NPFL099 Statistical Dialogue Systems
3. Neural Nets Basics

http://ufal.cz/npfl099

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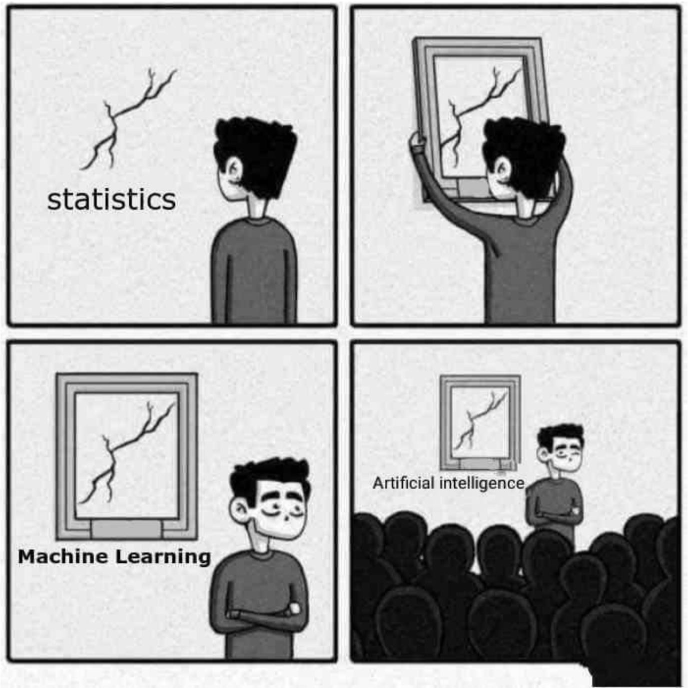
Machine Learning

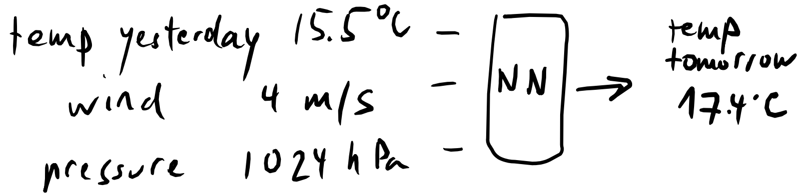
- ML is basically function approximation
- function: data (**features**)→ **labels**
- function shape:
  - this is where different ML algorithms differ
  - **neural nets**: compound non-linear functions
- training/learning = adjusting function parameters to minimize error (see next week)
  - **supervised learning** = based on data + labels given in advance
  - **reinforcement learning** = based on exploration & rewards given online



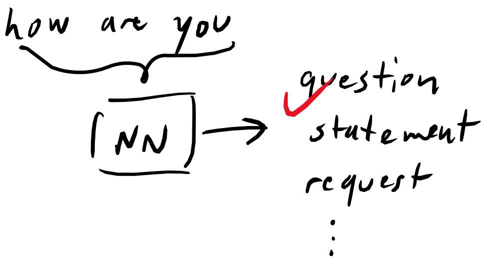
https://towardsdatascience.com/no-machine-learning-is-not-just-glorified-statistics-26d3952234e3

Typical machine learning problems in NLP

- **regression**
  - many inputs, 1 float output

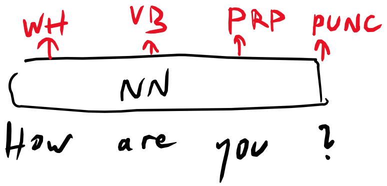


- **classification**
  - many inputs, 1 categorial output (k classes)

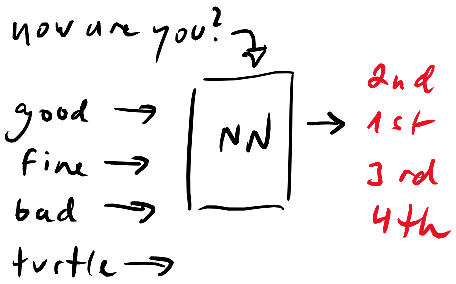


structured prediction

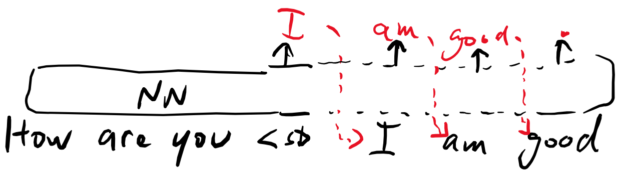
- **sequence labelling**
  - sequence of inputs, label each (~ repeated classification)
  - 1-to-1 input to output



- **ranking**
  - multiple inputs, choose best one (~ diff regression)



- **sequence prediction** (**autoregressive** generation)
  - some inputs (sequence/something else)
  - generate outputs, use previous output in predicting next one



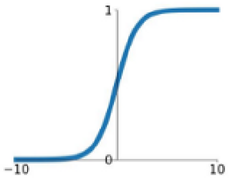
Neural networks

- **Non-linear functions**, composed of basic building blocks
  - stacked into **layers**
- Layers are made of **activation functions**:
  - linear functions (~basic, default)
  - nonlinearities – sigmoid, tanh, ReLU
  - softmax – probability estimates:

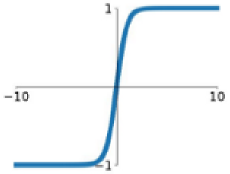
$$\mathrm{softmax}(\mathbf{x})_i = \frac{\exp(x_i)}{\sum_{j=1}^{|\mathbf{x}|} \exp(x_j)}$$

- Fully differentiable – training by **gradient descent**
  - network output incurs loss/cost
  - gradients **backpropagated** from loss to all parameters (composite function differentiation)

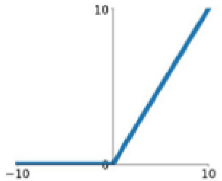
Sigmoid
$\sigma(x) = \frac{1}{1+e^{-x}}$



tanh
$\tanh(x)$



ReLU
$\max(0, x)$



https://medium.com/@shrutijadon10104776/survey-on-activation-functions-for-deep-learning-9689331ba092

