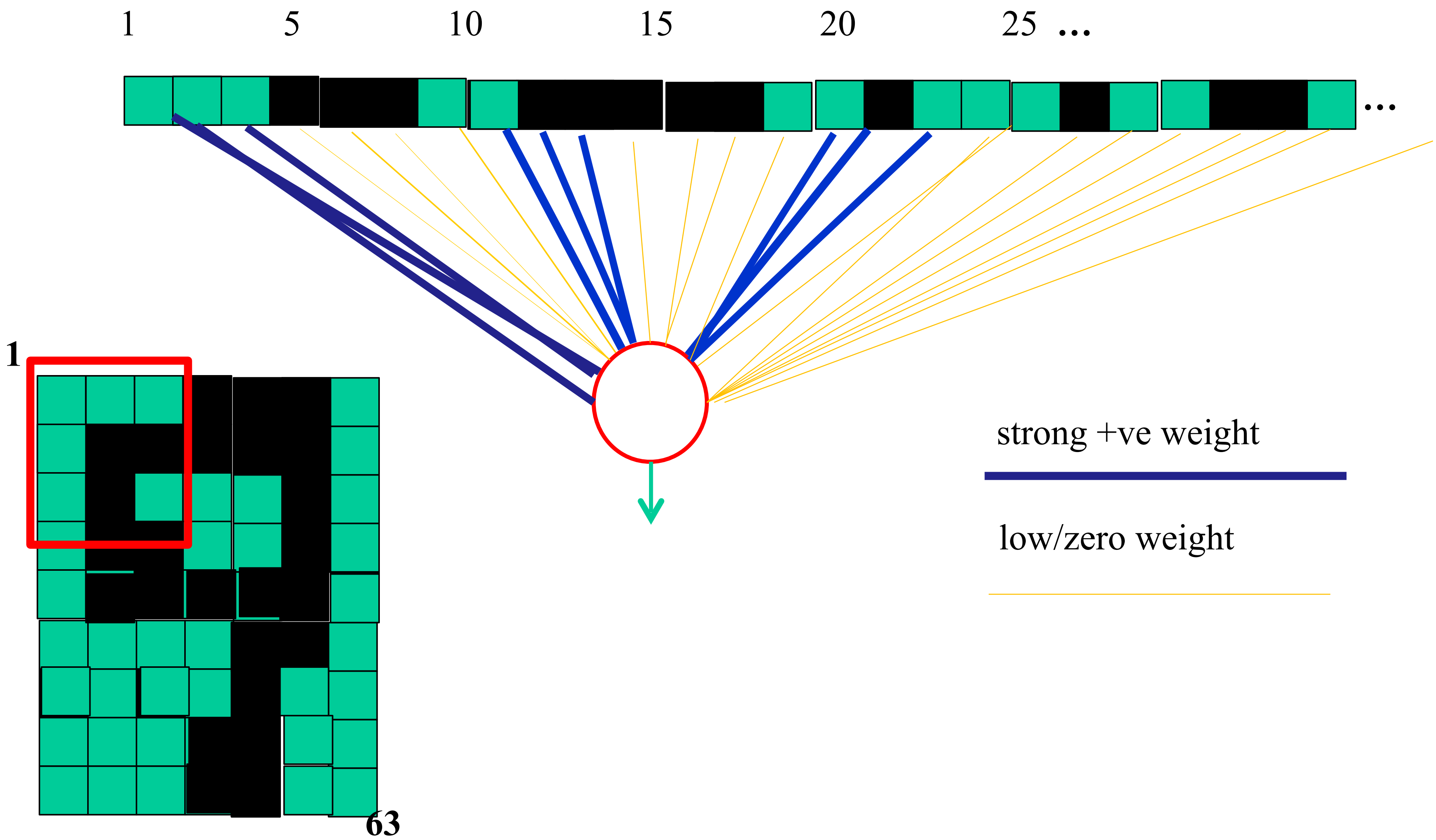


it will send strong signal for a horizontal line in the top row, ignoring everywhere else what does this unit detect?



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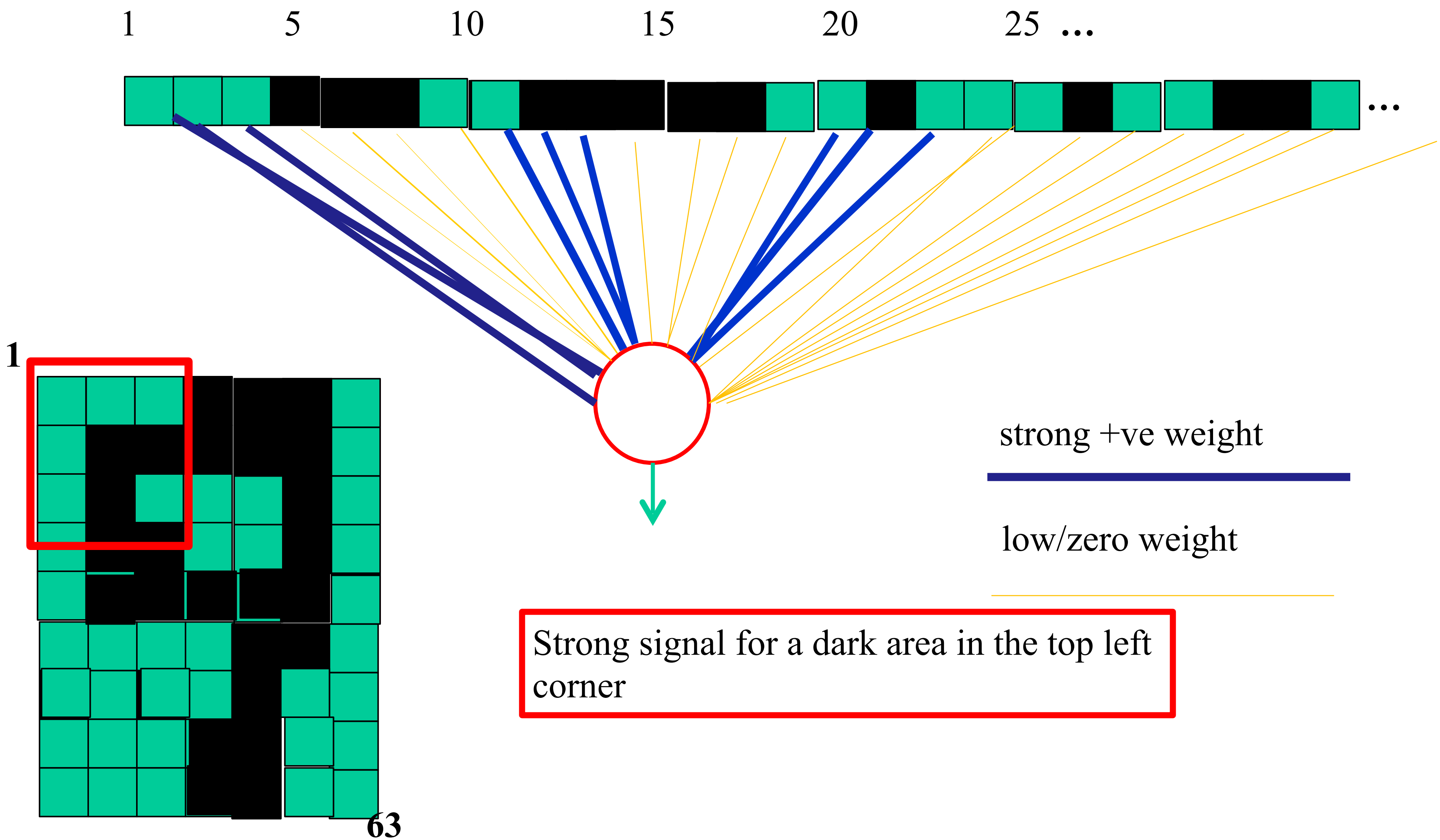


