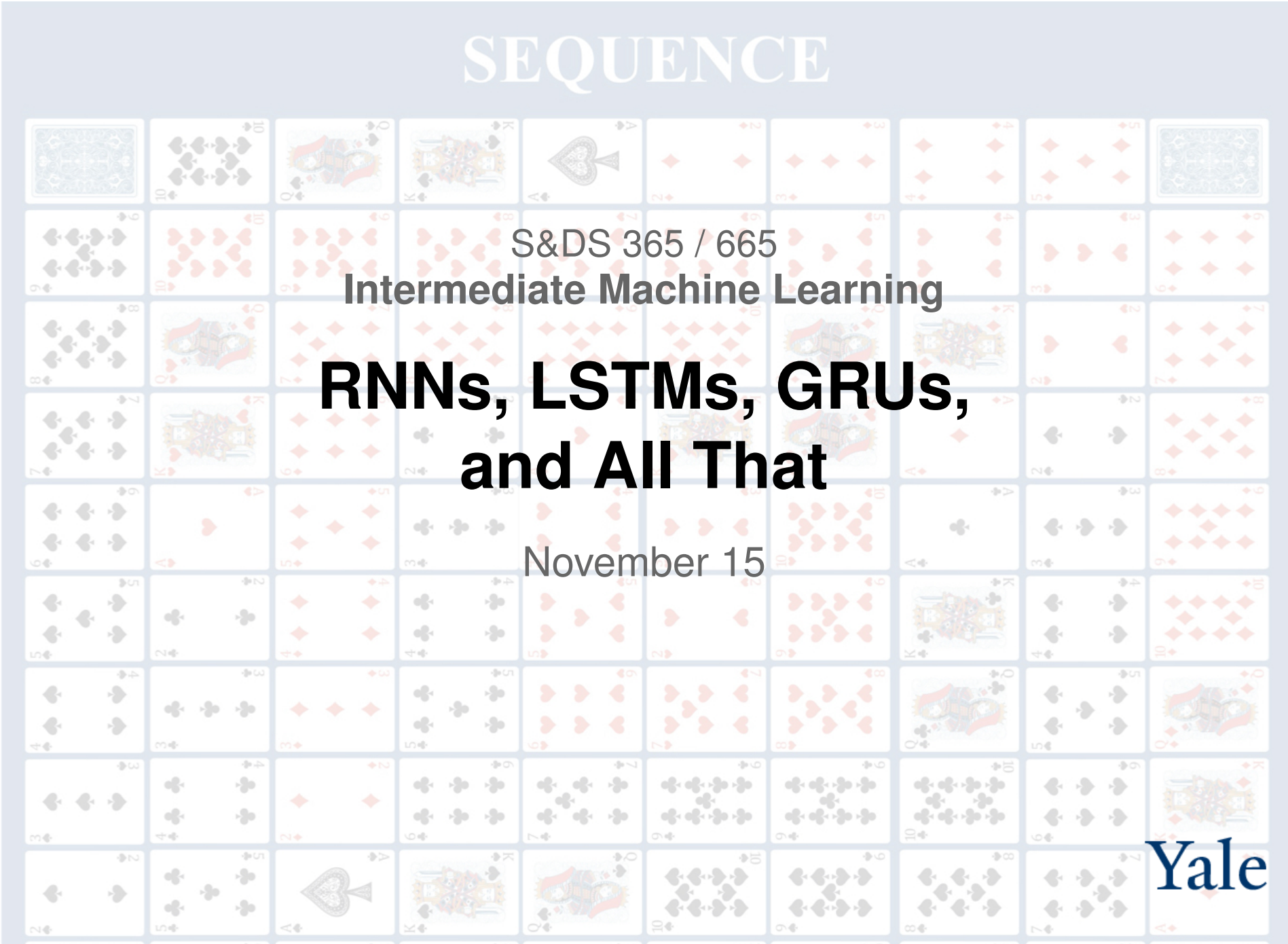


S&DS 365 / 665

Intermediate Machine Learning

RNNs, LSTMs, GRUs, and All That

November 15

Yale

Home stretch!

- Assignment 4 due tonight
- Assignment 5 (last!) posted today
  - Policy iteration
  - GRUs (today's topic)
- Quiz 5 (last!) November 30

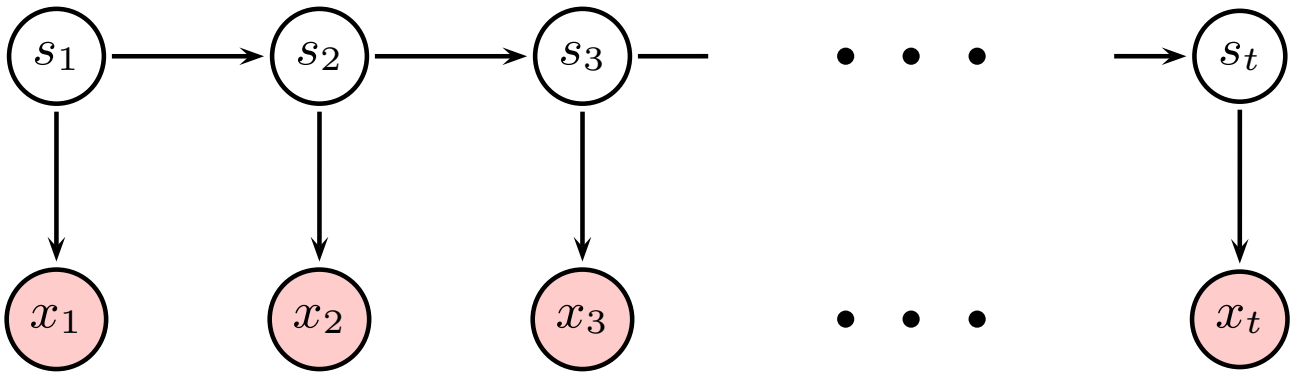
Recall: Hidden Markov Model

In an HMM, the next word is generated from a latent variable

- State is chosen stochastically (that is, probabilistically)
- Introduces dependence on earlier words that are further back than the previous time (non-Markov on observations)

Hidden Markov Model

The graphical model looks like this:



Here x_t is observable (word) at time t and s_t is unobserved state.