Layers visualization

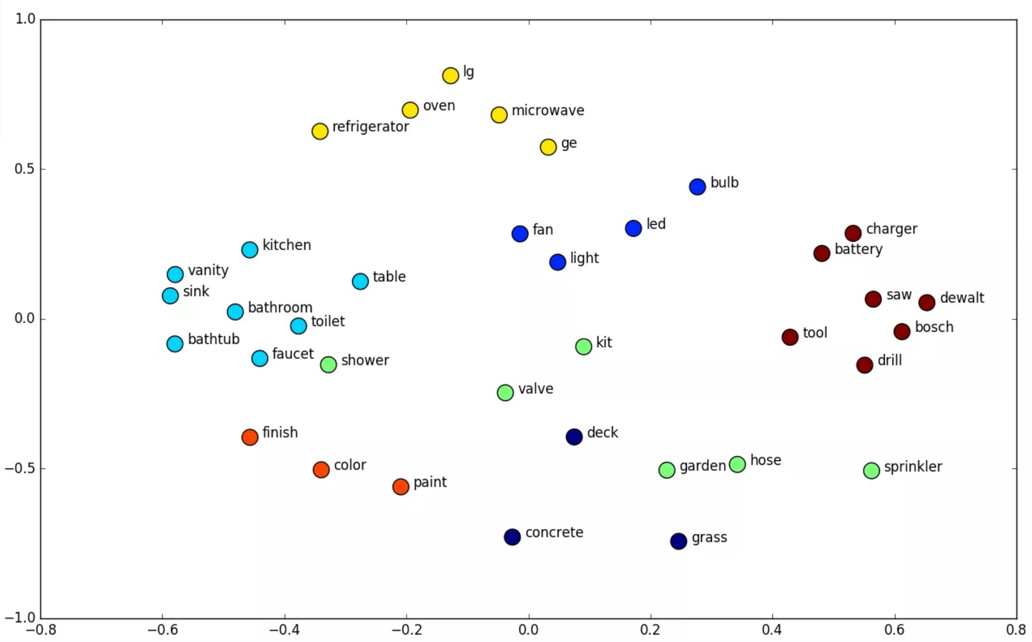
- https://playground.tensorflow.org/
  - 2 numeric features (=2 input variables) → binary classification (=1 output, 2 classes)
    - easiest case, but you can see the internals
    - more complex input features (→)
  - **feed-forward = fully connected = multi-layer perceptron** here
    - easiest case: connect everything & let the network figure it out
    - nice but gets too large very quickly, not good for variable-sized inputs
  - added layers & power to distinguish different classes
    - fits the training data Y/N ?
  - different activation functions
    - without them, it's just linear – no matter how many layers!
- best NN conceptualization – pipeline / flow (computational graph)
  - data flows through individual layers, gets changed
  - corresponds to a math formula, but flow graph can be easier to read

Feature representation

- technically can be anything, as long as it's meaningful
  - the network will learn to assign meaning/values itself
- **1-hot/binary**
  - words – numbered vocabulary
    - bigrams, n-grams, positional…
  - other features – especially handcrafted
    - word classes
    - various word combinations
    - outputs of other classifiers (sentiment, part-of-speech…)
    - is capitalized/is loud?
- **numeric** (floats)
  - best for continuous inputs: vision, audio
    - raw pixels, MFCCs…
- **vectors (embeddings)** →

Embeddings

- distributed (word) representation
  - **each word = a vector of floats**
  - basically an easy conversion of 1-hot → numeric
  - a dictionary of trainable features
- part of network parameters – trained
  a) random initialization
  b) pretraining
- the network learns which words are used similarly
  - they end up having close embedding values
  - embeddings end up different with different tasks & data & settings
- embedding size: ~100s-1000
- vocab size: ~50-100k

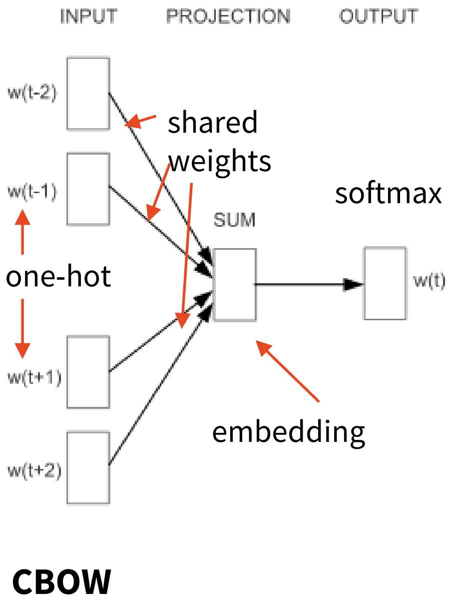


http://blog.kaggle.com/2016/05/18/home-depot-product-search-relevance-winners-interview-1st-place-alex-andreas-nurlan/

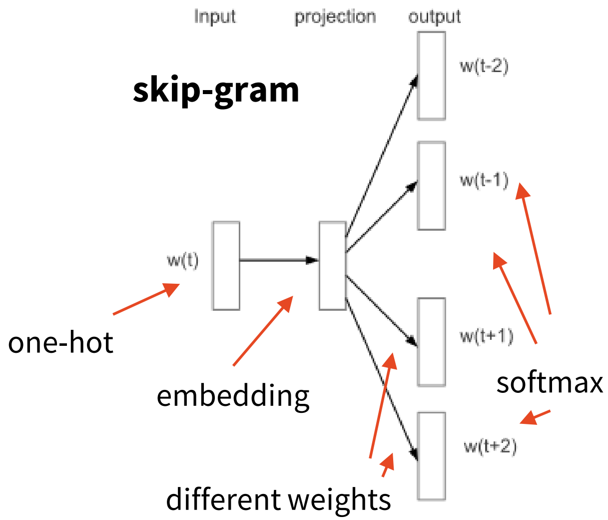
http://ruder.io/word-embeddings-2017/

Pretrained Word Embeddings

- **Word2Vec** https://projector.tensorflow.org/
  - Continuous Bag-of-Words (CBOW) (~ “masked LM”)
    - predict a word, given $\pm k$ words window
    - disregarding word order within the window
  - Skip-gram: reverse
    - given a word, predict its $\pm k$ word window
    - closer words = higher weight in training



(Mikolov et al., 2013)
http://arxiv.org/abs/1301.3781



- **GloVe**
  - optimized directly from corpus co-occurrences (= w_1 close to w_2)
  - target: $e_1 \cdot e_2 = \log(\#\text{co-occurrences})$
    - number weighted by distance, weighted down for low totals
  - trained by minimizing reconstruction loss on a co-occurrence matrix

(Pennington et al., 2014)
http://aclweb.org/anthology/D14-1162

https://geekyisawesome.blogspot.com/2017/03/word-embeddings-how-word2vec-and-glove.html
https://machinelearninginterview.com/topics/natural-language-processing/what-is-the-difference-between-word2vec-and-glove/

Word Embeddings

- Vocabulary is unlimited, embedding matrix isn't
  - + the bigger the embedding matrix, the slower your models
- Special **out-of-vocabulary token** *<unk>*
  - "default" / older option
  - all words not found in vocabulary are assigned this entry
  - can be trained using some rare words in the data
  - problem for generation – you don't want these on the output
- Using limited sets
  - **characters** – very small set
    - works, but makes for very long sequences (20 words ~ 80-100 characters)
    - slower, might be less accurate
  - **subwords** – compromise →

Subwords

- group of characters that:
  - make shorter sequences than using individual characters
  - cover everything
- **byte-pair encoding**
  - start from individual characters
  - iteratively merge most frequent bigram, until you get desired # of subwords
  - *sub@@ word* – the *@@* marks “no space after”

(Sennrich et al., 2016)
https://www.aclweb.org/anthology/P16-1162/

f a s t _
f a s t e r _
t a l l _
t a l l e r _

→

fast er _
tall er _
s l o w er _
tall e s t _

- **SentencePiece** – don’t pre-tokenize
  - criterium: likelihood of joined vs. separate
  - *sub word_* – the *_* marks a space
- 20-50k subwords for 1 language
  - ~250k subwords to cover them all

https://github.com/google/sentencepiece
https://blog.floydhub.com/tokenization-nlp/
https://d2l.ai/chapter_natural-language-processing-pretraining/subword-embedding.html

