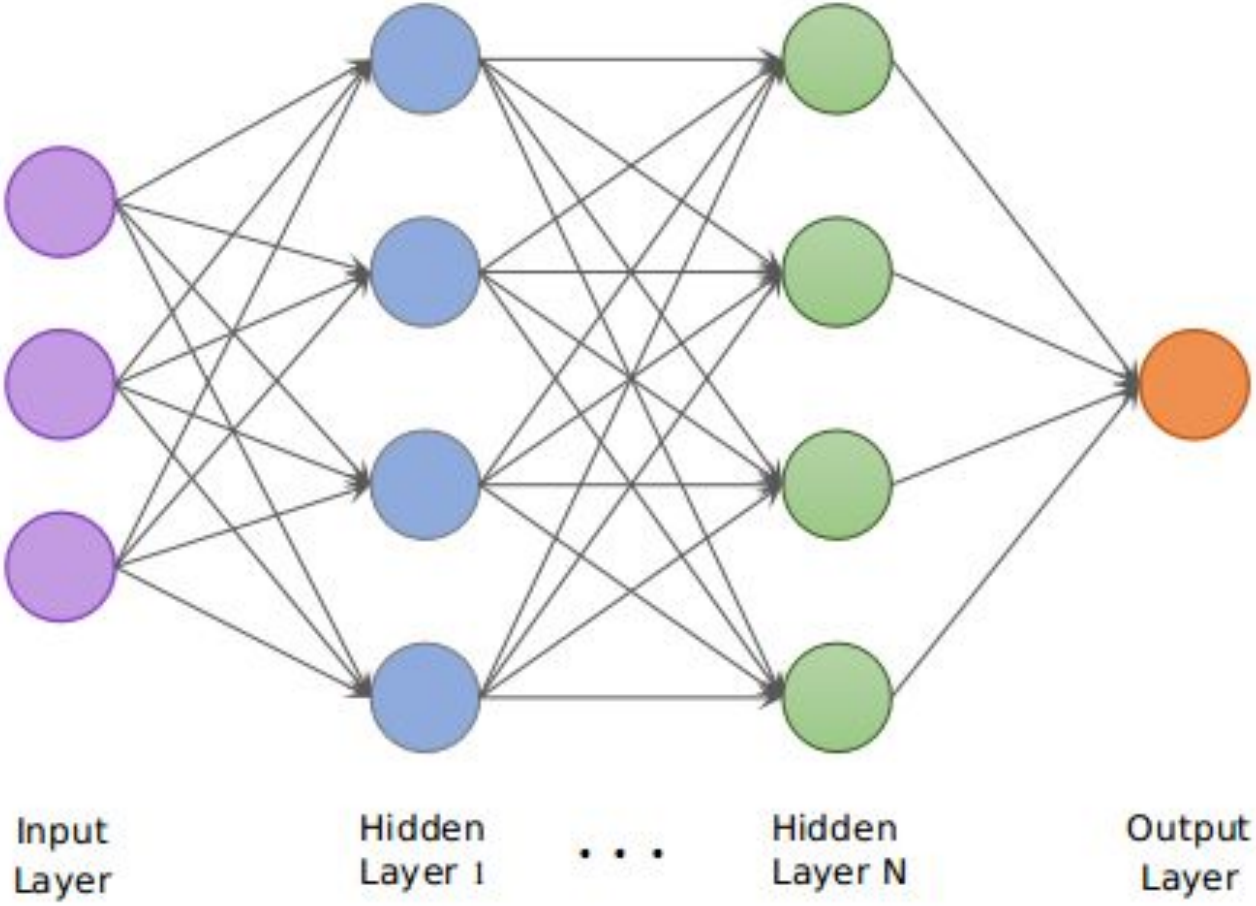
