CSI5180. Machine Learning for Bioinformatics Applications

Deep learning — practical issues

by

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Preamble

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Deep learning — practical issues

In this last lecture deep learning, we consider practical issues when using existing tools and libraries.

General objective :

- **Discuss** the pitfalls, limitations, and practical considerations when using deep learning algorithms.

Learning objectives

- **Discuss** the pitfalls, limitations, and practical considerations when using deep learning algorithms.
- **Explain** what is a dropout layer
- **Discuss** further mechanisms to regularize deep networks

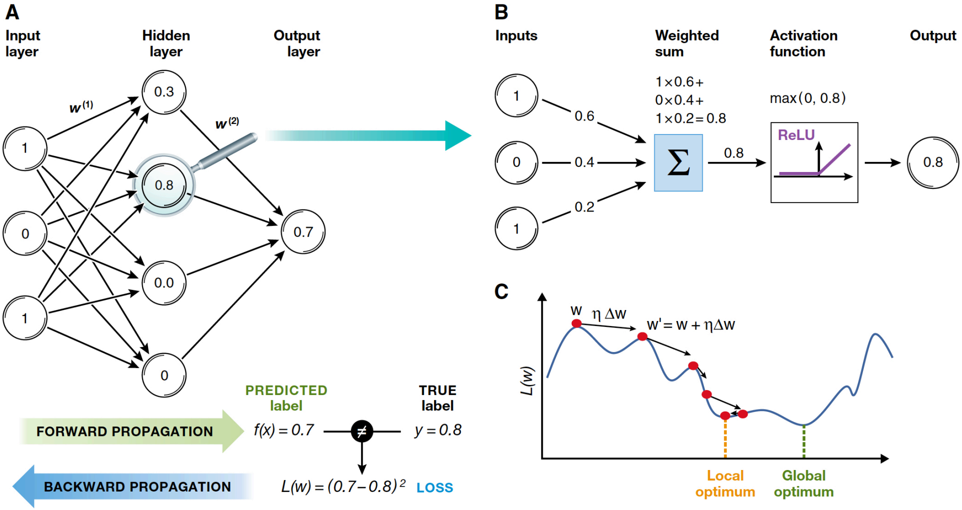
Reading:

- Christof Angermueller, Tanel Pärnamaa, Leopold Parts, and Oliver Stegle. Deep learning for computational biology. *Mol Syst Biol* **12**(7):878, 07 2016.

Plan

As mentioned previously

Overview



Source: [1] Box 1

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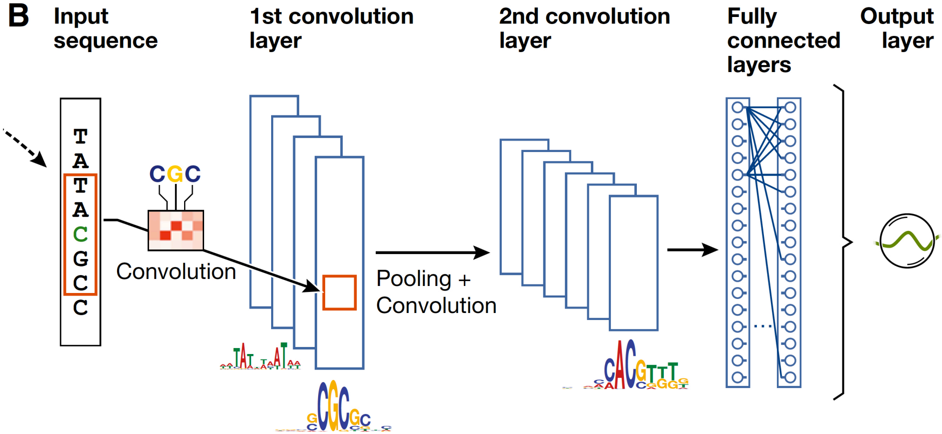
- **Local connectivity**. In a **convolutional layer** each neuron is connected to a small number of neurons from the previous layer. This small rectangular region is called the **receptive field**.
- **Parameter sharing**. All the neurons in a given **feature map** of a **convolutional layer** share the same **kernel** (**filter**).

Convolutional layer (Conv1D)



Source: [1] Figure 2B

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- **Convolutional Neural Networks** are able to detect patterns **irrespective** of their location in the input.
  - **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). They are also the most prevalent architecture.

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  - Literature suggests that RNNs are more difficult to train than other architectures.