Convolutional Networks

- Designed for computer vision – inspired by human vision
  - works for language in 1D, too!
- less parameters than fully connected – **filter/kernel**
- Apply (multiple) filter(s) repeatedly over the input
  - element-wise multiply window of input x filter
  - sum + apply non-linearity (ReLU) to result
  - => produce 1 element of output
  - can have more dimensions (~“set of filters”)
- **Stride** – how many steps to skip
  - less overlap, reducing output dimension
- **Pooling** – no filter, pre-set operation
  - **maximum**/average on each window
  - typical CNN architecture alternates convolution & pooling

input

1	1	1	0	0
0	1	1	1	0
0	0	1	1	1
0	0	1	1	0
0	1	1	0	0

filter

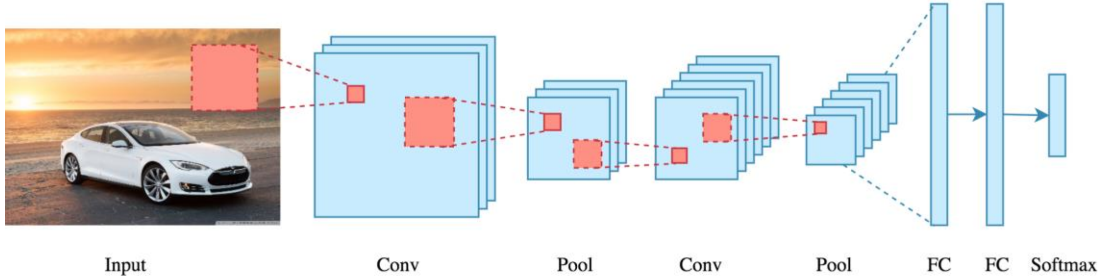
1	0	1
0	1	0
1	0	1

input x filter

1x1	1x0	1x1	0	0
0x0	1x1	1x0	1	0
0x1	0x0	1x1	1	1
0	0	1	1	0
0	1	1	0	0

4		

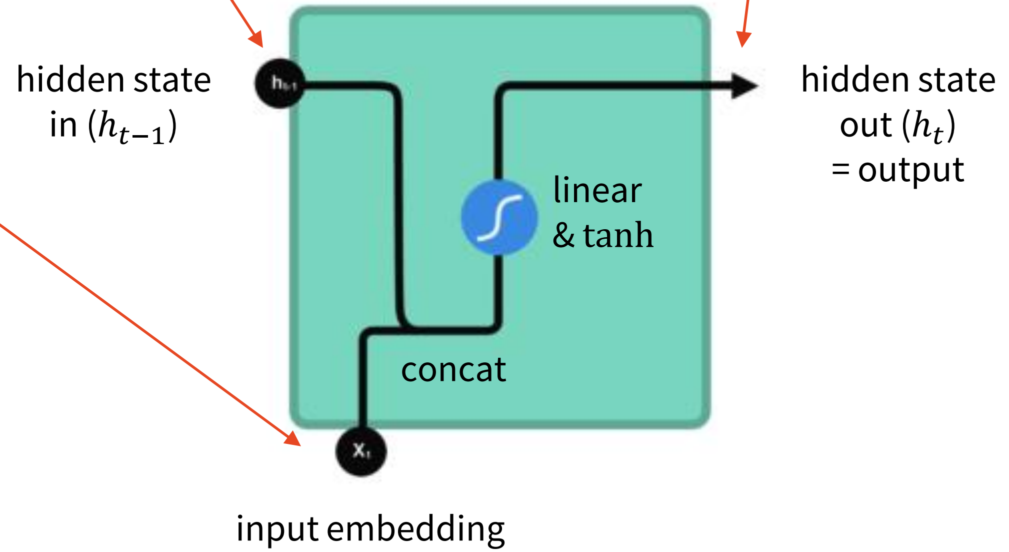
output

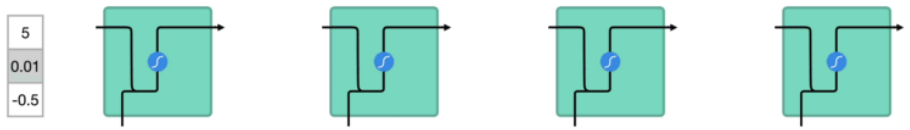


https://towardsdatascience.com/applied-deep-learning-part-4-convolutional-neural-networks-584bc134c1e2

Recurrent Neural Networks

- Identical layers with shared parameters (**cells**)
  - ~ the same layer is applied multiple times, taking its own outputs as input
    - ~ same number of layers as there are tokens
    - output = **hidden state** – fed to the next step
  - additional input – next token features
- **basic RNN**: linear + tanh
  - tanh: squashes everything to $[-1,1]$
    - good for repeated application
  - very simple structure
  - numeric problem: vanishing gradients
    - training updates get too small
    - can't hold long sequences well