Hidden Markov Model

Probability of word sequence:

$$p(x_1, \ldots, x_n) = \sum_{s_1,\ldots,s_n} \prod_{t=1}^{n} p(s_t \mid s_{t-1}) p(x_t \mid s_t)$$

Hidden Markov Model

Probability of word sequence:

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Probability of the next word:

$$p(x_t \mid x_1, \ldots, x_{t-1}) = \sum_{s_t} p(s_t \mid x_1, \ldots, x_{t-1})\, p(x_t \mid s_t)$$

This is efficiently computed using dynamic programming

Hidden Markov Model

- Next word x_t is predicted from the state s_t
- State is a summary of information from the past $x_1, \ldots, x_{t-1}$
- State evolves stochastically

Hidden Markov Models: Estimation

The usual algorithms for estimating the parameters are iterative:

- Use the forward-backward algorithm to compute the probability that the outputs are generated from each state
- Treat the data as labeled, with these weights, and compute the relative frequencies
- Repeat
- Maximum likelihood (or MAP) estimation

This is called the EM algorithm; “Expectation-Maximization”

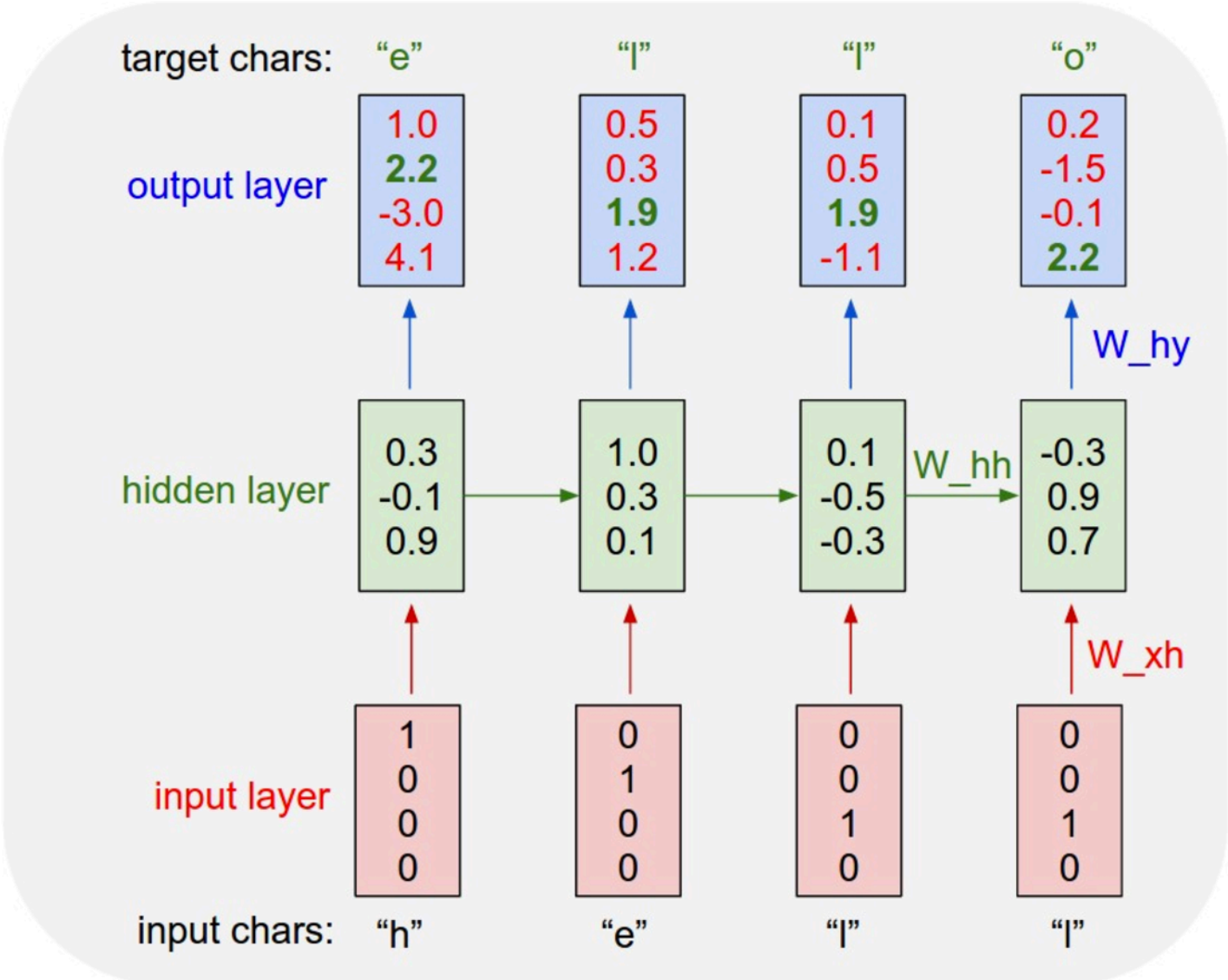
Recurrent neural networks

- Can be thought of as a type of language model
- Similar to hidden Markov models, but the *state evolves deterministically*, not stochastically
- HMMs are mixture models; RNNs are not
- The state is distributed, not categorical as for HMMs
- We'll describe this using characters rather than words — could do either

