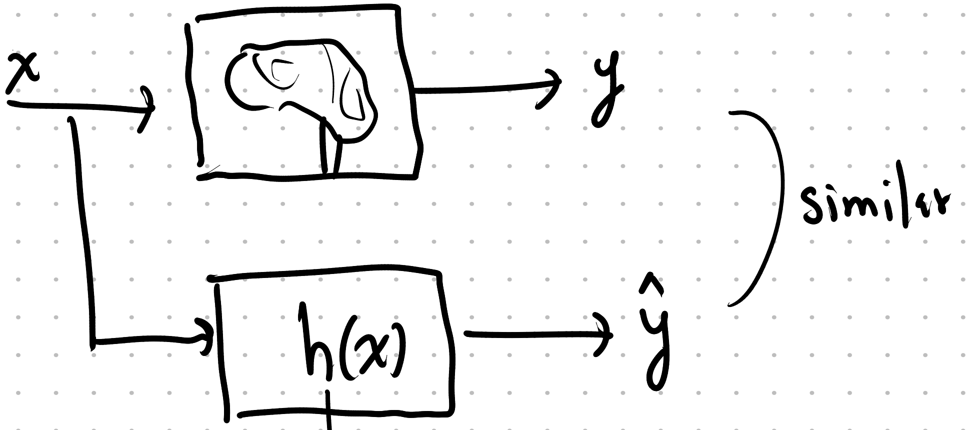
Statistics and Data Science for Engineers
E178 / ME276DS

Neural networks

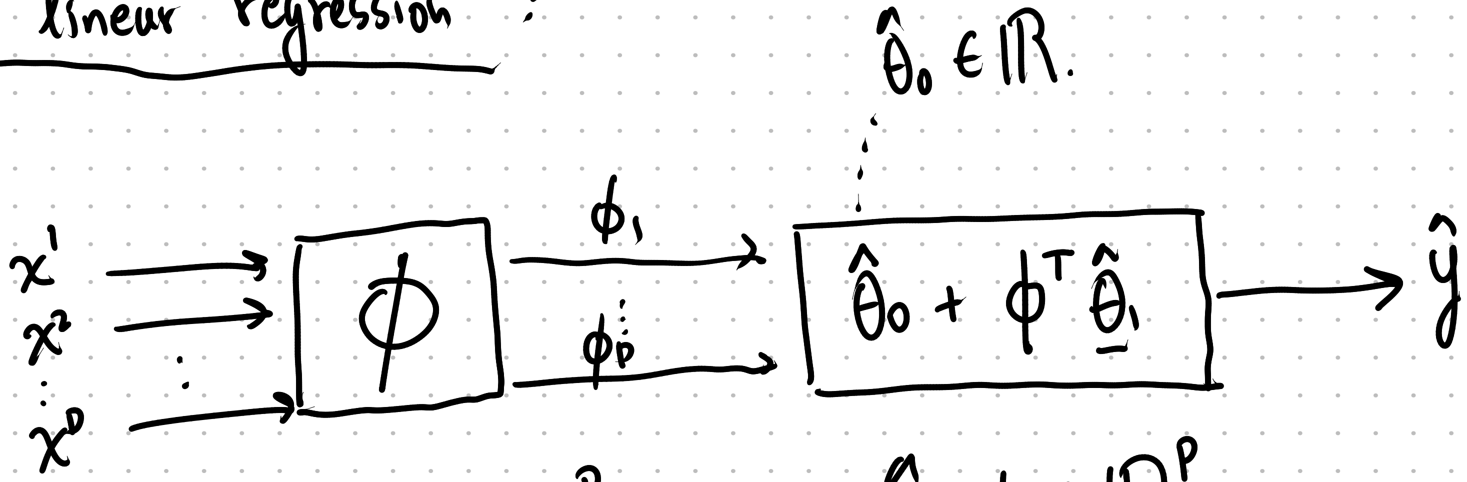


- Linear Regression (regression)
- Logistic regression (classification).

⋮

- Support Vector machine
- Decision trees
- Neural networks.

Recall linear regression:

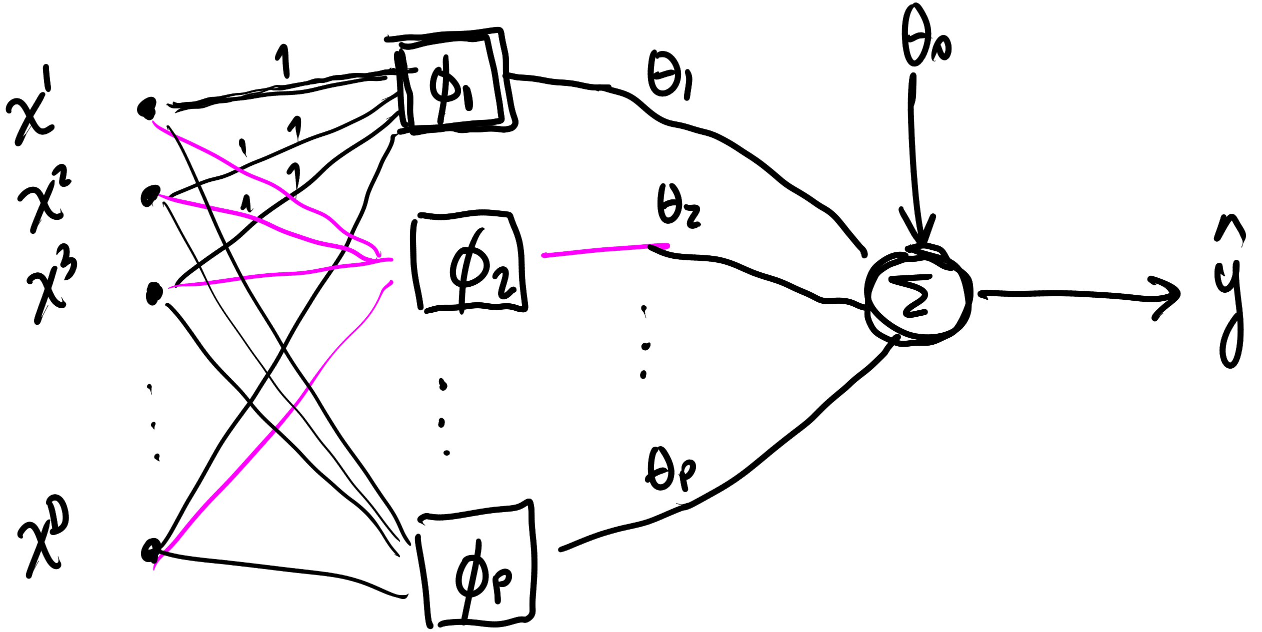


$\phi : \underbrace{\mathbb{R}^D}_{\text{inputs}} \to \underbrace{\mathbb{R}^P}_{\text{features}}$ $\qquad$ $\hat{\theta}_1, \phi \in \mathbb{R}^P$

- I have to manually design the features ϕ.
- Neural networks can be understood as a way to design the features automatically.