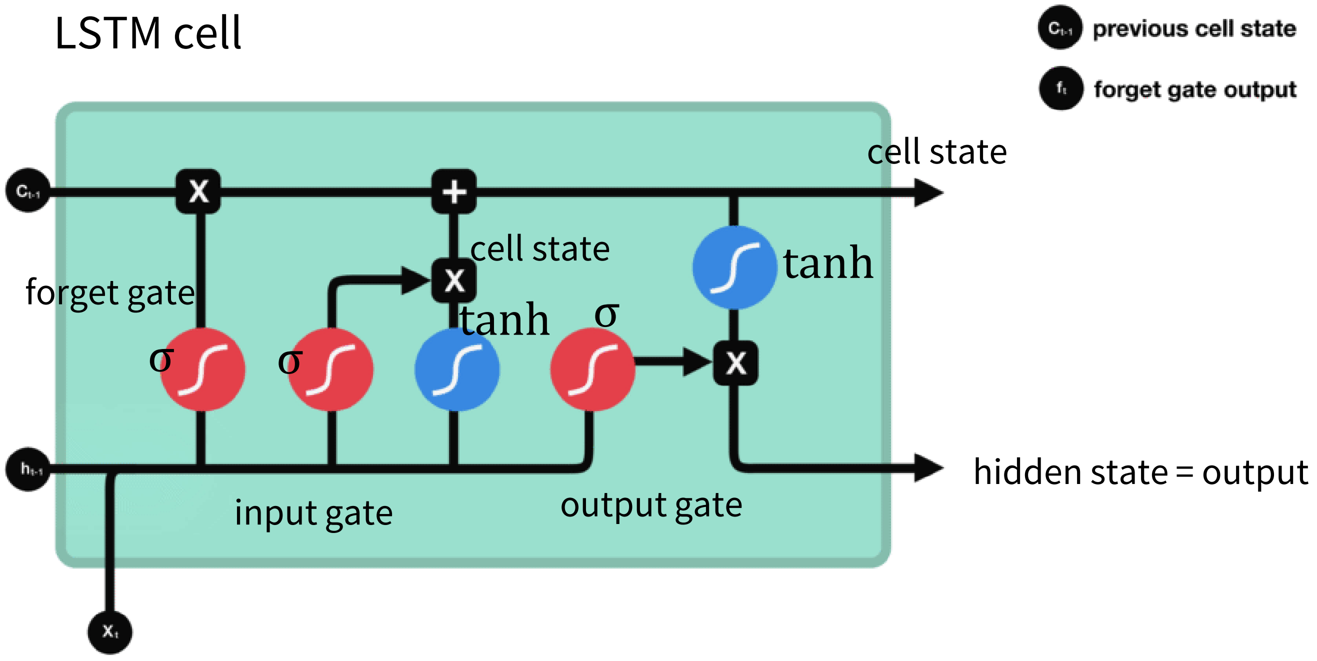


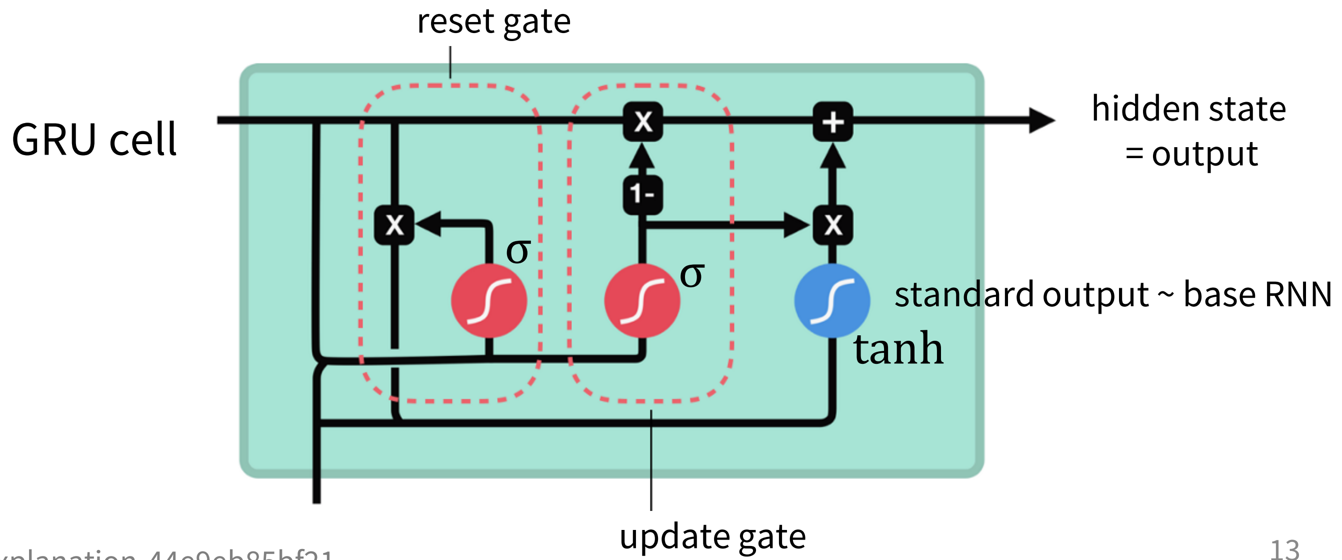


https://towardsdatascience.com/illustrated-guide-to-lstms-and-gru-s-a-step-by-step-explanation-44e9eb85bf21
https://medium.com/@saurabh.rathor092/simple-rnn-vs-gru-vs-lstm-difference-lies-in-more-flexible-control-5f33e07b1e57

LSTMs & GRUs

- **GRU, LSTM**: more complex, to make training more stable
  - “gates” to keep old values
  - $\sigma \sim [0,1]$ decisions:
    - forget stuff from previous?
    - take input into account?
    - put stuff onto output?
    - over individual dimensions (e.g. input has 100 dims, forget gate forgets dims 1-3 & 4-25)
    - all based on current input & state
  - LSTM is older & more complex
  - GRU almost as good but faster
  - both slower than base RNN
  - both handle long recurrences



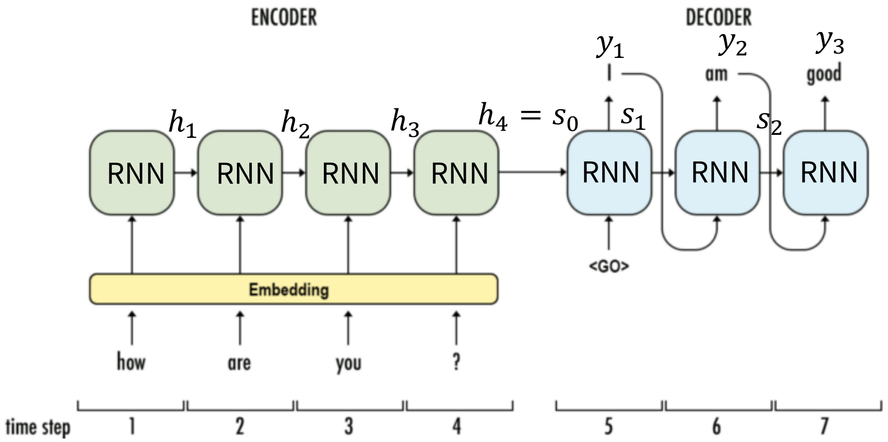


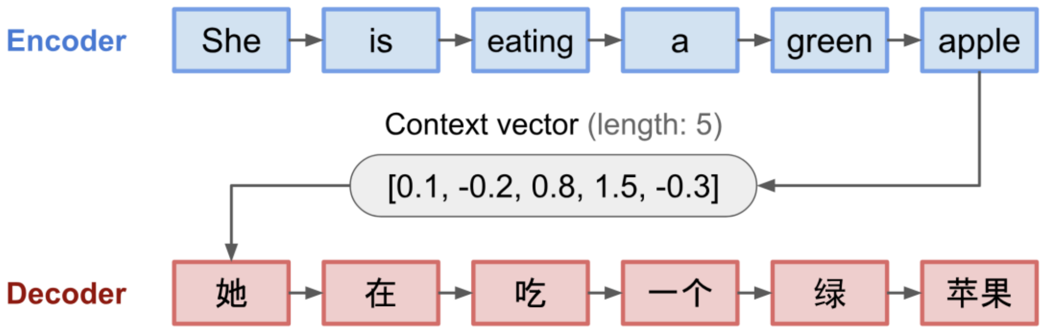
Encoder-Decoder Networks (Sequence-to-sequence)

