

Decoding Deep Learning Demystified and Codeless with KNIME

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This slide deck is available at https://kni.me/s/4-i5-EcLrZwf5cxN



Agenda

- Introduction to deep learning
 - Machinery of deep learning with KNIME
 - Artificial neural networks
 - Back propagation
 - Optimizing neural network models
 - Demo classification with a feedforward neural network (FFNN)
- Convolutional Neural Networks (CNN)
 - Computer vision
 - Convolution & pooling layers
 - Transfer learning
- Recurrent Neural Networks (RNN)
 - Sequential data & RNN
 - Long short-term memory (LSTM)



Target Audience

- Those interested in deep learning
 - With some background knowledge in machine learning
- No KNIME experience? No problem!
 - General introduction to deep learning
 - Some pointers to get started with DL with KNIME
 - Links to workflow examples on KNIME Hub







Machinery of deep learning with KNIME

What is KNIME Analytics Platform?

- A tool for data analysis, manipulation, visualization, and reporting
- Based on the graphical programming paradigm
- Provides a diverse array of extensions:
 - Text Mining
 - Network Mining
 - Cheminformatics
 - Many integrations, such as Java, R, Python, Weka, Keras, Plotly, H2O, etc.





Keras + KNIME



- KNIME Deep Learning Extension builds on top of the Keras Libraries
- The Keras libraries build on top of TensorFlow
- Deep Learning libraries from TensorFlow and Keras are accessible via Python ...
- ... And KNIME with the Deep Learning Keras Integration.



Installation

Deep Learning in KNIME Analytics Platform comes with a specific integration. A few simple steps are necessary to get it up and running.

- On your machine:
 - Anaconda with Python3 correctly installed
- Extensions installed on KNIME Analytics Platform
 - KNIME Deep Learning Keras Integration
 - KNIME Deep Learning TensorFlow Integration

NOTE: This is just a quick start guide to start using Deep Learning with your KNIME Analytics Platform. If you are experiencing issues or want to customize your installation, please refer to <u>KNIME Deep Learning Integration Installation Guide</u>



Artificial neural networks



Let's Start Simple

Single neuron





 $x_1w_1 + x_2w_2 + b$

Neural network





Frequently used Activation Functions



Non-linear activation functions enable modeling of non-linear problems





Minutes attended

Passed certification

Didn't pass certification



Input features: x_1 = minutes attended x_2 = workflows build Output: $\hat{y} =$ Probability that a person passed $\hat{y} \ge 0.5 \Rightarrow Passed$ and $\hat{y} < 0.5 \Rightarrow Failed$





Minutes attended

- Passed certification
- Didn't pass certification
- + New sample
 - x_1 = minutes attended = 170 x_2 = workflows build = 8





Input features: x_1 = minutes attended x_2 = workflows build Output: $\hat{y} = \text{Probability that a person passed}$ $\hat{y} \ge 0.5 \Rightarrow Passed \text{ and } \hat{y} < 0.5 \Rightarrow Failed$



Training a Neural Network = Finding Good Weights





Example of a Loss Landscape



Goal find w_1 and w_2 of the global minima of the loss landscape



Learning Rule from Gradient Descent

• Adjust the weight for the next step by the adjustment term $\Delta w(t)$





Idea Behind Gradient Descent

Mountain biking in foggy conditions

- 1. Start at your current position
- 2. Until you reached the valley
 - 1. Look for the direction of steepest ascent
 - 2. Cycle into the opposite direction for 2m
- 3. Update the current position

- 1. Initialize the weights W
- 2. Until we reach a minimum
 - 1. Calculate the gradient with respect to the weights $\nabla_W J(x, W)$

Gradient descent

algorithm

- 2. make a little step into the opposite direction $W \leftarrow W \eta \nabla_W J(x, W)$
- 3. Update the weights

Note: $\nabla_W J(x, W) = \begin{bmatrix} \frac{\partial J}{\partial w_1} \\ \frac{\partial J}{\partial w_2} \end{bmatrix}$, vector with the partial derivatives with respect to all weights.



