DSCI 572: Supervised Learning II

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Intro. to RNNs

RNNs (Rumelhart et al., 1986)

- A family of networks **classically specializing in sequential data**
- Most RNNs **can handle sequences of variable length**
- RNNs have the **advantage of sharing parameters**
- **Parameter sharing**: each member of the output is a function of the previous members of the output.
- Each output member is **produced using the same update rule applied to the previous outputs**.

Parameters Sharing

- Advantage of parameter sharing: makes it possible to apply the model to examples of different forms (e.g., different lengths).
- Parameter sharing: **specifically important when a piece of information occurs at different positions in time**

Example

- "In Vancouver I live".
- "I live in Vancouver".

Comparison to Feedforward Net

- A fully connected **feedforward network** would have separate parameters for each input feature, **needing to learn all the rules of the language separately at each position**
- By comparison, a **recurrent neural network** shares the same weights across several time steps

RNNs: Computational Graphs With Cycles

- **Operate on sequences** of $x^{(t)}$ with the time step t ranging from 1 to τ.
- The **time step can be the position of an item in the sequence**.
- **Can also be applied backward**
- An extension of the idea of a computational graph, to include **cycles**
- Cycles **represent the influence of the present value of a variable on its own value at a future time step**

Unfolding Computational Graphs I

- Consider the **classical form of a dynamical system**, with a state $s^{(t)}$:

1: A Dynamical System

$$s^{(t)} = f(s^{(t-1)}; \theta).$$

- For example, unfolding 3 times would give:

$$s^{(3)} = f(s^{(2)}; \theta).$$

$$= f(f(s^{(1)}; \theta); \theta).$$

- The **equation is recurrent** because the definition of s at time t refers back to the same definition at time $t - 1$.

Unfolding Computational Graphs II

- By repeatedly unfolding, we acquire an expression that does not involve recurrence.
- Such an expression can now be expressed by a traditional directed acyclic graph.

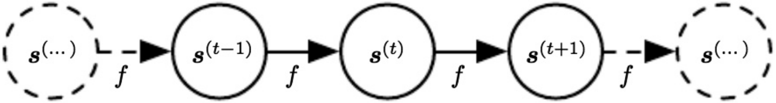


Figure: Each node represents the state at time t, and the function f maps the state at time t to the state at $t+1$. The same parameters are used for all time steps. [From Goodfellow et al., 2016]

RNNs as Computational Graphs

- Consider a dynamical system driven by an external signal $x^{(t)}$, where we observe the **state now contains information about the whole past sequence**:

2: Dynamical System With External Signal

$$s^{(t)} = f(s^{(t-1)}, x^{(t)}; \theta).$$

- Treating the **state as the hidden units** of the network:

3: Hidden State of RNN

$$h^{(t)} = f(h^{(t-1)}, x^{(t)}; \theta).$$

An RNN (Without Output)

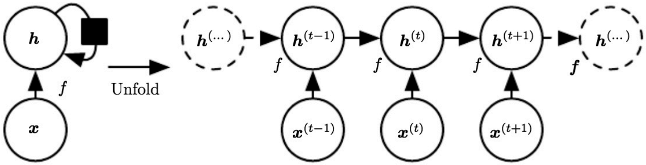


Figure: [From Goodfellow et al., 2016]

More on Unfolding

- **Unfolding** is the operation that maps a circuit as in the left side of the figure to a computational graph with repeated pieces as in the right side.
- The unfolded graph now has a **size** that depends on the sequence length.

RNNs as Generative Models

RNNs as Lossy Summarizers

- Typical RNNs would add **extra architectural features such as output layers** that read information from the state $\boldsymbol{h}$ to make predictions.
- Can be trained to **predict the future from the past** (e.g., predict the next word in a sequence).
- In these cases, the network typically learns to use $h^{(t)}$ as a kind of **lossy summary** of the task-relevant aspects of the past sequence of inputs up to t.
- Summary is necessarily **lossy**, since it maps an **arbitrary length sequence** $(x^{(t)}, x^{(t-1)}, x^{(t-2)}, \ldots, x^{(2)}, x^{(1)})$ to a **fixed length vector** $h^{(t)}$.