Pictorial representation of linear regression

$$\hat{y} = \theta_0 + \phi^T(x)\underline{\theta}_1 = \theta_0 + \sum_{j=1}^{P} \phi_j(x)\theta_j$$

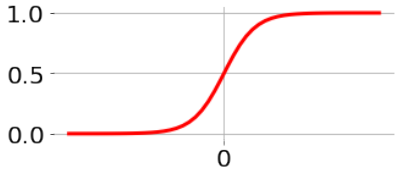


3 steps to NN:

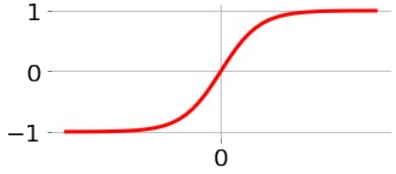
1. Replace the ϕ with "activation functions"
2. Put weights on all edges.
3. Replicate layers.

1) Generic nonlinearities, a.k.a. <u>*activation functions*</u>

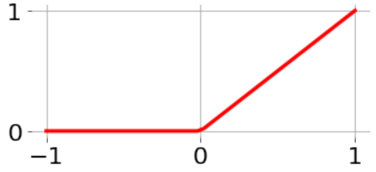
sigmoid: $$\phi(\xi) = \frac{1}{1+e^{-\xi}}$$



tanh: $$\phi(\xi) = \frac{e^{2\xi}-1}{e^{2\xi}+1}$$

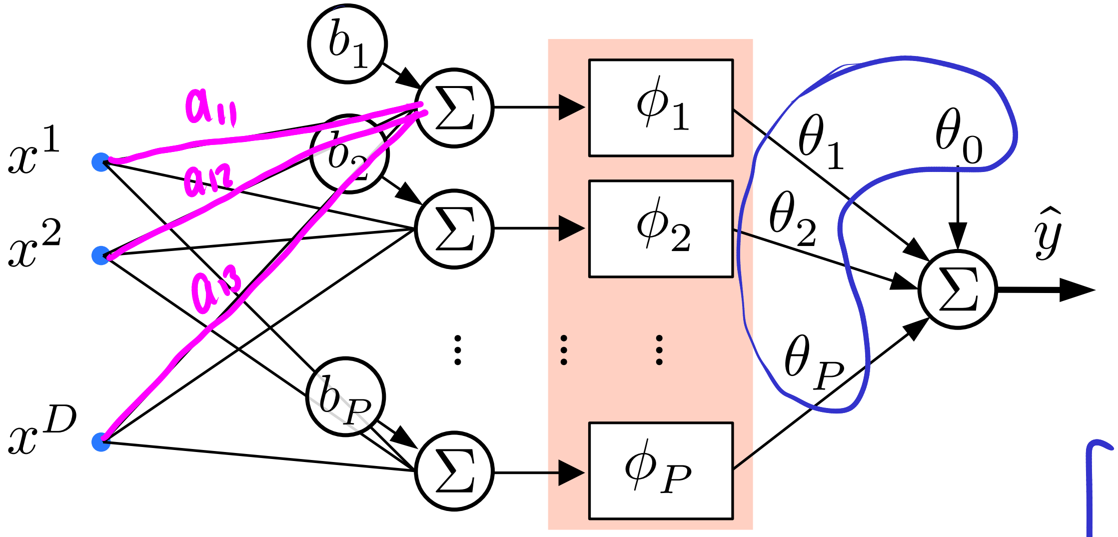


ReLU: $$\phi(\xi) = \mathsf{max}(0, \xi)$$



2) Weights on the inputs

$$\hat{y} = \theta_0 + \phi^T(b + Ax)\underline{\theta}_1 = \theta_0 + \sum_{j=1}^{P} \phi_j(b_j + A_j x)\theta_j$$



$P \times D$ "a" coeff.

P "b" coeff.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{P1} & \vdots & a_{P3} \end{bmatrix}$$

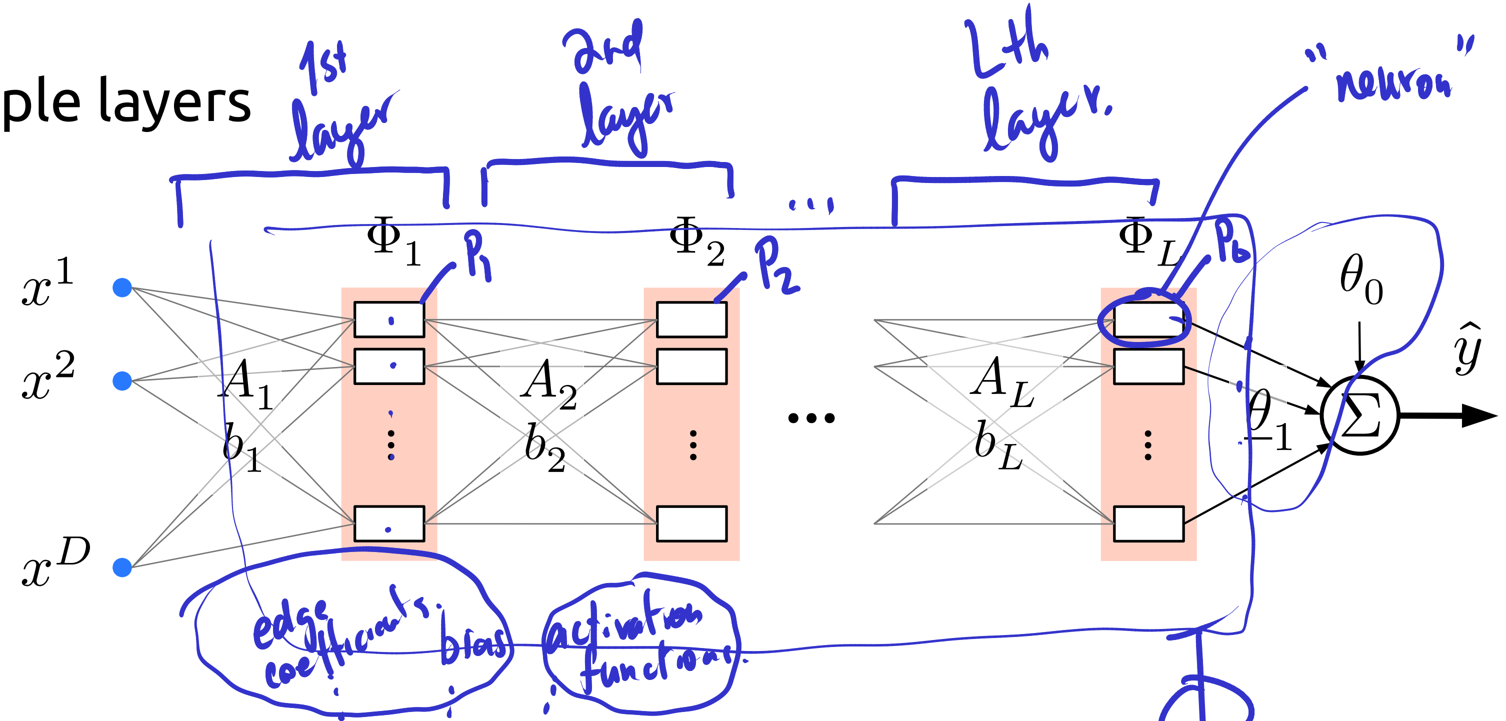
$$b = \begin{bmatrix} b_1 \\ \vdots \\ b_P \end{bmatrix}$$