---

Kalman filters also have distributed state, but use linear models

RNNs http://karpathy.github.io/2015/05/21/rnn-effectiveness/



RNNs

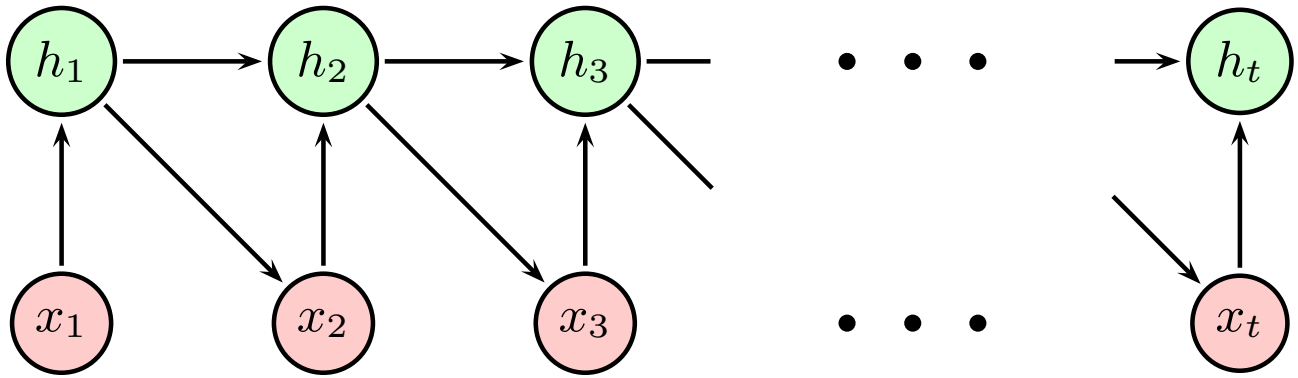
This means

$$
\begin{aligned}
h_t &= \tanh\left(W_{hh} h_{t-1} + W_{xh} x_t + b_h\right) \\
y_t &= W_{hy} h_t \\
x_{t+1} \mid y_t &\sim \text{Multinomial}(\pi(y_t))
\end{aligned}
$$

where $\pi(\cdot)$ is the soft-max function.

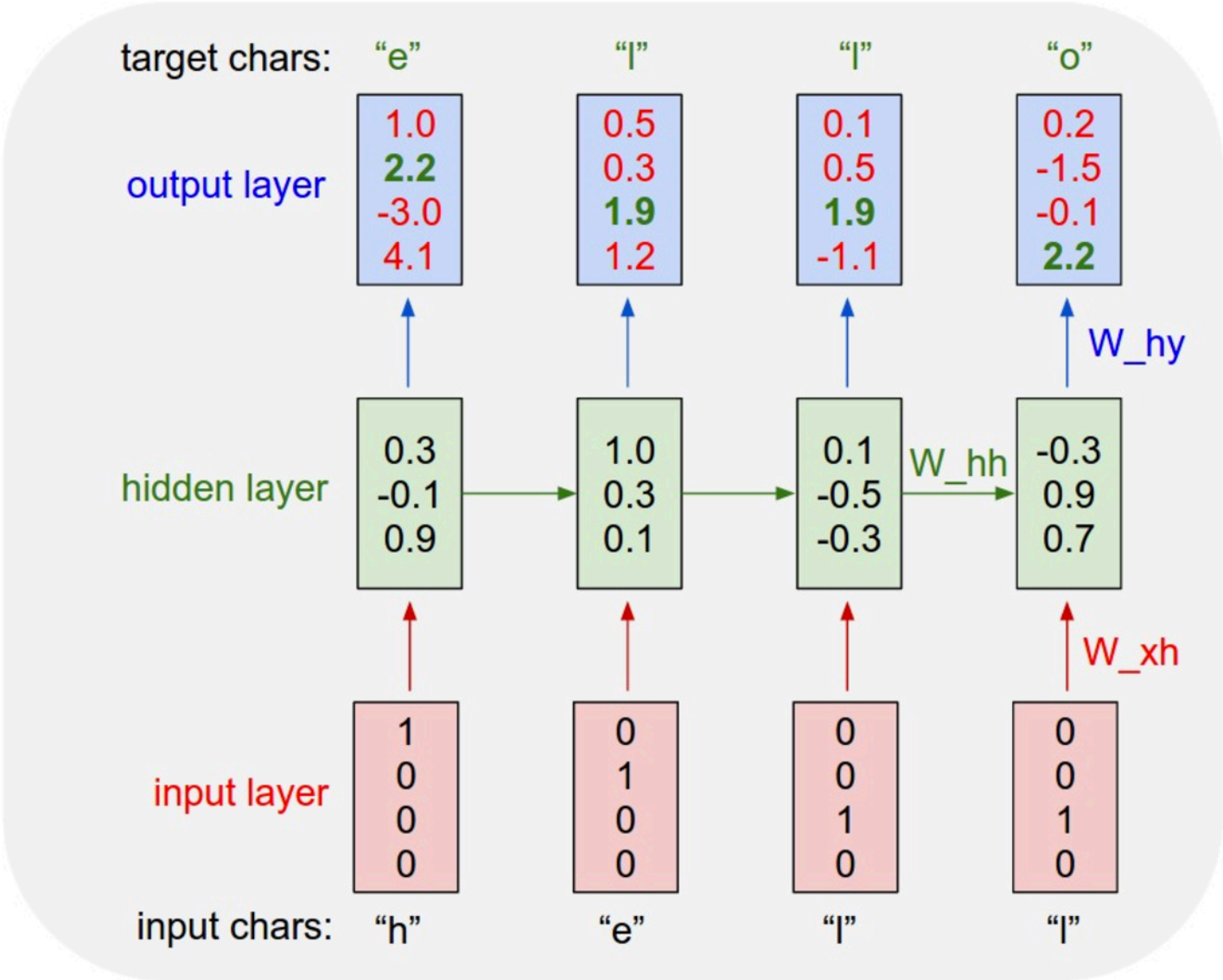
In this illustration, x_t is the "1-hot" representation of a character, $W_{xh} \in \mathbb{R}^{3\times 4}$, $W_{hh} \in \mathbb{R}^{3\times 3}$ and $W_{hy} \in \mathbb{R}^{4\times 3}$.