Strong signal for a dark area in the top left corner

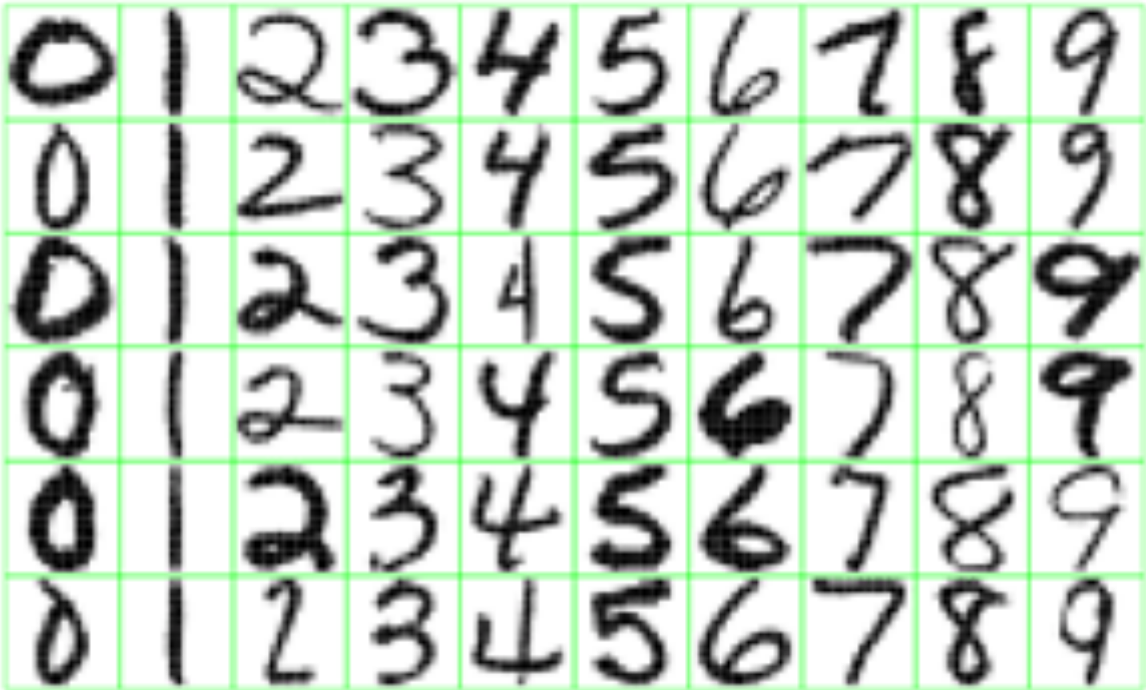
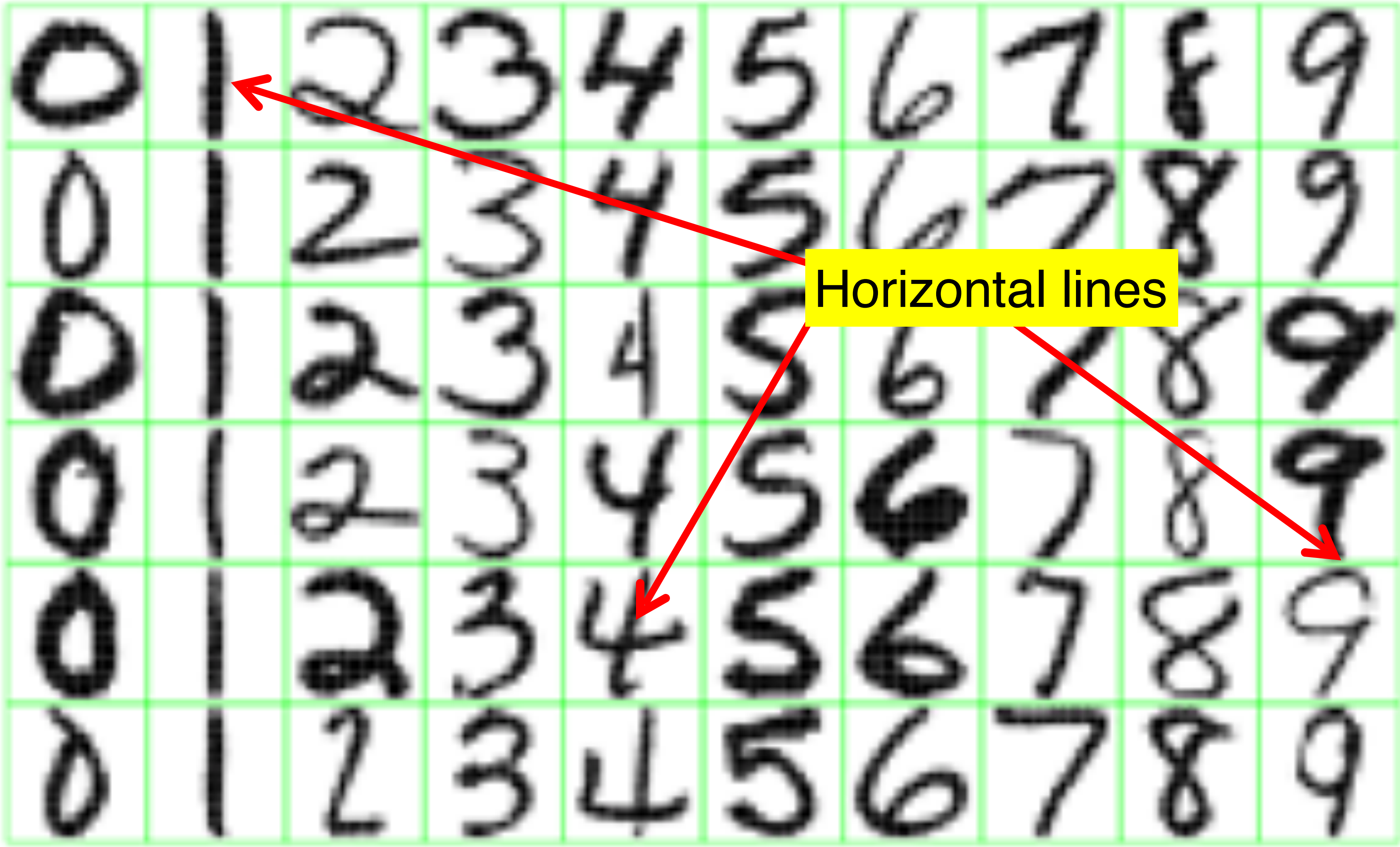


Figure 1.2: *Examples of handwritten digits from U.S. postal envelopes.*

What features might you expect a good NN to learn, when trained with data like this?

1



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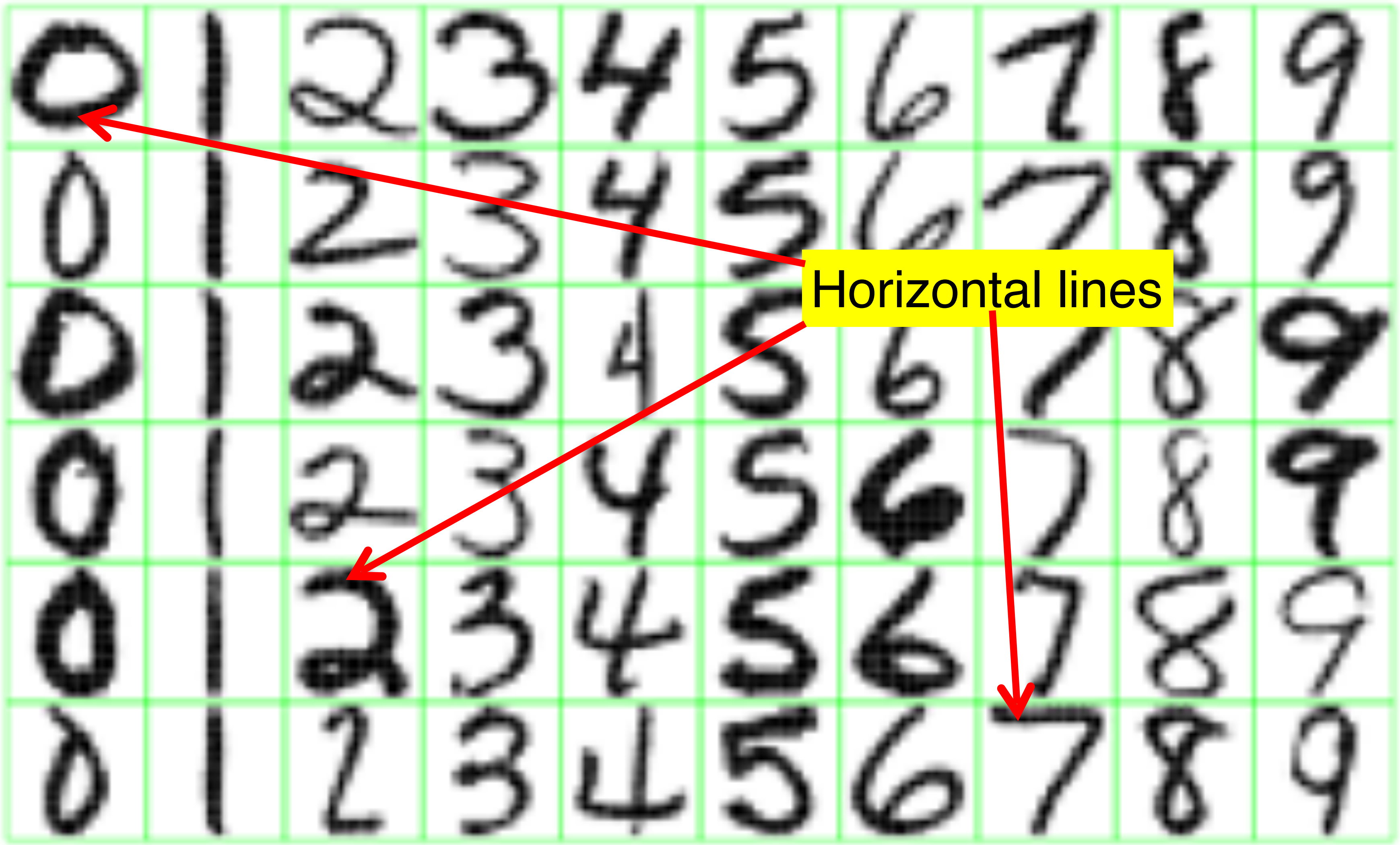

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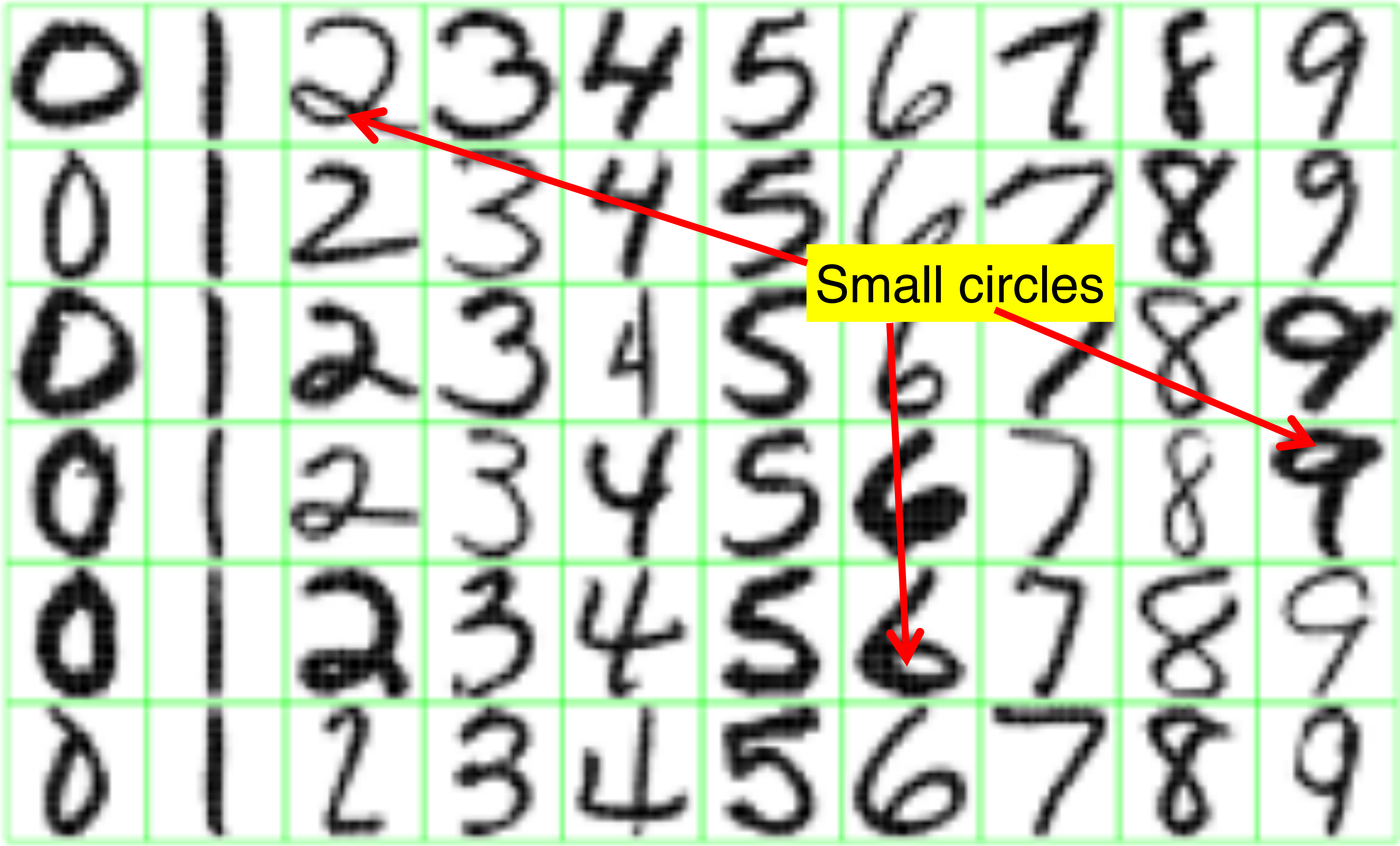