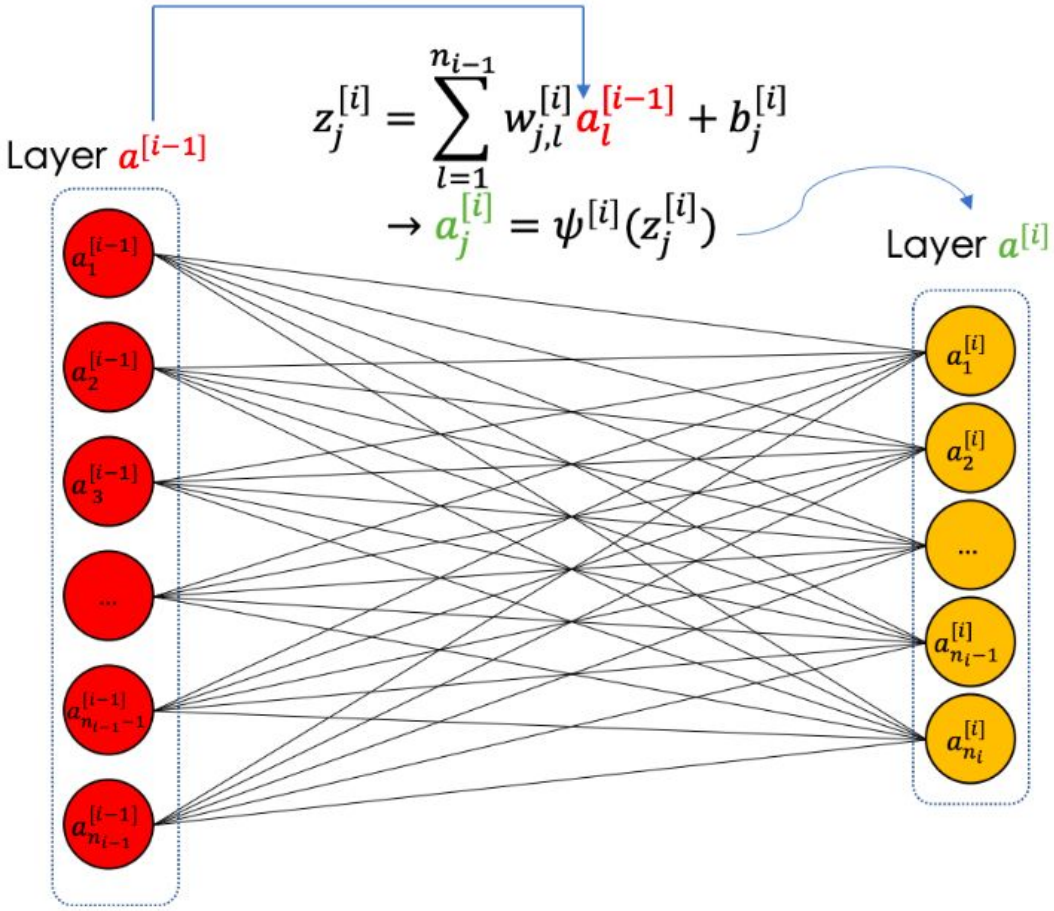
While waiting…

