Differentiable Neural Computers

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

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Logic and Computation

Overview: Probabilistic Programming

Cross-domain

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

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Intuition: "Rather than explicitly write a program, write some constraints on the behavior of the desired program and use computational tools to search the program space for models satisfying these constraints."

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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.

Overview: DNC

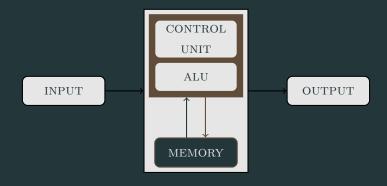
Differentiable Neural Computer

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

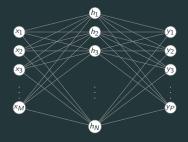
Introduction: Classic Computation

Von Neumann architecture



Introduction: Neural Networks

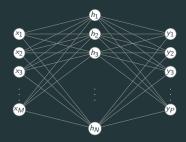
Simple Neural Net



 $\overline{NN}: \boldsymbol{x}_t \mapsto \boldsymbol{y}_t$ No memory

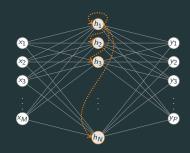
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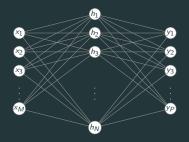
Simple Recurrent Net



 $RNN: \mathbf{x}_0 \otimes \mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_t \mapsto \mathbf{y}_t$ Finite memory

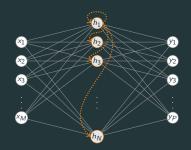
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"If training vanilla neural nets is optimization over functions, training recurrent nets is optimization over programs."

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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1. Content Lookup

- Attention over memory defined by weightings $w \in S^N$
- Compare controller output with memory objects (auto-associative memory)
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- Shift operations defined by Lw, $L^{\top}w$

3. Dynamic Allocation

- Mark memory locations with $\mathbf{u} \in [0,1]^N$ 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:

$$\boldsymbol{\mathcal{X}}_t = [\boldsymbol{x}_t; \boldsymbol{r}_{t-1}^1; \dots; \boldsymbol{r}_{t-1}^R]$$
 (timestep t)

and producing output:

$$(\mathbf{y}_t, \mathbf{\xi}_t) = \mathcal{N}([\mathbf{\chi}_1; \dots; \mathbf{\chi}_t]; \vartheta)$$
 (entire sequence)

where ${\cal N}$ a set of state equations and ${\it \vartheta}$ their trainable parameters.

LSTM: Overview

LSTM Network

Multiple stacked LSTM units.

LSTM Unit

A RNN that has an intrinsic memory cell c_t' and three gates.

LSTM: Overview

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Multiple stacked LSTM units.

ISTM Unit

A RNN that has an intrinsic memory cell c_t^l and three gates.

- 1. Input gate i_t^l
- 2. Forget gate f_t^l
- 3. Output gate o_t^l

LSTM: Signal-Flow (1/2)

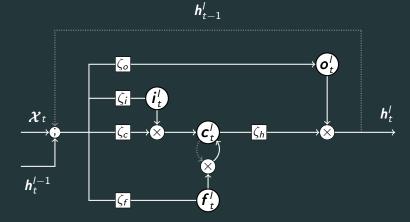
LSTM Unit (single layer)

- Input: $[X_t; h_{t-1}^l; h_t^{l-1}]$
- Output: h_t^I

LSTM: Signal-Flow (1/2)

LSTM Unit (single layer)

- Input: $[\boldsymbol{\chi}_t; \boldsymbol{h}_{t-1}^I; \boldsymbol{h}_t^{I-1}]$
- Output: **h**'_t



Controller: Signal-Flow (2/2)

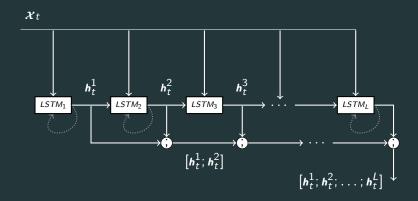
LSTM Network (multiple layers)

- Input: χ_t
- Output: $[\boldsymbol{h}_t^1; \boldsymbol{h}_t^2; \dots \boldsymbol{h}_t^L]$

Controller: Signal-Flow (2/2)

LSTM Network (multiple layers)

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



Controller: Outputs

$$(\mathbf{y}_t, \mathbf{\xi}_t) = \mathcal{N}([\mathbf{\chi}_1; \dots; \mathbf{\chi}_T]; \vartheta)$$

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User output
$$\boldsymbol{y}_t = W_y[\boldsymbol{h}_t^1; \dots; \boldsymbol{h}_t^L]$$

Controller: Outputs

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User output
$$\mathbf{y}_t = W_y[\mathbf{h}_t^1; \dots; \mathbf{h}_t^L]$$

