Differentiable Neural Computers

Hybrid Computing using a neural network with dynamic external memory (Graves et al. 2016)

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May 28, 2018

Logic and Computation

Overview: Probabilistic Programming

Cross-domain

- Data Flow Programming
- Bayesian Reasoning / Machine Learning
- Fuzzy Logic
- Functional Programming

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Program	Model
Discrete	Continuous
Deterministic	Stochastic
Static	Adaptive

Overview: DNC

Differentiable Neural Computer

A recurrent neural network coupled with an external memory.

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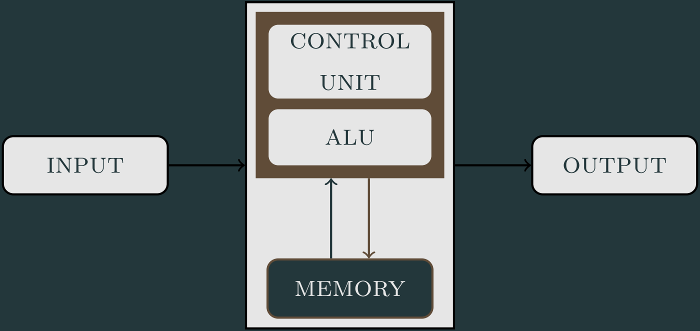
Differentiable Neural Computer

A recurrent neural network coupled with an external memory.

- Functional replication of biological memory
- Reimaging of classical concepts of computation
- Extension of NTMs
  - End-to-end differentiable
  - Auto-associative memory
  - Turing complete
  - \+ Computationally efficient memory management

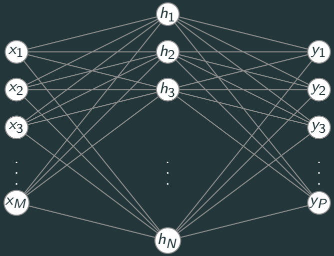
Introduction: Classic Computation

Von Neumann architecture



Introduction: Neural Networks

Simple Neural Net



$$NN : \boldsymbol{x}_t \mapsto \boldsymbol{y}_t$$

No memory

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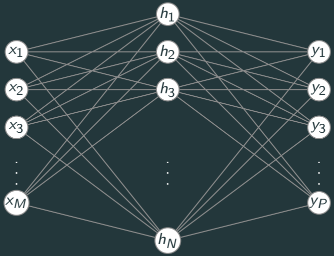

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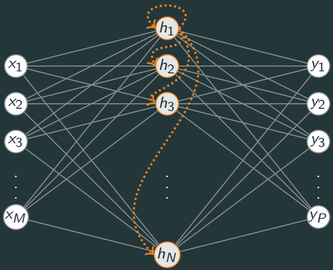

$RNN : \boldsymbol{x}_0 \otimes \boldsymbol{x}_1 \otimes \cdots \otimes \boldsymbol{x}_t \mapsto \boldsymbol{y}_t$

Finite memory

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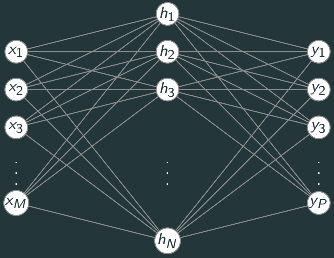

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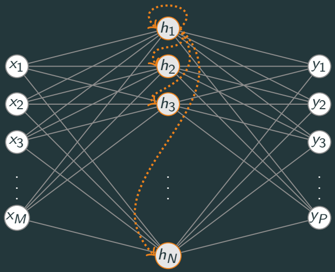

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Finite memory

"If training vanilla neural nets is optimization over functions, training recurrent nets is optimization over programs."

Approach

Train a RNN to act as the controller of a memory matrix $M \in \mathbb{R}^{N \times W}$ through R read heads and one write head.

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3. Dynamic Allocation
   - Mark memory locations with $\boldsymbol{u} \in [0,1]^N$ to signal usage
   - Manipulate signals during R/W operations to enable reallocation
   - Generalization to unbounded memory

Controller: Overview

A deep long short-term memory network receiving input:

$$\boldsymbol{\mathcal{X}}_t = [\boldsymbol{x}_t; \boldsymbol{r}^1_{t-1}; \ldots; \boldsymbol{r}^R_{t-1}] \qquad \text{(timestep t)}$$

and producing output:

$$(\boldsymbol{y}_t, \boldsymbol{\xi}_t) = \mathcal{N}([\boldsymbol{\mathcal{X}}_1; \ldots; \boldsymbol{\mathcal{X}}_t]; \vartheta) \qquad \text{(entire sequence)}$$

where $\mathcal{N}$ a set of state equations and ϑ their trainable parameters.

