Convolutional Neural Networks in High Energy Physics

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Overview

1. Basic concepts of neural networks
2. Convolutional neural networks
3. protoDUNE experiment results

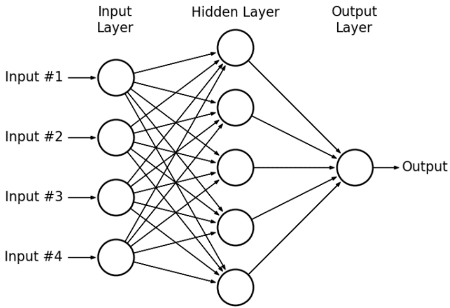
Basic concepts of neural networks

- supervised learning algorithm (imitation of biological neural network),
- let $\mathcal{T} = ((\boldsymbol{x}^{(1)}, y^{(1)}), \ldots, (\boldsymbol{x}^{(p)}, y^{(p)}))$, where $p \in \mathbb{N}$ is number of observations, $j \in \widehat{p} : \boldsymbol{x}^{(j)}$ is input vector and $j \in \widehat{p} : y^{(j)}$ is labeled output, be a dataset,
- $\mathcal{T}$ is further divided into training set, testing set and validation set (different techniques like k-fold cross-validation can be used),
- concept of neural networks is built upon universal approximation theorem

Most widely used architecture

- multilayer perceptron (MLP)

Figure: Multilayer perceptron with 4 inputs, 1 output and 1 hidden layer.



$$\text{in each layer for each neuron} : z = f\left(\sum_{i=1}^{|\mathcal{I}|} w_i x_i + \theta\right) \quad (1)$$

Optimization methods

- *loss function* measures the difference between output $\widehat{y}^{(j)}$ produced by neural network (with input $\boldsymbol{x}^{(j)}$) and labeled $y^{(j)}$ from $\mathcal{T}$,
  - regression: mean squared error as $L = \frac{1}{p}\sum_{j=1}^{p}\left(y^{(j)} - \widehat{y}^{(j)}\right)^2$,
  - classification:
    cross-entropy for binary classification as:

$$L = -\frac{1}{p}\sum_{j=1}^{p} y^{(j)}\log(\widehat{y}^{(j)}) + (1 - y^{(j)})\log(1 - \widehat{y}^{(j)}),$$

    cross-entropy for multi-class classification as:

$$L = -\frac{1}{p}\sum_{j=1}^{p}\sum_{i=1}^{\#\text{classes}} y_i^{(j)}\log(\widehat{y}_i^{(j)}),$$

  - categorical cross-entropy = softmax (on $\widehat{y}^{(j)}$) + cross-entropy,
- goal is to find global minimum of L with respects to weights matrix W

Optimization & Regularization methods

- gradient descent,
- stochastic gradient descent (randomly selected samples to compute gradients) and its numerous modifications, e. g. Adam (Adaptive Moment Estimation; adaptive change of step length etc.),
- backpropagation algorithm,
- *regularization* to loss function:
  - to loss function: e. g. $L = \underbrace{\frac{1}{p}\sum_{i=1}^{p} L_j}_{\text{data loss}} + \underbrace{\lambda \sum_{k}\sum_{l} W_{k,l}^2}_{\text{regularization loss}}$ (L_2 norm penalty),
  - in architecture: dropout (randomly excluding neurons)

Measures of classification goodness

- accuracy (simple correct predictions:all predictions on test set ratio)
- confusion matrix

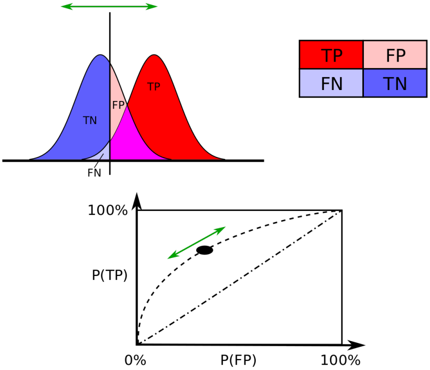
Figure: Confusion matrix definition.

Predicted Value (predicted by the test)		Actual Value (as confirmed by experiment): positives	Actual Value (as confirmed by experiment): negatives
	positives	**TP** True Positive	**FP** False Positive
	negatives	**FN** False Negative	**TN** True Negative

- F_1 score for binary classification, equals $2\frac{\text{Precision}\times\text{Recall}}{\text{Precision}+\text{Recall}}$, where Precision $= \frac{\text{TP}}{\text{TP}+\text{FP}}$ and Recall $=$ True Positive Rate (TPR) $= \frac{\text{TP}}{\text{TP}+\text{FN}}$.

- receiver operating characteristic (ROC), area under curve (AUC)

Figure: ROC and AUC vizualization.

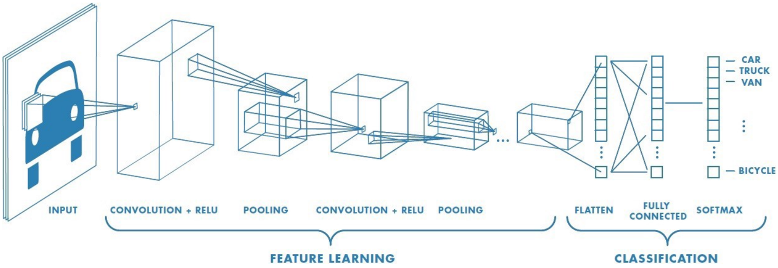


True Positive Rate (TPR) $= \frac{TP}{TP+FN}$, False Positive Rate (FPR) $= \frac{FP}{TN+FP}$

Convolutional neural network

- specially effective with visual data, widely used in computer vision
- layers typical for CNN: convolution and pooling layers (and flatten)
- consists of feature learning and classification

Figure: Demonstration of CNN architecture.