1. **Try to download data and codes:**
- GitHub repository: https://github.com/OBIWOW/OBiWoW-2025/tree/main/08-Monday/deep-learning-for-drug-target-interaction-prediction-and-drug-repurposing
2. **Download conda if you do not have it on your computer**
3. **Setup your environment (install necessary libraries)**
- We will run **Jupyter notebook**. We will need basic bioinformatics libraries such as **pandas, numpy, scikit-learn, matplotlib** and deep learning framework **PyTorch**, also **requests, pickle (or pickle5)**

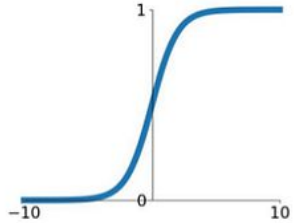

Input Layer
Hidden Layer 1
. . .
Hidden Layer N
Output Layer


$z_j^{[i]} = \sum_{l=1}^{n_{i-1}} w_{j,l}^{[i]} a_l^{[i-1]} + b_j^{[i]}$
$\rightarrow a_j^{[i]} = \psi^{[i]}(z_j^{[i]})$
Layer $a^{[i-1]}$
Layer $a^{[i]}$
$a_1^{[i-1]}$
$a_2^{[i-1]}$
$a_3^{[i-1]}$
...
$a_{n_{i-1}-1}^{[i-1]}$
$a_{n_{i-1}}^{[i-1]}$
$a_1^{[i]}$
$a_2^{[i]}$
...
$a_{n_i-1}^{[i]}$
$a_{n_i}^{[i]}$