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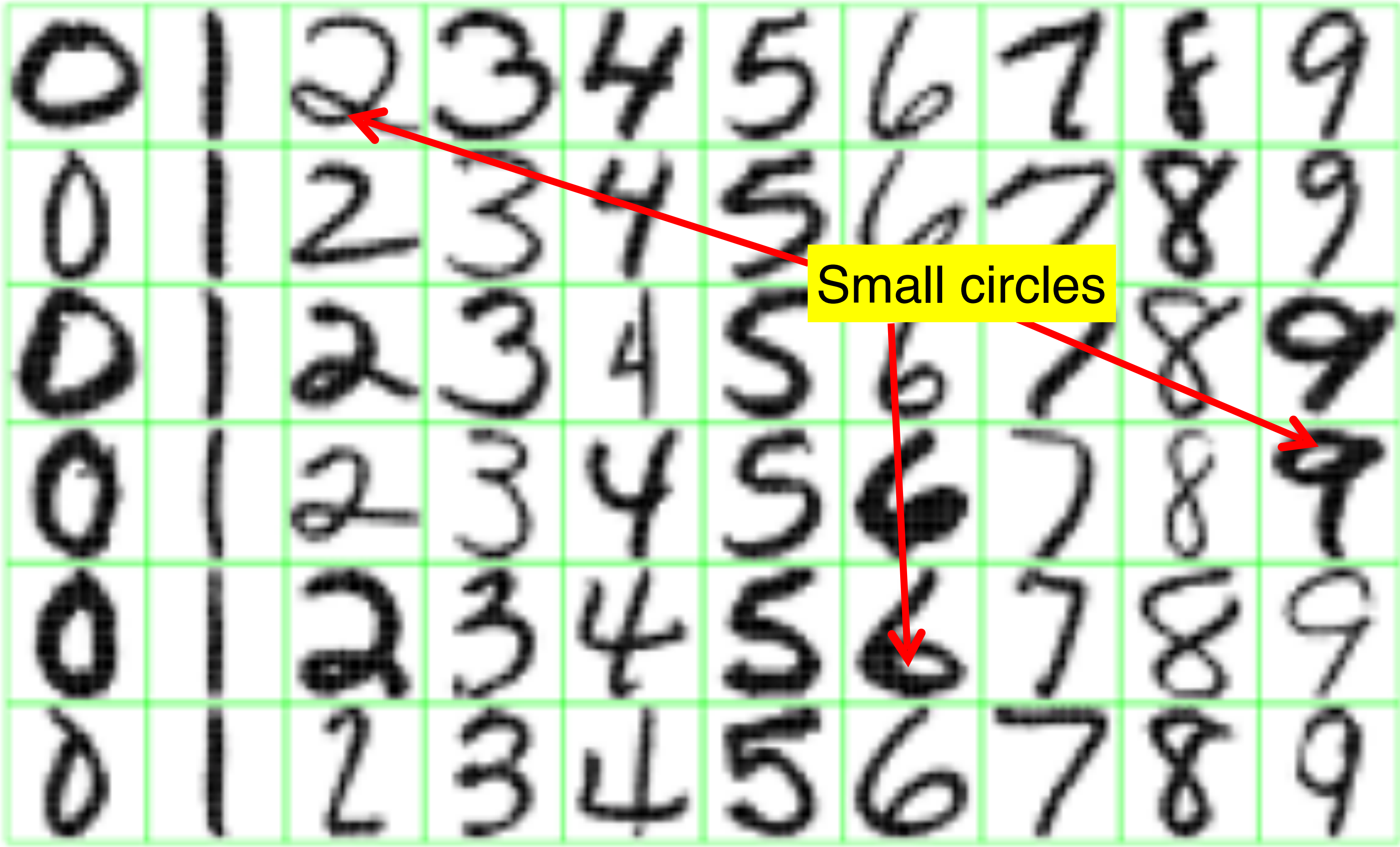
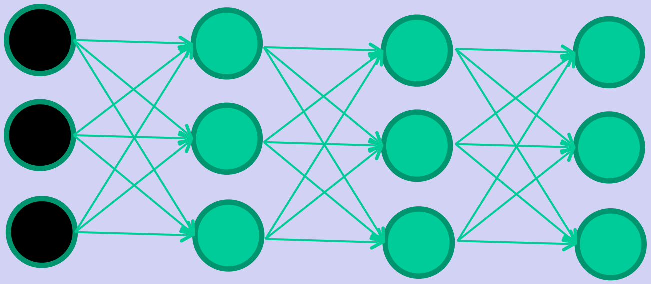


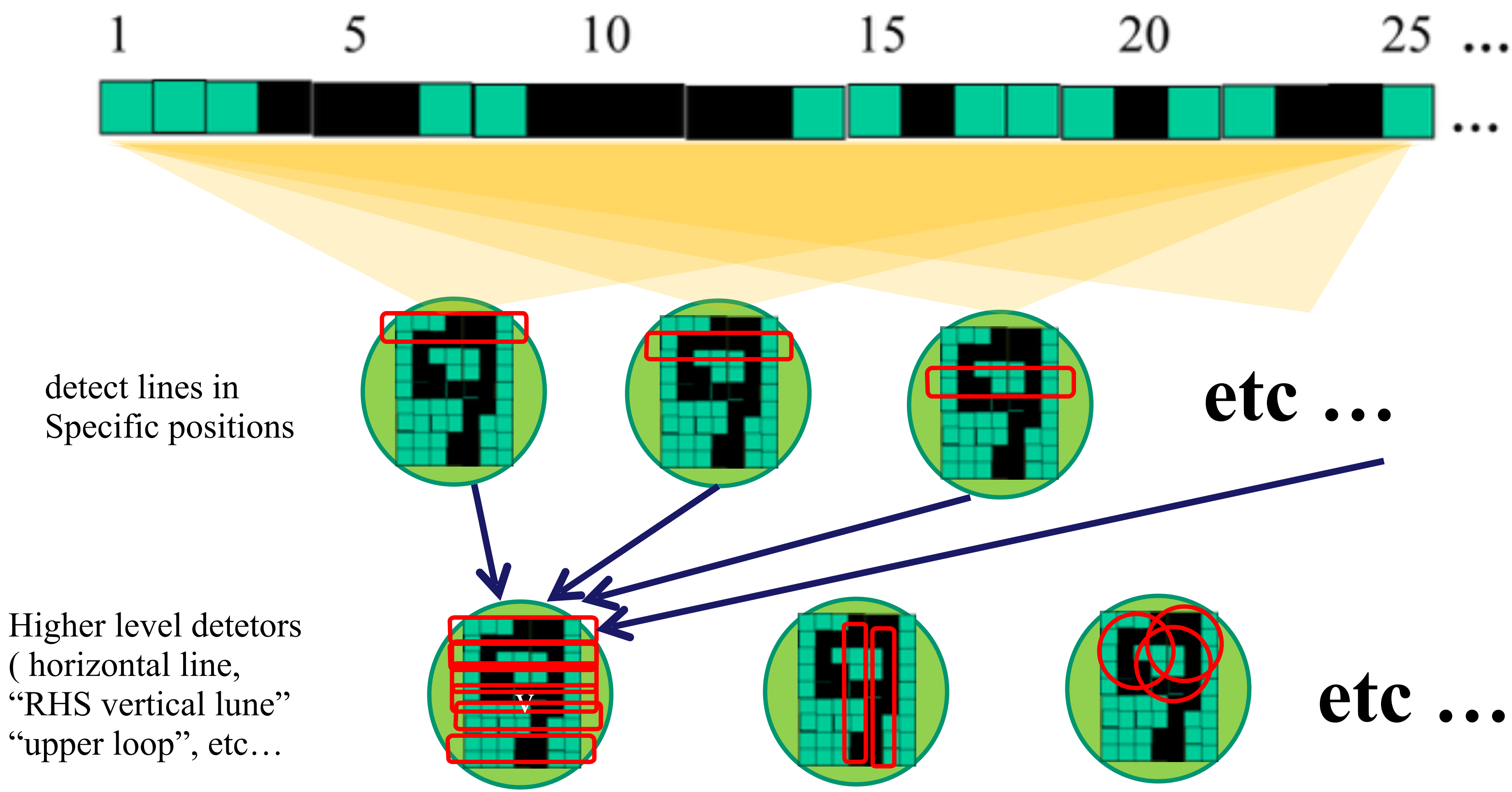
1

But what about position invariance?
Our example unit detectors were tied to specific parts of the image