LSTM: Overview

LSTM Network

Multiple stacked LSTM units.

LSTM Unit

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1. Input gate $\boldsymbol{i}_t^l$
2. Forget gate $\boldsymbol{f}_t^l$
3. Output gate $\boldsymbol{o}_t^l$

LSTM: Signal-Flow (1/2)

LSTM Unit (single layer)

- Input: $[\mathcal{X}_t; \boldsymbol{h}_{t-1}^{l}; \boldsymbol{h}_t^{l-1}]$
- Output: $\boldsymbol{h}_t^{l}$

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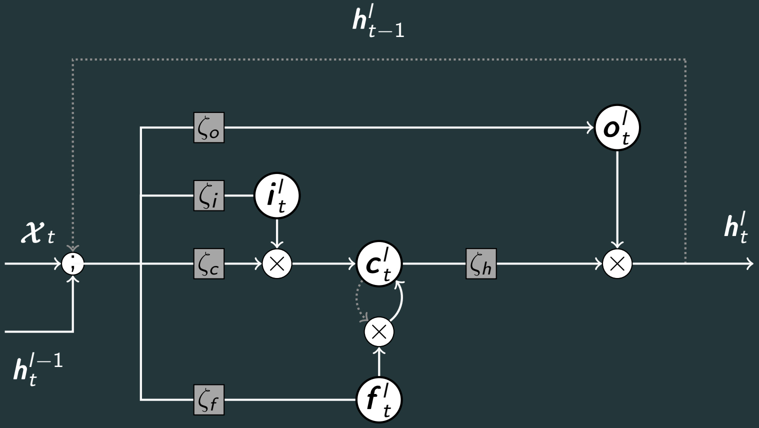

Controller: Signal-Flow (2/2)

LSTM Network (multiple layers)

- Input: $\boldsymbol{\mathcal{X}}_t$
- Output: $[\boldsymbol{h}_t^1; \boldsymbol{h}_t^2; \ldots \boldsymbol{h}_t^L]$

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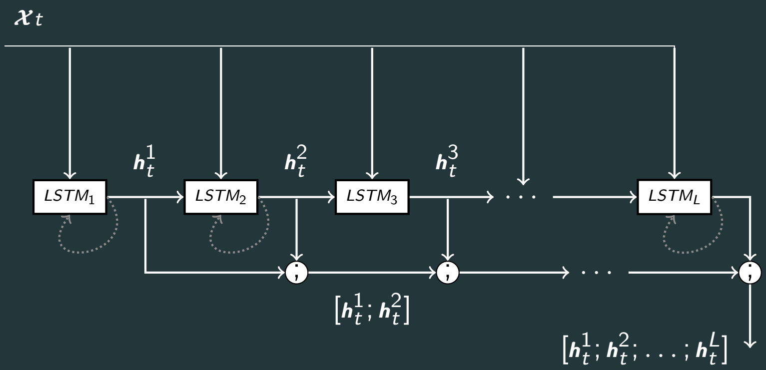

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Interface vector $\boldsymbol{\xi}_t = W_\xi[\boldsymbol{h}_t^1; \ldots; \boldsymbol{h}_t^L]$

- Read keys: $\boldsymbol{k}_t^{r,i}$
- Read strengths: $\beta_t^{r,i}$
- Write key: $\boldsymbol{k}_t^w$
- Write strength: β_t^w
- Erase vector: $\boldsymbol{e}_t$
- Write vector: $\boldsymbol{v}_t$
- Free gates: $\boldsymbol{\phi}_t^i$
- Allocation gate: g_t^a
- Write gate: g_t^w
- Read modes: $\boldsymbol{\pi}_t^i$

Memory Adressing: Content-Lookup

R read keys $\boldsymbol{k}^{r,i} \in \mathbb{R}^W, \ i = 1 \dots R$

R read strengths $\beta^{r,i} \in [1, \infty), \ i = 1 \dots R$

Write key $\boldsymbol{k}^w \in \mathbb{R}^W$

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Matching function $\mathcal{D}$ comparing memory contents

Weighting function $\mathcal{C}$ normalizing and sharpening matches

$$\mathcal{C}(M, \boldsymbol{k}, \beta)[i] = \frac{exp\{\beta \mathcal{D}(\boldsymbol{k}, M[i, :])\}}{\sum_j exp\{\beta \mathcal{D}(\boldsymbol{k}, M[j, :])\}}$$