RNN graphical structure



We shade the states because they are deterministic, not latent

RNN architecture



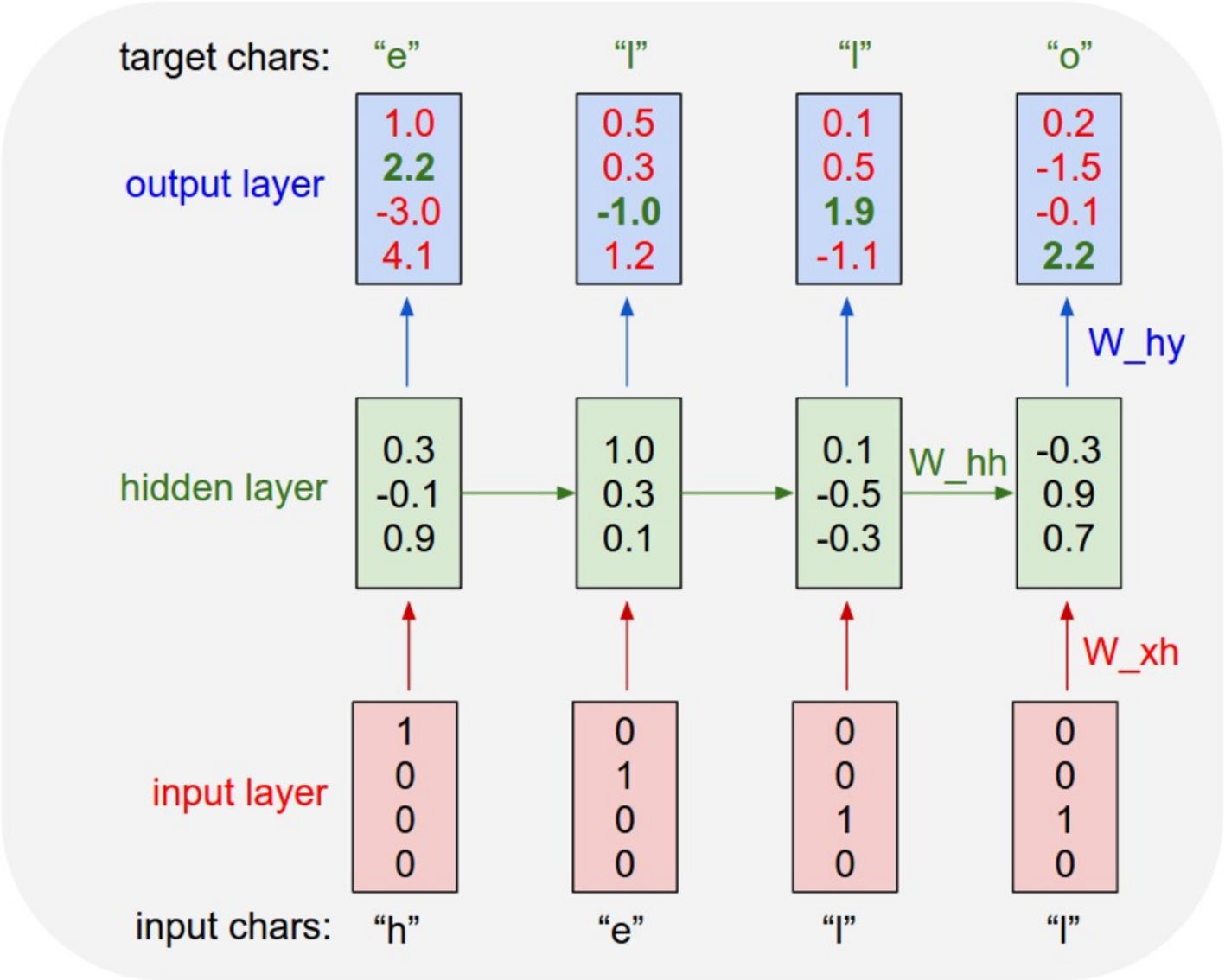
RNN Python Code

```
class RNN:
  # ...
  def step(self, x):
    # update the hidden state
    self.h = np.tanh(np.dot(self.W_hh, self.h) + np.dot(self.W_xh, x))
    # compute the output vector
    y = np.dot(self.W_hy, self.h)
    return y
```

One hidden layer:

```
rnn = RNN()
y = rnn.step(x) # x is an input vector, y is the RNN's output vector
```

One hidden layer



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    # compute the output vector
    y = np.dot(self.W_hy, self.h)
    return y
```

Two hidden layers:

```
y1 = rnn1.step(x)
y = rnn2.step(y1)
```

Hallucinated Shakespeare

```
PANDARUS:
Alas, I think he shall be come approached and the day
When little srain would be attain'd into being never fed,
And who is but a chain and subjects of his death,
I should not sleep.