Deep Networks



successive layers can detect higher-level features



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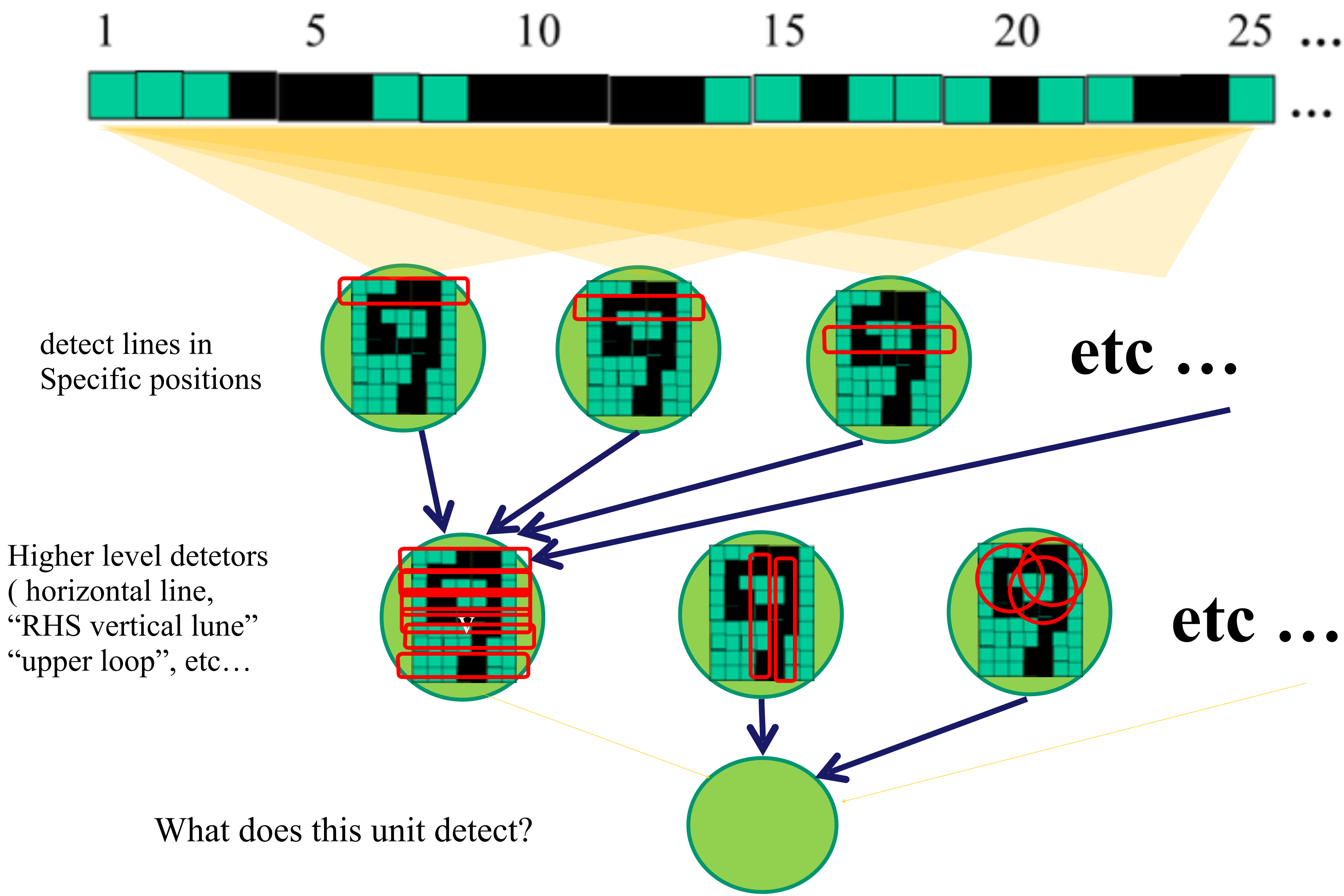
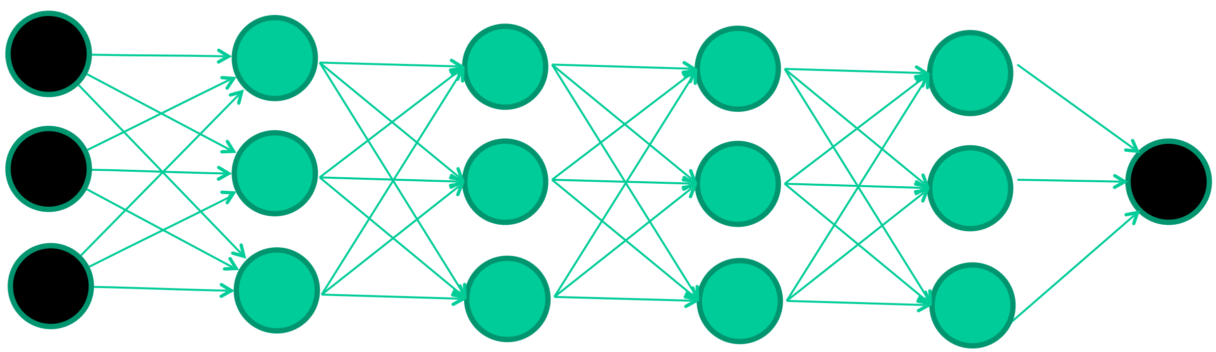
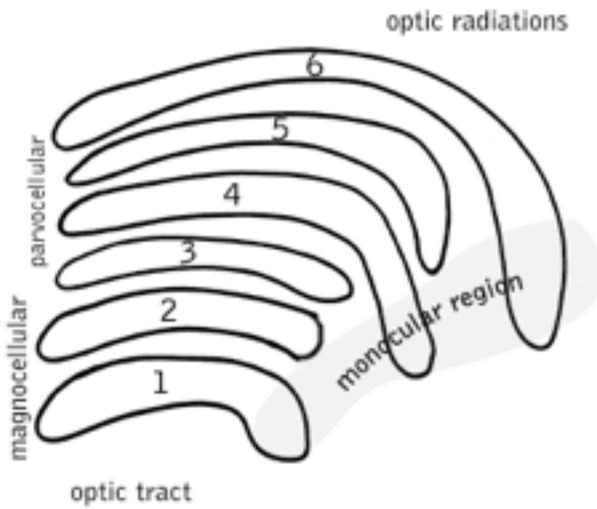


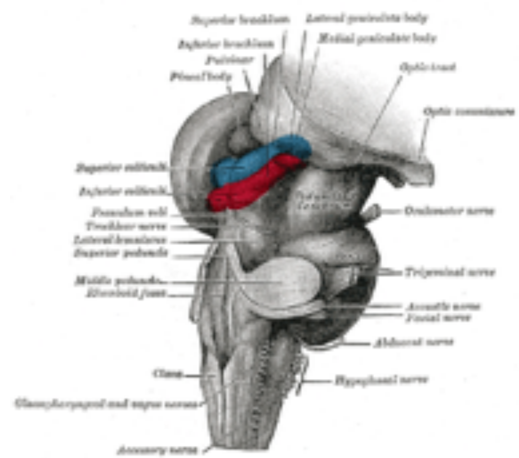
So: multiple layers make sense



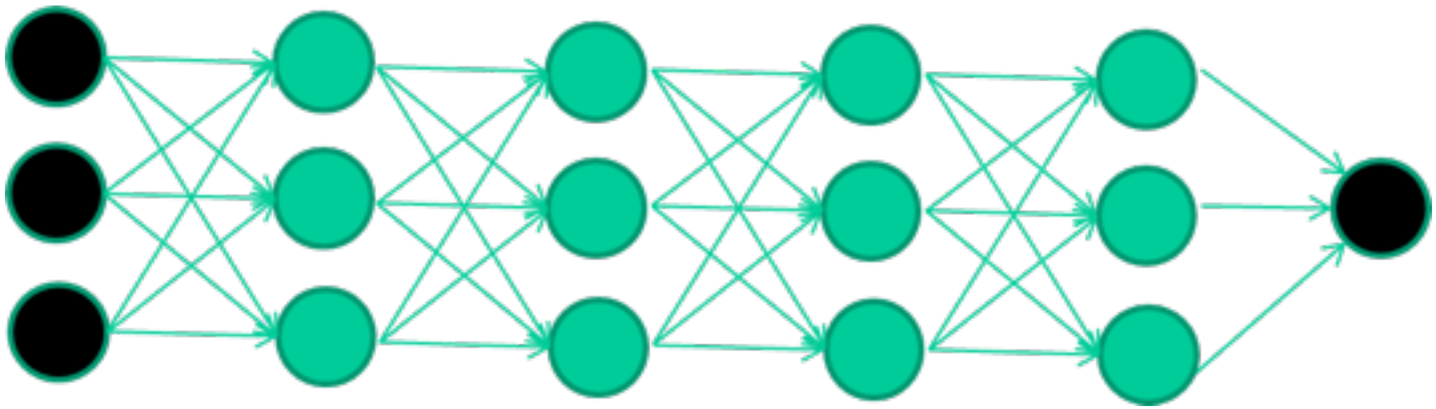
So: multiple layers make sense

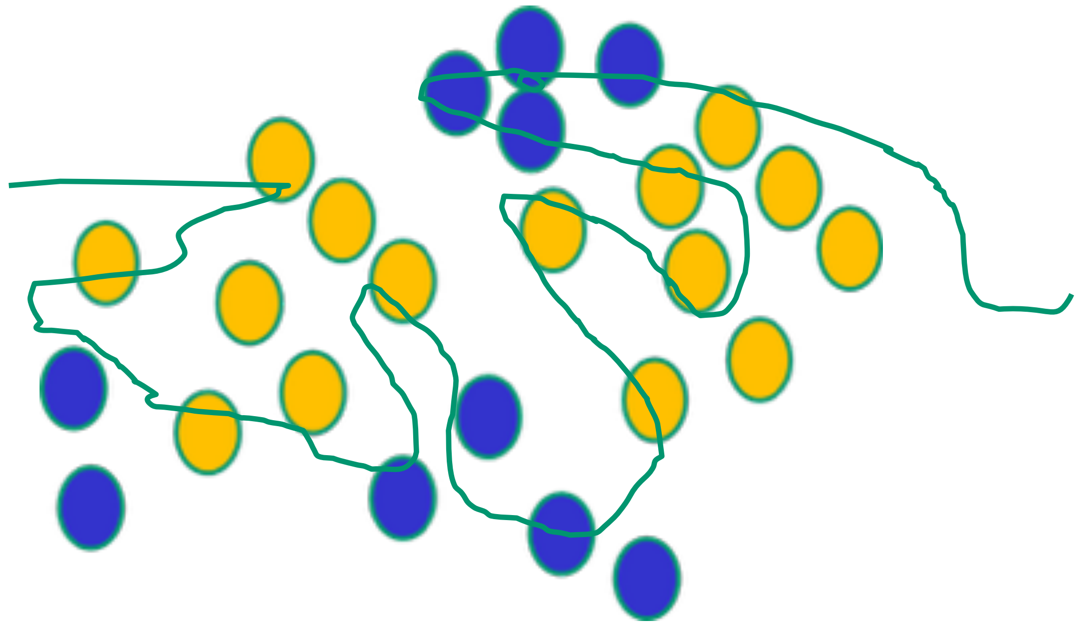
Multiple layers are also found in the brain, e.g. visual cortex