RNNs as Lossy Summarizers *Cont.*

Lossy Summarization Illustrated

- Summary might **selectively keep some aspects of the past sequence with more precision than other aspects**, depending on the training criterion
- Consider the case of statistical language modeling where the purpose is to **predict the next word**
- May not be necessary to keep all information up to time step t to predict next word
- Most demanding case is when we ask network to predict whole sequence (**auto-encoders**)

Unfolded Recurrence after t steps

- The unfolded recurrence after t steps can be represented with a function $g^{(t)}$:

4: A Function g

$$h^{(t)} = g^{(t)}(x^{(t)}, x^{(t-1)}, x^{(t-2)}, \ldots, x^{(2)}, x^{(1)}).$$
$$= f(h^{(t-1)}, x^{(t)}; \theta).$$

- The function g(t) takes the whole past sequence $(x^{(t)}, x^{(t-1)}, x^{(t-2)}, \ldots, x^{(2)}, x^{(1)})$ as input and produces the current state.
- The unfolded recurrent structure allows us to factorize $g^{(t)}$ into repeated application of a function f.

Learning a Single, Shared Model

- Two factors make it possible to learn a single model f that operates on `all time steps` and `all sequence lengths`:

Learning a Single Model

1. Regardless of the sequence length, the **learned model always has the same input size**. Why?
    - because it is specified in terms of transition from one state to another state, rather than specified in terms of a variable-length history of states.
2. It is possible to **use the same transition function f with the same parameters at every time step**.

Advantages of Learning a Single, Shared Model

- **Allows generalization** to sequence lengths that did not appear in the training set
- Allows the model to be **estimated with far fewer training examples** than would be required without parameter sharing.

Mapping input seq $\boldsymbol{x}$ to output seq $\boldsymbol{o}$

- Produce an **output at each time step**, with **recurrent connections between hidden units**

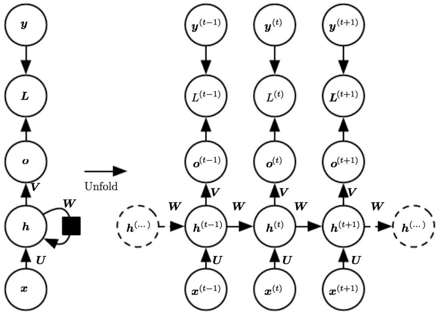


Figure: Three weight matrixes: **U**: input-to-hidden connections, **U**: hidden-to-hidden recurrent connections, **V**: hidden-to-output connections. Loss L compares how far each $\boldsymbol{o}$ is from its target $\boldsymbol{y}$. Loss internally computes $\hat{\mathbf{y}} = softmax(\mathbf{o})$ [From Goodfellow et al., 2016]

Mapping input seq $\boldsymbol{x}$ to output seq $\boldsymbol{o}$ *Cont.*

Notes on Previous Figure

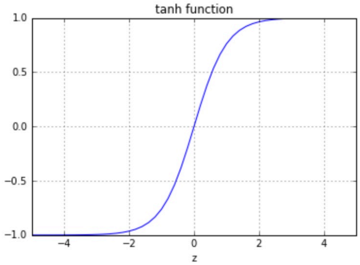
- Let's assume we will use a **hyperbolic tangent (tanh) as an activation function**.
- Figure **does not specify what form** the output and loss function take.
- Assume **output is discrete** (e.g., when the network predicts words or characters).
- Naturally, regard the output o as giving the **unnormalized log probabilities of each possible value of the discrete variable** (e.g., each word or character).
- **Apply the softmax** as a post-processing step to obtain a vector $\hat{y}$ of normalized probabilities over the output.

Hyperbolic Tangent Function I

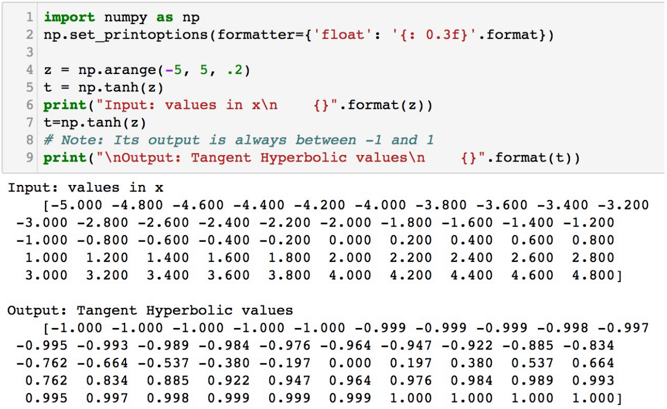
5: Hyperbolic Tangent

$$\tanh(z) = \frac{\sinh z}{\cosh z} = \frac{e^z - e^{-z}}{e^z + e^{-z}} = \frac{e^{2z} - 1}{e^{2z} + 1} = \frac{1 - e^{-2z}}{1 + e^{-2z}}$$

- Strongly neg inputs map to neg outputs; only zero-valued inputs map to near-zero outputs.



