CSI5180. Machine Learning for Bioinformatics Applications

Deep learning — architectures

by

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Preamble

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Deep learning — architectures

In this lecture, we focus our attention on the **architecture** of deep learning networks. On the back cover of their book “Deep Learning”, Goodfellow, Bengio and Courville present deep learning as a form of machine learning that enables computers to “**understand the world in terms of a hierarchy of concepts**”. This idea was implicit when we looked at the model behind feed forward networks: $h_{W,b}(X) = f_k(\ldots f_2(f_1(X))\ldots)$, where $f_l(Z) = \phi(W_l Z + b_l)$ for $l = 1 \ldots k$. This idea becomes much more concrete when examining the various architectures; namely, convolution neural networks and recurrent neural networks.

General objective :

- **Discuss** the relationships between the nature of the problems to be solved and the architecture of deep networks.

Learning objectives

- **Discuss** the relationships between the nature of the problems to be solved and the architecture of deep networks.
- **Explain** convolution neural networks (CNN).
- **Describe** recurrent neural networks (RNN).

Reading:

- Vanessa Isabell Jurtz, Alexander Rosenberg Johansen, Morten Nielsen, Jose Juan Almagro Armenteros, Henrik Nielsen, Casper Kaae Sønderby, Ole Winther, and Søren Kaae Sønderby, An introduction to deep learning on biological sequence data: examples and solutions, *Bioinformatics* **33**:22, 36853690, 2017.
- Seonwoo Min, Byunghan Lee, and Sungroh Yoon, Deep learning in bioinformatics, *Brief Bioinform* **18**:5, 851869, 2017.

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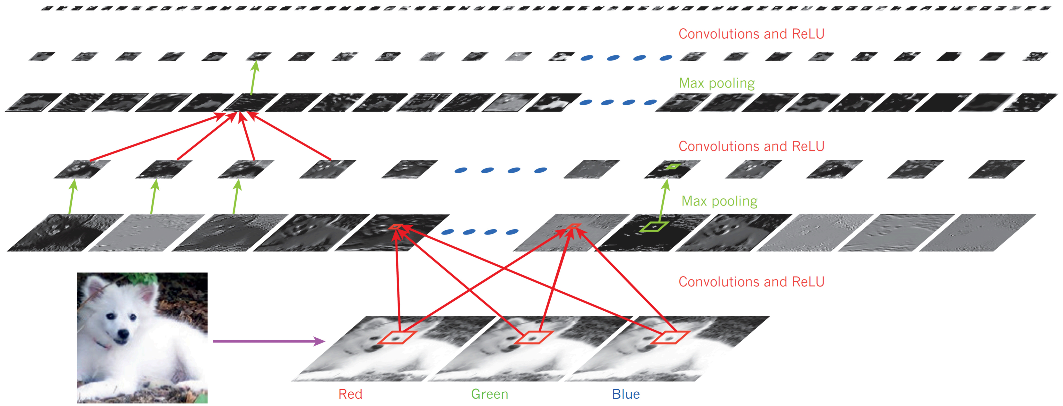
  - The authors solve **three (3) bioinformatics problems** using deep networks:
    - **Subcellular localization**
    - **Protein secondary structure**
    - **Peptide binding to MHCII molecules**
  - For each problem, they discuss the **pros** and **cons** of **convolutional networks** and **recurrent networks**.
  - `https://github.com/vanessajurtz/lasagne4bio`

Plan

Introduction

Hierarchy of concepts



- Yann LeCun, Yoshua Bengio, and Geoffrey Hinton, Deep learning, *Nature* **521**:7553, 43644, 2015.

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    - These are then combined to form **corners**, **crosses**, etc.
- This explains how **transfer learning** works and why selecting the bottom layers only.

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*"An MLP with just **one hidden layer** can theoretically model even the most **complex functions**, provided it **has enough neurons**. But for complex problems, **deep networks** have a much **higher parameter efficiency** than shallow ones: they can model complex functions **using exponentially fewer neurons** than shallow nets, allowing them to reach much **better performance** with the same amount of training data." [4] §10*

How many layers?

- Start with one layer, then **increase the number of layers** until the model starts **overfitting** the training data.
- **Finetune** the model adding regularization (dropout layers, regularization terms, etc.).

The number of neurons and other hyperparameters are determined using a grid search.

Remarks

- Consider a **feed-forward network** (FFN) and its model:

$$h_{W,b}(X) = f_k(\dots f_2(f_1(X))\dots)$$

where

$$f_l(Z) = \phi(W_l Z + b_l)$$

for $l = 1 \dots k$.

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- **Two layers 1,000-unit** implies **1,000,000** parameters!