But: until recently deep networks could not be efficiently trained

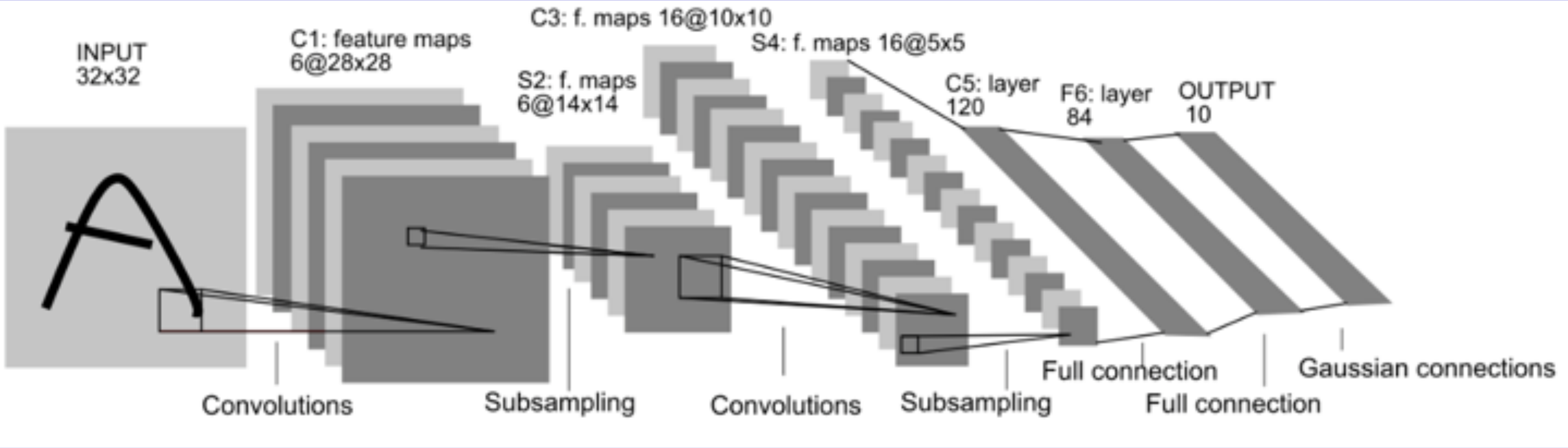




2006: The Deep Breakthrough

- Hinton, Osindero & Teh « A Fast Learning Algorithm for Deep Belief Nets », *Neural Computation*, 2006
- Bengio, Lamblin, Popovici, Larochelle « Greedy Layer-Wise Training of Deep Networks », *NIPS'2006*
- Ranzato, Poultney, Chopra, LeCun « Efficient Learning of Sparse Representations with an Energy-Based Model », *NIPS'2006*

Convolutional Neural Networks



Compared to standard feedforward neural networks with similarly-sized layers,

- CNNs have much fewer connections and parameters
- and so they are easier to train,
- while their theoretically-best performance is likely to be only slightly worse.

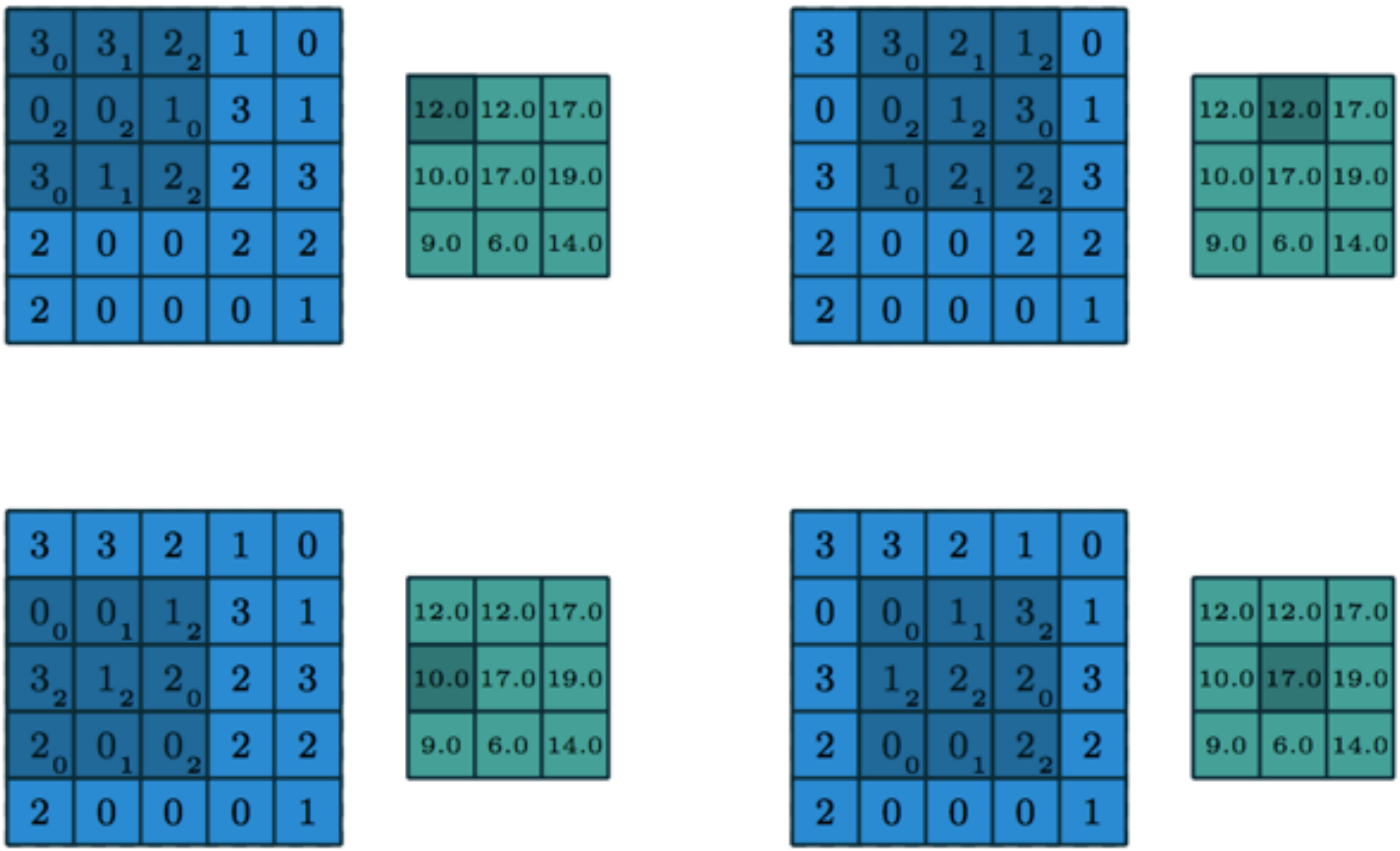
LeNet 5

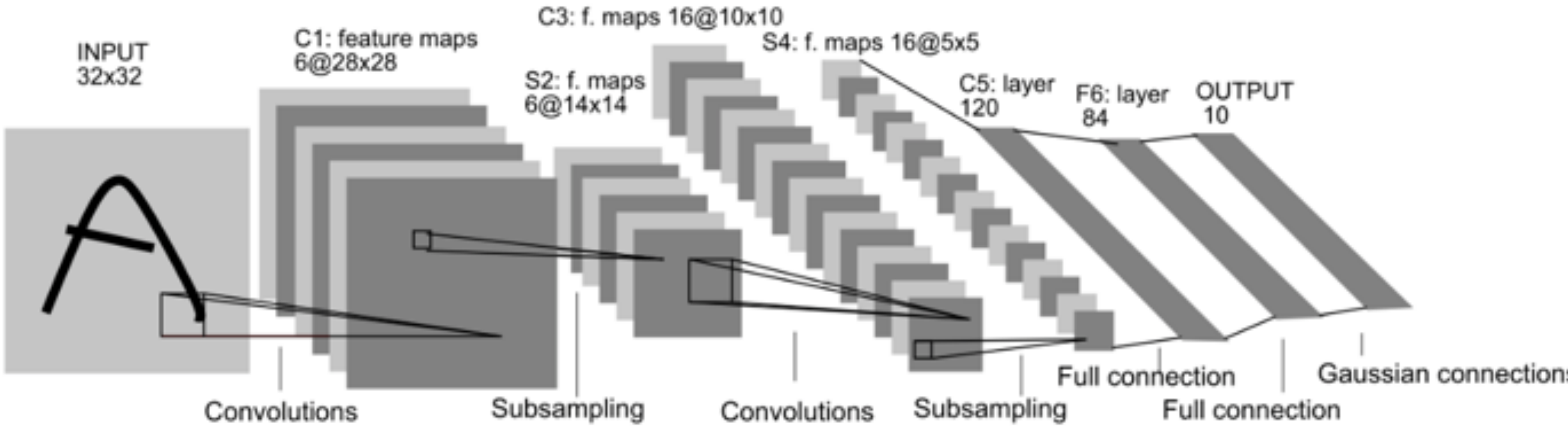
Y. LeCun, L. Bottou, Y. Bengio and P. Haffner: **Gradient-Based Learning Applied to Document Recognition**, *Proceedings of the IEEE, 86(11):2278-2324, November* ***1998***

Convolutional Kernel / Filter

0	1	2
2	2	0
0	1	2

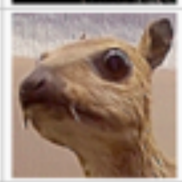
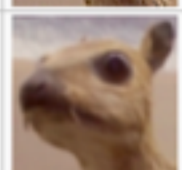
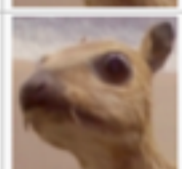
Apply convolutions