Idea Behind Gradient Descent



Back propagation



Backpropagation

Efficient way to calculate the gradient during optimization

Forward pass



Backward pass



























- Gradients can be determined one layer at a time by the chain rule
- To determine the gradient at a particular layer, you only need gradients from the subsequent layers → known as *back-propagation*







Input features: x_1 = minutes attended x_2 = workflows build Output: y = Probability that a person passed $y \ge 0.5 \Rightarrow Passed$ and $y < 0.5 \Rightarrow Failed$



Optimizing neural network models

Loss Functions

- Quantifies errors or deviations in the network outcome compared to the target
- We want to minimize the loss!!
- Different types of loss functions for classification and regression
- *Classification*: We want the predicted category to match the target
- *<u>Regression</u>*: We want to minimize deviation from the target



Different Loss Functions

- Binary classification
 - Binary cross entropy
- Multi-class classification
 - Categorical cross entropy
- Regression problem
 - Mean squared error (MSE)
 - Mean absolute error (MAE)





Loss Landscape of a Real Neural Network

- In reality, loss landscape may not be smooth
 - Possibly many local minima
- Different optimizer algorithms with
 - Varying learning rate η
 - History of gradients in previous iterations



Source: https://www.cs.umd.edu/~tomg/projects/landscapes/


Optimizers in Keras

Optimizer	How it works	Strengths	Weaknesses	When to use
SGD with momentum	Use the previous gradient to accelerate convergence	-Reduces oscillation near maxima	-Const learning rate	
NAG (Nesterov accelerated gradient)	Use the current gradient to predict gradient	-Increased responsiveness	-Additional hyperparameter	RNN
Adagrad	Updating by cumulating sum of sq gradients from past	-Different learning parameters for different features	-Computationally expensive -Shrinking learning rate	Sparse data (e.g. text)
Adadelta	Modified Adagrad with decaying average of sq gradients from past	-Learning rate not dramatically shrinking like Adagrad	-Computationally expensive	Sparse data (e.g. text)
RMSProp	Modified Adagrad with sq gradients added very slowly	-Learning rate not dramatically shrinking like Adagrad		
Adam (Adaptive Moment Estimation)	RMSProp plus decaying average of gradients from past	-Fast convergence	-Computationally expensive	



Which Activation Functions? Which Loss Functions?

Depends on the problem you are working on

	✓ Recommended		Activation Functions													
			Layers			Layer				Loss Functions						
	Prob	lems	Sigmoid	Tanh	ReLU	Sigmoid	Tanh	Linear	ReLU	Softmax	Binary CE	Hinge	Categorical CE	MSE	MSLE	MAE
	Binary cl	assification (0 vs 1)	\checkmark	\checkmark	\checkmark	✓					✓					
Classification Binary classification (-1 vs 1)		\checkmark	✓	✓		✓					✓					
Multi-class classification		\checkmark	✓	✓					~			✓				
	Regressi	on	✓	✓	✓	Δ	Δ	✓	Δ					✓		
Regression Regression (wide range)		✓	\checkmark	\checkmark			~							✓		
Regression (possible outliers)		\checkmark	\checkmark	\checkmark			~								✓	



Codeless Deep Learning with KNIME Analytics Platform



Download the workflow from the KNIME Hub



Demo – adult data classifier

- Adult data set: demographic data of 32k adults
- Goal: Binary classification whether the income is above \$50k
- 13 features numerical and nominal
- Train an ANN with 13-6-6-1 units

Demo with KNIME Analytics Platform



Demo – adult data classifier



Download the workflow from the KNIME Hub



Computer vision: Challenges working with image data

Why is Computer Vision Important?