Activation Functions

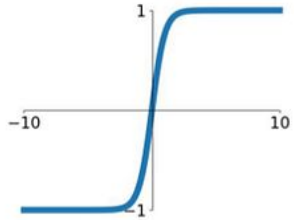
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



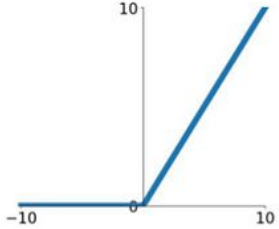
tanh

$$\tanh(x)$$



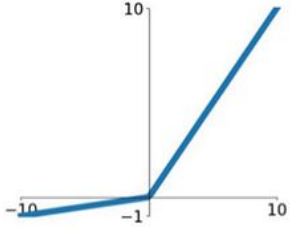
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

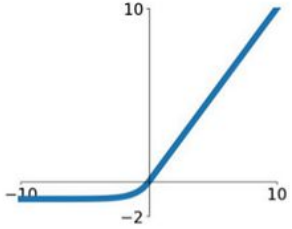


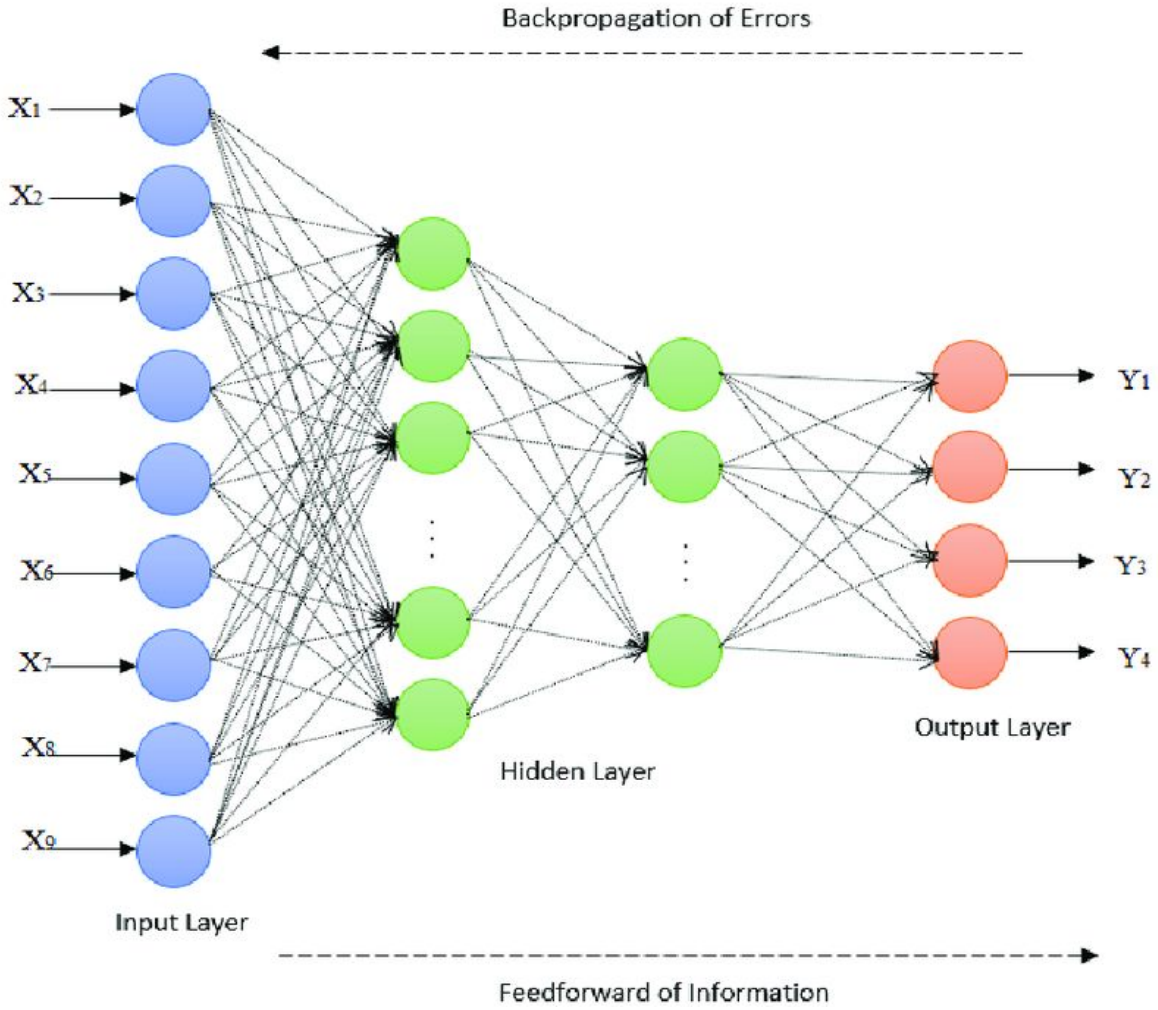
Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