- Input: 32x32 pixel image. Largest character is 20x20
  (All important info should be in the center of the receptive field of the highest level feature detectors)
- Cx: Convolutional layer
- Sx: Subsample layer
- Fx: Fully connected layer
- Black and White pixel values are normalized:
  E.g. White = -0.1, Black =1.175 (Mean of pixels = 0, Std of pixels =1)

Convolutional filters perform image processing

Operation	Filter	Convolved Image
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	
Edge detection	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Box blur (normalized)	$\frac{1}{9}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	
Gaussian blur (approximation)	$\frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	

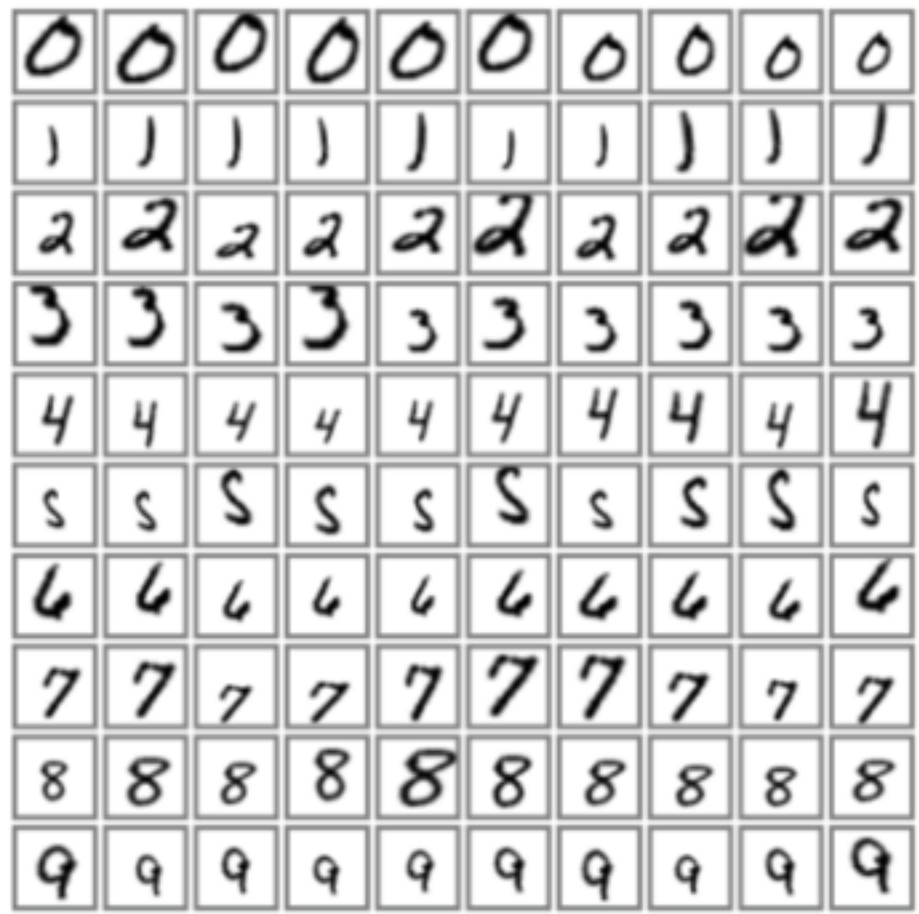
Example: filters in face recognition

First Layer Representation   Second Layer Representation   Third Layer Representation

MNIST dataset

60,000 original datasets

Test error: 0.95%



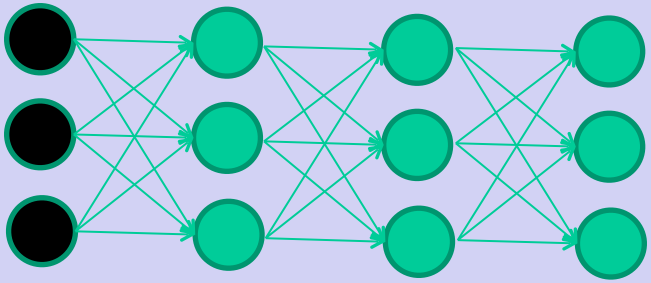
540,000 artificial distortions

+ 60,000 original

Test error: 0.8%

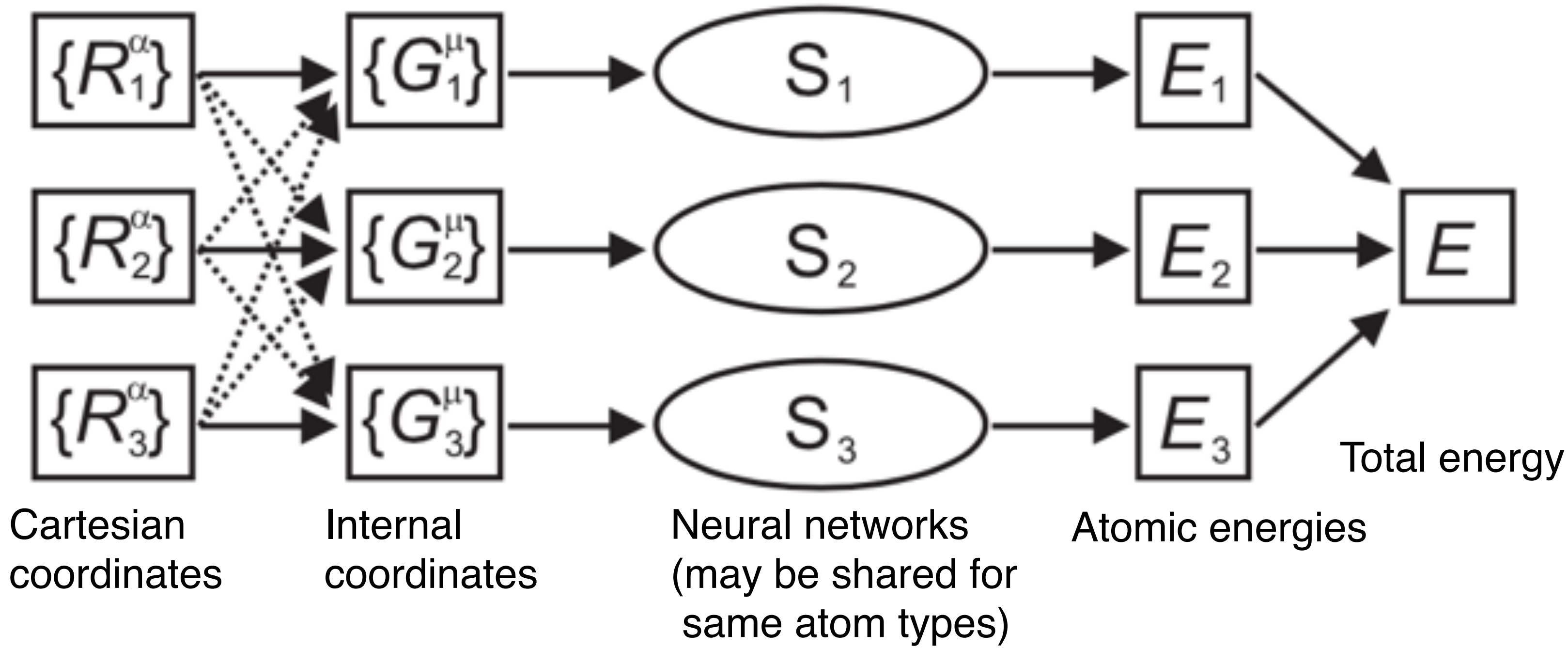
Misclassified examples

Applications to molecular systems



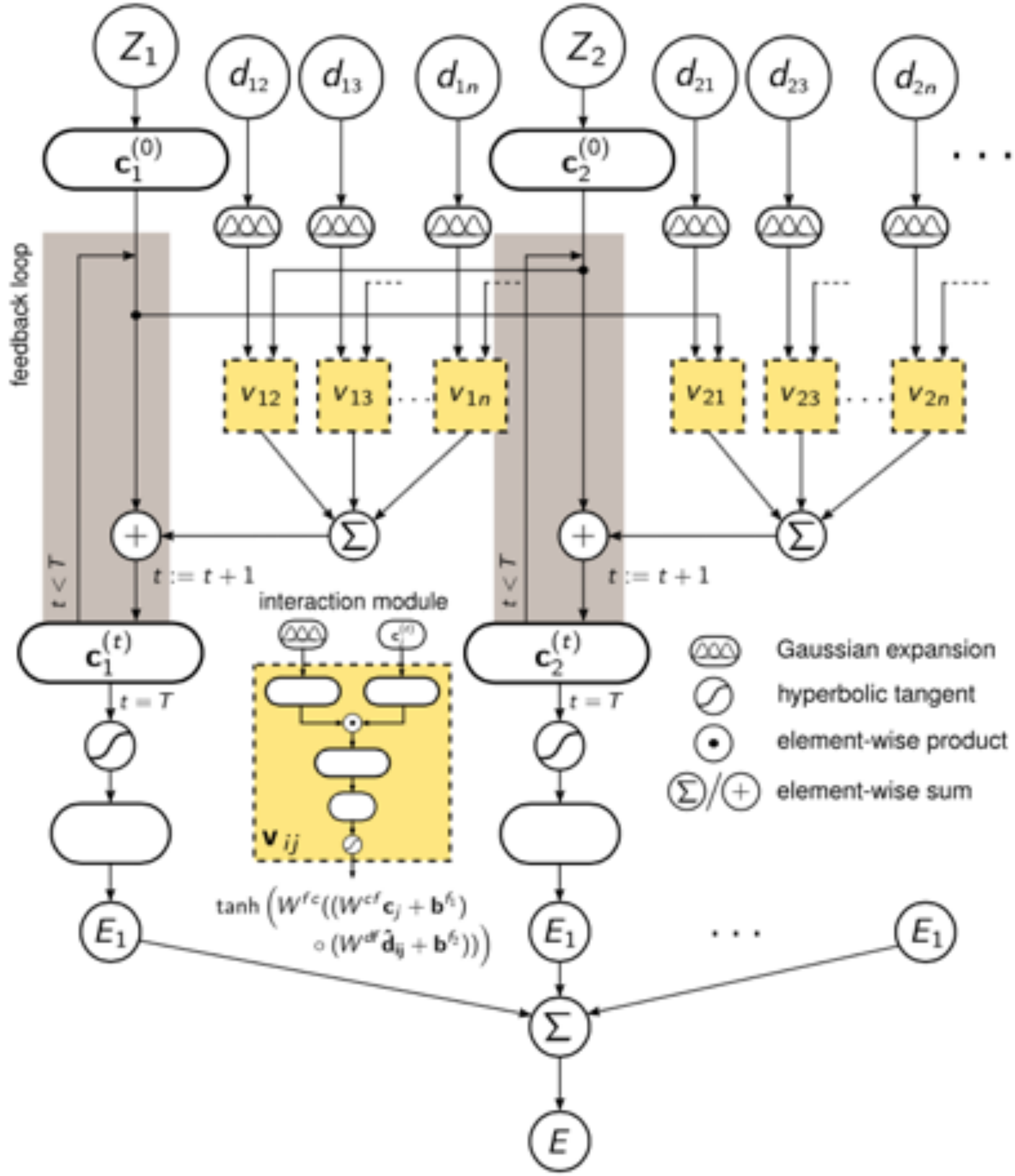
1) Learning to represent (effective) energy function

