Gated Recurrent Models

Stephan Gouws & Richard Klein



Part 1: Intuition, Inference and Training

- Building intuitions: From Feedforward to Recurrent Models
- Inference in RNNs: Fprop
- Training in RNNs: Backpropagation-through-time (BPTT)

SHORT BREAK



Part 2: Gated models & Applications

- Long Short-term Memory (LSTMs)
- Gated Recurrent Units (GRUs)
- Applications:
 - Image captioning
 - Sequence classification (Practical 4: MNIST)
 - Language modeling
 - Sequence-labeling (lots of NLP tasks, e.g. POS tagging, NER, ...)
 - Sequence-to-sequence learning (Machine translation, Dialogue modeling, ...)

Recurrent Models

PART 1: Intuition, Inference and Training







We need to be able to <mark>remember</mark> information from previous time steps

Recurrent neural networks: Intuition



Long-term dependencies: Why do they matter?

Michel C. was born in Paris, France. He is married and has three children. He received a M.S. in neurosciences from the University Pierre & Marie Curie and the Ecole Normale Supérieure in 1987, and and then spent most of his career in Switzerland, at the Ecole Polytechnique de Lausanne. He specialized in child and adolescent psychiatry and his first field of research was severe mood disorders in adolescent, topic of his PhD in neurosciences (2002). **His mother tongue is** <u>?????</u>

















one to one



one to many Image

Captioning





We'll talk about this a little later. We'll also implement this in today's practical!

FFNs













FFNs



Image

Captioning

one to many



many to one



MNIST predictor



many to many





I-ORG I-PER I-LOC U.N. official Ekeus for Baghdad heads

0 0

0

many to many



Sequence labeling (e.g. NER)



Classify following examples:











But what if these were not digits, but longer numbers?



Problem? Variable length inputs.









The RNN Computation Graph



"Feedback loop" / state / memory / stack (previous time-step)







"Unrolled" over *n* time-steps.





class FeedForwardModel():

...

def forward(self, x):
 # Compute activations on the hidden Layer.

hidden_layer = self.act_fn(np.dot(self.W_xh, x) + b)

Compute the (linear) output layer activations.
y = np.dot(self.W_hy, hidden_layer)





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class RecurrentModel():

...

def recurrent_fn(self, x, prev_state):

Compute the new state based on the previous state and current input.

new_state = self.act_fn(np.dot(self.W_xh, x) + np.dot(self.W_hh, prev_state) + b)

Compute the output vector.

y = np.dot(self.W_hy, new_state)

return new_state, y





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Input at

current

time-step

class RecurrentModel():

 $y_t = W_{hy}h_t$

Recurrent

function

...

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New

state

Compute the output vector.
y = np.dot(self.W_hy, new_state)

return new_state, y



The RNN API



```
def forward(self, data_sequence, initial_state):
    state = initial_state
    all_states, all_ys = [state], []
    cache = []
```

```
for x, y in data_sequence:
    new_state, y_pred = recurrent_fn(x, state)
    loss += cross_entropy(y_pred, y)
```

```
cache.append((new_state, y_pred))
state = new_state
```

```
return loss, cache
```

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NOTATION: W_{xh} is a matrix that maps a vector x into a vector h.

$h = f_{\theta}(W_{xh}x + b)$



NOTATION: W_{xh} is a matrix that maps a vector x into a vector h.

<mark>Math: FFNs v RNNs</mark>

$$h = f_{\theta}(W_{xh}x + b)$$

Input



NOTATION: W_{xh} is a matrix that maps a vector x into a vector h.

 $h = f_{\theta}(W_{xh}x + b)$

Activation function

Input



Hidden layer

$$h = f_{\theta}(W_{xh}x + b)$$

Activation function

Input

NOTATION: W_{xh} is a matrix that maps a vector x into a vector h.



Hidden layer

$$\begin{split} h &= \int_{\theta} (W_{xh} x + b) \\ \text{Activation} & \text{Input} \end{split}$$

$$\begin{split} h_t &= \int_{\theta} (W_{xh} x_t + b) \\ \text{Input} & \text{Input} \end{cases}$$

$$\end{split}$$

$$\begin{split} h_t &= \int_{\theta} (W_{xh} x_t - b) \\ \text{New state} & \text{Input at current} \\ \end{split}$$

time-step

. . .

NOTATION: W_{xh} is a matrix that maps a vector x into a vector h.







Inference & Training

- How do we make predictions using RNNs?
 - Forward propagation: "Fprop"
 - Essentially a composition of functions: $a_2 = f_2(f_1(x))$.
 - We "unroll" the computational graph over time-steps.
- How do we train RNNs?
 - Backward propagation: "Backprop-through time"
 - We need to consider predictions over several time-steps!
 - Credit assignment over time.
 - We work backwards in time from the last state to the first.

Training: Ways to Train RNNs

- Echo State Networks: Initialize W_{xh} , W_{hh} , W_{ho} , carefully, then only train W_{ho} !
- **Backpropagation through time (BPTT)**: Propagate errors backwards through the unrolled graph.
- There are other options.