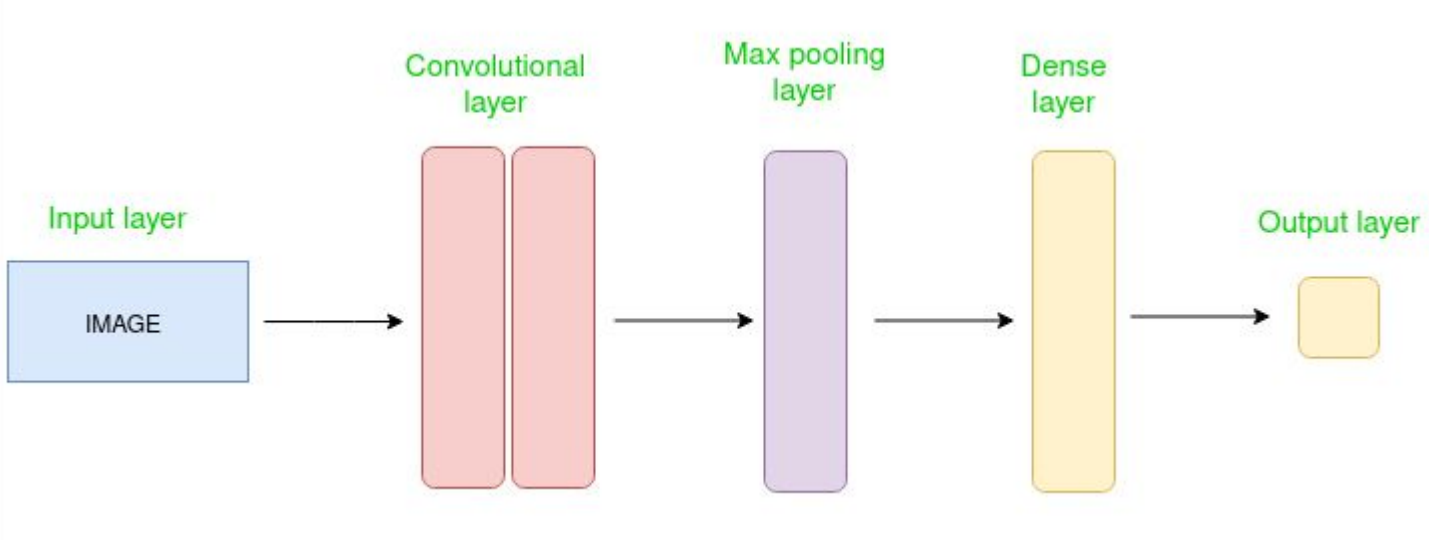
ELU

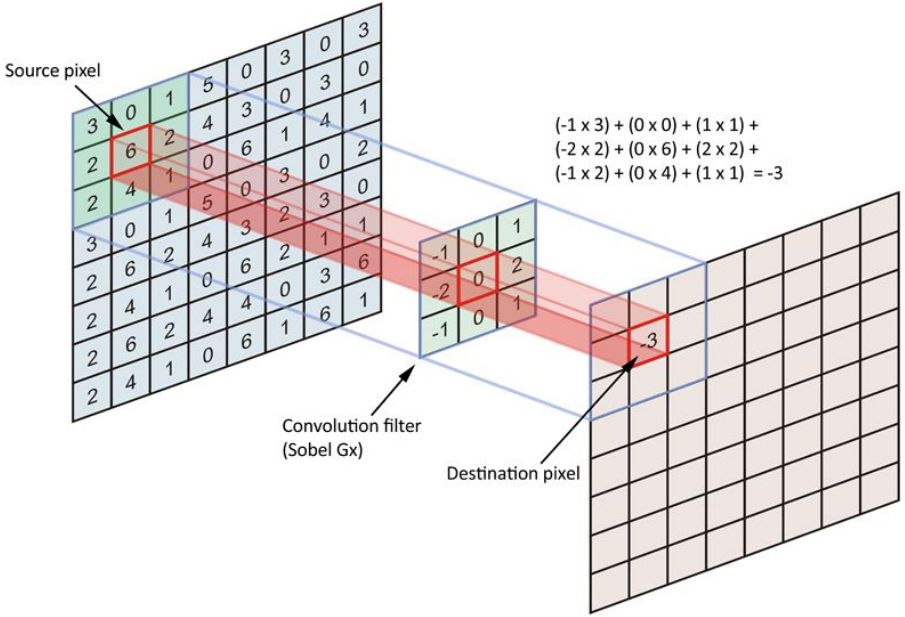
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



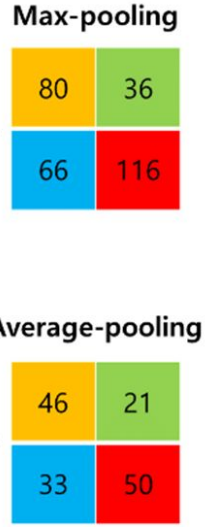

Backpropagation of Errors
X1
X2
X3
X4
X5
X6
X7
X8
X9
Y1
Y2
Y3
Y4
Input Layer
Hidden Layer
Output Layer
Feedforward of Information