- Increasing amount of video and image data
 - 30 000 minutes of video are uploaded to YouTube every minute
- Many application areas and use cases:
 - Image classification / image recognition
 - Detecting of diseases
 - Detecting of anomalies
 - Face recognition to unlock a phone or door
 - Object detection
 - Marking objects in an image, e.g., traffic signs
 - Semantic segmentation
 - Neural style transfer







How Can We Represent a Gray-Scale Image?



- A gray-scale image can be stored in a matrix
- Each cell represents one pixel of the image



How Can We Represent a Colored Image?



- A colored image can be encoded via the intensity of red, green, and blue for each pixel.
 - → It can be stored in a tensor with one channel for each color
 - Example: n x m pixel image with k channels can be stored in a tensor of size n x m x k.

Problems with FFNN for Image Classification

- Goal: Train network to recognize x's
- Approach: Flatten the image and apply a feed forward neural network



- Problem: A lot of variables / weights
 - Example: Image with 224 x 224 pixels with 3 channels and 100 neurons in the next layer
 → 150,528 inputs → 15,052,800 weights in the first layer.
 - Unmanageable and likely leads to overfitting during training



Problems with FFNN for Image Classification

- Goal: Train network to recognize x's
- Approach: Flatten the image and apply a feed forward neural network



Problem: Loss of spatial dependencies



Challenge: Different Variations

Goal: Train network to recognize x's









Different Variations

Viewpoint variations



Illumination conditions



Source: http://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L3.pdf

Deformations



Intra-class variations





Use Filter to Check for Different Features

Check for arms going from lower right to top left

Check for crosses

Check for arms going from lower left to top right













Convolution & pooling layers



How Can We Apply a Filter

- Goal of a filter:
 - High value if the feature is in an image patch
 - Low value if the feature is not in an image patch
- Idea:
 - Use a kernel / matrix and place it on top of different parts of the image
 - Multiply the pixel value with the according kernel value and sum up the values



Note: In the deep learning community this operation is called a convolution and is represented via an asterisk *. Strictly mathematical it is a cross correlation.



Applying Multiple Filters

		Kernel / Filter		Output	Feature map
	*	1 -1 -1 -1 1 -1 -1 -1 1	=	9 -3 1 -3 5 -3 1 -3 9	
1 -1 -1 -1 1 -1 1 1 -1 -1 -1 1 1 -1 -1 -1 1 1 -1 -1 -1 1 -1 1 -1 1 -1 -1 1 -1	*	1 -1 1 -1 1 -1 1 -1 1	=	5 -7 5 -7 9 -7 5 -7 5	9 -3 1 -3 5 -7 5 1 -7 1 -3 9 1 -7 1 -3 9 5 -3 5 -3 9 -3 1
	*	-1 -1 1 -1 1 -1 1 -1 -1	=	1 -3 9 -3 5 -3 9 -3 1	

Impact of Handcrafted Kernel



Edge detection



$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$





One Way to Classify Images

- 1. Use domain knowledge to define important features
- 2. Try to detect these features
- Problem: Handcrafting different filters is hard
- Solution: Use a Convolutional Neural Network (CNN)
 - Kernel / filters trained as part of the network to extract features
 - Extracted features are used by the network for the classification task





Cat



Convolutional Neural Network (CNN)

- A CNN is a neural network with at least one convolutional layer.
- Instead of handcrafting different features a CNN learns a hierarchy of features using multiple convolution layers that detect different features.

Low level features



Edges, dark spots

Mid level features



Eyes, ears, nose

High level features



Facial structure

Images from: <u>http://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L3.pdf</u>



How Do Convolutional Layers Works?

 Idea: Instead of connecting every neuron to the new layer, a sliding window is used.



Image from: <u>https://towardsdatascience.com/a-comprehensive-</u> guide-to-convolutional-neural-networks-the-eli5-way-<u>3bd2b1164a53</u>



How Do Convolutional Layers Work?