$$\phi_1\left(a_{11}x^1 + a_{12}x^2 + a_{13}x^3 + b_1\right) \quad \theta_1$$

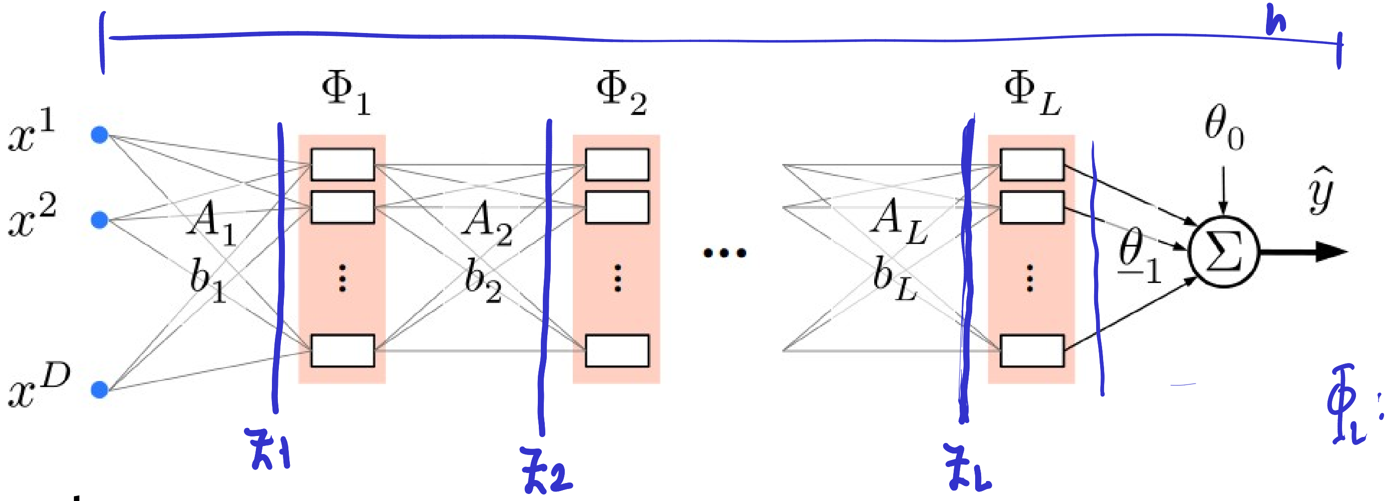
$$\phi_1\left(A_1 x + b_1\right)$$

$$A_1 = \left[a_{11}, a_{12}, a_{13}\right]$$

3) Multiple layers



- Hidden layers: $(A_\ell, b_\ell, \Phi_\ell, P_\ell)$ $\ell = 1 \dots L$
- Output layer: $(\theta_0, \underline{\theta}_1)$ ... final linear regression. (regression problem)



$\Phi_L : \mathbb{R}^{p_L} \to \mathbb{R}^{p_L}$.

Put it all together :

$$\hat{y} = h(x) = \theta_0 + \underline{\theta}_1^T \, \Phi_L\Big(b_L + A_L \cdot \Phi_{L-1}\big(\underbrace{b_{L-1} + A_{L-1}\,\Phi_{L-2}(\dots \Phi_1(b_1 + A_1 x)\dots)}_{z_{L-1}}\big)\Big).$$

... complicated nested. function.

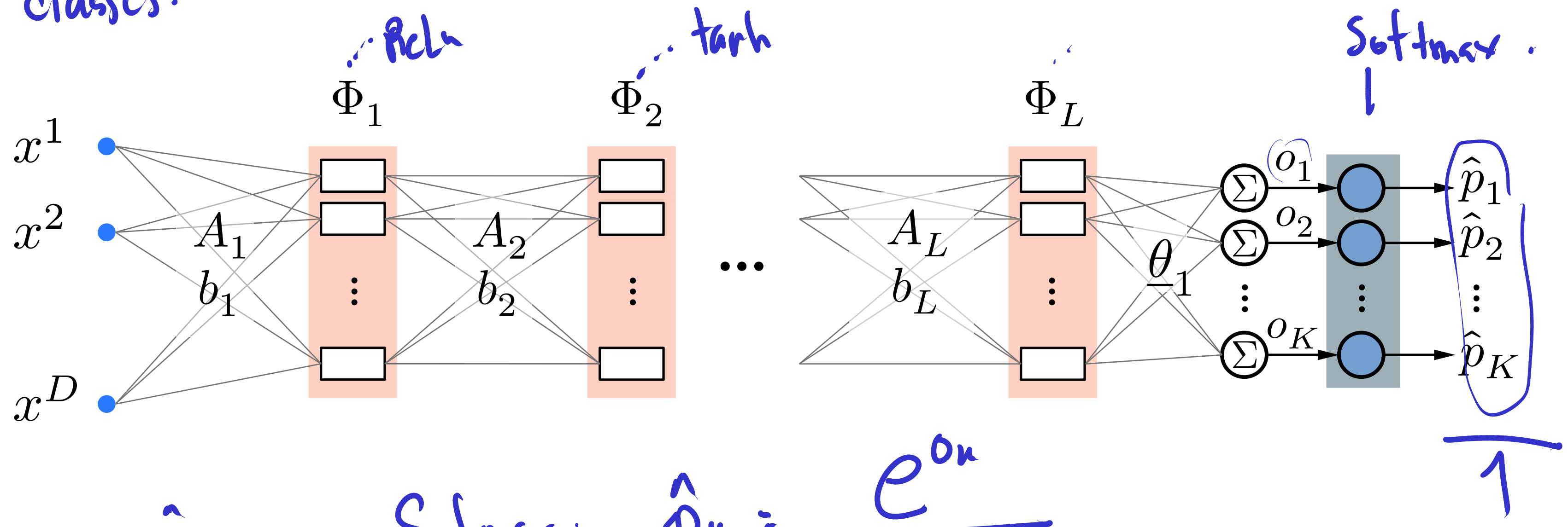
... perceptron.