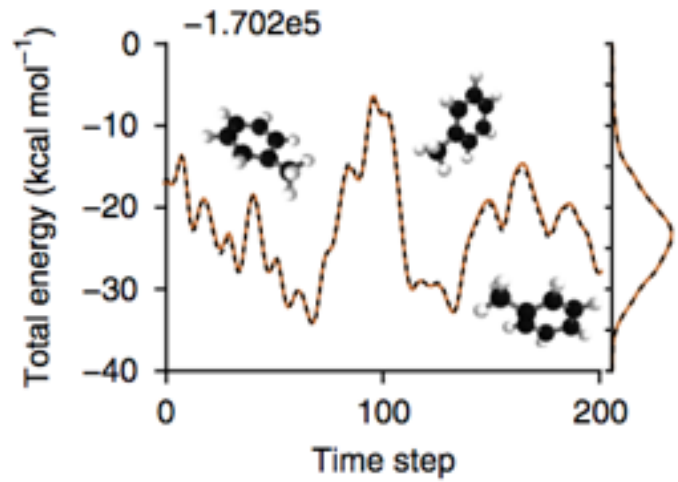
Behler-Parrinello network

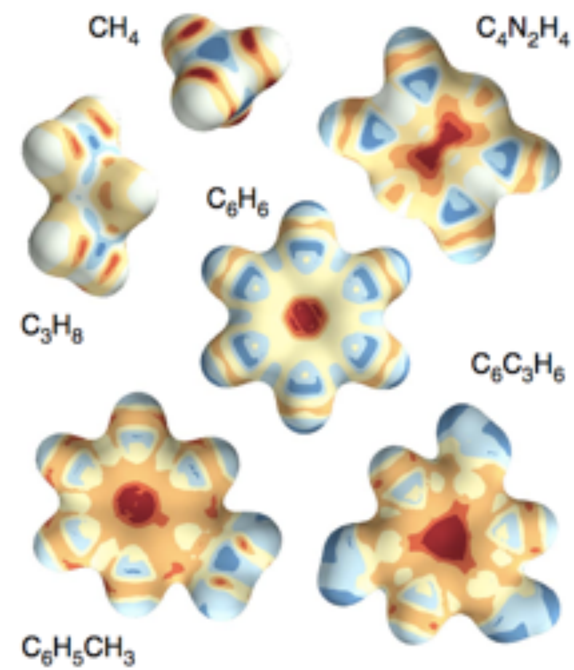


Behler and Parrinello, PRL 98, 146401 (2007)

1) Learning to represent (effective) energy function

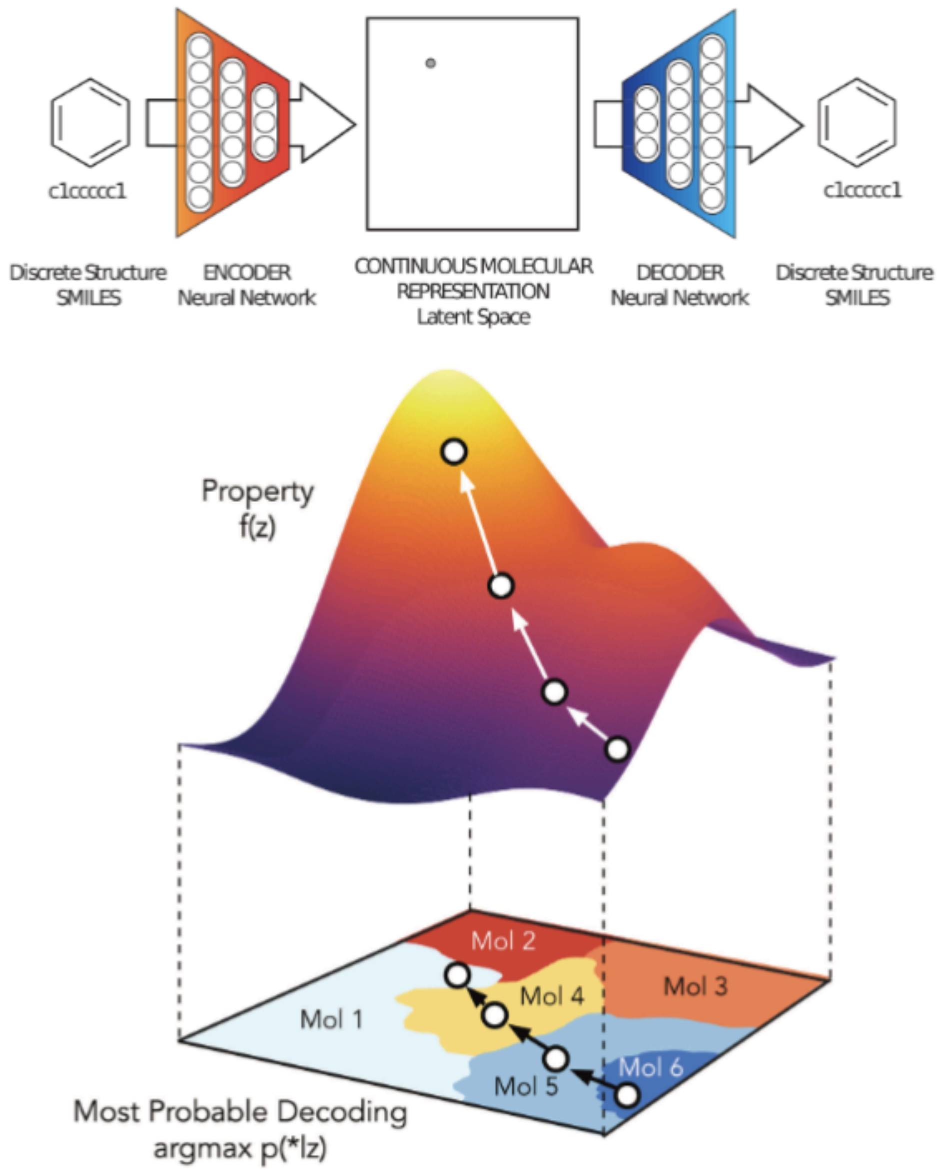






Schuett, Arbabzadah, Chmiela, Müller & Tkatchenko, Nature Communications 8, 13890 (2017)

2) Generator networks



Gómez-Bombarelli, …, Aspuru-Guzik: Automatic Chemical Design using Variational Autoencoders (2016)

2) Generator networks

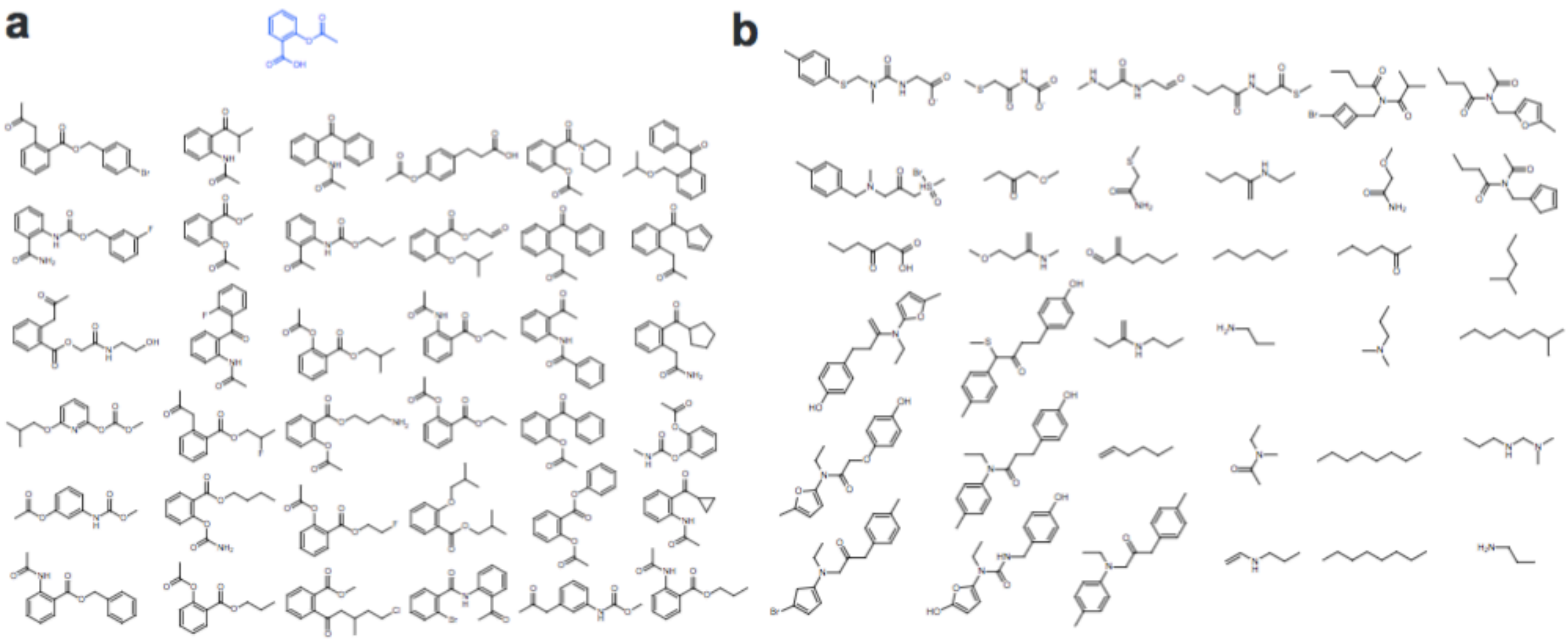
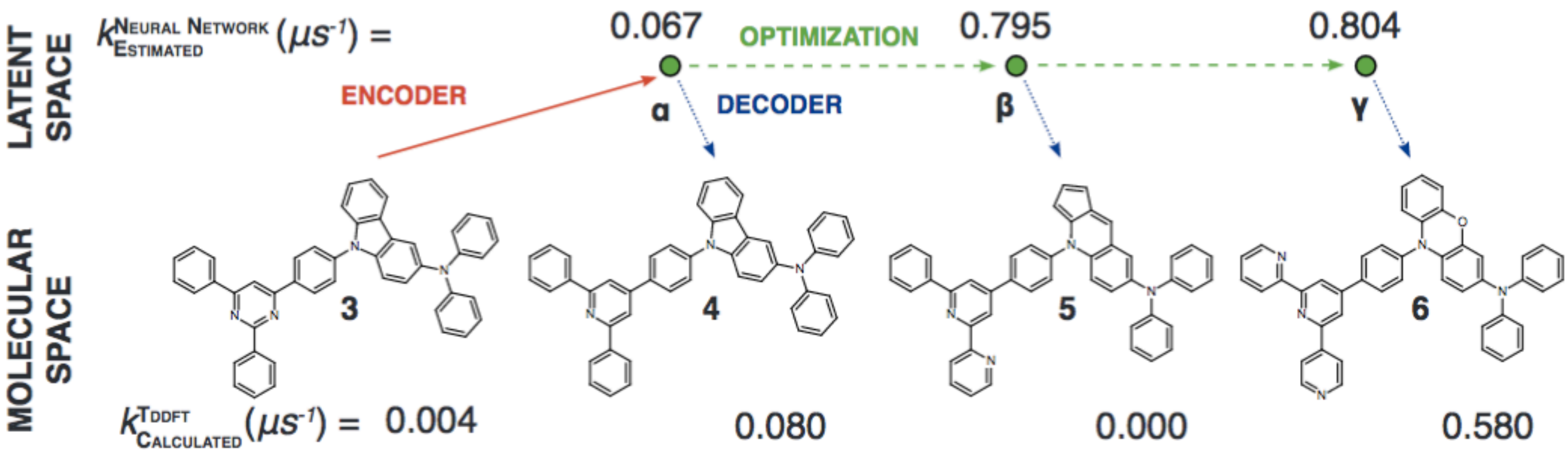