Second Senator:
They are away this miseries, produced upon my soul,
Breaking and strongly should be buried, when I perish
The earth and thoughts of many states.

DUKE VINCENTIO:
Well, your wit is in the care of side and that.

Second Lord:
They would be ruled after this chamber, and
my fair nues begun out of the fact, to be conveyed,
Whose noble souls I'll have the heart of the wars.

Clown:
Come, sir, I will make did behold your worship.

VIOLA:
I'll drink it.
```

Interpreting RNNs

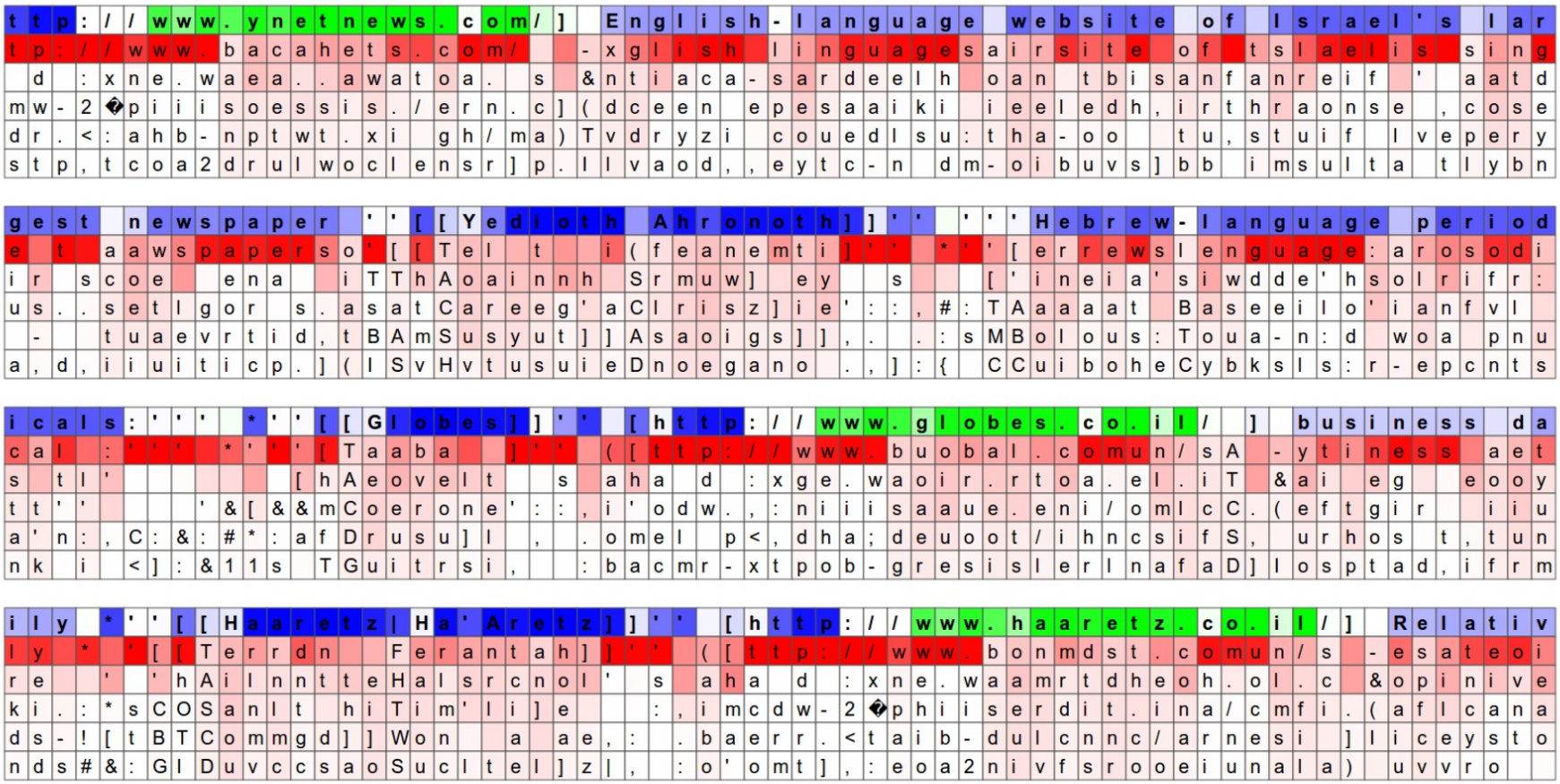
Each component is a tanh-thresholded linear function of the previous states and current input—a “neuron”

If the jth neuron h_{tj} is close to ± 1 then it is very “excited.” This is colored green in the following illustration. If it is near zero, then it is “not excited” or cool—this is colored blue.

Below the neuron color, the five most probable characters c are shown — ordered in decreasing order of y_{tc} and hence $\pi(y_t)_c$.

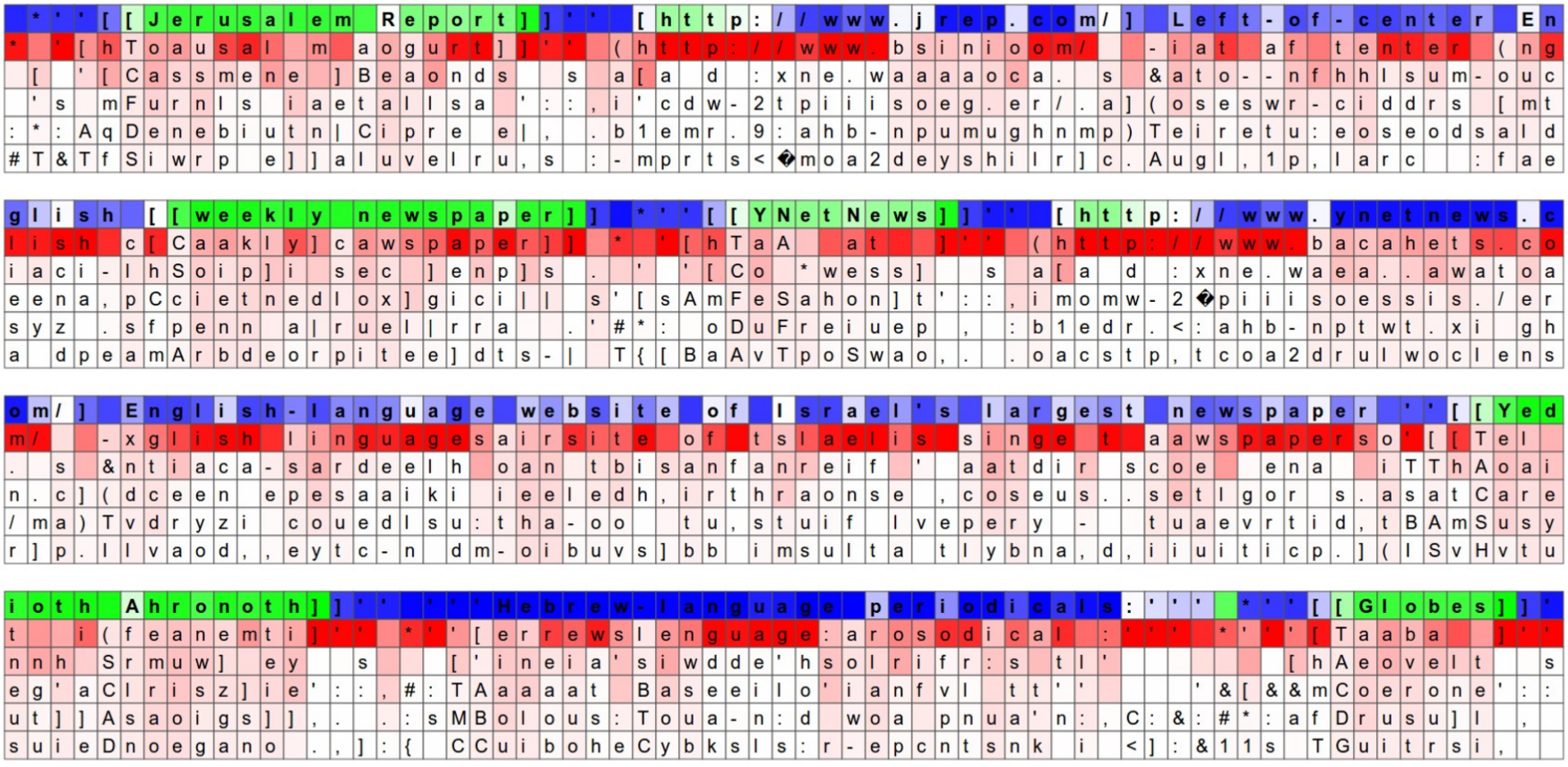