- Default RNN paradigm for sequences/structure prediction
  - **encoder** RNN: encodes the input token-by-token into **hidden states** h_t
    - next step: last hidden state + next token as input
  - **decoder RNN**: constructs the output token-by-token
    - initialized by last encoder hidden state
    - output: hidden state & softmax over output vocabulary + argmax
    - next step: last hidden state + last generated token as input
  - LSTM/GRU cells over vectors of ~ embedding size
  - used in MT, dialogue, parsing…
    - more complex structures linearized to sequences

$$\boldsymbol{h}_0 = \mathbf{0}$$
$$\boldsymbol{h}_t = \mathrm{cell}(\boldsymbol{x}_t, \boldsymbol{h}_{t-1})$$

$$\boldsymbol{s}_0 = \boldsymbol{h}_T$$
$$p(y_t | y_1, \dots y_{t-1}, \mathbf{x}) = \mathrm{softmax}(\boldsymbol{s}_t)$$
$$\boldsymbol{s}_t = \mathrm{cell}(\boldsymbol{y}_{t-1}, \boldsymbol{s}_{t-1})$$



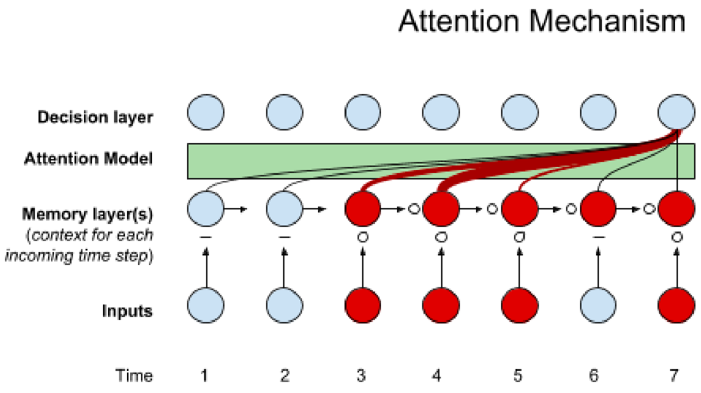


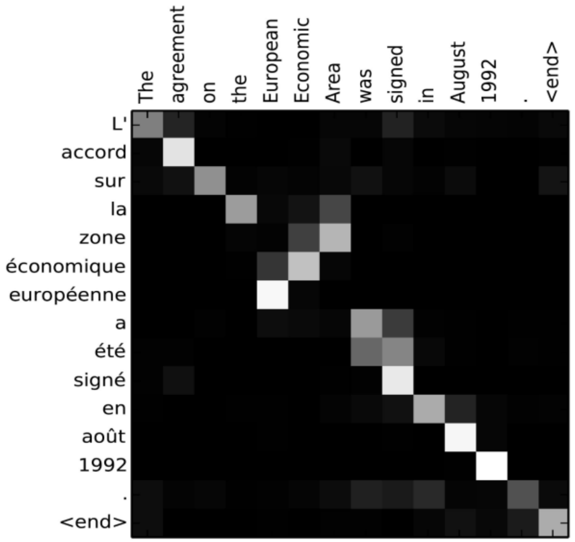
https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html

https://medium.com/syncedreview/a-brief-overview-of-attention-mechanism-13c578ba9129

Attention

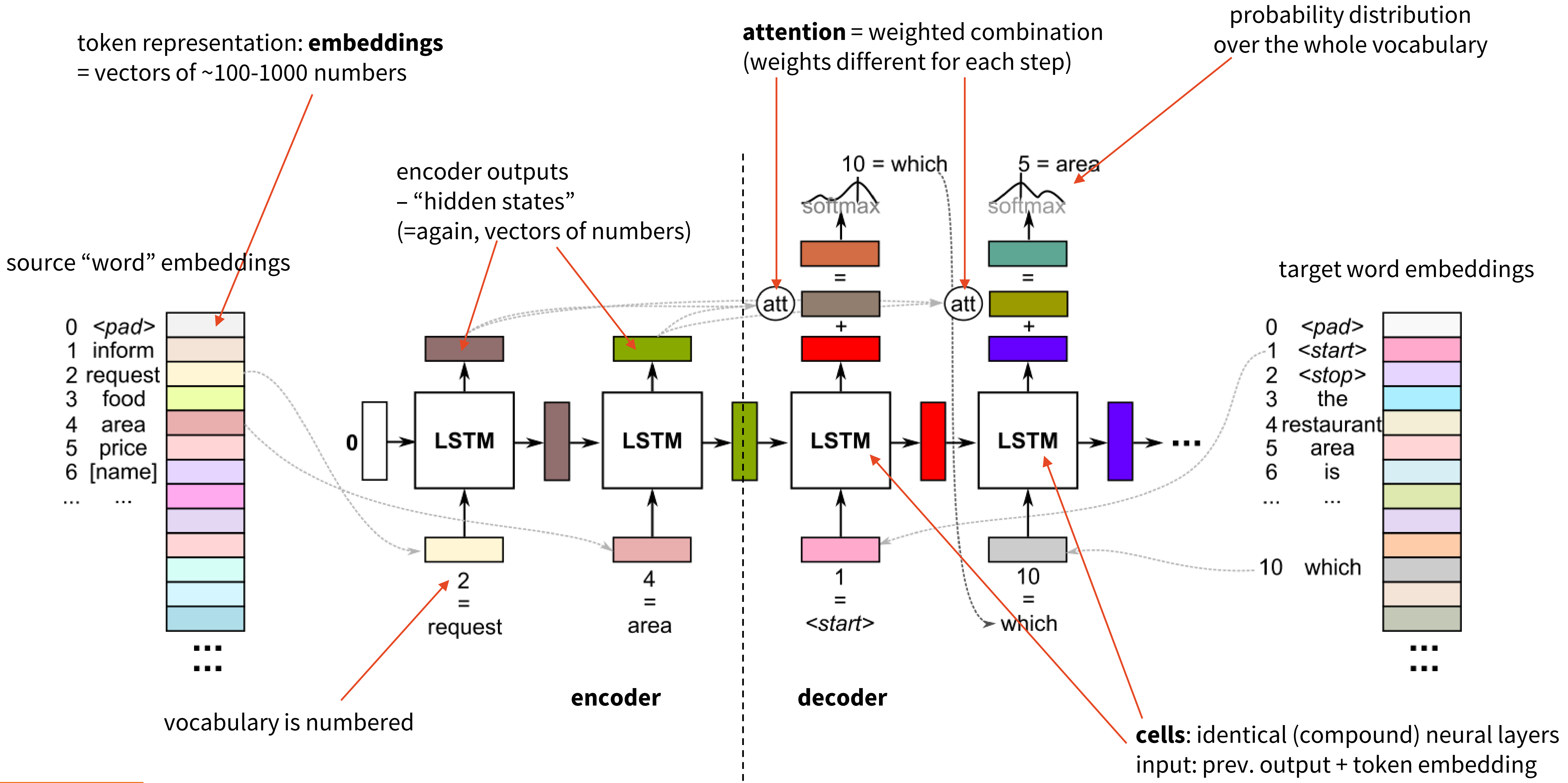
- Encoder-decoder is too crude for complex sequences
  - the whole input is crammed into a fixed-size vector (last hidden state)
- **Attention** = “memory” of **all encoder** hidden states
  - weighted combination, re-weighted for every decoder step
    → can focus on currently important part of input
  - fed into decoder inputs + decoder softmax layer
- **Self-attention** – over **previous decoder steps**
  - increases consistency when generating long sequences