Memory Adressing: R/W

Attention dictated by weightings $\boldsymbol{w} \in \mathcal{S}_N$

Erase vector $\boldsymbol{e}_t \in [0,1]^W$

Write vector $\boldsymbol{v}_t \in \mathbb{R}^W$

Read operations

$$\boldsymbol{r}_t^i = M_t^\top \boldsymbol{w}_t^{r,i}$$

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$$M_t = \underbrace{M_{t-1} \circ (\mathbf{1} - \boldsymbol{w}_t^w \boldsymbol{e}_t^\top)}_{\text{erased memory}} + \underbrace{\boldsymbol{w}_t^w \boldsymbol{v}_t^\top}_{\text{new write}}$$

Memory Adressing: Dynamic Allocation

Free gates $\phi_t^i \in [0,1]$
Allocation gate $g_t^a \in [0,1]$
Write gate $g_t^w \in [0,1]$

"Free list" scheme

$$\boldsymbol{\psi}_t = \prod_{i=1}^{R}(\mathbf{1} - \phi_t^i w_{t-1}^{r,i}) \qquad \text{(memory retention)}$$

$$u_t = (\boldsymbol{u}_{t-1} + \boldsymbol{w}_{t-1}^w - \boldsymbol{u}_{t-1} \circ \boldsymbol{w}_{t-1}^w) \circ \boldsymbol{\psi}_t \qquad \text{(usage tracking)}$$

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Attention shift

- Obtain the allocation vector $\boldsymbol{a}_t$ by normalizing $\boldsymbol{u}_t$
- Shift $\boldsymbol{w}_t$ by $g_t^a \boldsymbol{a}_t$ and scale by g_t^w

Memory Adressing: Temporal Linking

Read modes: $\boldsymbol{\pi}_t^i \in \mathcal{S}_3$

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Temporal Transition $\boldsymbol{L}_t \in [0,1]^{N\times N}$

$$\boldsymbol{L}[i,j] = \underbrace{(1 - w_t^W[i] - w_t^W[j])\boldsymbol{L}_{t-1}[i,j]}_{\text{Part of last transition}} + \underbrace{w_t^w[i]w_{t-1}^w[j]}_{\text{Current transition}}$$

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Mode Interpolation

$$\boldsymbol{w}_t^{r,i} = \underbrace{\boldsymbol{\pi}_t^i[1]L\boldsymbol{w}_t^{r,i}}_{\text{Forward shift}} + \underbrace{\boldsymbol{\pi}_t^i[2]\boldsymbol{w}_t^{r,i}}_{\text{No shift}} + \underbrace{\boldsymbol{\pi}_t^i[3]L^\top\boldsymbol{w}_t^{r,i}}_{\text{Backward shift}}$$

Experiments

- Language Tasks
  - Inference
  - Logical Reasoning

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- Language Tasks
  - Inference
  - Logical Reasoning
- Graph Tasks
  - Network Traversal
  - Policy Learning

Conclusion

Recap

- We can simulate computation and expand upon it by using differentiable, continuous operations.
- Simple programs (over complex data structures) can now be automagically inferred.

Thank you!

Questions?

Appendix: LSTM Equations

$$\boldsymbol{i}_t^l = \sigma(W_i^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t-1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_i^l) \qquad \text{(input gate)}$$

$$\boldsymbol{f}_t^l = \sigma(W_f^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t-1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_f^l) \qquad \text{(forget gate)}$$

$$\boldsymbol{s}_t^l = \boldsymbol{f}_t^l \boldsymbol{s}_{t-1}^l + \boldsymbol{i}_t^l \, tanh(W_s^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t_1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_s^l) \qquad \text{(state)}$$

$$\boldsymbol{o}_t^l = \sigma(W_o^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t-1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_o^l) \qquad \text{(output gate)}$$

$$\boldsymbol{h}_t^l = \boldsymbol{o}_t^l \, tanh(\boldsymbol{s}_t^l) \qquad \text{(hidden)}$$

$$\boldsymbol{\upsilon}_t = W_y[\boldsymbol{h}_t^1; \ldots; \boldsymbol{h}_t^L] \qquad \text{(output vector)}$$

$$\boldsymbol{\xi}_t = W_\xi[\boldsymbol{h}_t^1; \ldots; \boldsymbol{h}_t^L] \qquad \text{(interface vector)}$$

Appendix: Further Reading

Neural Architectures

- Learning to Forget (Gers, Schmidhuber, Cummins)
- Neural Turing Machines (Graves, Wayne, Danihelka)
- Entity Networks (Henaff, Weston, Szlam, Bordes, LeCun)
- End-to-End Memory Networks (Sukhbaatar, Szlam, Weston, Fergus)
- Jointly Learning to Align and Translate (Bahdanau, Cho, Bengio)

Probabilistic Programming

- Principles of Probabilistic Programming Languages (Goodman)
- Backprop as a Functor (Fong, Spivak, Tuyras)
- Formal Methods for Probabilistic Programming (Selsam, Liang, Dill)