LSTM: A Search Space Odysseys

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Recurrent Neural Networks - RNNs

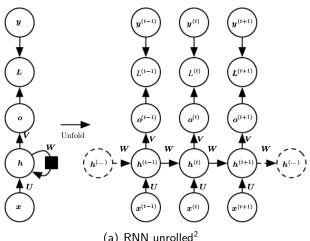
- Used to deal with sequential data, where there is a temporal dependence from a time instance to another
- Mathematically, they model a conditional distribution of the form $P(x_t|x_{t-1},...,x_2,x_1)$, where x_t is the current input at time t
- The output of a vanilla RNN cell at each time step is computed using the current input x_t and also the previous cell state h_{t-1}^{-1} as:

$$y_t = tanh(Ux_t + Wh_{t-1} + b),$$

where $U \in R^{M \times N}$, $W \in R^{N \times N}$ are the shared parameter matrices for the RNN cells and $b \in R^N$ is the bias

¹Meant to encompass a summary of the past information

Recurrent Neural Networks Unrolled



(a) RNN unrolled²

²Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. http://www.deeplearningbook.org. MIT Press, 2016.

Vanishing/Exploding Gradient

- The main algorithm for learning the weights of an RNN is called Backpropagation Through Time (BPTT)
- When computing the gradients with respect to the weights of the network, W depends on a recurrent connection from a previous timestep and so the partial derivative w.r.t. W becomes:

$$\frac{\partial L^{(t)}}{\partial W} = \sum_{k=0}^t \frac{\partial L^{(t)}}{\partial o^{(t)}} \frac{\partial o^{(t)}}{\partial h^{(t)}} \bigg(\prod_{j=k+1}^t \frac{\partial h^{(j)}}{\partial h^{(j-1)}} \bigg) \frac{\partial h^{(k)}}{\partial W},$$

where $L^{(t)}$ is the error and $o^{(t)}$ is the predicted value at the t^{th} output step

• If the number of timesteps is big, the product from the formula above will either diminish to 0 or explode to ∞ , thus prohibiting the learning process further on

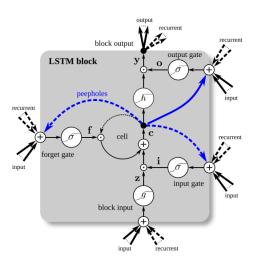
Long Short-Term Memory - LSTM

- LSTM³ solves the problem of vanishing/exploding gradients
- The LSTM architecture is a memory cell, which can maintain its state over time, and nonlinear gating units, which regulate the information flow into and out of the cell
- Further experiments have proven that no other variants that differ from the vanilla LSTM by adding, removing or modifying exactly one aspect can obtain a much better performance⁴

³Sepp Hochreiter and Jürgen Schmidhuber. "Long Short-term Memory". In: 9 (Dec. 1997), pp. 1735–80.

⁴Klaus Greff et al. "LSTM: A Search Space Odyssey". In: *CoRR* abs/1503.04069 (2015). arXiv: 1503.04069. URL: http://arxiv.org/abs/1503.04069.

LSTM Cell



Legend unweighted connection weighted connection connection with time-lag branching point 0 mutliplication sum over all inputs gate activation function (always sigmoid) input activation function (usually tanh) output activation function (usually tanh)

(b) LSTM cell

LSTM Cell Computation

The formulas for a vanilla LSTM layer forward pass can be written as:

$$\begin{split} & \bar{z}^t = W_z x^t + R_z y^{t-1} + b_z \\ & z^t = g(\bar{z}^t) & \text{block input} \\ & \bar{i}^t = W_i x^t + R_i y^{t-1} + p_i \odot c^{t-1} + b_i \\ & i^t = \sigma(\bar{i}^t) & \text{input gate} \\ & \bar{f}^t = W_f x^t + R_f y^{t-1} + p_f \odot c^{t-1} + b_f \\ & f^t = \sigma(\bar{f}^t) & \text{forget gate} \\ & c^t = z^t \odot i^t + c^{t-1} \odot f^t & \text{cell} \\ & \bar{o}^t = W_o x^t + R_o y^{t-1} + p_o \odot c^{t-1} + b_o \\ & o^t = \sigma(\bar{o}^t) & \text{output gate} \\ & y^t = h(c^t) \odot o^t & \text{block output} \end{split}$$