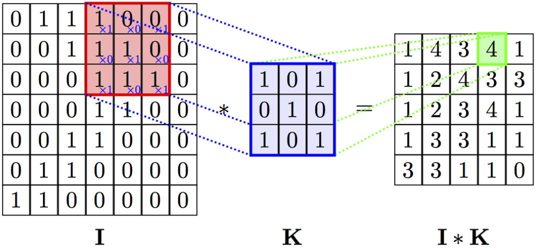
Convolution layer

- 2D convolution with kernel K

$$(I * K)(i,j) = \sum_{m=-k}^{k} \sum_{n=-k}^{k} I(m,n)K(i-m, j-n)$$

- stride corresponds to pixel shift
- padding (e. g. zero padding) used for not lowering dimension (information loss prevention)

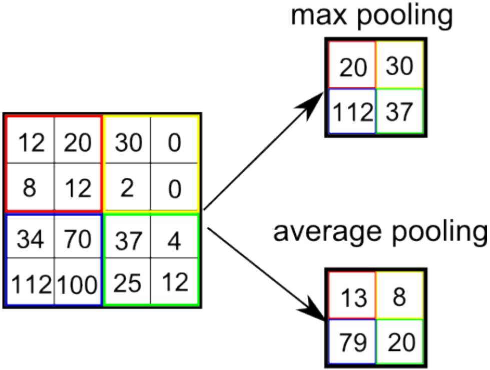
Figure: Convolution visualization (with stride 1).



Pooling

- method for dimensionality reduction
- max pooling (most used), average pooling

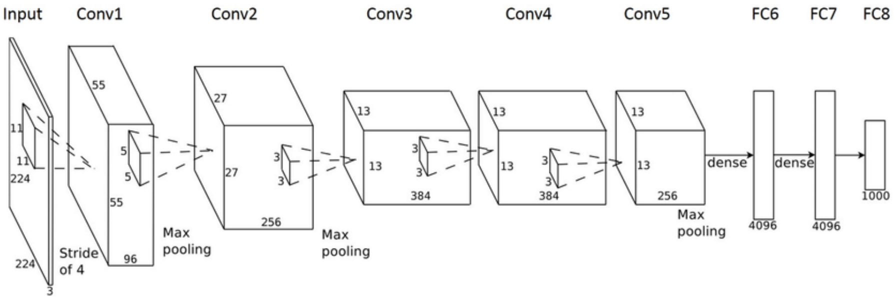
Figure: Pooling.



Convolutional neural network architectures

- kernels in the first convolutional layer detect low-level features (edges and curves),
- kernels in higher layers encode more abstract features,
- by stacking several convolutional and pooling layers, higher-level feature representations could be gradually extracted,

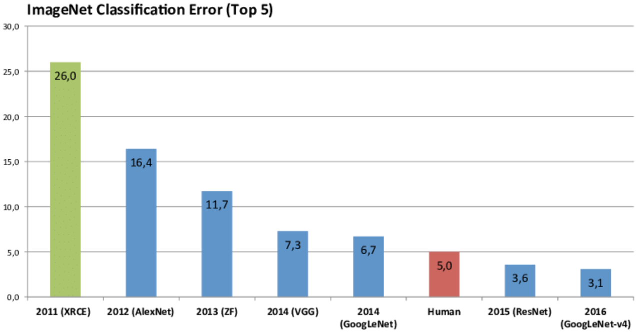
Figure: Example of CNN architecture (AlexNET).



Convolutional neural network architectures

- benchmark datasets: MNIST, cifar10, ImageNet (ILSVRC challenge)
- breakthrough in 2012 (AlexNet)
- great successes in next years: LeNet (Inception), VGG, ResNet, ResNext; more in Mira's presentation

Figure: Different CNN architectures.



Experiment protoDUNE

- Liquid Argon Time Projection Chambers (LArTPC) experiment
- DUNE, protoDUNE: Fermilab, CERN collaboration
- dataset primarily focused on classification of electron, muon and tau neutrino; secondarily on other variables' classification (interaction type, number of particles in the process)
- optimizer: SGD
- binary cross-entropy (for binary classification of neutrino/antineutrino) and categorical cross-entropy (for multi-class classification for others)
- architecture: ResNet18 with primarily with one output layer, secondarily with seven output layers
- in Tensorflow 1.13.1, Python 3.6

Experiment protoDUNE

Overall results by DUNE CNN team (accuracies in %) tested on protoDUNE Monte Carlo samples (MCC8.1):

- neutrino/antineutrino: 73.5,
- flavour: 90.3,
- interaction type: 71.5,
- # protons: 81.2 (0, 1, 2, 3+),
- # pions: 84.1 (0, 1, 2, 3+),
- # pizeros: 90.9 (0, 1, 2, 3+),
- # neutrons: 99.1 (0, 1, 2, 3+; but almost all the events have 0 neutrons)

Future goals & Conclusion

Future goals:

- other metrics
- 3D convolutional neural network
- sparse convolutional network

Conclusion:

- we have given a brief introduction into neural network and its convolution aspects
- we have discussed protoDUNE experiment classification results

Thank you for your attention

Variables' classes

- neutrino/antineutrino
- flavour: CC (charged current) ν_μ, CC ν_e, CC ν_τ, NC (neutral current),
- interaction type: CC quasi electric, CC Res, CC DIS, CC other
- # protons: 0, 1, 2, 3+,
- # pions: 0, 1, 2, 3+,
- # pizeros: 0, 1, 2, 3+,
- # neutrons: 0, 1, 2, 3+; but almost all the events have 0 neutrons