Recurrent Neural Networks

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Common ways for classic ML application for time series data

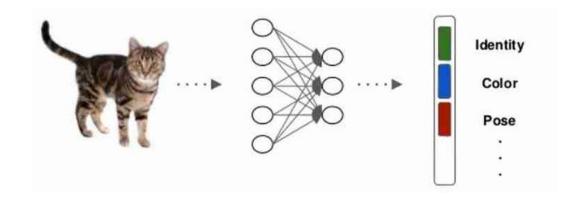
- 1. Take input data including history for the target variable
- Add differences, combinations, rolling means, medians, etc.
- 3. Add one-hot-encoding for important categorical features (day of week, holiday or not)
- Now we have input features for all points
- Let's apply our favorite ML regression algorithm



Deep Learning problems with sequential data: we need representations

Input Output "The quick brown fox jumped over Speech recognition the lazy dog." "There is nothing to like in Sentiment classification this movie." Voulez-vous chanter Machine translation Do you want to sing with me? avec moi? Video activity Running recognition

One example problem: why do we need Neural networks?



Textbook example: next word prediction

The most complicated and difficult part of it was only just beginning.

Textbook example: next word prediction

Idea 1: use previous word(s)

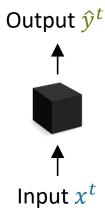
<u>Problem 1:</u> long-term dependencies

"France is where I grew up, but I now live in Boston. I speak fluent ____."

The most complicated and difficult part of it was only just beginning.



Feature representation: [0, 0, 0, 1, 0, 0]



Textbook example: next word prediction

Idea 1: use previous word(s)

Problem 1: long-term dependencies

Idea 2: use bag of words model

The most complicated and difficult part of it was only just beginning.



Feature representation: [0, 3, 0, 2, 0, 0]

Bag of words: number of occurrences of each word

Textbook example: next word prediction

<u>Idea 1:</u> use previous word(s)

Idea 2: use bag of words model

<u>Problem 1:</u> long-term dependencies

<u>Problem 2:</u> order preservation

The food was good, not bad at all.

VS.

The food was bad, not good at all.

The most complicated and difficult part of it was only just beginning.

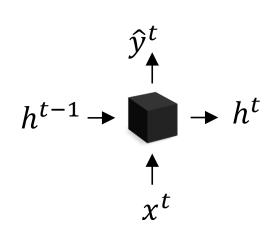


Feature representation: [0, 3, 0, 2, 0, 0]

Bag of words: number of occurrences of each word (see also TF-IDF features)

Model Design Criteria

- Variable-length sequences processing
- 2. Long-term memory
- 3. Maintain order information
- 4. Natural preprocessing



Recurrent Neural Networks are the solution!

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Sequence processing with classic ML models

- Variable-length sequences processing
- 2. Long-term memory
- 3. Maintain order information
- 4. Natural preprocessing

YES (if one to one)





NO



a kind of

Examples of texts generated by LSTM (Long Short Term Memory NN)

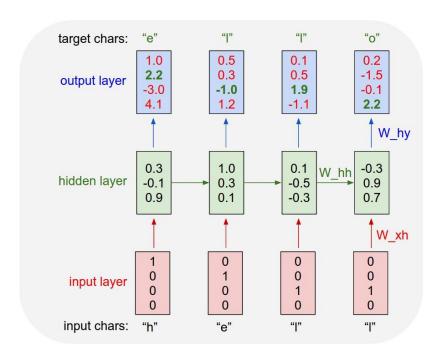
- Shakespeare
- Wiki
- Algebraic geometrics articles
- Linux Source Code
- Dinosaurs names

For $\bigoplus_{n=1,...,m}$ where $\mathcal{L}_{m_*} = 0$, hence we can find a closed subset \mathcal{H} in \mathcal{H} and

see Descent, Lemma ??. Namely, by Lemma ?? we see that R is geometrically

any sets F on X, U is a closed immersion of S, then $U \to T$ is a separated algebraic Suppose $X = \lim |X|$ (by the formal open covering X and a single map $Proj_{_{Y}}(A) =$ $\operatorname{Spec}(B)$ over U compatible with the complex Proof. Proof of (1). It also start we get $Set(A) = \Gamma(X, O_{X,O_X}).$ $S = \operatorname{Spec}(R) = U \times_X U \times_X U$ When in this case of to show that $Q \to C_{Z/X}$ is stable under the following result and the comparicoly in the fibre product covering we have to prove the lemma in the second conditions of (1), and (3). This finishes the proof. By Definition ?? generated by $\coprod Z \times_U U \to V$. Consider the maps M along the set of points (without element is when the closed subschemes are catenary. If T is surjective we Sch_{Ippf} and $U \rightarrow U$ is the fibre category of S in U in Section, ?? and the fact that may assume that T is connected with residue fields of S. Moreover there exists a any U affine, see Morphisms, Lemma ??. Hence we obtain a scheme S and any closed subspace $Z \subset X$ of X where U in X' is proper (some defining as a closed subset of the uniqueness it suffices to check the fact that the following theorem open subset $W \subset U$ in Sh(G) such that $Spec(R') \to S$ is smooth or an f is locally of finite type. Since S = Spec(R) and Y = Spec(R). which has a nonzero morphism we may assume that f_i is of finite presentation over Proof. This is form all sheaves of sheaves on X. But given a scheme U and a S. We claim that $\mathcal{O}_{X,x'}$ is a scheme where $x, x', s'' \in S'$ such that $\mathcal{O}_{X,x'} \to \mathcal{O}'_{X',x'}$ is surjective étale morphism $U \to X$. Let $U \cap U = \coprod_{i=1,...,n} U_i$ be the scheme X over separated. By Algebra, Lemma ?? we can define a map of complexes $GL_{S'}(x'/S'')$ S at the schemes $X_i \rightarrow X$ and $U = \lim_i X_i$. The following lemma surjective restrocomposes of this implies that $F_{x_0} = F_{x_0} =$ To prove study we see that $\mathcal{F}|_{U}$ is a covering of \mathcal{X}' , and \mathcal{T}_{c} is an object of $\mathcal{F}_{X/S}$ for i > 0 and F_p exists and let F_i be a presheaf of O_X -modules on C as a F-module. Lemma 0.2. Let X be a locally Noetherian scheme over S, $E = F_{Y/2}$. Set I =In particular F = U/F we have to show that $\mathcal{J}_1 \subset \mathcal{I}'_n$. Since $\mathcal{I}^n \subset \mathcal{I}^n$ are nonzero over $i_0 \leq \mathfrak{p}$ is a subset of $\mathcal{J}_{n,0} \circ \overline{A}_2$ works. $\widetilde{M}^{\bullet} = \mathcal{I}^{\bullet} \otimes_{\operatorname{Spec}(k)} \mathcal{O}_{S,s} - i_X^{-1} \mathcal{F})$ Lemma 0.3. In Situation ??. Hence we may assume q' = 0. is a unique morphism of algebraic stacks. Note that $Arrows = (Sch/S)_{fppf}^{opp}, (Sch/S)_{fppf}$ Proof. We will use the property we see that p is the mext functor (??). On the other hand, by Lemma ?? we see that $V = \Gamma(S, \mathcal{O}) \longmapsto (U, \operatorname{Spec}(A))$ is an open subset of X. Thus U is affine. This is a continuous map of X is the where K is an F-algebra where δ_{n+1} is a scheme over S. inverse, the groupoid scheme S. Proof. See discussion of sheaves of sets. The result for prove any open covering follows from the less of Example ??. It may replace S by $X_{spaces, étale}$ which gives an open subspace of X and T equal to S_{Zar} ,