Hyperbolic Tangent Function II



```python
import numpy as np
np.set_printoptions(formatter={'float': '{: 0.3f}'.format})

z = np.arange(-5, 5, .2)
t = np.tanh(z)
print("Input: values in x\n    {}".format(z))
t=np.tanh(z)
# Note: Its output is always between -1 and 1
print("\nOutput: Tangent Hyperbolic values\n    {}".format(t))
```

```
Input: values in x
    [-5.000 -4.800 -4.600 -4.400 -4.200 -4.000 -3.800 -3.600 -3.400 -3.200
 -3.000 -2.800 -2.600 -2.400 -2.200 -2.000 -1.800 -1.600 -1.400 -1.200
 -1.000 -0.800 -0.600 -0.400 -0.200  0.000  0.200  0.400  0.600  0.800
  1.000  1.200  1.400  1.600  1.800  2.000  2.200  2.400  2.600  2.800
  3.000  3.200  3.400  3.600  3.800  4.000  4.200  4.400  4.600  4.800]

Output: Tangent Hyperbolic values
    [-1.000 -1.000 -1.000 -1.000 -1.000 -0.999 -0.999 -0.999 -0.998 -0.997
 -0.995 -0.993 -0.989 -0.984 -0.976 -0.964 -0.947 -0.922 -0.885 -0.834
 -0.762 -0.664 -0.537 -0.380 -0.197  0.000  0.197  0.380  0.537  0.664
  0.762  0.834  0.885  0.922  0.947  0.964  0.976  0.984  0.989  0.993
  0.995  0.997  0.998  0.999  0.999  0.999  1.000  1.000  1.000  1.000]
```

RNN Update Equations I

- **Forward propagation** begins with a specification of the initial state $h^{(0)}$. Then, for each time step from $t = 1$ to $t = \tau$, we apply the following update equations:

6: RNN Equations

$$\mathbf{a}^{(t)} = \mathbf{b} + \mathbf{W}\ \mathbf{h}^{(t)} + \mathbf{U}\ \mathbf{x}^{(t)}$$
$$\mathbf{h}^{(t)} = \tanh(\mathbf{a}^{(t)})$$
$$\mathbf{o}^{(t)} = \mathbf{c} + \mathbf{V}\ \mathbf{h}^{(t)}$$
$$\hat{\mathbf{y}}^{(t)} = softmax(\mathbf{o}^{(t)})$$

- where the parameters are the bias vectors **b** and **c** along with the weight matrices **U**, **V**, and **W**, respectively for input-to-hidden, hidden-to-output and hidden-to-hidden connections.

RNN Update Equations II

Mapping Sequences of Same Length

- This RNN **maps an input sequence to an output sequence of the same length**.
- The total loss for a given sequence of x values paired with a sequence of y values would then be just the **sum of the losses over all the time steps**.
- For example, if $L^{(t)}$ is the negative log-likelihood of $y^{(t)}$ given $x^{(1)}, \dots, x^{(t)}$, then: See next slide...

RNN Loss

7: RNN Loss

$$L = \left(x^{(1)}, \ldots, x^{(\tau)}, y^{(1)}, \ldots, y^{(\tau)}\right)$$

$$= \sum_t L^{(t)}$$

$$= -\sum_t \log p_{model}\left(y^{(t)} | x^{(1)}, \ldots, x^{(t)}\right)$$

Expensive Gradient

- Computing the gradients for the loss described earlier involves a forward pass and a backward pass, with a **costly runtime:** $O(\tau)$
- Cannot be parallelized due to sequential process: Each time step may be computed only after the previous one

Back-propagation Through Time (BPTT)

BPTT

- States computed during forward pass **must be stored until re-used** during the backward pass
- So, the **memory cost is also** $O(\tau)$
- The back-propagation algorithm applied to this unrolled graph with $O(\tau)$ is called **back-propagation Through Time (BPTT)**.
- To sum up, this network trained with recurrent connections between hidden units is **very powerful**, yet **expensive to train**.
- Are there other options? (Yes, as we will see. . .)