- Idea:
 - Use a kernel / weight matrix and slide it over the image
 - At each position: Apply the convolution and a non-linear activation, e.g. ReLU



- The weights of the kernel are learned during training
- Note: These are similar steps like in a feed forward neural network



Keras Convolution 2D Layer

	Dialog - 0:91 - Keras Convolution 2D Layer (Filters: 32)
	Options Advanced Flow Variables Job Manager Selection
	Name prefix
	Input tensor input_1_0:0 [28, 28, 1] float ᅌ
	Filters 32 C
	Kernel size 3, 3
Keras Convolution	Strides 1, 1
2D Layer	
	Padding Valid ᅌ

	Dilation rate 1, 1
	Activation function ReLU
	OK Apply Cancel



Pooling Layer

- Idea: Replace the area of an image or feature map with a summary statistic.
- Example: Replace each 2x2 area with the
 - Maximum value (Max pooling)
 - Mean value (Average pooling)
- Pooling layers are often used in between convolutional layers to
 - Increase the receptive field of the following layers
 - Reduce computational complexity
- No parameters to learn





Keras Max Pooling 2D Layer Node

	Dialog - 0:92 - Keras Max Pooling 2D Layer (Pool size: 2, 2)
	Options Flow Variables Job Manager Selection
Keras Max Pooling 2D Layer	Name prefix Input tensor conv2d_1_0:0 [26, 26, 32] float Pool size 2, 2 Strides 2, 2 Padding Valid
	OK Apply Cancel



CNN for Image Classification



Image from: https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53



Image Classification: Cats & Dogs Data

Kaggle Dogs vs Cats Challenge https://www.kaggle.com/c/dogs-vs-cats/overview







Classification with KNIME





Simple CNN for Image Classification





Transfer learning



Standard vs. Transfer Learning





Cancer Cell Classification with Transfer Learning

- Transfer learning can be adapted to a wide range of image classification problems
- Task: Classify histopathology slide images and about the type of lymphoma
 - chronic lymphocytic leukemia (CLL)
 - follicular lymphoma (FL)
 - mantle cell lymphoma (MCL)
- Reuse VGG16 network





Popular CNN: VGG-16 (2015)





Transfer Learning for Image Classification





Transfer Learning for Image Classification





Transfer Learning for Image Classification: Option 2



Download the workflow from the KNIME Hub



Sequential data & RNN


- Text is a sequence of words or characters → sequential data
- Task: Predict the next word in a sequence

• The last word in the sequence is "the". What is the next word?



Requirement 1: The network must be able to take context information into account





- This made our vacation
- The hotel was good, not bad at all. The hotel was bad, not good at all. This made our vacation ____

Requirement 2: The network must be able to take order into account





Requirement 3: The network needs to handle different sequence lengths



 Time information can be either in the beginning, the middle, or the end of a sentence



Requirement 4: The network must be position independent



Feed Forward Neural Network for Sequential Data

- Idea: Use a feed forward neural network to handle sequential data
- Doesn't meet the requirements of sequential data
 - Doesn't take word order into account
 - Fixed input → can't handle different sequence length
 - Doesn't share parameters
 → not position invariant

Solution: Recurrent Neural Network (RNN)





Recurrent Neural Networks

- Recurrent Neural Networks (RNNs) are a family of neural networks suitable for processing of sequential data
- Key idea: use a loop connection
- RNNs are used for all sorts of tasks:
 - Language modeling / Text generation
 - Text classification
 - Neural machine translation
 - Text summarization
 - Image captioning
 - Speech to text
 - Demand prediction
 - Stock price prediction



From Feed Forward to Recurrent Neural Networks









From Feed Forward to Recurrent Neural Networks





RNN Rolled and Unrolled Representation





Memory of an RNN





Example: Language model



A = A feed forward network with one or multiple layers



The Math Behind An RNN





RNN Architectures: Many to Many (Seq2Seq)



Language model

Neural machine translation



RNN Architectures: Many-to-One & One-to-Many





Limitation of Simple RNNs

The "memory" of simple RNNs is sometimes too limited to be useful:

- "Cars drive on the ____" (road)
- "I love the beach.