- Simple solution: don't train the recurrent weights $(W_{hh} \otimes W_{xh})!$
- Initialization very important.
- Super simple. However, with recent improvements in initialization etc, BPTT does better!



[Scholarpedia]

Inference & Training

- y_{1} y_{2} y_{n} y_{n
- How do we make predictions using RN
 - Forward propagation: "Fprop"
 - Essentially a composition of functions: $a_2 = f_2(f_1(x))$.
 - We "unroll" the computational graph over time-steps.
- How do we train RNNs?
 - Propagate errors backwards through unrolled graph: "Backprop-through time" (BPTT).
 - We need to consider predictions over several time-steps!
 - Credit assignment over time.
 - \circ ~ We work backwards in time from the last state to the first.

Training: BPTT Intuition



Training: Truncated BPTT



Run forward and backward through chunks of the sequence instead of whole sequence

Training: **Truncated** BPTT



Carry hidden states forward in time forever, but only backpropagate for some smaller number of steps







<u>Step 1</u>: Compute all errors.

Unrolling the RNN Computation Graph



<u>Step 1</u>: Compute all errors. <u>Step 2</u>: Pass error back for each time-step from n back to 1.



<u>Step 1</u>: Compute all errors. <u>Step 2</u>: Pass error back for each time-step from n back to 1. <u>Step 3</u>: Update weights.



Unrolling the RNN Computation Graph













θ











$$\begin{split} \frac{\partial E_{t}}{\partial \theta} &= \sum_{t'=1}^{t} \frac{\partial E_{t}}{\partial h_{t}} \frac{\partial h_{t}}{\partial h_{t'}} \frac{\partial h_{t'}}{\partial \theta} \\ & \text{where} \\ \frac{\partial h_{t}}{\partial h_{t'}} &= \Pi_{k=t'+1}^{t} \frac{\partial h_{k}}{\partial h_{k-1}} \end{split}$$
Unrolling the RNN Computation Graph



Training: Truncated BPTT Code

```
def bptt(modeL, X_train, y_train, initial_state):
    # Forward
    Loss, caches = forward(X_train, y_train, model, initial_state)
    avg_loss /= y_train.shape[0]
    # Backward
    dh_next = np.zeros((1, last_state.shape[0]))
    grads = {k: np.zeros_like(v) for k, v in model.items()}
```

```
for t in reversed(range(len(X_train))):
    grad, dh_next = cell_fn_backward(ys[t], y_train[t], dh_next, caches[t])
    for k in grads.keys():
        grads[k] += grad[k]
```



"Lego block"!

return grads, avg_loss

Training: Truncated BPTT Code

```
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for k in grads.keys():
    grads[k] += grad[k]
```

return grads, avg_loss



"Lego block"!

Total gradient = Sum of these lego-gradients over time!

```
\frac{\partial E_{TOTAL}}{\partial \theta} = \frac{\partial \sum_{t} E_{t}}{\partial \theta}= \sum_{t} \frac{\partial E_{t}}{\partial \theta}
```



$$h_{t} = \tanh(W_{hh}h_{t-1} + W_{xh}x_{t})$$
$$= \tanh\left(\left(W_{hh} \quad W_{hx}\right) \begin{pmatrix}h_{t-1}\\x_{t}\end{pmatrix}\right)$$
$$= \tanh\left(W\begin{pmatrix}h_{t-1}\\x_{t}\end{pmatrix}\right)$$

Backpropagation from h_t to h_{t-1} multiplies by W (actually W_{hh}^{T})



$$h_{t} = \tanh(W_{hh}h_{t-1} + W_{xh}x_{t})$$
$$= \tanh\left(\begin{pmatrix}W_{hh} & W_{hx}\end{pmatrix}\begin{pmatrix}h_{t-1}\\x_{t}\end{pmatrix}\right)$$
$$= \tanh\left(W\begin{pmatrix}h_{t-1}\\x_{t}\end{pmatrix}\right)$$



Computing gradient of h₀ involves many factors of W (and repeated tanh)



Computing gradient of h₀ involves many factors of W (and repeated tanh) Largest singular value > 1: **Exploding gradients**

Largest singular value < 1: **Vanishing gradients**



Computing gradient of h₀ involves many factors of W (and repeated tanh) Largest singular value > 1: Exploding gradients

Largest singular value < 1: Vanishing gradients **Gradient clipping**: Scale gradient if its norm is too big

grad_norm = np.sum(grad * grad)
if grad_norm > threshold:
 grad *= (threshold / grad_norm)



Computing gradient of h₀ involves many factors of W (and repeated tanh) Largest singular value > 1: Exploding gradients

Largest singular value < 1: Vanishing gradients

Gated Recurrent Models

PART II: Gated Architectures & Applications





Implementing a memory cell in a neural network

To preserve information for a long time in the activities of an RNN, we use a circuit that implements an analog memory cell.

- A linear unit that has a self-link with a weight of 1 will maintain its state.
- Information is stored in the cell by activating its write gate.
- Information is retrieved by activating the read gate.
- We can backpropagate through this circuit because logistics are have nice derivatives.