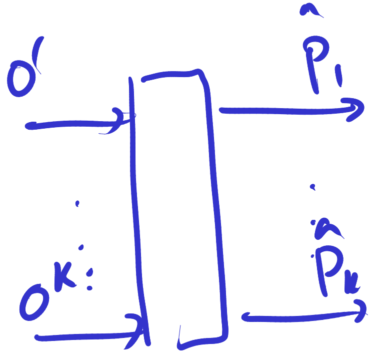
Write this in a recursive form.

$$
\begin{cases}
\hat{y} = \theta_0 + \underline{\theta}_1^T \Phi_L(z_L) \\
z_L = b_L + A_L \cdot \Phi_{L-1}(z_{L-1}) \\
z_{L-1} = b_{L-1} + A_{L-1} \Phi_{L-2}(z_{L-2}) \\
\quad \vdots \\
z_\ell = b_\ell + A_\ell \Phi_{\ell-1}(z_{\ell-1}) \qquad \text{(general form)} \\
\quad \vdots \\
z_1 = b_1 + A_1 x
\end{cases}
$$

Classification networks

K ... classes.





Softmax: $\hat{p}_k = \dfrac{e^{o_k}}{\sum e^{o_k}}$

Properties:
- $\hat{p}_k > 0$.
- $\sum_k \hat{p}_k = 1$
- preserves order: $o_i > o_j \implies \hat{p}_i > \hat{p}_j$

K entries.

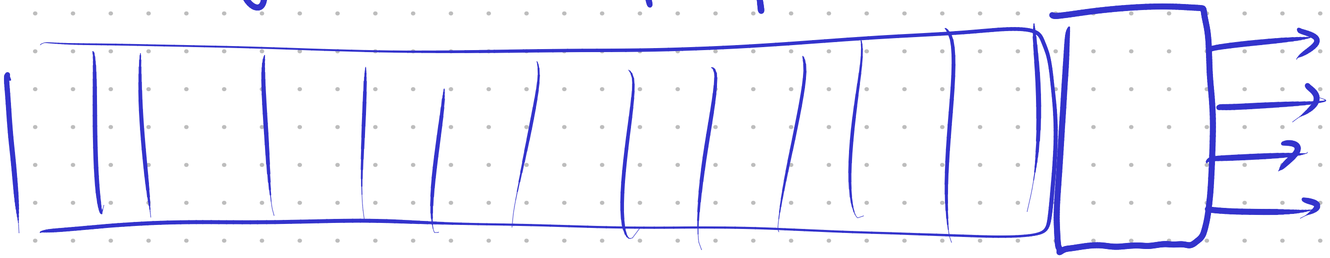
One-hot encoding (OHE)

$$c_1 \longrightarrow \begin{bmatrix}1\\0\\\vdots\\0\\0\end{bmatrix} \qquad c_2 \longrightarrow \begin{bmatrix}0\\1\\\vdots\\0\\0\end{bmatrix} \qquad \cdots \qquad c_{K-1} \longrightarrow \begin{bmatrix}0\\0\\\vdots\\1\\0\end{bmatrix} \qquad c_K \longrightarrow \begin{bmatrix}0\\0\\\vdots\\0\\1\end{bmatrix}$$

Example:
Binary output

	0-1 encoding	OHE
y_i	$y_i = 0$ for c_1 $y_i = 1$ for c_2	$y_i = \begin{bmatrix}y_i^1\\y_i^2\end{bmatrix}$ $\nearrow = \begin{bmatrix}1\\0\end{bmatrix}$ for c_1 $\searrow = \begin{bmatrix}0\\1\end{bmatrix}$ for c_2
$\hat{p}_i$	$\hat{p}_i \in [0,1]$. 0.3 ... c1	$\hat{p}_i = \begin{bmatrix}\hat{p}_i^1\\\hat{p}_i^2\end{bmatrix} = \begin{bmatrix}1-\hat{p}_i\\\hat{p}_i\end{bmatrix}$ ..... $\begin{bmatrix}0.7\\0.3\end{bmatrix}$ ... c1.

Recall on neural networks.

- From linear regression → perceptron.
- 
  - Regression : Linear regression
  - Classification : Softmax.
- Classification
  - Output: K probabilities over classes
    - → OHEncode y.
  - Loss function: Multiclass CE.

Loss function: Multi-class cross entropy

0 or 1

$$\text{CE}(y_i, \hat{p}_i) = \boxed{-\sum_{k=1}^{K} y_i^k \log \hat{p}_i^k}$$

OHE
multiclass

Recall: Binary cross entropy under 0-1 encoding (logistic regression)

$$\text{CE}(y_i, \hat{p}_i) = -y_i \log(\hat{p}_i) - (1 - y_i) \log(1 - \hat{p}_i)$$

Example

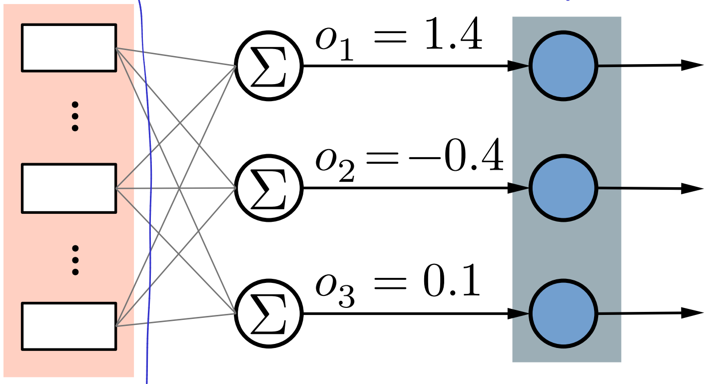
3-class classification.

final layer has K outputs.

Softmax.

Φ_L

x_i



$\hat{p}^1 = 0.695$

$\hat{p}^2 = 0.115$

$\hat{p}^3 = 0.190$

1

OHE class 3.