Lemma 0.1. Assume (3) and (3) by the construction in the description.



Conclusions

- Classic ML can't handle semistructured data common in sequential data processing
- We should *learn representations* via Neural Networks
- Results are nice even for relatively simple models

Problem statements

We want to model the conditional distribution:

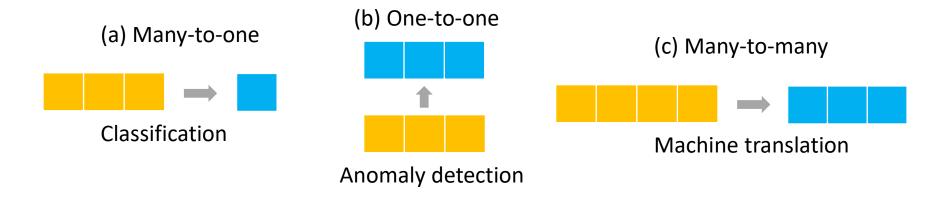
$$p(y_t|y_1,...,y_{t-1},x_1,...,x_t)$$



Our goal would be to propose such model

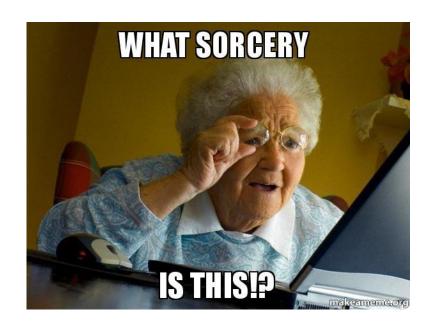
Problem statements

We also look at similar models and problems.

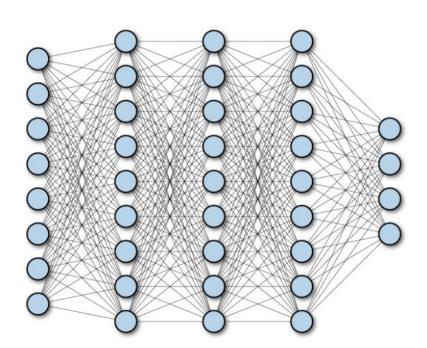


Model Design Criteria

- 1. Variable-length sequences processing
- 2. Long-term memory
- 3. Maintain order information
- 4. Natural preprocessing
- 5. General end2end approach

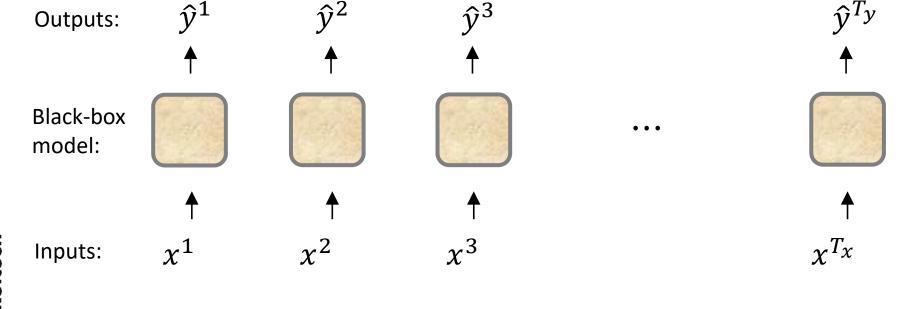


Fully connected neural networks?



Separate Fully-Connected Neural Networks or other separate models

We model $p(y_t|x_t)$ instead of $p(y_t|y_1,...,y_{t-1},x_t)$



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Why not a standard fully-connected network?



- Inputs, outputs can be different lengths in different examples
- Huge number of parameters (for length 512 it is about 256 000)
- Doesn't share features learned across different positions of text
- Not easy to separate contribution from different y-s ...think about it as a problem to think about e.g. p(y

SOTA options

Recurrent Neural Networks	Today	SOTA in some problem
One dimensional convolutions (1D CNN)	Next lecture (also see ROCKET)	SOTA in another problems
Transformers	After them	SOTA in most NLP problems

SOTA results for scoring problem

		Micro Precision
Two RNN architectures	LSTM	0.762
	GRU	0.765
	1D CNN	0.745
	Transformer	0.755
	Gradient boosting	0.697

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A vanilla Recurrent Neural Network



Simple RNN model

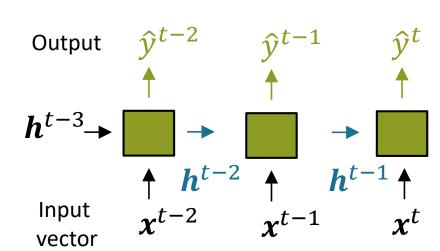
At each step:

 \hat{y}^t - output / model prediction

 x^t - input vector / new information

 h^t - cell / hidden state

Representation state



Main idea:

The model inside dark green block is the same for all time moments!

$$p(y_t|y_1,...,y_{t-1},x_1,...,x_t) = p(y_t|h_{t-1},x_t) = p(y_t|h_t)$$

Simple RNN model block

General form:

$$\boldsymbol{h}^t = f_h(\boldsymbol{x}^t, \boldsymbol{h}^{t-1})$$

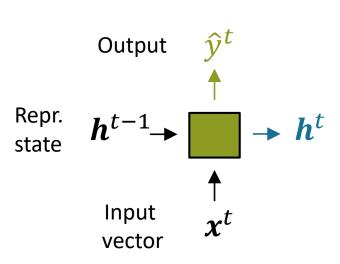
$$\hat{y}^t = f_y(\boldsymbol{h}^t)$$

Vanilla RNN model for classification:

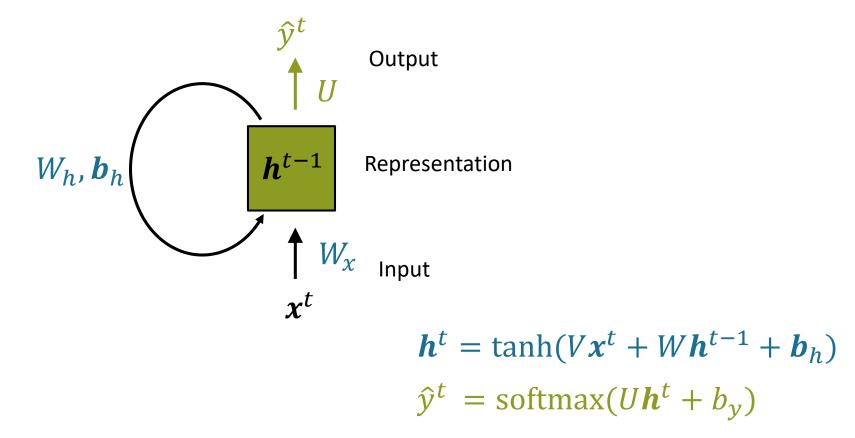
$$h^{t} = \tanh(Vx^{t} + Wh^{t-1} + b_{h})$$

$$\hat{y}^{t} = \operatorname{softmax}(Uh^{t} + b_{y})$$

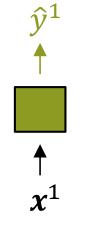
Parameters: V, W, U



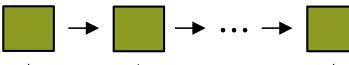
Compressed form of RNN







Sequence to a single output







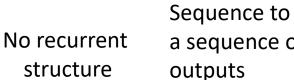












a sequence of

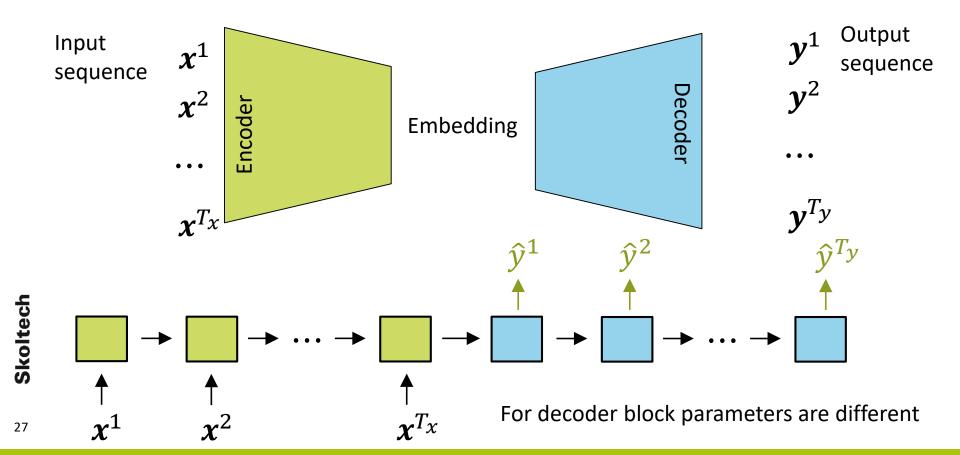








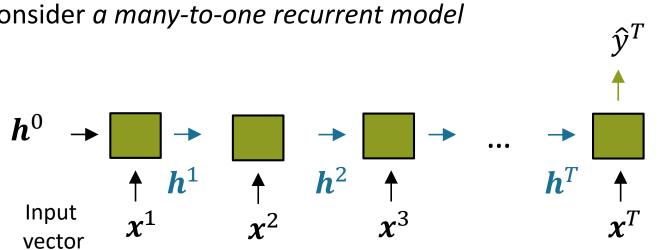
A sequence to sequence model



Details on Recurrent **Neural** Networks

An RNN model

Let us consider a many-to-one recurrent model



Output

Forward propagation through RNN

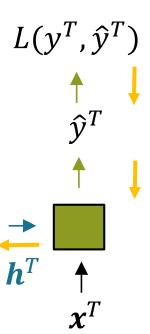
Composition of functions to get the output Output Input vector

Processing block is the same for all time moments. The processing time is linear in T: it is O(T).

Backward propagation through RNN

Composition of functions to get the output and calculate loss and its derivatives

Let's discuss pros and cons for this model



Loss function

Backpropagation w.r.t. U

$$L_{t} = L^{t}(\hat{y}^{t}, y^{t})$$

$$\uparrow$$

$$\uparrow$$

$$h^{t-1} \rightarrow \qquad \uparrow$$

$$\uparrow$$

$$\uparrow$$

$$\frac{\partial L_T}{\partial U} = \frac{\partial L_T}{\partial \hat{y}^T} \frac{\partial \hat{y}^T}{\partial U}$$

Recall the formula for the output

$$\hat{y}^t = \operatorname{softmax}(Uh^t + b_y)$$

Backpropagation w.r.t. W

$$\frac{\partial L_T}{\partial W} = \frac{\partial L_T}{\partial \hat{y}^T} \frac{\partial \hat{y}^T}{\partial W}$$

$$\frac{\partial L_t}{\partial \hat{y}^t} \frac{\partial \hat{y}^t}{\partial W} = \frac{\partial L_t}{\partial \hat{y}^t} \frac{\partial \hat{y}^t}{\partial h^t} \left(\frac{\partial h^t}{\partial W} + \frac{\partial h^t}{\partial h^{t-1}} \frac{\partial h^{t-1}}{\partial W} + \cdots \right)$$

$$\frac{\partial L_t}{\partial \hat{y}^t} \frac{\partial \hat{y}^t}{\partial W} = \frac{\partial L_t}{\partial \hat{y}^t} \frac{\partial \hat{y}^t}{\partial h^t} \sum_{i=0}^t \frac{\partial h^i}{\partial W} \left(\prod_{j=i+1}^t \frac{\partial h^j}{\partial h^{j-1}} \right)$$

We have a product of derivatives It can be a problem.

$$\boldsymbol{h}^t = \tanh(V\boldsymbol{x}^t + W\boldsymbol{h}^{t-1} + \boldsymbol{b}_h)$$

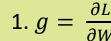
Problem: gradient explosion

$$\frac{\partial L_t}{\partial W} = \frac{\partial L_t}{\partial \hat{y}^t} \frac{\partial \hat{y}^t}{\partial h^t} \sum_{i=0}^t \frac{\partial h^i}{\partial W} \left(\prod_{j=i+1}^t \frac{\partial h^j}{\partial h^{j-1}} \right)$$

Solution:

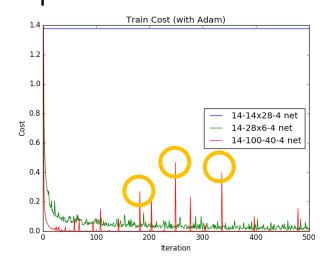
Gradient clipping to scale big gradients

$$\left| \frac{\partial h^j}{\partial h^{j-1}} \right| > 1$$
, nonstationary (c.t. ARIMA lecture)



2. If g > t for some threshold t:

$$g = \frac{t}{\|g\|} g$$

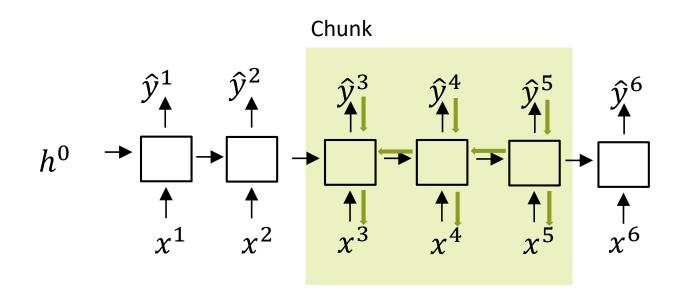


Threshold t is selected given the dynamic of loss function over iterations

Problem: gradient explosion

Solutions:

- Gradient clipping to scale big gradients
- Truncated backpropagation through time



Problems of classic RNN: gradient vanishing

A more serious problem

Many values < 1

Product << 1

$$\left| \left| \frac{\partial h^j}{\partial h^{j-1}} \right| \right| < 1$$

Can't learn long range dependences

Bias parameters to capture long-term dependencies

Tricks:

Activation functions

Use ReLU

Parameter initialization

- Initialize weights to identity matrix
- Initialize biases to zero

Hard to detect!

Another big problem of classic RNN

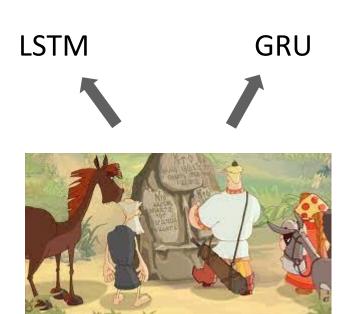
Problem: Neural networks forget fast, and it is hard to learn long-term dependencies

Solution: Gated architectures

More complex recurrent units with gates to control what information is passed through

- GRU: Gated Recurrent Unit
- LSTM Long-Short Term Memory
- Other?

Selection of RNN architecture



Better RNN units: LSTM and GRU

LSTM: long short term memory [1]

GRU: Gated recurrent unit [2]

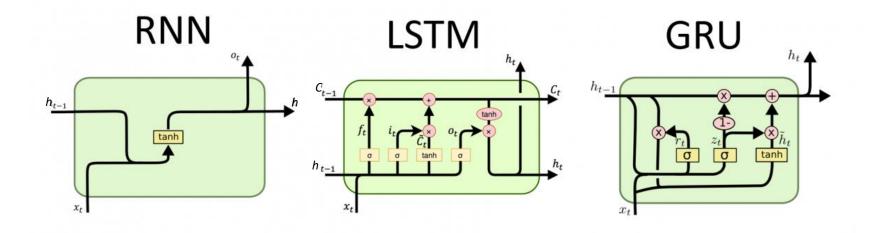


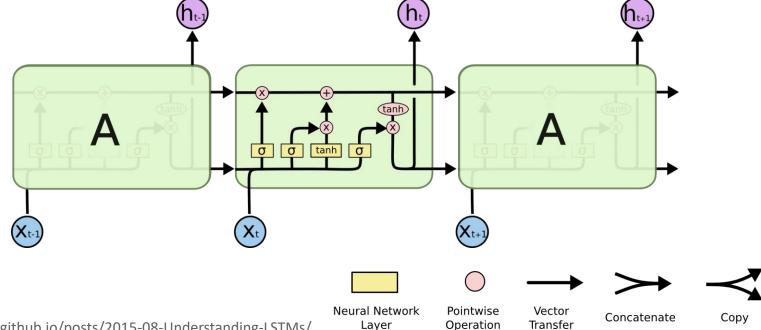
Image source: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

1. Schmidhuber, J., & Hochreiter, S. Long short-term memory. Neural Computations. 1997.

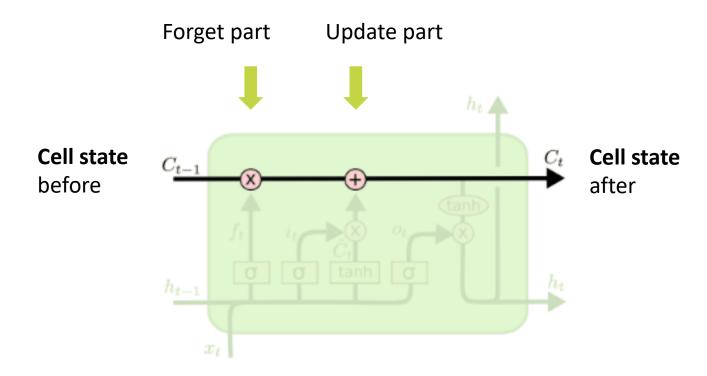
2. Cho, K., Van Merriënboer et al. Learning phrase representations using RNN encoder-decoder for statistical machine translation. EMNLP. 2014.

Details on how LSTM works

"Remembering information for long periods of time is practically the default behavior of LSTM" Temporal representation = Cell representation (long term) + Hidden state (short term)