LSTM Gates

- Each gate is computed in terms of the current input, the previous output, a peephole connection to the previous cell state and a bias
- i^t, f^t and o^t are called the input, forget and output gates and their role is to determine how much information flows from previous and current timesteps. This effect is achieved by squashing the gates through a sigmoid function. Then an element wise multiplication is performed such that the input gate determines how much of the current information is used, the forget gate deals with the information flow from the previous cell state and finally, the output gate specifies how much information to send to the output y
- The peephole connections were added such that the network can learn precise timings easier⁵

⁵Felix A. Gers, Nicol N. Schraudolph, and Jürgen Schmidhuber. "Learning Precise Timing with Lstm Recurrent Networks". In: *J. Mach. Learn. Res.* 3 (Mar. 2003), pp. 115–143. ISSN: 1532-4435. DOI: 10.1162/153244303768966139. URL: https://doi.org/10.1162/153244303768966139.

Evaluation Setup

- The vanilla LSTM is used as a baseline and evaluated together with eight of its variants
- Random search was used to obtain good-performing hyperparameters
- Three datasets were used to evaluate the performance
 - The TIMIT Speech corpus
 - The IAM Online Handwriting Database
 - JSB Chorales
- The interaction between hyperparameters was observed using the fANOVA framework⁶

⁶F. Hutter, H. Hoos, and K. Leyton-Brown. "An Efficient Approach for Assessing Hyperparameter Importance". In: *Proceedings of International Conference on Machine Learning 2014 (ICML 2014)*. June 2014, 754762.

LSTM Variants

- **NIG:** No Input Gate: $i^t = 1$
- **NFG:** No Forget Gate: $f^t = 1$
- **NOG:** No Output Gate: $o^t = 1$
- **NIAF:** No Input Activation Function: g(x) = x
- **NOAF:** No Output Activation Function: h(x) = x
- CIFG: Coupled Input and Forget Gate: $f^t = 1 i^t$
- NP: No Peepholes:

$$\bar{t}^t = W_i x^t + R_i y^{t-1} + b_i$$

$$\bar{f}^t = W_f x^t + R_f y^{t-1} + b_f$$

$$\bar{o}^t = W_o x^t + R_o y^{t-1} + b_o$$

LSTM Variants

• FGR: Full Gate Recurrence:

$$\bar{i}^{t} = W_{i}x^{t} + R_{i}y^{t-1} + p_{i} \odot c^{t-1} + b_{i}
+ R_{ii}i^{t-1} + R_{fi}f^{t-1} + R_{oi}o^{t-1}
\bar{f}^{t} = W_{f}x^{t} + R_{f}y^{t-1} + p_{f} \odot c^{t-1} + b_{f}
+ R_{if}i^{t-1} + R_{ff}f^{t-1} + R_{of}o^{t-1}
\bar{o}^{t} = W_{o}x^{t} + R_{o}y^{t-1} + p_{o} \odot c^{t-1} + b_{o}
+ R_{io}i^{t-1} + R_{fo}f^{t-1} + R_{oo}o^{t-1}$$

- The CIFG variant is also known as Gated Recurrent Unit (GRU)⁷
- The FGR variant adds recurrent connections between all the gates, thus significantly increasing the number of parameters

⁷Kyunghyun Cho et al. "Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation". In: *CoRR* abs/1406.1078 (2014). arXiv: 1406.1078. URL: http://arxiv.org/abs/1406.1078.