My favorite sound is the crashing of _____" (cars? glass? waves?)



Long short-term memory (LSTM)

Long Short-Term Memory (LSTM) Units

Special type of unit with

- an additional cell state
- three gates
 - Forget gate
 - Input gate
 - Output gate



Image Source: Christopher Olah, https://colah.github.io/posts/2015-08-Understanding-LSTMs/





Idea of a Gate

• A gate can be ...





LSTM Units

- Additional cell state makes it easier to remember information
- At each time step
 - 1. The forget gate removes irrelevant information from the cell state
 - 2. The input gate decides which information should be added to the cell state
 - 3. The cell state is updated
 - 4. The output gate decides which information to output and to send to the next time step



Image Source: Christopher Olah, https://colah.github.io/posts/2015-08-Understanding-LSTMs/



LSTM Layer Node

	•••	Dialog - 4:51 - Keras LSTM Layer		
	Options Initializers	Regularizers Constrain	nts Flow Variables >	Size of the hidden
	Name prefix	0		state vectors
	Input tensor First hidden state tensor	Offset_1_0:0 [51, 1] float	O	
	Second hidden state tensor Units		3 100 C	
Keras LSTM Layer	Activation	Tanh		
	Recurrent activation	Hard sigmoid	•	
	Use bias Dropout		0, 3	Activate "Return
	Recurrent dropout		0 0	sequences" for
	Implementation	1		seq2seq models
	Return sequences			A stimula "Detum
	Go backwards Unroll			state" to use it
Optional input ports				during deployment
for the hidden state tensors	OK Apply Cancel 🕡			



Example: Text Classification

- Task: Assigning tags or categories to text according to its content
- Examples:
 - Identify the underlying sentiment of movie / restaurant / product reviews, tweets etc.
 - Positive
 - Negative
 - Classify vacation reviews. What is the review about?
 - Hotel
 - Flight
 - Booking process



Use Case: Sentiment Analysis of Movie Reviews



Preprocessing:

- Different sequence lengths
 - Sequences within the same training batch must have the same length
 - Solution: Truncate too long sequences and zero pad too short sequences
- Encoding
 - Index encoding plus embedding layer
 - Large number of different words: Define a fixed dictionary size and assign default ("unknown") value to all other words



Use Case: Sentiment Analysis of Movie Reviews

Preprocessing

This film is mediocre at best. Angie Harmon is as funny as a bag of hammers. Her bitchy demeanor from Law and Order carries over in a failed attempt at comedy. Charlie Sheen is the only one to come out unscathed in this horrible anti-comedy. The only positive thing to come out of this mess is Charlie and Denise's marriage. Hopefully that effort produces better results.



Dict Replacer (2 In-Ports)

52 29 8 1488 35 130 1 11794 18869 8 20 187 20 3 2984 6 20001 1 883 8167 8409 39 3791 4 8384 2716 148 9 3 1154 585 35 258 1 1987 5781 8 2 65 30 7 221 44 13964 9 10 552 20001 1 18 65 1124 159 7 221 44 6 10 931 8 1987 4 10239 14 1570 1 5136 12 741 7256 131 1829 1

Network







Text Classification: Sentiment Analysis



Download the workflow from the KNIME Hub



To learn more...

- Codeless Deep Learning with KNIME— Packt, 2020
 - By Rosaria Silipo & Kathrin Melcher





Upcoming Online Courses

- Introduction to Text Processing
 - Nov 28 Dec 2, 10-11:30am CST
 - https://www.knime.com/events/introduction-text-processing-2211
- Introduction to Time Series Analysis
 - Nov 29 Dec 2, 10-11:30am CST
 - https://www.knime.com/events/introduction-time-series-analysis-2211

Use Code Joinus10 to get 10% discount on your registration



Thank you!

This slide deck is available at https://kni.me/s/4-i5-EcLrZwf5cxN