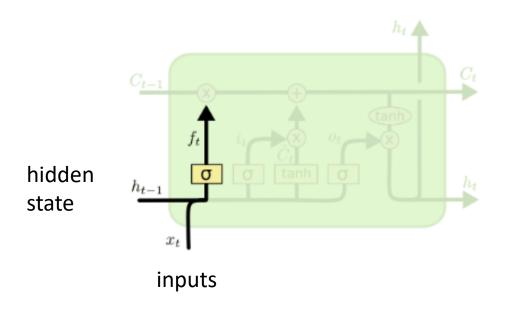


Long term memory part – Cell state



Forget part

Identify how much should we forget

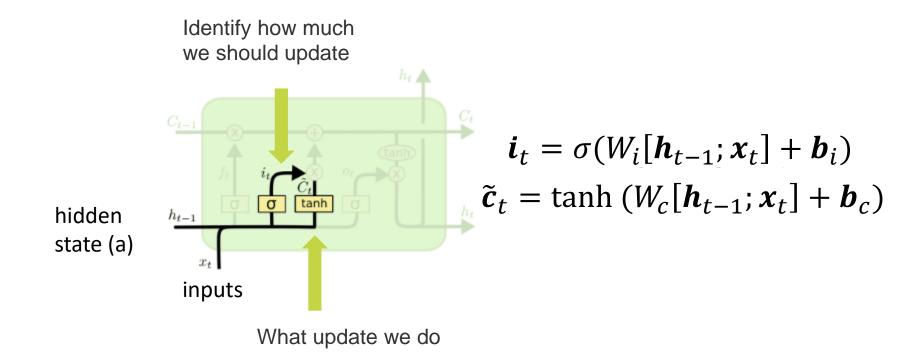


$$f_t = \sigma(W_f[\boldsymbol{h}_{t-1}; \boldsymbol{x}_t] + \boldsymbol{b}_f)$$

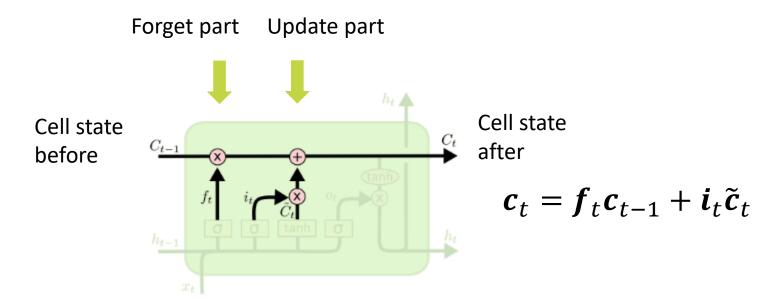
 $[\boldsymbol{h}_{t-1}; \boldsymbol{x}_t]$ is the concatenation

 W_f , \boldsymbol{b}_f are forget parameters σ is the sigmoid function, so the output is between 0 and 1

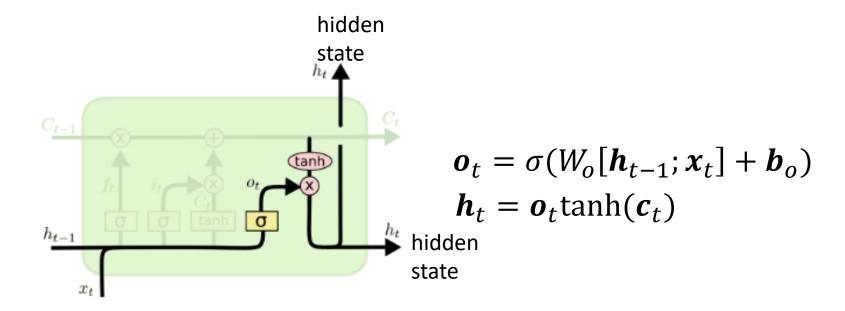
Update part



Long term memory part – Cell state

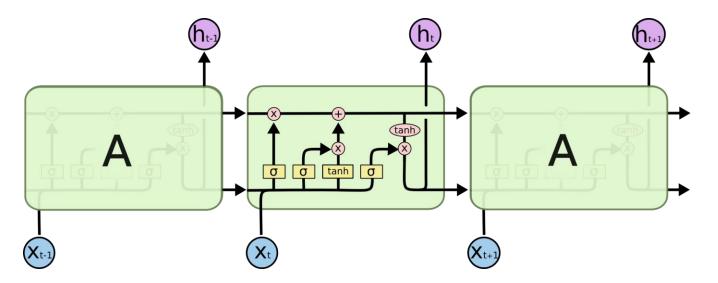


Update everything else



Details on how LSTM works

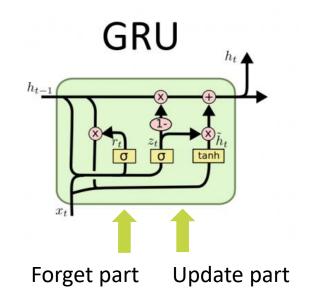
- There are cell and hidden (activation) states
- LSTM block forgets and updates cell state during processing at one block



GRU – Gated Recurrent Unit

- Update gate what to pay attention to
- Reset gate what to forget

$$\mathbf{r}^{t} = \sigma(W_{xr}\mathbf{x}^{t} + W_{hr}\mathbf{h}^{t-1} + b_{r})$$
$$\mathbf{z}^{t} = \sigma(W_{xz}\mathbf{x}^{t} + W_{hz}\mathbf{h}^{t-1} + b_{z})$$

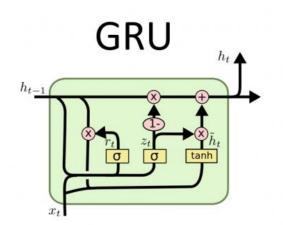


$$\widetilde{\boldsymbol{h}}^{t} = \tanh(W_{xh}\boldsymbol{x}^{t} + W_{hr}(\boldsymbol{r}^{t} \odot \boldsymbol{h}^{t-1}) + b_{h})$$

$$\boldsymbol{h}^{t} = \boldsymbol{z}^{t} \odot \boldsymbol{h}^{t-1} + (1 - \boldsymbol{z}^{t}) \odot \widetilde{\boldsymbol{h}}^{t}$$

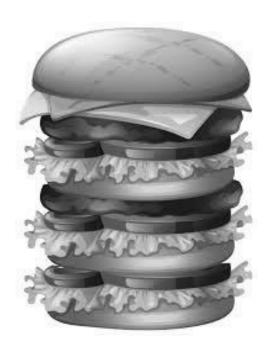
GRU – Gated Recurrent Unit

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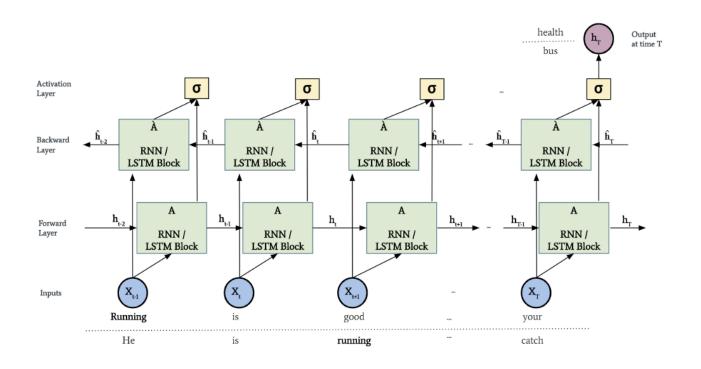


- Slightly worse than LSTM for NLP but not in all problems
- Simpler and cheaper than LSTM