https://skymind.ai/wiki/attention-mechanism-memory-network

Seq2seq RNNs with Attention

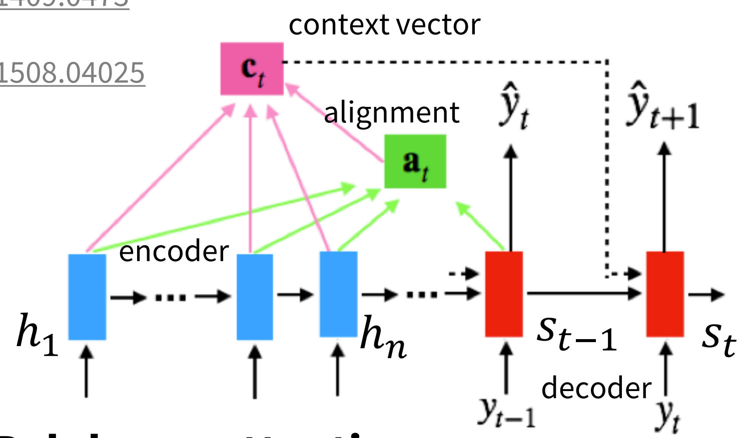


(Bahdanau et al., 2015) http://arxiv.org/abs/1409.0473

Bahdanau & Luong Attention

- different combination with decoder state
  - Bahdanau: use on input to decoder cell
  - Luong: modify final decoder state
- different weights computation
- both work well – exact formula not important

(Bahdanau et al., 2015)
http://arxiv.org/abs/1409.0473
(Luong et al., 2015)
http://arxiv.org/abs/1508.04025



Bahdanau attention

attention value = context vector

sum of encoder hidden states
weighted by attention weights α_{ti}

$$\boldsymbol{c}_t = \sum_{i=1}^{n} \alpha_{ti} \boldsymbol{h}_i$$

attention weights = alignment model

decoder state
trained parameters

Bahdanau:

$$\alpha_{ti} = \mathrm{softmax}(\boldsymbol{v}_\alpha \cdot \tanh(\mathbf{W}_\alpha \cdot \boldsymbol{s}_{t-1} + \mathbf{U}_\alpha \cdot \boldsymbol{h}_i))$$

encoder hidden state

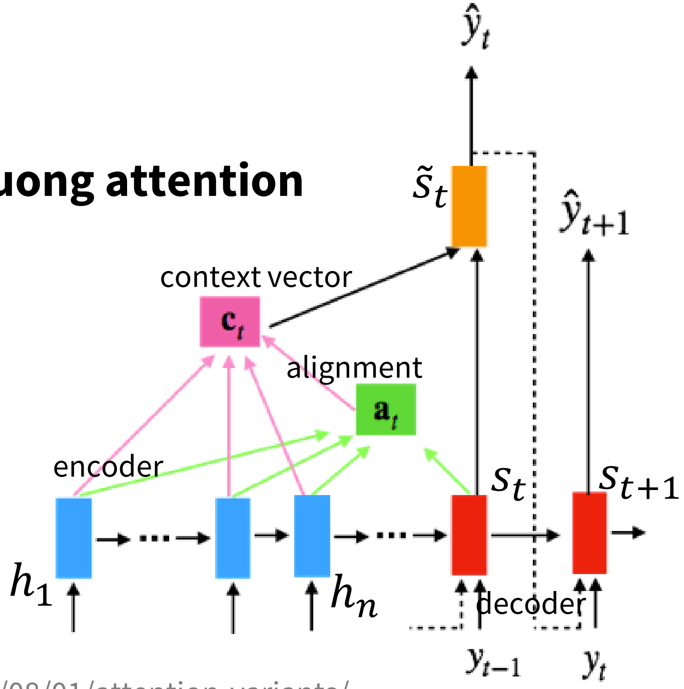
Luong:

$$\alpha_{ti} = \mathrm{softmax}(\boldsymbol{h}_i^\top \cdot \boldsymbol{s}_t)$$

decoder state

encoder hidden state

Luong attention

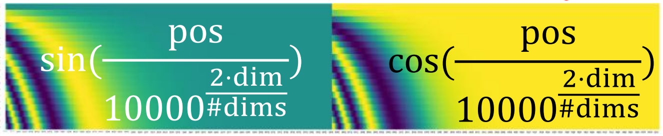


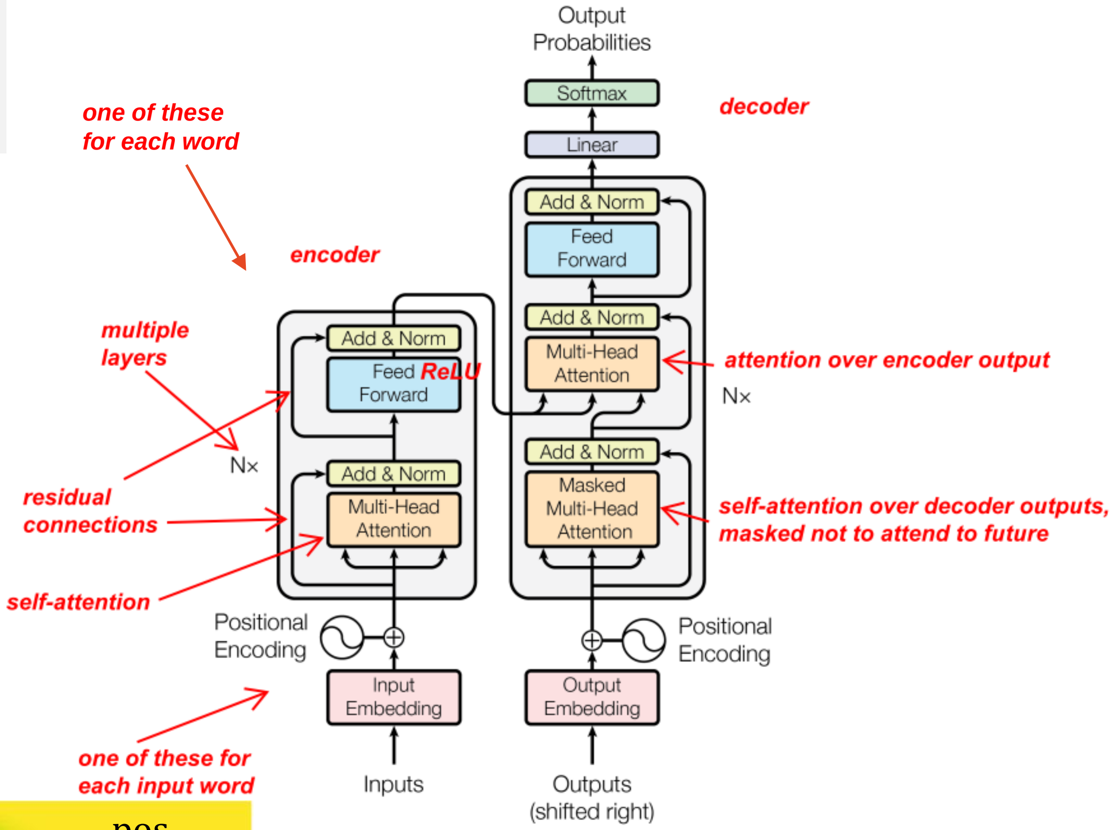
http://cnyah.com/2017/08/01/attention-variants/