Convolutional Neural Network

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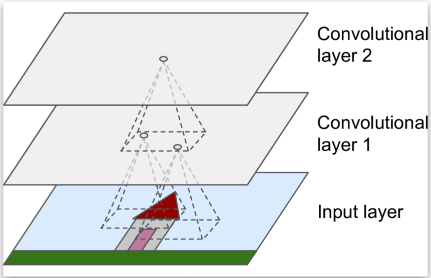
Convolutional networks come from the field of **machine vision**. Hence their close connection to **grid-like inputs**.

CNN - receptive field



Source: [4] Figure 14.2

- Each unit is connected to neurons in its **receptive fields**.
  - Unit i, j in layer l is connected to the units i to $i + f_h - 1$, j to $j + f_w - 1$ of the layer $l - 1$, where f_h and f_w are respectively the **height** and **width** of the **receptive field**.

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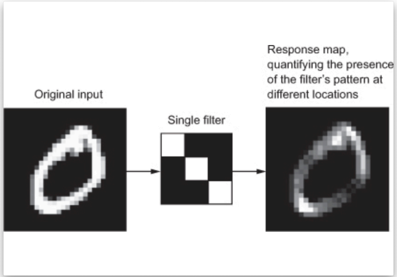
- **Stride**. It is possible to connect a large larger $(l-1)$ to a smaller one (l) by skipping units. The number of units skipped is called **stride**, s_h and s_w.
  - Unit i, j in layer l is connected to the units $i \times s_h$ to $i \times s_h + f_h - 1$, $j \times s_w$ to $j \times s_w + f_w - 1$ of the layer $l-1$, where f_h and f_w are respectively the **height** and **width** of the **receptive field**, s_h and s_w are respectively the **height** and **width strides**.

CNN - filters


Original input
Single filter
Response map, quantifying the presence of the filter's pattern at different locations

Source: [3] Figure 4.3

- A **window** of size $f_h \times f_w$ is moved over the output of the layers $l-1$ (this is called the **input feature map**) position by position.

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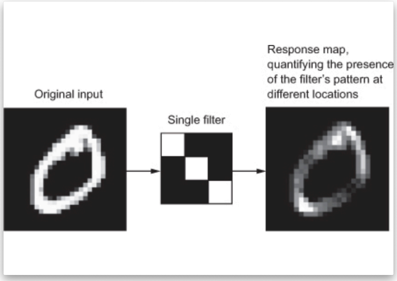
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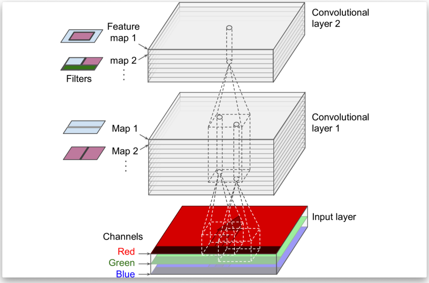
- A **window** of size $f_h \times f_w$ is moved over the output of the layers $l - 1$ (this is called the **input feature map**) position by position.
- **For each location**, it calculates the product between the extracted patch and a matrix of the same size, called a **convolution kernel** or **filter**. The **sum** of the values of the resulting matrix is the **output** for that location.

CNN - model



Source: [4] Figure 14.6

$$z_{i,j,k} = b_k + \sum_{u=0}^{f_h-1} + \sum_{v=0}^{f_w-1} + \sum_{k'=0}^{f_{n'}-1} x_{i',j',k'} \cdot w_{u,v,k',k}$$

where $i' = i \times s_h + u$ and $j' = j \times s_w + v$; see [4] §14.

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- "Of course, you do not have to define the filters manually: instead, **during training the convolutional layer will automatically learn the most useful filters for its task**,"
- "(. . .) and **the layers above will learn to combine them** into more complex patterns."
- "The fact that **all neurons in a feature map share the same parameters** dramatically reduces the number of parameters in the model."

CNN - convolution (ressources)

- **A guide to convolution arithmetic for deep learning**
- Vincent Dumoulin and Francesco Visin
- Last revised 11 Jan 2018
    - https://arxiv.org/abs/1603.07285
    - https://github.com/vdumoulin/conv_arithmetic/

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- This (subsampling) has the effect of **shrinking the network**, each window of size $f_h \times f_w$ is reduced to a single value, **max** or **mean** of that window.
- "[A] max pooling layer also introduces some level of **invariance to small translations**." [4] §14

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  - Let $h_{u,l}$ be the state of the unit u in layer l.
- **Each unit** has two inputs, as before the output of the units from the **previous layer** ($l-1$), but also the vector of states for this layer (l) at the **previous time step**.