y_i	y^k	$-y^k \log \hat{p}^k$
y^1	0	0
y^2	0	0
y^3	1	$-\log 0.19$

$\text{CE}(y, \hat{p}) = -\log 0.19 = 1.66.$

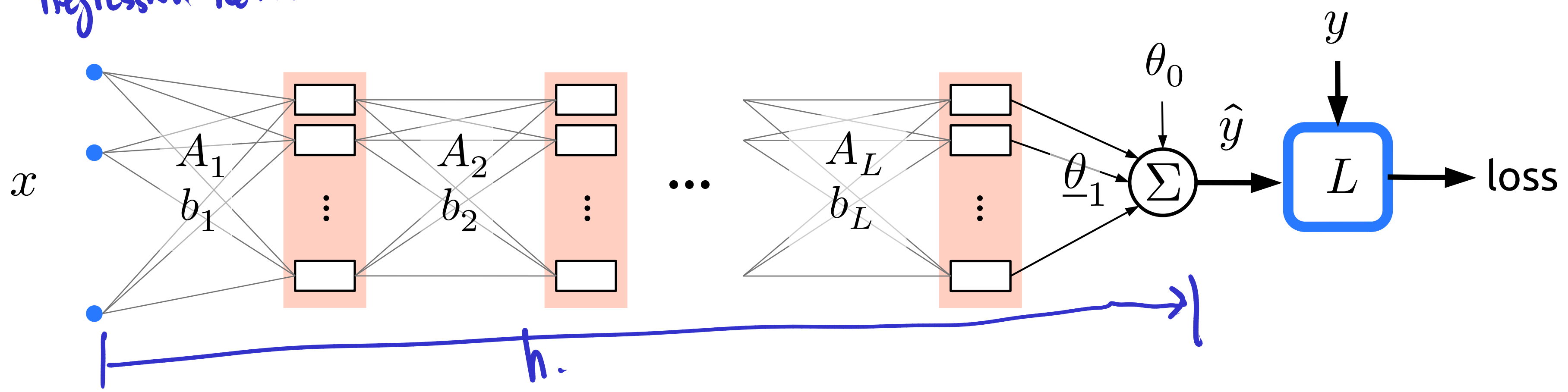
c3

$CE(c1, \hat{p}) = -\log 0.695$: smaller than 1.66

Training the neural network

- Hyper-parameters
  - # of layers L
  - # of "neurons" in each layer p_ℓ
  - activation function for each layer
- Tunable parameters   ... Backpropagation of the loss.
  - All edge weights

Regression network



$$\theta = (A_1, b_1, A_2, b_2, \dots, A_L, b_L, \theta_0, \underline{\theta}_1)$$

$$\hat{\theta} = \arg\min_{\theta} \underbrace{\sum_{i=1}^{N} L(y_i, h(x_i; \theta))}_{= \, \mathbb{L}}$$

$$\theta_{k+1} = \theta_k - \gamma \nabla_\theta \mathbb{L}(\theta_k).$$

$$L = (\hat{y} - y)^2 \longrightarrow \frac{dL}{d\hat{y}} = 2(\hat{y} - y).$$

$$\nabla_\theta \mathbb{L} = \sum \frac{dL}{d\hat{y}} \cdot \nabla_\theta h.$$

... **Regression**

scalar

vector.

$$\text{or} = \sum \frac{dL}{d\hat{p}} \cdot \nabla_\theta h$$

... Classification

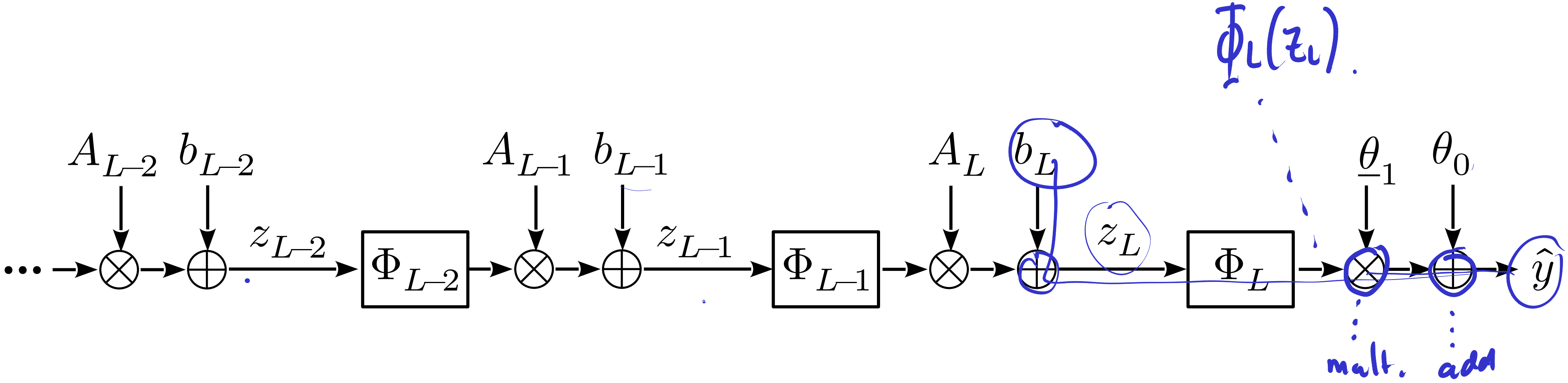
vector

matrix

Gradient of the ~~loss~~ $\nabla_\theta h$.

Computing $\nabla_\theta h$ with back-propagation

$$
\begin{aligned}
h : \hat{y} &= \theta_0 + \Phi_L^T(z_L)\theta_1 \\
z_L &= \boxed{b_L} + A_L \Phi_{L-1}(z_{L-1}) \\
z_{L-1} &= b_{L-1} + A_{L-1}\Phi_{L-2}(z_{L-2}) \\
&\vdots
\end{aligned}
$$



$$\nabla_\theta h = \left[\frac{\partial h}{\partial \theta_0}, \frac{\partial h}{\partial \underline{\theta}_1}, \frac{\partial h}{\partial b_L}, \frac{\partial h}{\partial A_L}, \dots \right]$$

✓ ✓

$$\frac{\partial h}{\partial \theta_0} = 1.$$

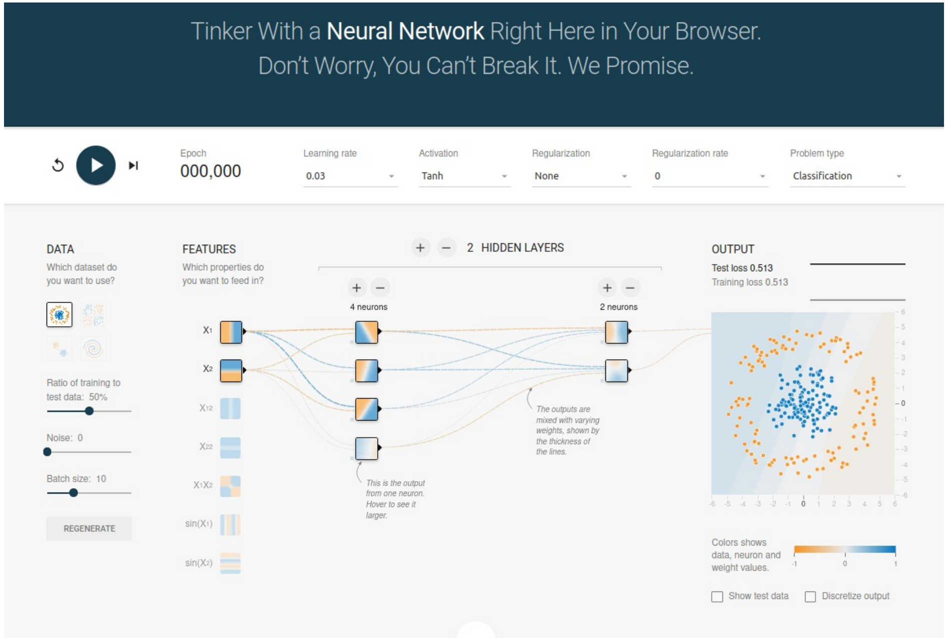
$$\frac{\partial h}{\partial \underline{\theta}_1} = \Phi_L(z_L).$$