Three layers, with 512 neurons on each level. Most will be completely uninterpretable. Recall—it’s generally even hard to interpret coefficients in a least squares linear regression model!

Interpretation



The neuron highlighted in this image seems to get very excited about URLs and turns off outside of the URLs. The LSTM is likely using this neuron to remember if it is inside a URL or not.

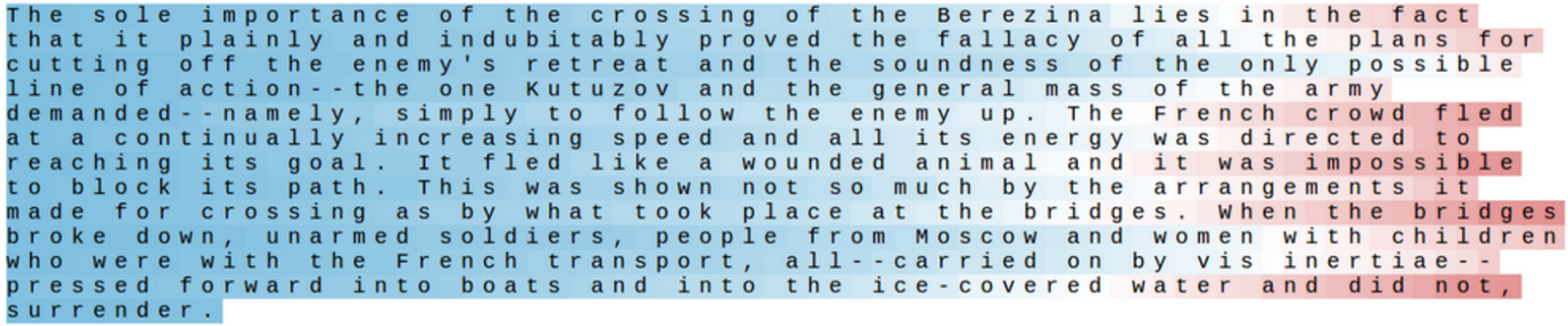
Interpretation



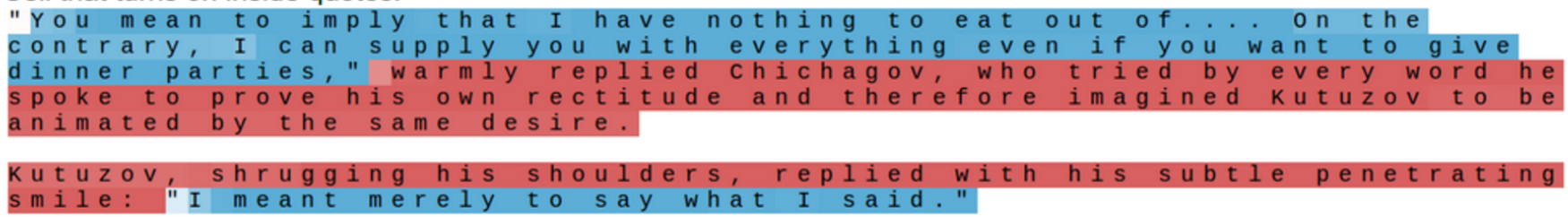
The highlighted neuron here gets very excited when the RNN is inside the [[ ]] markdown environment and turns off outside of it. Interestingly, the neuron can't turn on right after it sees the character "[", it must wait for the second "[" and then activate. This task of counting whether the model has seen one or two "[" is likely done with a different neuron.

Interpretation

Cell sensitive to position in line:



Cell that turns on inside quotes:



Cell that robustly activates inside if statements:

```
static int __dequeue_signal(struct sigpending *pending, sigset_t *mask,
        siginfo_t *info)
{
  int sig = next_signal(pending, mask);
  if (sig) {
    if (current->notifier) {
      if (sigismember(current->notifier_mask, sig)) {
        if (!(current->notifier)(current->notifier_data)) {
          clear_thread_flag(TIF_SIGPENDING);
          return 0;
        }
      }
    }
    collect_signal(sig, pending, info);
  }
  return sig;
}
```

rnn-demo.ipynb: numpy version

We'll train an "np-complete" RNN on the complete works of William Shakespeare, downloaded from Project Gutenberg (specifically, this link).

This uses a simple, direct implementation of backpropagation for RNNs, paralleling what we did for simple feedforward networks.

In [ ]:

```
def lossFun(inputs, targets, hprev):
  """
  inputs,targets are both list of integers.
  hprev is Hx1 array of initial hidden state
  returns the loss, gradients on model parameters, and last hidden state
  """
  xs, hs, ys, ps = {}, {}, {}, {}
  hs[-1] = np.copy(hprev)
  loss = 0

  # forward pass
  for t in range(len(inputs)):
    xs[t] = np.zeros((vocab_size,1)) # encode in 1-of-k representation
    xs[t][inputs[t]] = 1
    hs[t] = np.tanh(np.dot(Wxh, xs[t]) + np.dot(Whh, hs[t-1]) + bh) # hidden state
    ys[t] = np.dot(Why, hs[t]) + by # unnormalized log probabilities for next chars
    ps[t] = np.exp(ys[t]) / np.sum(np.exp(ys[t])) # probabilities for next chars
    loss += -np.log(ps[t][targets[t],0]) # softmax (cross-entropy loss)

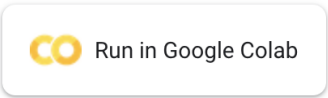
  # backward pass: compute gradients going backwards
  dWxh, dWhh, dWhy = np.zeros_like(Wxh), np.zeros_like(Whh), np.zeros_like(Why)
  dbh, dby = np.zeros_like(bh), np.zeros_like(by)
  dhnext = np.zeros_like(hs[0])
  for t in reversed(range(len(inputs))):
    dy = np.copy(ps[t])
    dy[targets[t]] -= 1 # backprop into y. see http://cs231n.github.io/neural-networks-case-stu
    dWhy += np.dot(dy, hs[t].T)
    dby += dy
    dh = np.dot(Why.T, dy) + dhnext # backprop into h
    dhraw = (1 - hs[t] * hs[t]) * dh # backprop through tanh nonlinearity
    dbh += dhraw
    dWxh += np.dot(dhraw, xs[t].T)
    dWhh += np.dot(dhraw, hs[t-1].T)
    dhnext = np.dot(Whh.T, dhraw)

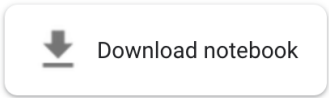
  for dparam in [dWxh, dWhh, dWhy, dbh, dby]:
    np.clip(dparam, -5, 5, out=dparam) # clip to mitigate exploding gradients

  return loss, dWxh, dWhh, dWhy, dbh, dby, hs[len(inputs)-1]
```

Tensorflow implementation

Text generation with an RNN





This tutorial demonstrates how to generate text using a character-based RNN. You will work with a dataset of Shakespeare's writing from Andrej Karpathy's The Unreasonable Effectiveness of Recurrent Neural Networks. Given a sequence of characters from this data ("Shakespear"), train a model to predict the next character in the sequence ("e"). Longer sequences of text can be generated by calling the model repeatedly.

Note: Enable GPU acceleration to execute this notebook faster. In Colab: *Runtime > Change runtime type > Hardware accelerator > GPU*. If running locally make sure TensorFlow version >= 1.11.

This tutorial includes runnable code implemented using tf.keras and eager execution. The following is sample output when the model in this tutorial trained for 30 epochs, and started with the string "Q":

```
QUEENE:
I had thought thou hadst a Roman; for the oracle,
Thus by All bids the man against the word,
Which are so weak of care, by old care done;
Your children were in your holy love,
And the precipitation through the bleeding throne.