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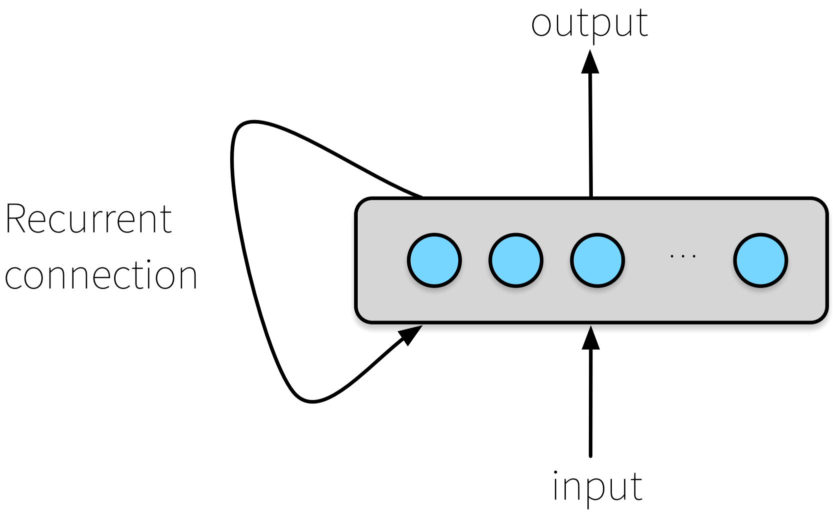

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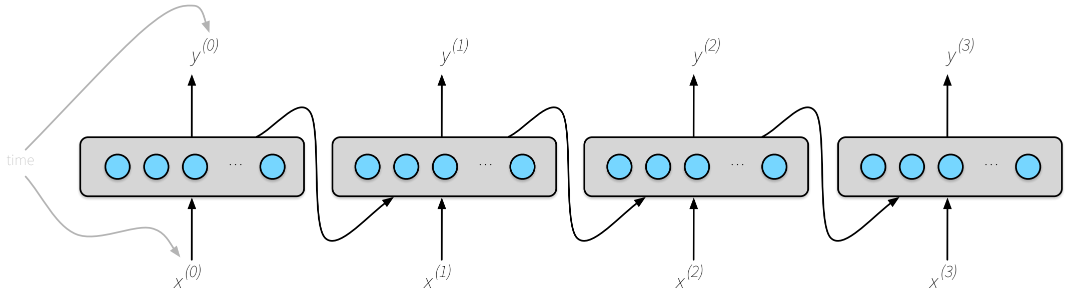

$$Y^{(t)} = \phi(X^{(t)} W_X + Y^{(t-1)} W_Y + b)$$

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- **Long Short-Term Memory** (**LSTM**) are networks with long-term memory.

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model = keras.models.Sequential([
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- **Bidirectional LSTM** cells also exist.

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- Hinton and colleagues say that they are "**preventing co-adaptation**".
- **Dropout layers** can make the network converging more slowly. However, the resulting network is expected to make **fewer generalization errors**.

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  - **Pooling** makes the network less sensitive to small translations.
  - In bioinformatics, **CNN** networks are ideally suited to detect local (sequence) motifs, independent of their position within the input (sequence).
- **Recurrent networks (RNN)** and **LSTM** can input sequences of varying length.

Keras

```
model = keras.models.Sequential([
    keras.layers.Conv2D(64, 7, ..., input_shape=[28, 28, 1]),
    keras.layers.MaxPooling2D(2),
    keras.layers.Conv2D(128, 3, activation="relu", padding="same"),
    keras.layers.Conv2D(128, 3, activation="relu", padding="same"),
    keras.layers.MaxPooling2D(2),
    keras.layers.Conv2D(256, 3, activation="relu", padding="same"),
    keras.layers.Conv2D(256, 3, activation="relu", padding="same"),
    keras.layers.MaxPooling2D(2),
    keras.layers.Flatten(),
    keras.layers.Dense(128, activation="relu"),
    keras.layers.Dropout(0.5),
    keras.layers.Dense(64, activation="relu"),
    keras.layers.Dropout(0.5),
    keras.layers.Dense(10, activation="softmax")
])
```

[4] §14:

Further considerations

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We obviously barely scratched the surface of deep learning. Here are some important concept that we did not consider:

- The **vanishing** and **exploding** gradient.
- Initialization.
- **Data augmentation**.
- **Attention** layer.
- Understanding what the network has learnt.

Prologue

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- **RNN** and **LSTM** handle sequence information, where the input sequences can be of different lengths. They can detect patterns along the sequence.
- **Dropout** layers are an effective regularization mechanism.

Next module

- **Concept**- and **rule**-based

References

Vanessa Isabell Jurtz, Alexander Rosenberg Johansen, Morten Nielsen, Jose Juan Almagro Armenteros, Henrik Nielsen, Casper Kaae Sønderby, Ole Winther, and Søren Kaae Sønderby.
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O'Reilly Media, 2nd edition, 2019.

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