Tensors generalization of a matrix.

$$\frac{\partial h}{\partial b_L} = \frac{\partial h}{\partial \underline{\Phi}_L} \cdot \frac{\partial \Phi_L}{\partial z_L} \frac{\partial z_L}{\partial b_L}. = \underline{\theta}_1^T \left[\Phi_L' \right]$$

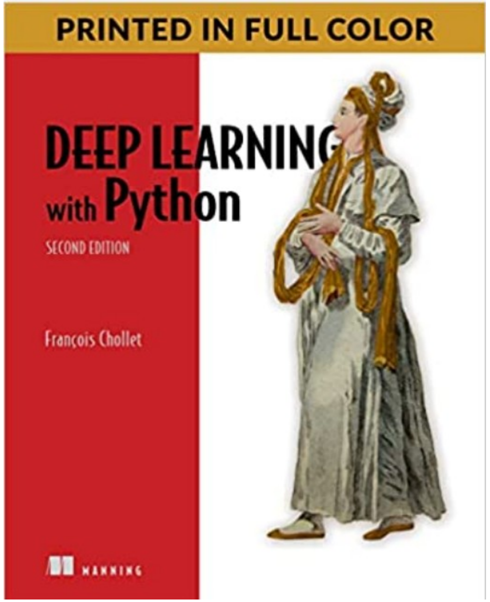
$$\frac{\partial h}{\partial A_L} = \frac{\partial h}{\partial \underline{\Phi}_L} \cdot \frac{\partial \Phi_L}{\partial z_L} \frac{\partial z_L}{\partial A_L}. = \underline{\theta}_1^T \left[\Phi_L' \right] [[\underline{\Phi}_{L-1}]]$$