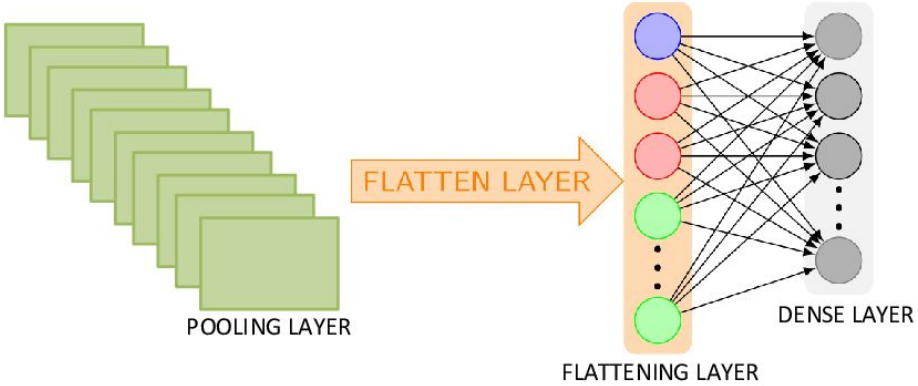
Convolutional Neural Networks

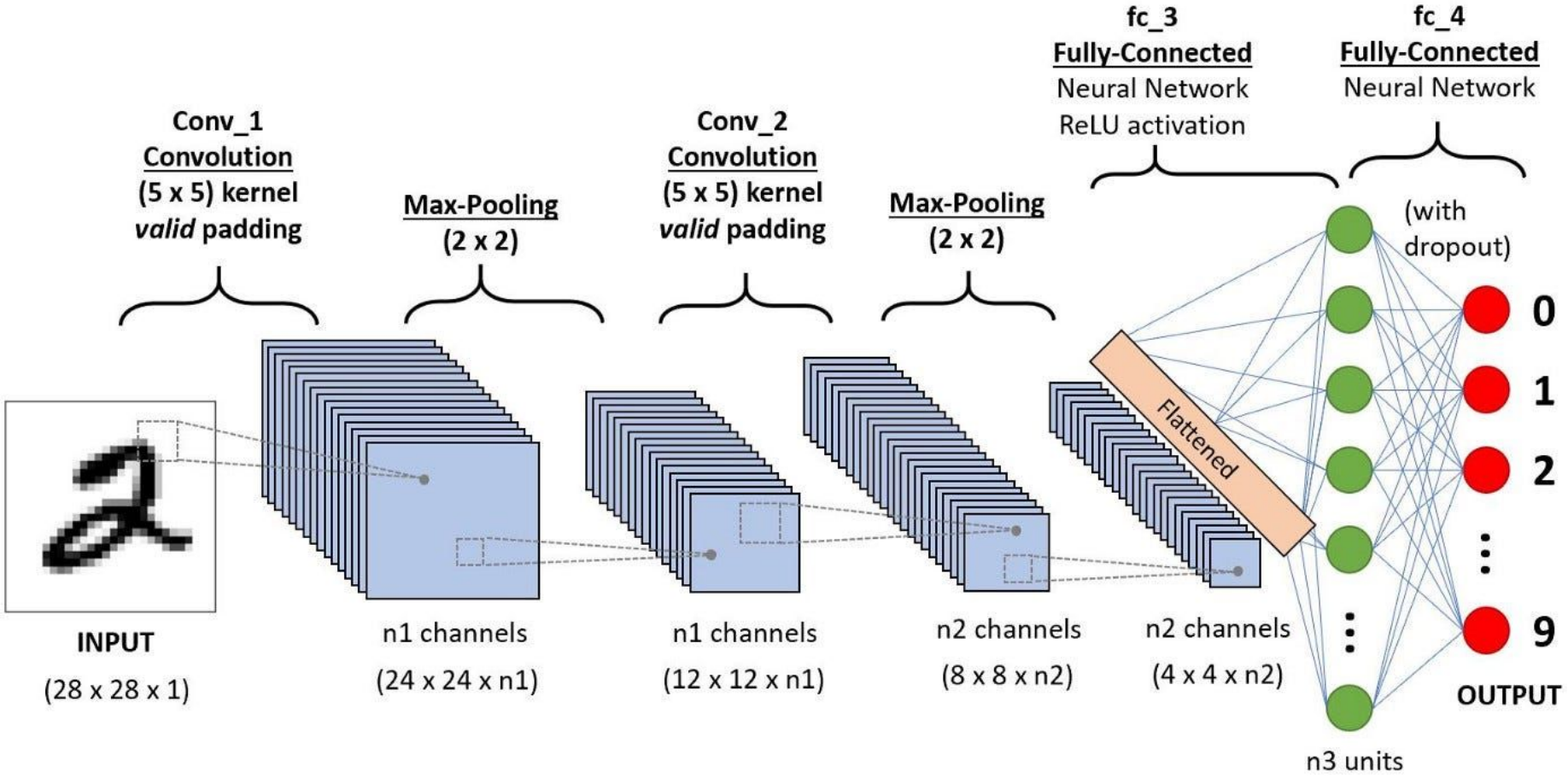



Source pixel
(-1 x 3) + (0 x 0) + (1 x 1) +
(-2 x 2) + (0 x 6) + (2 x 2) +
(-1 x 2) + (0 x 4) + (1 x 1) = -3
Convolution filter
(Sobel Gx)
Destination pixel

80 56 25 36
6 42 21 2
66 8 22 116
34 24 50 12


Max-pooling
80 36
66 116
Average-pooling
46 21
33 50


FLATTEN LAYER
POOLING LAYER
FLATTENING LAYER
DENSE LAYER


fc_3
Fully-Connected
Neural Network
ReLU activation
fc_4
Fully-Connected
Neural Network
Conv_1
Convolution
(5 x 5) kernel
valid padding
Max-Pooling
(2 x 2)
Conv_2
Convolution
(5 x 5) kernel
valid padding
Max-Pooling
(2 x 2)
(with
dropout)
Flattened
0
1
2
9
INPUT
(28 x 28 x 1)
n1 channels
(24 x 24 x n1)
n1 channels
(12 x 12 x n1)
n2 channels
(8 x 8 x n2)
n2 channels
(4 x 4 x n2)
n3 units
OUTPUT

Evaluation form