Figure 3: **a)**. Random sampling. Molecules decoded from randomly-sampled points in the latent space of a variational autoencoder, near to a given molecule (aspirin [2-(acetyloxy)benzoic acid], highlighted in blue). **b)**. Interpolation. Two-dimensional interpolation between four random points in in drug-like VAE. Decodings of interpolating linearly between the latent representations of the four molecules in the corners.

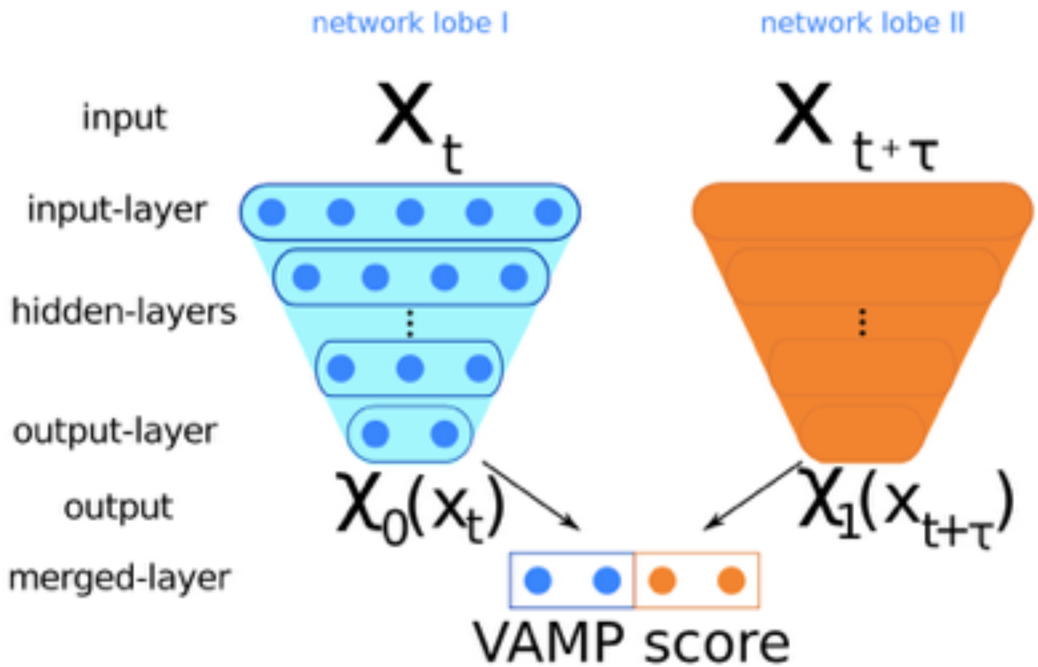
Gómez-Bombarelli, …, Aspuru-Guzik: Automatic Chemical Design using Variational Autoencoders (2016)

2) Generator networks



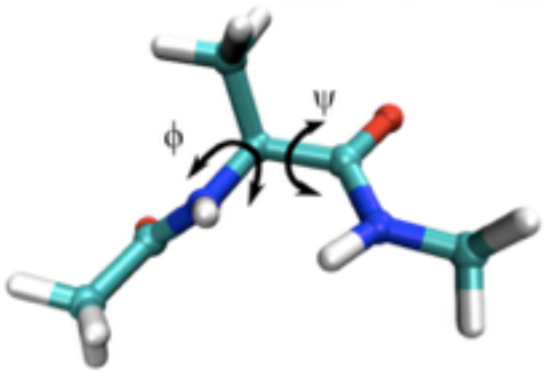
Gómez-Bombarelli, …, Aspuru-Guzik: Automatic Chemical Design using Variational Autoencoders (2016)

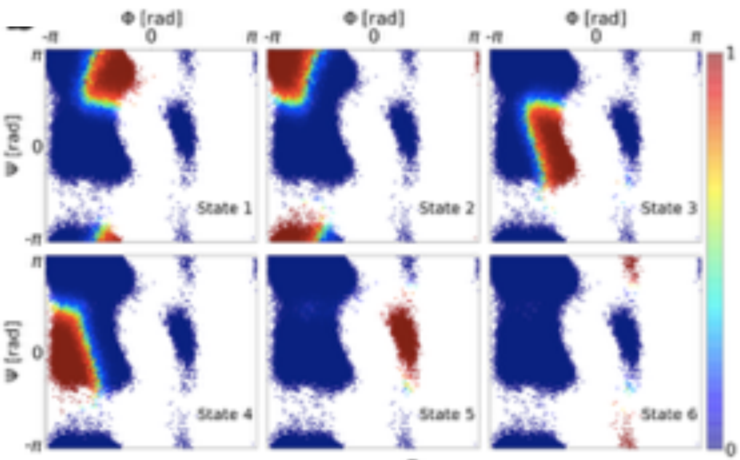
3) VAMPnets

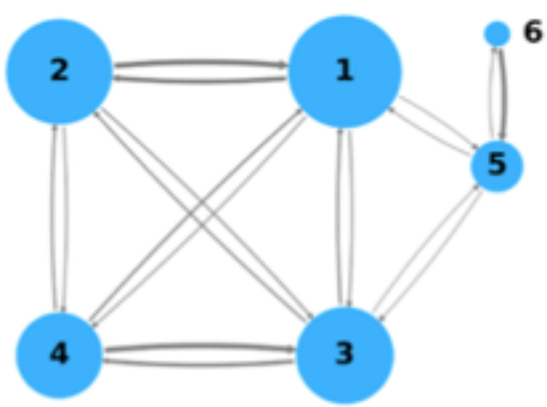


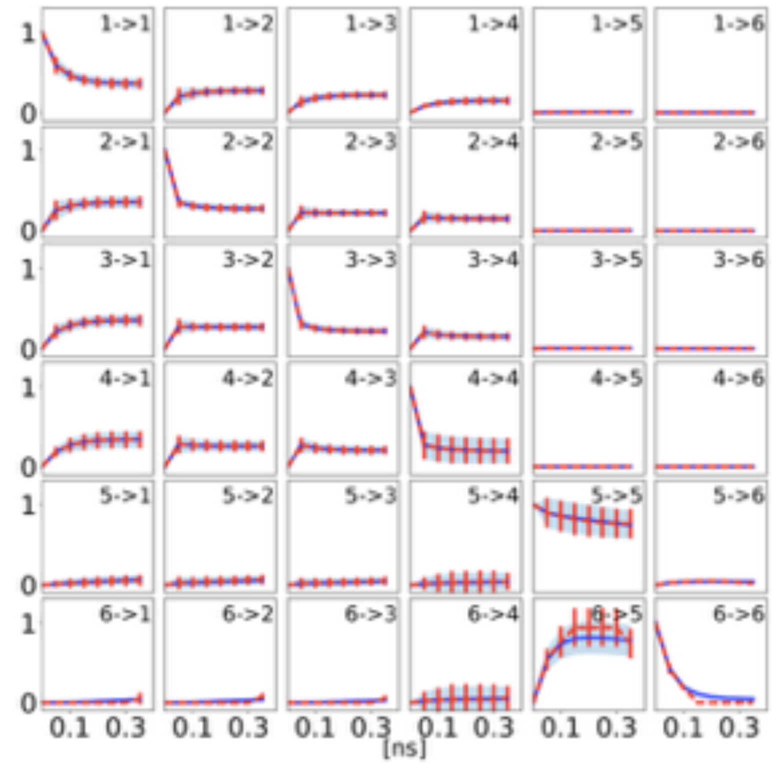
Mardt, Pasquali, Wu & Noé: VAMPnets - deep learning of molecular kinetics (2017)

3) VAMPnets









Mardt, Pasquali, Wu & Noé: VAMPnets - deep learning of molecular kinetics (2017)