https://playground.tensorflow.org

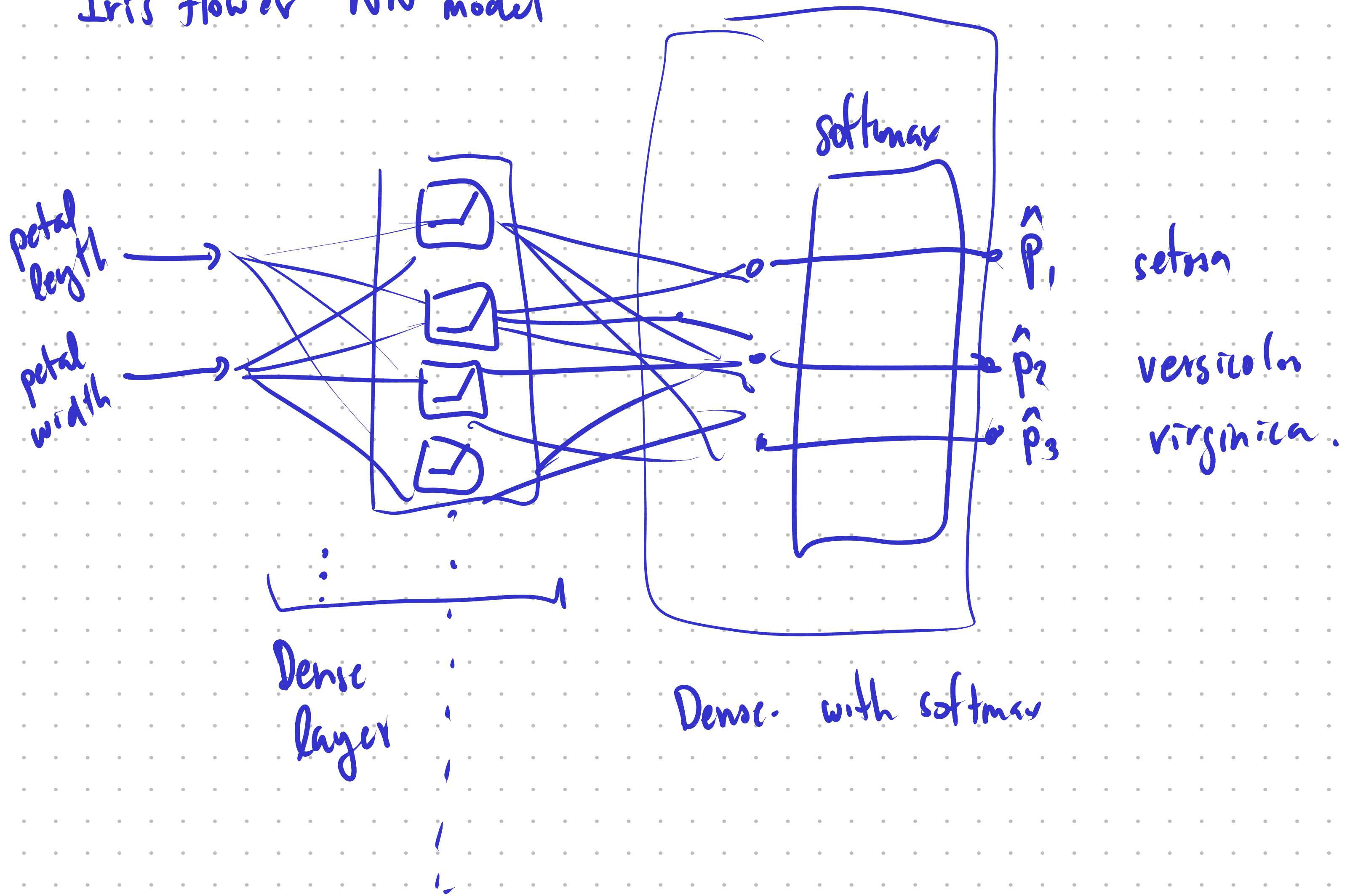


Keras

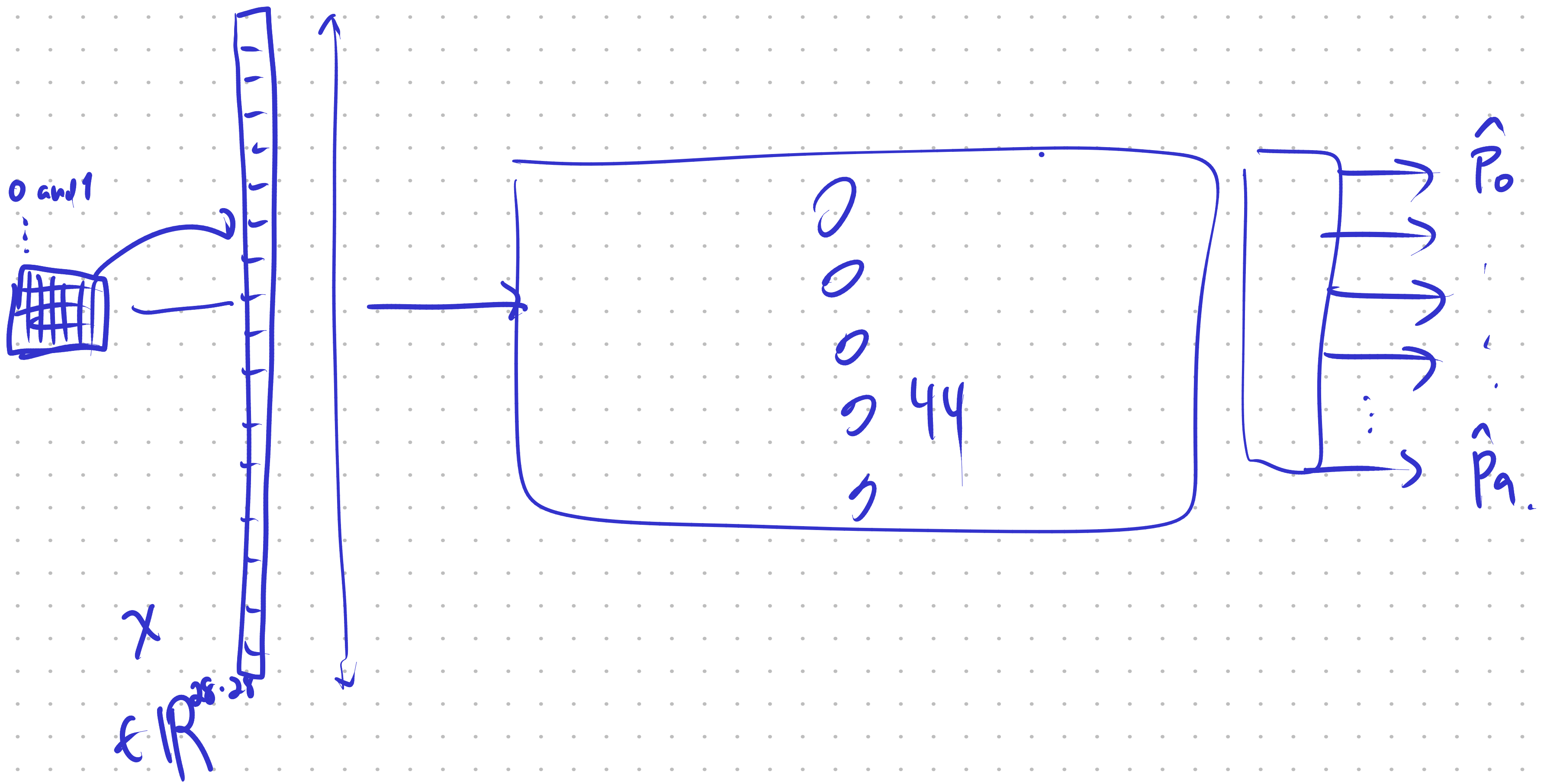
TensorFlow



Iris flower NN model



MNIST demo

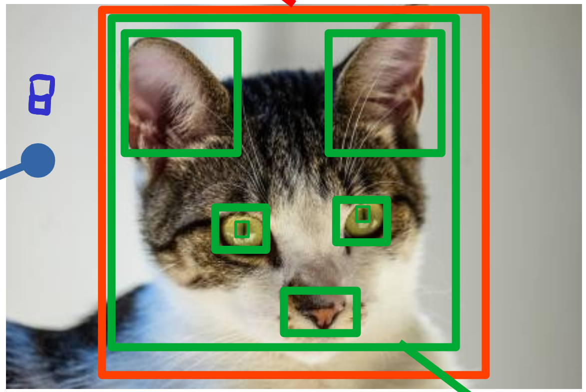


0 and 1
x
$\in \mathbb{R}^{28 \cdot 28}$
44
$\hat{p}_0$
$\hat{p}_9$

Neural networks for images

Convolutional Neural Networks.

translational
invariance



spatial
correlations

hierarchical
structure

Convolution operator

$$\overbrace{\text{kernel , bias , activation}}^{\text{filter}}$$

$$\overset{\text{pixels}}{\begin{array}{|c|c|c|}\hline p_1 & p_2 & p_3 \\ \hline p_4 & p_5 & p_6 \\ \hline p_7 & p_8 & p_9 \\ \hline \end{array}} \quad \overset{\substack{\text{convolution}\\\text{operator}\\\downarrow}}{*} \quad \left\{ \begin{array}{|c|c|c|}\hline f_1 & f_2 & f_3 \\ \hline f_4 & f_5 & f_6 \\ \hline f_7 & f_8 & f_9 \\ \hline \end{array} \;,\; b \;,\; \phi(\cdot) \right\} = \phi\left(b + \sum_{i=1}^{9} p_i \, f_i \right)$$

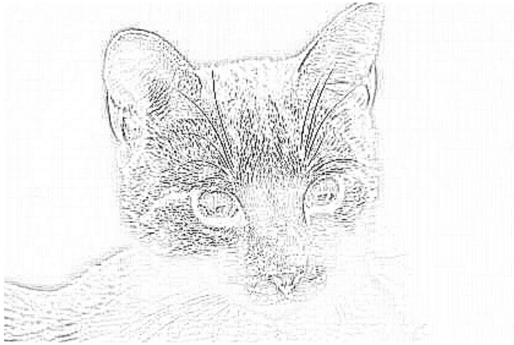
Example

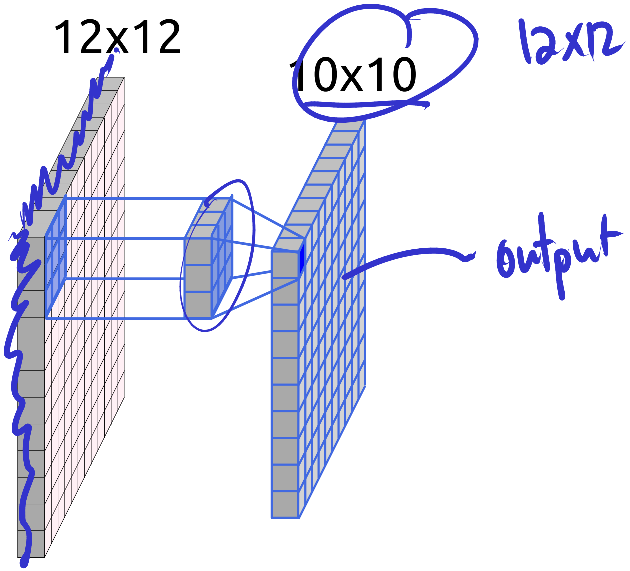
$$\begin{bmatrix} 1.0 & 0.0 & 0.8 \\ 0.1 & 0.3 & 0.5 \\ 0.1 & 0.1 & 0.0 \end{bmatrix} * \left\{ \begin{bmatrix} -0.2 & 1.2 & 0.2 \\ -0.3 & 0.5 & 0.5 \\ 0.0 & 0.0 & 0.1 \end{bmatrix}, \; b = 1, \; \phi = \text{ReLU} \right\}$$

$$\begin{aligned} &= \phi\left(b + \sum_i p_i \, f_i\right) \\ &= \text{ReLU}(1 + (1.0)(-0.2) + (0.0)(1.2) + \ldots) \\ &= \text{ReLU}(1.33) \\ &= 1.33 \end{aligned}$$

