Sequence modeling

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Sequence modeling

Basic ideas
• Sequences of vectors, e.g. frames in an audio stream
• Learn about subsequences
Unfolding computational graphs

• Consider a function that relies on previous state: \( s^{(t)} = f(s^{(t-1)}|\theta) \)

• Next step:
  \[
  s^{(t+1)} = f(s^{(t)}|\theta) \\
  s^{(t+1)} = f(f(s^{(t-1)}|\theta)|\theta)
  \]

• We can think of this as a graph

Add an input

• \( s^{(t)} = f(s^{(t-1)}, x^{(t)}|\theta) \)

• \( s^{(t)} \) has past history of input

• Consider this occurring in a hidden unit:
  \( h^{(t)} = f(h^{(t-1)}, x^{(t)}|\theta) \)
Recursive neural networks (RNNs)

- Prior knowledge of $x^{(t)}$ tends to be lossy, as one usually does not need the entire history

RNNs

Examples of how RNNs can be used. In each case, we describe the output and its dependencies
1. Output for each input; depends on previous inputs
2. Output for each input; depends on last output
3. Single output for sequence

Recurrence in the hidden layers can result in Turing complete networks.
Notation

We are using compact network representation (chapter 6), networks can have breadth.

Case 1 example
one output/input, depends on previous inputs
Case 1 example contd.

discrete (e.g. categorical) outputs

one node/category
unnormalized log P(category|history)
For classification, can add a softmax
layer for normalized probabilities,
unnecessary for training

Loss(y,o) – Needed for training

Case 1 example contd.

Forward propagation

Initialize state $h^{(0)}$

For each time $t$

\[
\alpha^{(t)} = b + Wh^{(t-1)} + Ux^{(t)}
\]

\[
h^{(t)} = \tanh(\alpha^{(t)})
\]

\[
o^{(t)} = c + Vh^{(t)}
\]

\[
\hat{y}^{(t)} = \text{softmax}(o^{(t)}) \quad \text{(postprocessing step)}
\]
Loss of a sequence

- Sequence loss is sum of losses

\[ L(\{x^{(1)}, x^{(2)}, \ldots, x^{(r)}\}, \{y^{(1)}, y^{(2)}, \ldots, y^{(r)}\}) = \sum_t L^{(t)} \]

- Suppose we use a negative log likelihood loss (e.g. MLE approach), this becomes

\[ \sum_t L^{(t)} = -\sum_t \log P_{model}(y^{(t)} | x^{(1)}, x^{(2)}, \ldots, x^{(t)}) \]

Gradient of sequence

(overview)

- Forward pass – Compute gradient of each step
- Backward pass – Use stored states and gradients to back-propogate through time
- Expensive in time and space
Case 2
output depends on previous output

Case 3
labeling a sequence
More on output recurrences

- Dependence on solely the output is not Turing complete
- Loss function minimizes difference between target and output; nothing will drive it to capture information about network state

Output recurrences: Teacher forcing

When training for output recurrences, we could use a MLE approach to find the model which maximizes:

$$\log P(o^{(1)}, y^{(2)} | x^{(1)}, x^{(2)})$$

but we know what we want for $o^{(1)}$: $y^{(1)}$
Teacher forcing

If we use the previous label

\[ \log P(y^{(1)}, y^{(2)} | x^{(1)}, x^{(2)}) \]

we can parallelize the backpropagation as we don’t need to compute the previous dependency.

Teacher forcing

We can rewrite the MLE target (Bayes rule):

\[
\log P(y^{(1)}, y^{(2)} | x^{(1)}, x^{(2)}) = \log \left( P(y^{(2)} | y^{(1)}, x^{(1)}, x^{(2)}) P(y^{(1)} | x^{(1)}, x^{(2)}) \right) \\
= \log \left( P(y^{(2)} | y^{(1)}, x^{(2)}) P(y^{(1)} | x^{(1)}) \right) \\
= \log P(y^{(2)} | y^{(1)}, x^{(2)}) + \log P(y^{(1)} | x^{(1)})
\]

\[ \text{independent of } x^{(t)} \text{ where } t \neq \tau \]

since there are no hidden recurrences
Teacher forcing

Teacher forcing can be used in networks with output and hidden layer recurrences, but…

we can no longer parallelize training and must use back-propagation through time

RNN gradient computation

- Assume loss at time $t$: $\frac{\partial L}{\partial L(t)} = 1$
- Consider network of Fig. 10.5:

$$o^{(t)} = c + Vh^{(t)}$$
$$h^{(t)} = f(b + Ux^{(t)} + Wh^{(t-1)})$$
RNN gradient computation