Regularization

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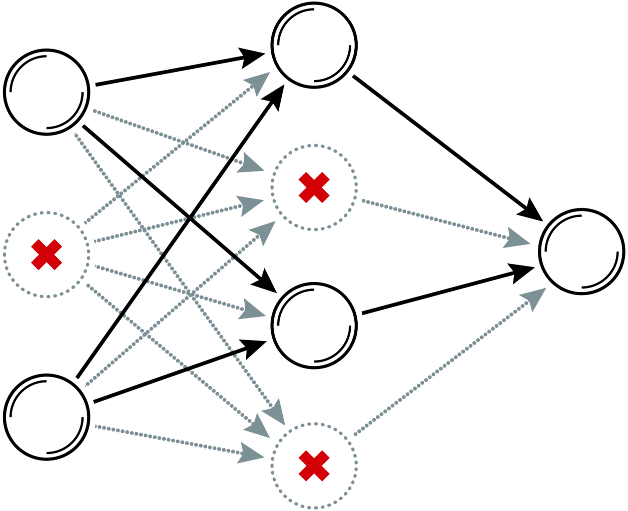


Source: [1] Figure 5F

Regularizers

- Applying penalties on layer parameters
- https://keras.io/regularizers/

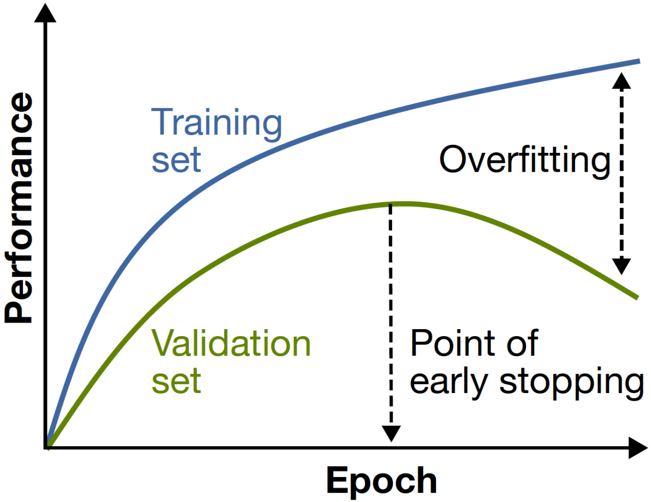
```
# other import directives are here
from keras import regularizers

model = Sequential()
model.add(Dense(32, input_shape=(16,)))
model.add(Dense(64, input_dim=64,
                kernel_regularizer=regularizers.l2(0.01)))
```

Available penalties

```
keras.regularizers.l1(0.)
keras.regularizers.l2(0.)
keras.regularizers.l1_l2(l1=0.01, l2=0.01)
```

Early stopping



Source: [1] Figure 5E

Hyperparameters

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  - **Nesterov Accelerated Gradient**, **AdaGrad**, **RMSProp**, **Adam** and **Nadam**.
  - **Adam** is a good default choice.

Loss function

- **Regression**
  - **mean_squared_error** (MSE) or **mean_absolute_error** (MAE)
- **Classification**
  - **Binary classification** : binary_crossentropy
  - **Multiclass classification** : categorical_crossentropy
- https://keras.io/losses/

```
from keras import losses

model.compile(loss=losses.mean_squared_error, optimizer='sgd')
```

Output layer activation

- **Regression** [3] Table 10.1:
  - ReLU/softplus (if positive outputs)
  - logistic/tanh (if bounded outputs)
- **Classification**
  - **Binary classification** : logistic
  - **Multiclass classification** : softmax
- https://keras.io/activations/

```
model = keras.models.Sequential([
    ...
    Dense(64, activation="relu"),
    ...
])
```

Hyperparameters

Name	Range	Default value
Learning rate	0.1, 0.01, 0.001, 0.0001	0.01
Batch size	64, 128, 256	128
Momentum rate	0.8, 0.9, 0.95	0.9
Weight initialization	Normal, Uniform, Glorot uniform	Glorot uniform
Per-parameter adaptive learning rate methods	RMSprop, Adagrad, Adadelta, Adam	Adam
Batch normalization	Yes, no	Yes
Learning rate decay	None, linear, exponential	Linear (rate 0.5)
Activation function	Sigmoid, Tanh, ReLU, Softmax	ReLU
Dropout rate	0.1, 0.25, 0.5, 0.75	0.5
L1, L2 regularization	0, 0.01, 0.001	

Source: [1] Table 2

Keras

Keras

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

[3] §14:

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- **Attention** layer
- Multi-tasks (not multi-class, not multi-labels)

Of deep neural networks

- The see the world as a **hierarchy of concepts**, effectively bypassing the need to create features (features engineering).
  - “Deep neural networks can help **circumventing the manual extraction of features** by **learning them** from data.” [1]
- **Transfer learning** is a possibly unique to deep learning.
- **Hundreds of papers** in bioinformatics alone.

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

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