Propagating through a memory cell



Backpropagating through a memory cell?







σ





σ





σ







σ







Element-wise operations tanh



σ





Element-wise operations tanh







Gated Recurrent Units (GRUs)

X,

GRU

VH⁺

►H₊

 H_{t-1}

$$GRV = Gated X = X_t | H_{t-1} P+n$$

$$Recurrent Unit$$

$$X' = X_t | r * H_{t-1}$$
 p+n

$$X'' = tanh(X'.W_c + b_c) \qquad "$$

Ht = (1-z) * Ht-1 + z * X'' "

$$Y_t = softmax(H_t.W + b)$$
 m

Gated Recurrent Units (GRUs)

$$GRU = Gated X = X_t | H_{t-1} P+n$$

$$Recurrent Unit$$

$$z_{gates instead} = \sigma(X.W_z + b_z)$$

$$r = \sigma(X.W_r + b_r)$$

$$n$$

$$X' = X_t | r * H_{t-1}$$
 ρ_{+n}

$$X'' = tanh(X'.W_{c} + b_{c}) \qquad n$$

Ht = (1-z) * Ht-1 + z * X'' n

$$Y_t = softmax(H_t.W + b)$$
 m



Long Short-term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]



Backpropagation from c_t to c_{t-1} only elementwise multiplication by f, no matrix multiply by W

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$

$$h_t = o \odot \tanh(c_t)$$

Long Short-term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]

Uninterrupted gradient flow!



Applications/Tasks

- Image captioning
- Sequence classification (Practical 4: MNIST)
- Language modeling
- Sequence-labeling (lots of NLP tasks, e.g. POS tagging, NER, ...)
- Sequence-to-sequence learning (Machine translation, Summarization, ...)



One-to-Many: Image captioning

GOAL: Given image, generate a sentence to describe its content.



One-to-Many: Image captioning



GOAL: Given image, generate a sentence to describe its content.



"man in black shirt is playing guitar."



"construction worker in orange safety vest is working on road."



"two young girls are playing with lego toy."



"boy is doing backflip on wakeboard."

Many-to-one: Sequence Classifier (Prac 4)

GOAL: Given a sequence of inputs, predict the label for the whole sequence.

Examples:

- Given a sentence, say if it is **{negative, neutral, positive}**
- Given the words in an email, predict if it is a **spam message**.
- Given "pieces" of an image, predict **what number** is in the image.
Many-to-1: Polarity/Sentiment Classifer

We feed all the words into the model one at a time, and make one prediction at the end:



Pos/Neg?

Many-to-1: Spam Classifer



Many-to-1: Image Classifier (Prac 4)

We chop up the image and feed all the pieces through the model, and then make one prediction at the end:



y_{imag}

е

Next-token Prediction: Language modeling



Next-token Prediction: Language modeling



- Mapping each input $x_1, x_2, ..., x_n$ to its own label $y_1, y_2, ..., y_n$
- (Notice: Same length m; each input has an output.)
- A lot of NLP Tasks fall in this category, e.g.:
 - **Part-of-speech tagging**: map words to their parts-of-speech (noun, verb, etc).
 - **Named-entity Recognition**: identify mentions of people, places, etc in text
 - Semantic Role Labeling: find the main actions, and who performs them on whom/what

• Part-of-speech tagging



• Part-of-speech tagging



Heat water in a large vessel.



- Mapping input sequences $\{x_1, x_2, ..., x_m\}$ to output sequences $\{y_1, y_2, ..., y_n\}$.
- Note: Arbitrary m and n.
- Many applications, most notably Machine Translation.
- Also: POS tagging, Parsing, Summarization, Dialog

MACHINE TRANSLATION



Prompt: You can't eat pasta every day. You can't live only on Italian food.

System: I don't eat Italian food, but I do eat a lot of Italian food.

Prompt: What do you have planned tonight?

Baseline: I have no idea what I want to do with my life. I have no idea what I want to (Bad, Mediocre, Bad)

Ours: I was planning on doing a few of these, but I'm not sure what to choose. I need to find a place to camp, and I don't have a lot of time to make a plan. (Excellent, Good, Mediocre)

Prompt: Have you seen *Suicide Squad*?

Baseline: I have not, but I will check it out. (Good, Good, Good)

Ours: I saw it in a theater once and it was great. It was very... I don't know, a little dark. I like the psychological effects and the way it portrays the characters in the movie. (Excellent, Excellent, Excellent)

Key take-aways

- RNNs have memory/state that evolve over time.
- We unroll the graph over time to do forward propagation.
- Backprop-through-time (BPTT):
 - Perform Chain Rule over the unrolled graph efficiently by saving and reusing previous computations.
 - dE/dW is sum over all time-steps (b/c of tied weights)
- Vanishing/exploding gradients
- Gated architectures
 - State is *selectively* overwritten per time-step
 - Uninterrupted gradient flow through time: no vanishing/exploding gradients!
- Lots of cool applications!



Thank-you to the following resources, from which some of these slides were drawn and adapted.

- <u>Stanford CS231n</u>
- <u>TensorFlow without a PhD</u>

The end.