• Assume \( o \) feeds softmax layer \( \hat{y} \)
• Use negative log likelihood loss function.
  – Our first use of this loss on a softmax layer
    (we usually use cross entropy)
  – Gradients computed recursively

\[
\frac{\partial L}{\partial o_i(t)} = \hat{y}_i \log(\hat{y}_i) - \log(1 \cdot \hat{y}_i)
\]

RNN gradient computation

• In general, the gradient is \( \frac{\partial L}{\partial o_i(t)} \)

• Consider the last step, time \( t \)
  – Define change of overall loss with respect to
    loss at time \( t \) as \( 1: \frac{\partial L}{\partial o_i(t)} = 1 \)
  – then

\[
\begin{align*}
(V_o, L) &= \frac{\partial L}{\partial o_i(t)} = \frac{\partial L}{\partial \hat{y}_i} \frac{\partial \hat{y}_i}{\partial o_i(t)} \\
&= \frac{\partial L}{\partial \hat{y}_i} (\log(\hat{y}_i) - \log(1 \cdot \hat{y}_i)) \\
&= \frac{\partial L}{\partial \hat{y}_i} \left( \log(\hat{y}_i) - \log(1 \cdot \hat{y}_i) \right) \\
&= \hat{y}_i \log(\hat{y}_i) - \log(1 \cdot \hat{y}_i)
\end{align*}
\]
RNN gradient computation

- Given the output gradient at time $\tau \nabla_{o(\tau)} L$, compute gradient of the hidden node
  \[ \nabla_{h(t)} L = V \nabla_{o(t)} L \]
- Previous time steps $t < \tau$ need to consider history
  \[ \nabla_{h(t)} L = \left( \frac{\partial h^{(t+1)}}{\partial h^{(t)}} \right)^T \nabla_{h^{(t+1)}} L + \left( \frac{\partial h^{(t)}}{\partial h^{(t)}} \right)^T \nabla_{h^{(t)}} L \]
  Further simplification depends on activation function derivative

Parameter updates

We need to learn how the loss should be applied to each of the parameters. General idea:

- Create copies of parameters at each time step (avoids introducing dependencies)
- Average over time

Example:
\[ \nabla_w L = \sum_t \sum_i \left( \frac{\partial L}{\partial h^{(t)}_i} \right) \nabla_{w^{(t)} h_i^{(t)}} \]
Marginal distributions

Integrate/sums over elements of a joint distribution to find $P$ of desired random variable

$$X, Y \sim P(X, Y)$$

$$P(X = x) = \int P(x, y) dy$$

$$P(Y = y) = \int P(x, y) dx$$

Graphical models

• Networks of nodes can be used for inference/belief, frequently on latent (unobservable) variables
• Weights inform relationships between nodes
• Allows us to think about probabilities by marginalizing what we don’t know

$$P(F \mid A, B) = \frac{\sum \sum \sum \sum \sum P(A, B, C, D, E, F)}{\sum \sum \sum \sum \sum P(A, B, C, D, E, F)}$$
RNNs as directed graphical models

- Simple case: RNN of a sequence where only recursion is previous output and there are no inputs

\[ P(y^{(1)}, \ldots, y^{(t)}) = \prod_{i=1}^{t} P(y^{(i)} | y^{(i-1)}, y^{(i-2)}, \ldots, y^{(0)}) \]  

by chain rule of \( P \)

- With a negative log likelihood loss,

\[ L = \sum_{t} L^{(t)} \]

\[ L^{(t)} = -\log P(y^{(i)} | y^{(i-1)}, y^{(i-2)}, \ldots, y^{(0)}) \]

RNNs as directed graphical models

- Graphical models with a long dependency require many edges

- These become difficult to estimate
RNNs as directed graphical models

Ways to deal with large # of parameters

• Remove weak dependencies

• Assume a Markov property, values more than $\tau$ time steps in the past no longer matter, e.g. $\tau = 2$:

$$P(y^{(t)} | y^{(t-1)}, \ldots, y^{(2)}, y^{(1)})$$

$$= P(y^{(t)} | y^{(t-1)}, y^{(t-2)})$$

---

RNNs as directed graphical models

• Introduce a state variable that captures the dependency

• Assumption: Relationship stationary, does not change over time
RNNs
as directed graphical models

Use as a sequence generator introduces a new problem: How to stop…
- Can introduce a stop symbol, or
- Train a node to predict end of sequence
- Train a node to predict sequence length