Interface vector $\boldsymbol{\xi}_t = W_{\mathcal{E}}[\mathbf{h}_t^1; \dots; \mathbf{h}_t^L]$

- Read keys: $\mathbf{k}_{t}^{r,i}$
- Read strengths: $\beta_t^{r,i}$
- Write key: \mathbf{k}_t^w
- Write strength: β_t^w
- Erase vector: e_t

- Write vector: \mathbf{v}_t
- Free gates: ϕ_t^i
- Allocation gate: g_t^a
- Write gate: g_t^w
- Read modes: π_t^i

Memory Adressing: Content-Lookup

```
R read keys \mathbf{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 \mathbf{k}^w \in \mathbb{R}^W
Write strength \beta^w \in [1,\infty)
```

Memory Adressing: Content-Lookup

R read keys $\mathbf{k}^{r,i} \in \mathbb{R}^W, i = 1...R$ R read strengths $\beta^{r,i} \in [1,\infty), i = 1...R$ Write key $\mathbf{k}^w \in \mathbb{R}^W$ Write strength $\beta^w \in [1,\infty)$

Matching function $\mathcal D$ comparing memory contents

Memory Adressing: Content-Lookup

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

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Write key $\mathbf{k}^w \in \mathbb{R}^W$
Write strength $\beta^w \in [1,\infty)$

Matching function $\mathcal D$ comparing memory contents

Weighting function $\mathcal C$ normalizing and sharpening matches

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

Memory Adressing: R/W

Attention dictated by weightings $\mathbf{w} \in \mathcal{S}^N$ Erase vector $\mathbf{e}_t \in [0,1]^W$ Write vector $\mathbf{v}_t \in \mathbb{R}^W$

Read operations

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

Memory Adressing: R/W

Attention dictated by weightings $\mathbf{w} \in \mathcal{S}^N$

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Read operations

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

Write operations

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

Memory Adressing: Dynamic Allocation

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

"Free list" scheme

$$oldsymbol{\psi}_t = \prod_{i=1}^K (1 - oldsymbol{\phi}_t^i oldsymbol{w}_{t-1}^{r,i})$$
 (memory retention)

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

Memory Adressing: Dynamic Allocation

Free gates
$$\phi_t^i \in [0, 1]^W$$

Allocation gate $g_t^a \in [0, 1]$
Write gate $g_t^w \in [0, 1]$

"Free list" scheme

$$m{\psi}_t = \prod_{i=1}^R (\mathbf{1} - m{\phi}_t^i m{w}_{t-1}^{r,i})$$
 (memory retention) $u_t = (m{u}_{t-1} + m{w}_{t-1}^w - m{u}_{t-1} \circ m{w}_{t-1}^w) \circ m{\psi}_t$ (usage tracking)

Attention shift

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

Memory Adressing: Temporal Linking

Read modes: $\pi_t^i \in \mathcal{S}_3$

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Temporal Transition $L_t \in [0,1]^{N \times N}$

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

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Mode Interpolation

$$m{w}_t^{r,i} = \underbrace{m{\pi}_t^i[1]Lm{w}_t^{r,i}}_{ ext{Forward shift}} + \underbrace{m{\pi}_t^i[2]m{w}_t^{r,i}}_{ ext{No shift}} + \underbrace{m{\pi}_t^i[3]L^{ op}m{w}_t^{r,i}}_{ ext{Backward shift}}$$

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.

Takeaway

We can automatically infer simple functions over complex data structures in the form of probability distributions, just by using examples!

Thank you!

Questions?

Appendix: LSTM Equations

$$\begin{split} &\boldsymbol{i}_t^l = \sigma(W_i^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t-1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_i^l) & \text{(input gate)} \\ &\boldsymbol{f}_t^l = \sigma(W_f^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t-1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_f^l) & \text{(forget gate)} \\ &\boldsymbol{s}_t^l = \boldsymbol{f}_t^l \boldsymbol{s}_{t-1}^l + \boldsymbol{i}_t^l \tanh(W_s^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t_1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_s^l) & \text{(state)} \\ &\boldsymbol{o}_t^l = \sigma(W_o^l[\boldsymbol{\mathcal{X}}_t; \boldsymbol{h}_{t-1}^l; \boldsymbol{h}_t^{l-1}] + \boldsymbol{b}_o^l) & \text{(output gate)} \\ &\boldsymbol{h}_t^l = \boldsymbol{o}_t^l \tanh(\boldsymbol{s}_t^l) & \text{(hidden)} \\ &\boldsymbol{v}_t = W_y[\boldsymbol{h}_t^1; \dots; \boldsymbol{h}_t^l] & \text{(output vector)} \\ &\boldsymbol{\xi}_t = W_{\mathcal{E}}[\boldsymbol{h}_t^l; \dots; \boldsymbol{h}_t^l] & \text{(interface vector)} \end{split}$$

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)