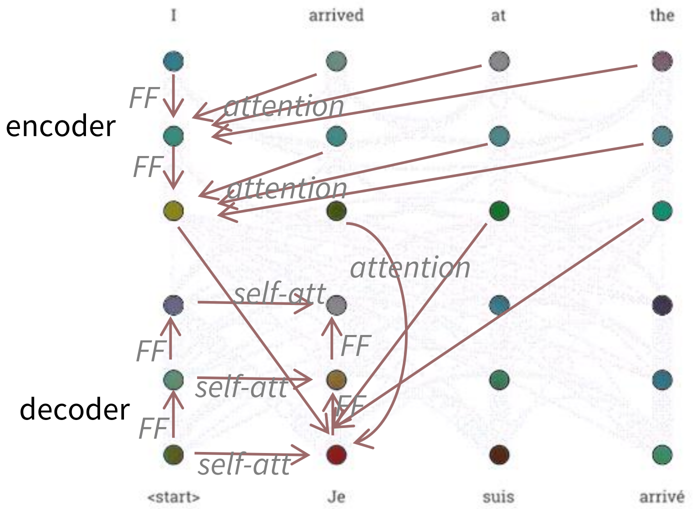
Transformer

(Waswani et al., 2017)
https://arxiv.org/abs/1706.03762

- getting rid of (encoder) recurrences
  - making it faster to train, allowing bigger nets
  - replace everything with attention
    + feed-forward networks
  - ⇒ needs more layers
  - ⇒ needs to encode positions
- positional encoding
  - adding position-dependent patterns to the input
- attention – dot-product (Luong style)
  - scaled by $\frac{1}{\sqrt{\#\mathrm{dims}}}$ (so values don't get too big)
  - **more heads** (attentions in parallel)
    – focus on multiple inputs





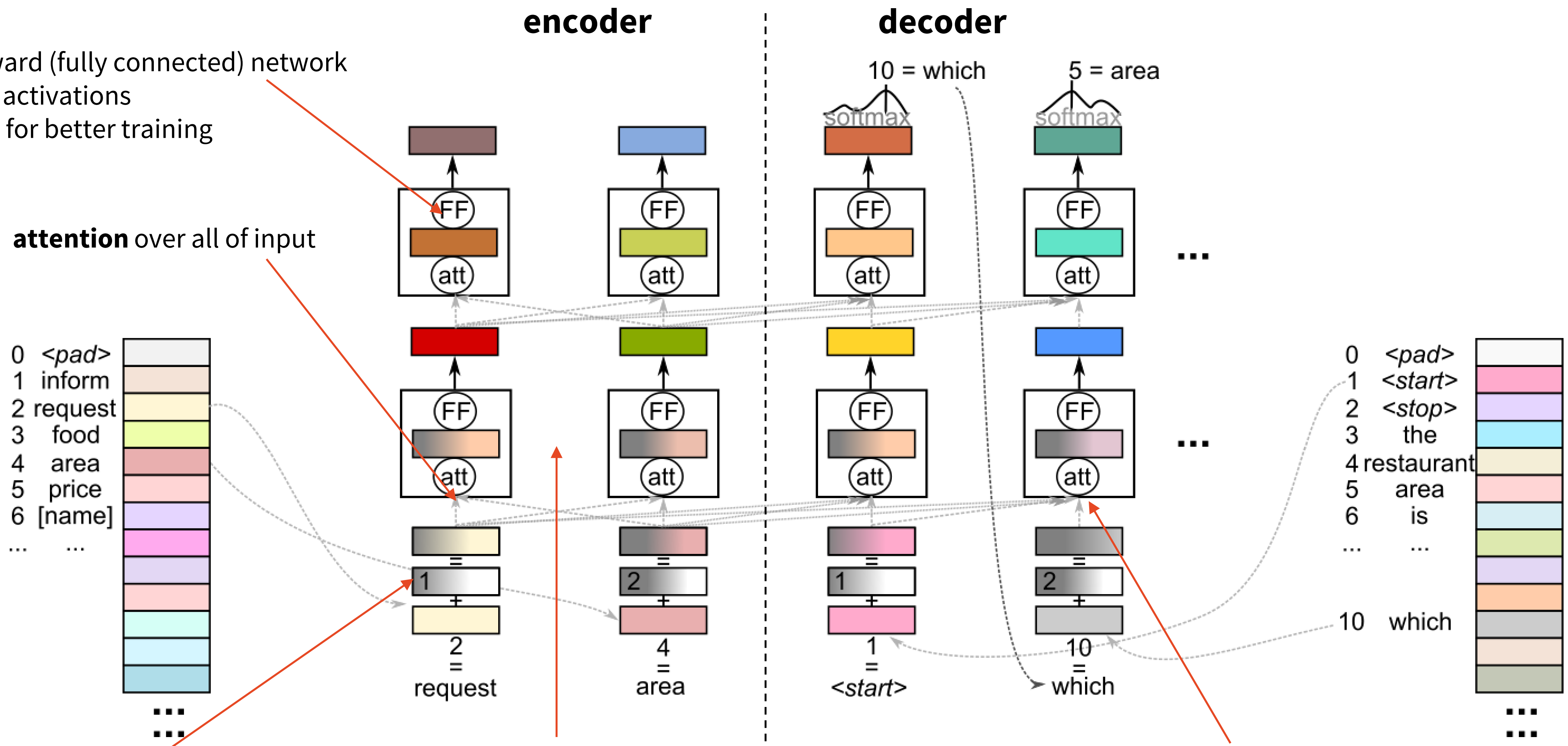


http://jalammar.github.io/illustrated-transformer/ https://ai.googleblog.com/2017/08/transformer-novel-neural-network.html

Transformer

feed-forward (fully connected) network
- ReLU activations
- tricks for better training

attention over all of input



no recurrent connections

attention over all of input
& output generated so far (**self-attention**)

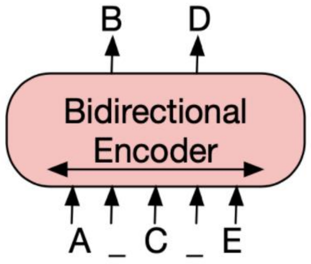
positional encoding
(indicate position in sentence)

(Vaswani et al., 2017) http://arxiv.org/abs/1706.03762

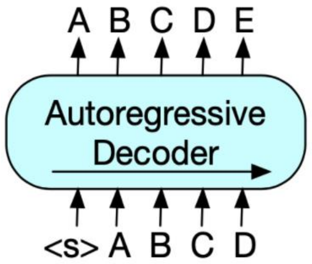
Pretrained Language Models

https://lilianweng.github.io/posts/2019-01-31-lm/
https://github.com/jessevig/bertviz