Multilayer architectures



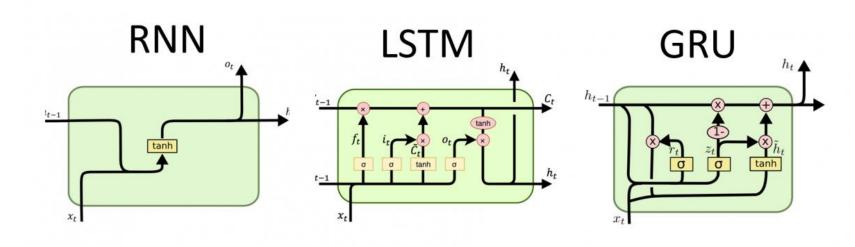
Other architectures: bidirectional LSTM



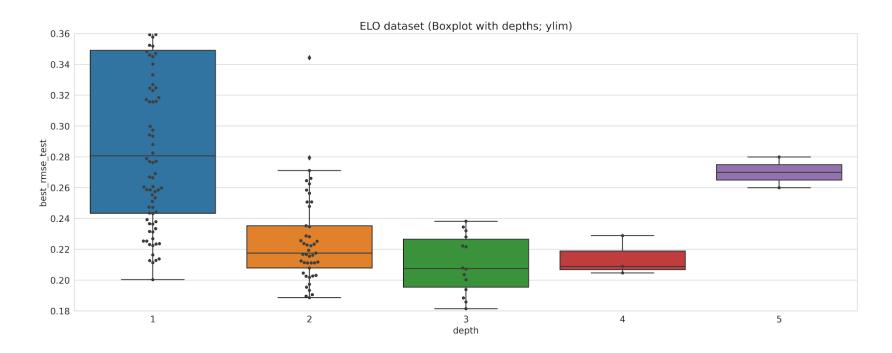
Other architectures: bidirectional LSTM

Bidirectional LSTM are useful when we benefit from the future data or can use it:

- Handwriting Recognition
- Speech Recognition
- Protein Structure Prediction (Bioinformatics)



Multiple layers RNN performance



Does a better recurrent block exist?



Towards a better recurrent block

- LSTM architecture is ad-hoc and has a substantial number of components whose purpose is not immediately apparent
- Like the LSTM, it is hard to tell, at a glance, which part of the GRU is essential for its functioning.
- Let's compare 10 000 different architectures on 3 problems with 1 000 of them pass the initial filtering stage: genetic algorithm
- Each architecture has been evaluated on about 220 hyperparameter settings.
- 230 000 hyperparameter configurations in total!



Best found architectures MUTx are close to GRU

GRU:

$$r_{t} = \operatorname{sigm}(W_{xr}x_{t} + W_{hr}h_{t-1} + b_{r})$$

$$z_{t} = \operatorname{sigm}(W_{xz}x_{t} + W_{hz}h_{t-1} + b_{z})$$

$$\tilde{h}_{t} = \operatorname{tanh}(W_{xh}x_{t} + W_{hh}(r_{t} \odot h_{t-1}) + b_{h})$$

$$h_{t} = z_{t} \odot h_{t-1} + (1 - z_{t}) \odot \tilde{h}_{t}$$

Arch.	N	N-dropout	P
Tanh	3.612	3.267	6.809
LSTM	3.492	3.403	6.866
LSTM-f	3.732	3.420	6.813
LSTM-i	3.426	3.252	6.856
LSTM-o	3.406	3.253	6.870
LSTM-b	3.419	3.345	6.820
GRU	3.410	3.427	6.876
MUT1	3.254	3.376	6.792
MUT2	3.372	3.429	6.852
MUT3	3.337	3.505	6.840

Table 2. Negative Log Likelihood on the music datasets. N stands for Nottingham, N-dropout stands for Nottingham with nonzero dropout, and P stands for Piano-Midi.

MUT1:

$$z = \operatorname{sigm}(W_{xz}x_t + b_z)$$

$$r = \operatorname{sigm}(W_{xr}x_t + W_{hr}h_t + b_r)$$

$$h_{t+1} = \tanh(W_{hh}(r \odot h_t) + \tanh(x_t) + b_h) \odot z$$

$$+ h_t \odot (1 - z)$$

MUT2:

$$z = \operatorname{sigm}(W_{xz}x_t + W_{hz}h_t + b_z)$$

$$r = \operatorname{sigm}(x_t + W_{hr}h_t + b_r)$$

$$h_{t+1} = \operatorname{tanh}(W_{hh}(r \odot h_t) + W_{xh}x_t + b_h) \odot z$$

$$+ h_t \odot (1 - z)$$

MUT3:

$$z = \operatorname{sigm}(W_{xz}x_t + W_{hz} \tanh(h_t) + b_z)$$

$$r = \operatorname{sigm}(W_{xr}x_t + W_{hr}h_t + b_r)$$

$$h_{t+1} = \tanh(W_{hh}(r \odot h_t) + W_{xh}x_t + b_h) \odot z$$

$$+ h_t \odot (1 - z)$$

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Towards a better recurrent block

- LSTM architecture is ad-hoc and has a substantial number of components whose purpose is not immediately apparent
- Like the LSTM, it is hard to tell, at a glance, which part of the GRU is essential for its functioning.
- Let's compare 8 LSTM variants and hope for the best by search over the space of hyperparameters with 5400 runs in total
- No significant improvement over the common LSTM
- Some advices on hyperparameters selection



Neural architecture search for a better Recurrent block

- Linear: $f(x_1,...,x_n) = W_1x_1 + ... + W_nx_n + b$,
- Blending (element wise): $f(z, x, y) = z \odot x + (1 z) \odot y$,
- Element wise product and sum,
- Activations: Tanh, Sigmoid, and LeakyReLU.

- Number of nodes < 25
- Number of hidden states < 4
- Number of linear input vectors < 4

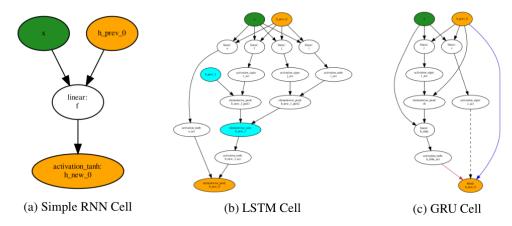
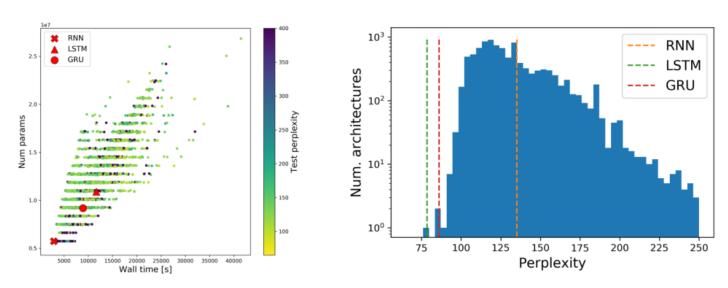


Figure 2: Examples of conventional RNN cells. Colors of nodes highlight the corresponding previous and new hidden states, green color also highlights the input vector. Black dashed, blue and red edges indicate blending arguments z, x and y respectively.