Convolution of full images

$* \{$  $, \; b \; , \; \phi(\cdot) \} =$

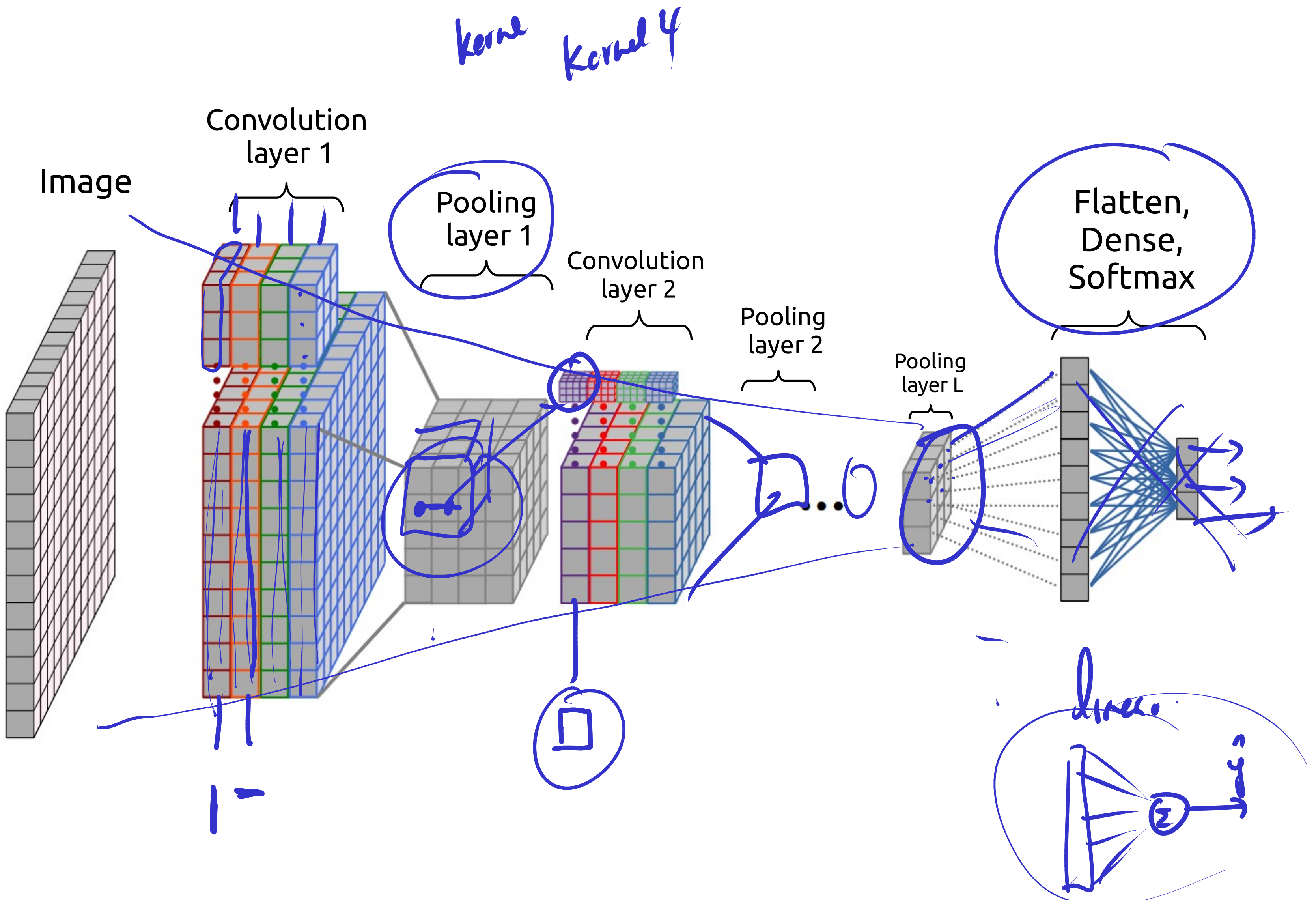




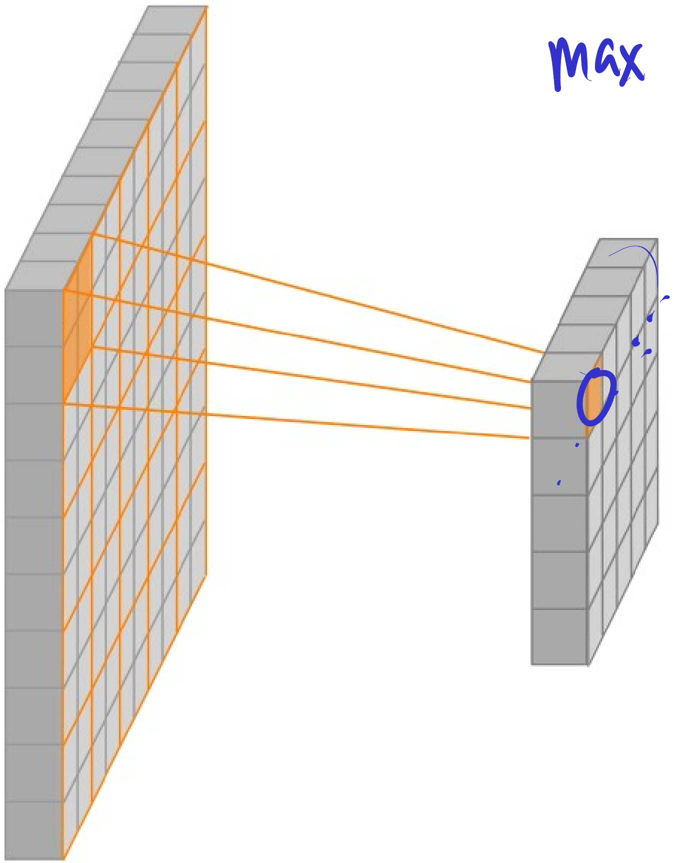
Padding $\left\{ \; , \; b \; , \; \phi(\cdot) \; , \; p = \text{True} \; \right\}$

Stride $\left\{ \; , \; b \; , \; \phi(\cdot) \; , \; s = 2 \right\}$

$* \left\{ \; , \; b \; , \; \phi(\cdot) \; , \; s = 2 \right\} \quad =$


kerne
Kernel 4
Convolution layer 1
Image
Pooling layer 1
Convolution layer 2
Pooling layer 2
Pooling layer L
Flatten, Dense, Softmax

Pooling



max pooling.