Sequences conditioned on context

- RNNs can serve as graphical models that depend on input & output history
- When the input sequence is of fixed size (usually not the case for speech) can provide
  - sequence as input to initial state
  - sequence as input at each time step
Bidirectional RNNs

- Sometimes, observing features in the future helps us know what occurred in the past…

\[ P(x^{(2)} = e | x^{(1)} = b) \]

vs.

\[ P(x^{(2)} = e | x^{(1)} = b, x^{(3)} = d) \]

- Very useful for speech recognition where coarticulation & phonotactics can play a large role
Bidirectional RNNs

- Compute two RNNs, one moving forward, the other backwards

- Avoids need for fixed length window required for feed-forward nets or RNNs with a look-ahead buffer
Recap so far

- Map sequence to fixed size vector
- Fixed vector to sequence
- N inputs to N outputs

What about this?

10 ms advance
M to N sequences

Many applications require sequences of length M to be mapped to sequences of length N, e.g.
- speech recognition
- language translation
- query handling

How can I get to Logan Heights?

M to N sequences

- Neural nets that handle this are known as sequence to sequence, or encoder-decoder architectures

- Basic idea:
  - Encoder RNN outputs a state or sequence representing the concept
  - Decoder RNN maps the concept onto another sequence
**M to N sequences**

Concept is typically final state or vector

Can use fixed vector to sequence architecture to generate new sequence

Deep recurrent networks

What happens when the recursions pass through multiple layers?

Layer $n$ (could be multiple layers) serves the role of building a representation to feed into the hidden state layer $h$
Deep recurrent networks

- If layer n is deep, this creates a long path between h and the information that loops back through it
- Long paths make learning difficult (more on this next)
- Can introduce a delay loop to assist

Long-term dependencies

- Recurrence involves computing the same function over and over
- Let us simplify to think about implications
  - Use identity function as activation function
  - Recurrence becomes $h^{(t)} = W^T h^{(t-1)}$
  - Unwinding the recursion $h^{(t)} = (W^t)^T h^{(0)}$
Long-term dependencies

• Suppose \( W \) has an eigenvalue decomposition (2.7)
  \[ W = Q\Lambda Q^T \]
  – \( Q \) is a matrix of eigenvectors, \( QQ^T = I \)
  – \( \Lambda \) is a diagonal matrix of eigenvalues

\[
\begin{align*}
\text{Long-term dependencies} \\
\text{h} &= (W^t)^T h^{(0)} \\
&= (Q^T \Lambda Q)^t h^{(0)} \quad \text{as} \quad W^T = (Q\Lambda Q^T)^T = Q^T\Lambda Q \\
&= Q^T \Lambda^t Q h^{(0)} \quad \text{as} \quad Q^T\Lambda Q Q^T\Lambda Q = Q^T\Lambda I\Lambda Q = Q^T\Lambda\Lambda Q \\
\end{align*}
\]

What happens if eigen values are
  – small?
  – large?
Long-term dependencies

- In a non-recurrent net, weights will vary, but in RNNs the same weights are used over and over again.

- Techniques must be applied to keep gradients from vanishing or exploding (see references in Goodfellow et al 10.7 for further details)

Long-term dependence strategies

Skip connections
- Create networks with longer delays
- Reduces number of times weight is applied
- Delay of $d$ reduces gradient vanishing by factor of $1/d$ (in our simplified example: $Q\Lambda^{t/d}Q^T h^{(0)}$)
- Problems if what was skipped was important
Long-term dependence strategies

- Gated RNNs
  - Long-term dependence problem due to using the same weights at each step
  - What if the weights were dynamic?
  - Dynamic weights allow us to respond to input

Long short term memory (LSTM)

- Popular gated architecture
- Weights are conditioned on context
- Can be interpreted as an attention mechanism
LSTM

LSTM adds one or more gates to control input and output as well as reset the state.

LSTM forward propagation

Forget gate

\[ f_i^{(t)} = \sigma \left( b_i^d + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right) \]
**LSTM forward propagation**

**external input gate**

\[ g_i^{(t)} = \sigma \left( b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right) \]

\[ s_i^{(t)} = f_i^{(t)} s_i^{(t-1)} + g_i^{(t)} \sigma \left( b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right) \]

Fig. 10.16 Goodfellow et al.
LSTM forward propagation

\[
h_i^{(t)} = \tanh(s_i^{(t)})d_i^{(t)}
\]

\[
q_i^{(t)} = \sigma \left( h_i^{(t)} + \sum_j U_{ij}x_i^{(t)} + \sum_j W_{ij}h_j^{(t-1)} \right)
\]