Neural architecture search for a better Recurrent block



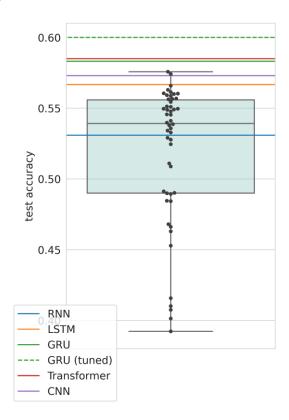
(a) Joint distribution of metrics.

(b) Best test perplexity distribution.

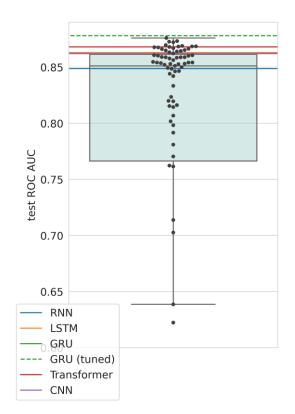
Figure 4: Architectures metrics on PTB.

Best architecture for Transactions data

Age prediction



Gender prediction



Architecture performance transferability

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0.81

0.82

0.83

0.84

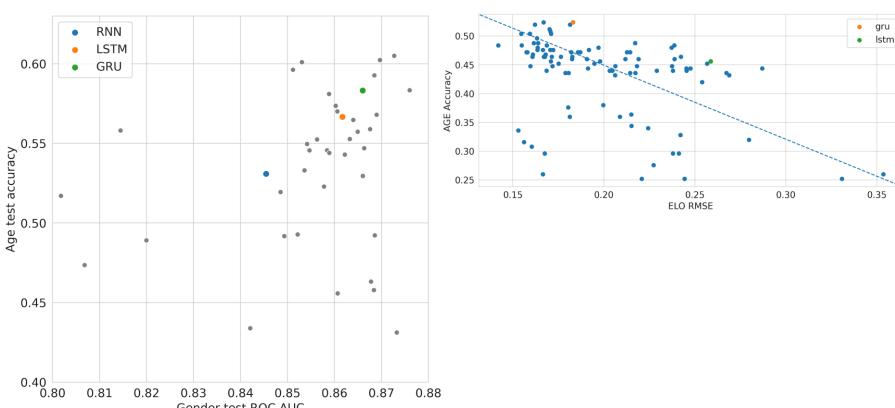
Gender test ROC AUC

0.85

0.86

0.87

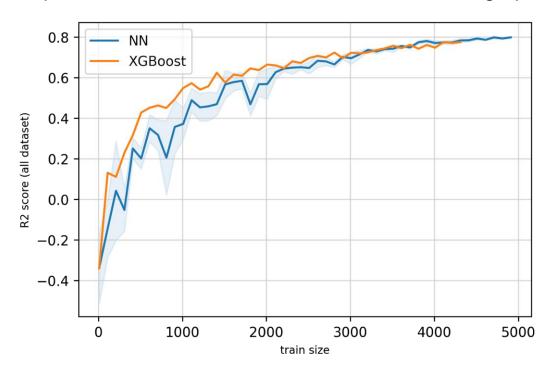
0.88



Can we predict the performance of an architecture?

We can, but we need large samples

For path features and NLP NAS bench with 11000 graph2vec features

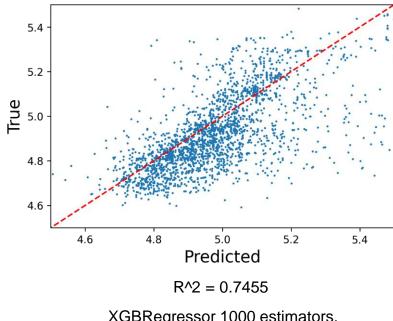


A. Narayanan, M. Chandramohan, R. Venkatesan, L. Chen, Y. Liu, and S. Jaiswal. graph2vec: Learning distributed representations of graphs. arXiv preprint arXiv:1707.05005, 2017.

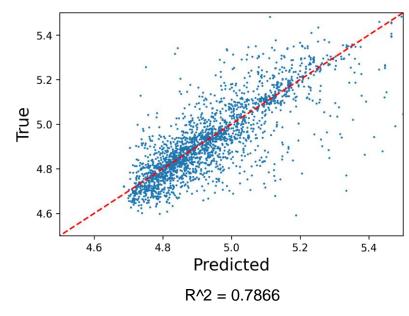
Skoltech

We can, but we need large samples

For path features and NLP NAS bench with 11000 features

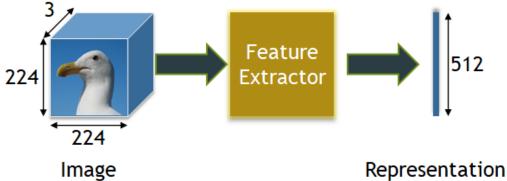


XGBRegressor 1000 estimators, Ir=0.05, default parameters

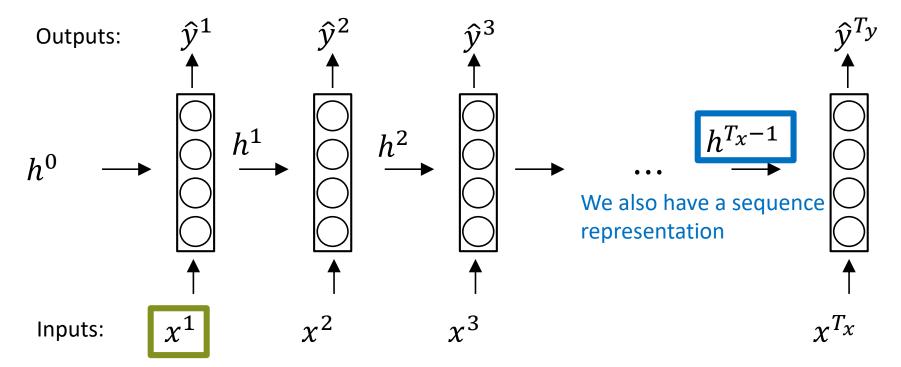


Dense NN, 10 layers with dim=20, ELU Ir=0.005, 120 epochs

Representation
learning is the core
feature of Neural
Networks



Representation learning is still here for Recurrent Neural Networks



Most of the time we also learn representations of objects in an end2end manner with backpropagation