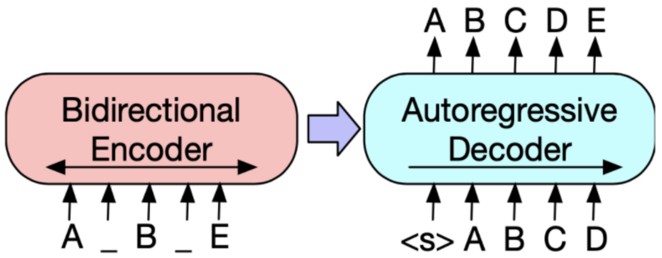
- Beyond pretrained word embeddings
  - reflects different word meanings in sentence context (~contextual embeddings)
  - used as input to added layers on top / base for model finetuning (next week)
- LSTM-based: **ELMo** (trained on language modelling)
  - weighted sum of static word embeddings & LSTM outputs



- **Transformer encoders**: **BERT**, **RoBERTa**…
  - for classification, sequence tagging
  - any Transformer layer used (typically the last one)

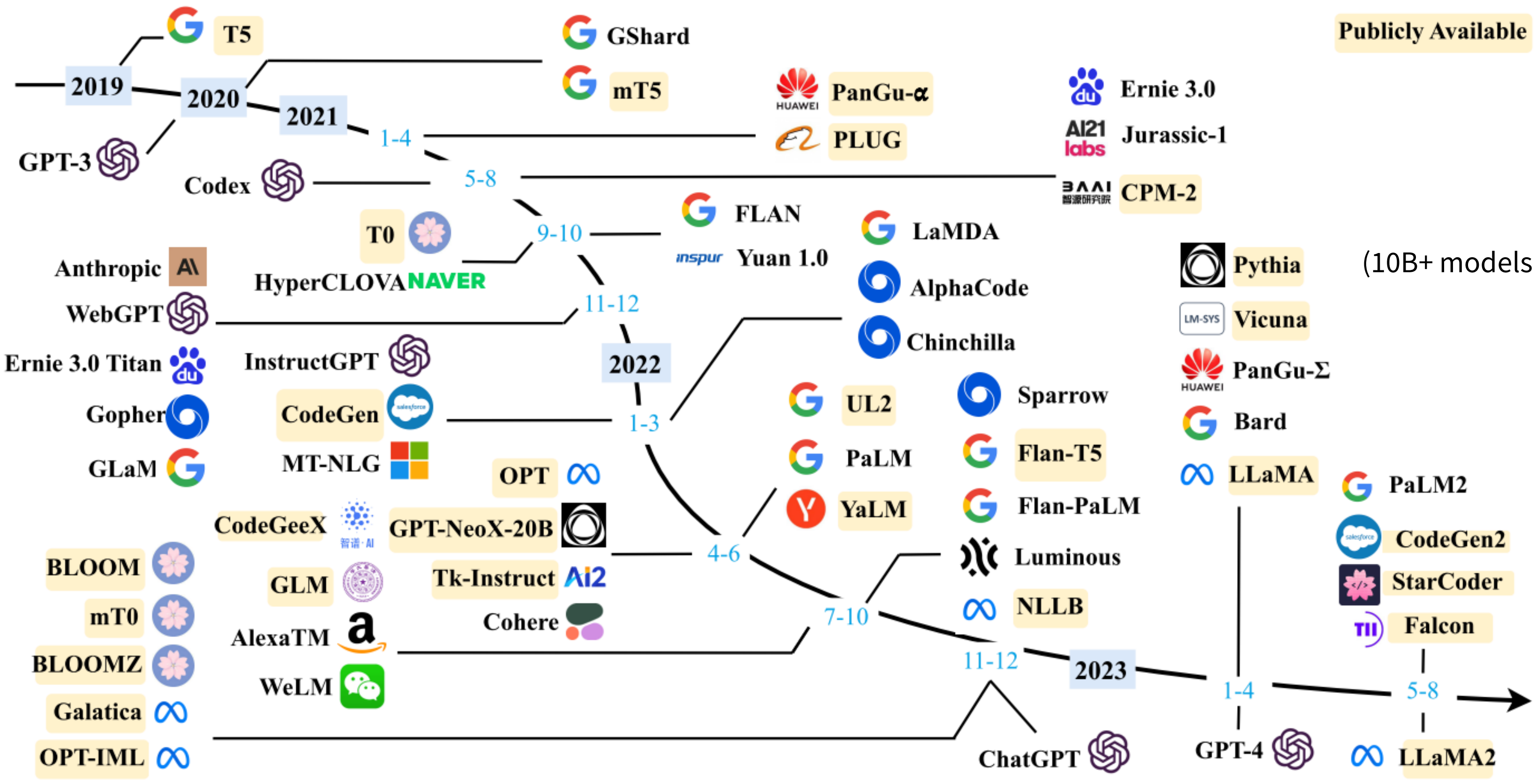


- **Transformer decoders**: **GPT-2**, **GPT-3**…
  - for generation, language modelling
  - input: **force-decoding**
- **Transformer encoder-decoders**: **BART**, **T5**…
  - same as ↑, explicit input



Large Language Models

- Most are just Transformer decoders
- Only difference w.r.t. previous: **size** (& training methods – see next time)
  - BERT/GPT2/T5 etc.: typically 100M-1B params
  - LLMs: 7B-60B (LlaMa), 100B+ (GPT3, PaLM…), unknown (ChatGPT, GPT4…)



(10B+ models shown here)

(Zhao et al., 2023)
http://arxiv.org/abs/2303.18223

Summary

- ML as a function mapping in → out
  - input features – 1-hot, numeric, **embeddings**
    - pretrained embeddings
  - function: layers ~ pipeline, data flows through (= complicated function)
  - outputs: classification (category), regression (float)
    - structured prediction – sequence tagging, ranking, generation
- Neural networks (~function shapes)
  - feed-forward/fully connected
  - CNNs (filters, pooling)
  - RNNs (LSTMs, GRUs)
  - encoder-decoder (seq2seq)
  - attention, **Transformer** (positional encoding & feed-forward & attention)
    - **pretrained models**
- Next week: how to train this stuff

Thanks

Contact us:

https://ufaldsg.slack.com/
odusek@ufal.mff.cuni.cz
Zoom/Skype/Troja

No lab today
Next week: lecture & lab
Tue 9:50

Get the slides here:

http://ufal.cz/npfl099

References/Further:

Goodfellow et al. (2016): Deep Learning, MIT Press (http://www.deeplearningbook.org)
Kim et al. (2018): Tutorial on Deep Latent Variable Models of Natural Language (http://arxiv.org/abs/1812.06834)
Milan Straka's Deep Learning slides: http://ufal.mff.cuni.cz/courses/npfl114/1819-summer

Neural nets tutorials:

- https://codelabs.developers.google.com/codelabs/cloud-tensorflow-mnist/#0
- https://minitorch.github.io/index.html
- https://objax.readthedocs.io/en/latest/

LLM intro: https://www.understandingai.org/p/large-language-models-explained-with