Take-home messages

- For some types of data classic methods fail:
 we need to learn a representation i.e. extract features automatically
- Neural Networks provide enough flexibility for this problem for various data types
- The basic architecture is Recurrent Neural Network (RNN)
- But we can do better in terms of keeping the necessary information with LSTM and GRU blocks/architectures

Sources

- Recurrent Neural Networks | in Deep learning course by MIT 6.S191
- Coursera course on Sequence models https://www.coursera.org/learn/nlp-sequence-models
- http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Machine translation: application example









War and Peas

Dog Translation Machine

koltech

Machine translation, 50-s

Cold war child: translator from Russian to English IBM 701 Translator

Doctor Dostert predicted that "five, perhaps three years hence, interlingual meaning conversion by electronic process in important functional areas of several languages may well be an accomplished fact." (1954)

Rule-based approach that uses English-Russian dictionary



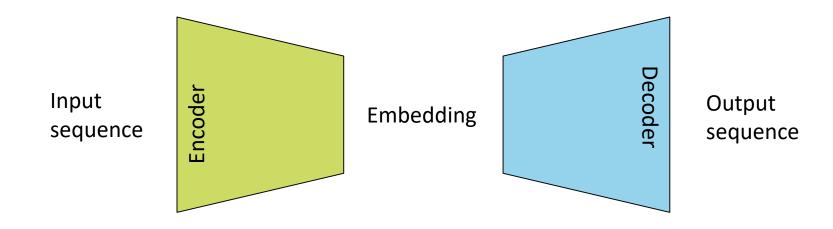
Project shut-down in 5 years: no significant progress

https://www.ibm.com/ibm/history/exhibits/701/701_translator.html https://youtu.be/8ZtdVUB007A

Statistical approach – the leading one before 2014

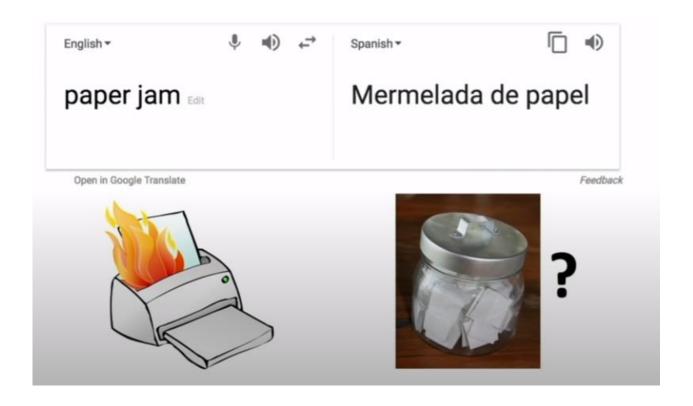
- Complicated and heavy model
- Many separate components
- Complex generation of inputs
- Support of a sophisticated system
- Quality is not great

Neural network for machine translation

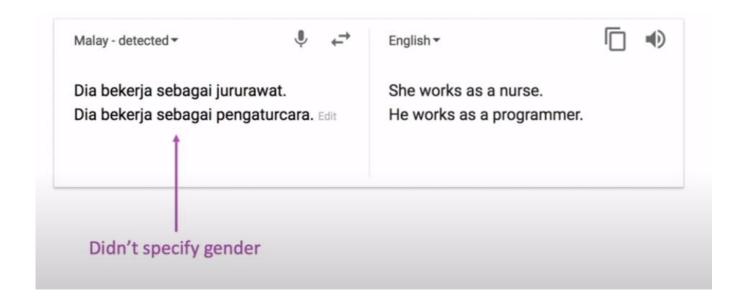


seq2seq (sequence to sequence) architecture

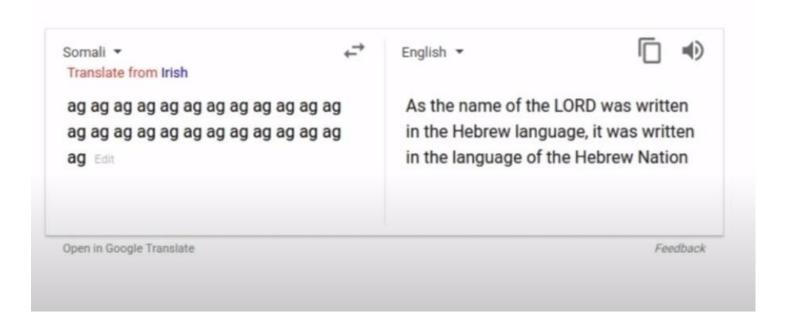
Not a perfect solution with little control over result



Contains biases from learning sample

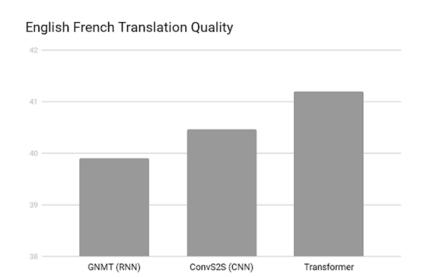


Output strange results



Attention/transformer – new state-of-the art for Machine translation

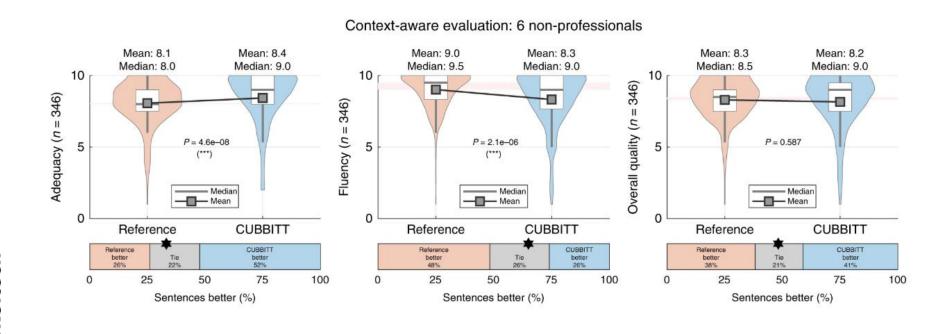
English German Translation quality 28 26 24 29 GNMT (RNN) ConvS2S (CNN) SliceNet (CNN) Transformer



- Maximize BLEU translation quality metric
- The best model is **Transformer**

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NLP deep learning models: CUBBITT is comparable to reference human translation for a selected dataset on News translation



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Conclusions

- Machine translation problem was attacked by many problems during a long period of time
- Right now the state-of-the-art is Neural Networks Transformers
- They can even improve over human-translation

Another semi-structured data problems

Credit scoring: default prediction

Money Transactions data



Fraud detection in healthcare insurance

A history of visits

→

Is there a fraud?

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