BISHOP OF ELY:
Marry, and will, my lord, to weep in such a one were prettiest;
Yet now I was adopted heir
Of the world's lamentable day,
To watch the next way with his father with his face?

ESCALUS:
The cause why then we are all resolved more sons.
```

Memory circuits

A variant called “Long Short-Term Memory” RNNs has a special hidden later that “includes” or “forgets” information from the past.

Intuition: In language modeling, may be useful to remember/forget gender or number of subject so that personal pronouns (“he” vs. ”she” vs. ”they”) can be used appropriately.

Useful for things like matching parentheses, etc.

A simpler alternative to the LSTM circuit is called the *Gated Recurrent Unit* (GRU)

“Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation”, Cho et al. 2014
https://arxiv.org/pdf/1406.1078v3.pdf

Vanilla RNNs

In principle the state h_t can carry information from far in the past.

In practice, the gradients vanish (or explode) so this doesn't really happen

We need other mechanisms to "remember" information from far away and use it to predict future words

Vanilla RNNs

State is updated according to

$$h_t = \tanh\left(W_{hh}h_{t-1} + W_{hx}x_t + b_h\right)$$

We'll modify this with two types of "neural circuits" for storing information to be used downstream

LSTMs and GRUs

Both LSTMs and GRUs have longer-range dependencies than vanilla RNNs.

We'll go through this in detail for GRUs, which are simpler, more efficient, and more commonly used.

(And this is what you'll use on Assignment 5!)

Hadamard product

We'll need to use pointwise products. This is given the fancy name "Hadamard product" and written $\odot$:

$$\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \odot \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} = \begin{pmatrix} 4 \\ 10 \\ 18 \end{pmatrix}$$

Nothing more than the `numpy` $\star$ operation.

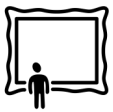
Hadamard product

We'll need to use pointwise products. This is given the fancy name "Hadamard product" and written $\odot$:

$$\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \odot \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 0 \\ 4 \end{pmatrix}$$

Nothing more than the `numpy` $\star$ operation.

Gated recurrent units (GRUs)



High level idea:

- Learn when to update hidden state to “remember” important pieces of information
- Keep them in memory until they are used
- Reset or “forget” this information when no longer useful

GRUs

GRUs make use of “gates” denoted by Γ (Greek G for “Gate”)

$\Gamma = 1$: “the gate is open” and information flows through

$\Gamma = 0$: “the gate is closed” and information is blocked

GRUs

Two types of gates are used:

Γ^u: When open, information from long-term memory is propagated. When closed, information from local state is used.

Γ^r: When closed, the local state is reset. When open, the state is updated as in a “vanilla” RNN.

Note: These are usually called the “update” and “reset” gates. I find this terminology super confusing. More suggestive names might be the long distance memory gate (Γ^u) and the short distance memory gate (Γ^r).

GRUs

The state evolves according to

$$c_t = \tanh\left(W_{hx} x_t + W_{hh}\left(\Gamma_t^r \odot h_{t-1}\right) + b_h\right)$$

$$h_t = (1 - \Gamma_t^u) \odot c_t + \Gamma_t^u \odot h_{t-1}$$

GRUs

The state evolves according to

$$c_t = \tanh\left(W_{hx}x_t + W_{hh}\left(\Gamma^r_t \odot h_{t-1}\right) + b_h\right)$$

$$h_t = (1 - \Gamma^u_t) \odot c_t + \Gamma^u_t \odot h_{t-1}$$

- c_t is the "candidate state" computed using the usual "vanilla RNN" state, after possibly resetting some components.
- When the long-term memory gate is open ($\Gamma^u = 1$), the information gets sent through directly. *This deals with vanishing gradients*.
- The gates are multi-dimensional, applied componentwise
- Prediction of the next word is made using h_t.

GRUs

Everything needs to be differentiable, so the gate is actually "soft" and between zero and one.

The gates are computed as

$$\Gamma_t^u = \sigma\left(W_{ux} x_t + W_{uh} h_{t-1} + b_u\right)$$

$$\Gamma_t^r = \sigma\left(W_{rx} x_t + W_{rh} h_{t-1} + b_r\right)$$

where σ is the sigmoid function.

Putting it together

GRU state update equations

$$\Gamma_t^u = \sigma\left(W_{ux} x_t + W_{uh} h_{t-1} + b_u\right)$$

$$\Gamma_t^r = \sigma\left(W_{rx} x_t + W_{rh} h_{t-1} + b_r\right)$$

$$c_t = \tanh\left(W_{hx} x_t + W_{hh}\left(\Gamma_t^r \odot h_{t-1}\right) + b_h\right)$$

$$h_t = \left(1 - \Gamma_t^u\right) \odot c_t + \Gamma_t^u \odot h_{t-1}$$

There are minor variants on this architecture that are sometimes used.

Putting it together

The reset gate is sometimes moved outside the linear map:

GRU state update equations

$$\Gamma_t^u = \sigma\left(W_{ux} x_t + W_{uh} h_{t-1} + b_u\right)$$

$$\Gamma_t^r = \sigma\left(W_{rx} x_t + W_{rh} h_{t-1} + b_r\right)$$

$$c_t = \tanh\left(W_{hx} x_t + \Gamma_t^r \odot W_{hh} h_{t-1} + b_h\right)$$

$$h_t = (1 - \Gamma_t^u) \odot c_t + \Gamma_t^u \odot h_{t-1}$$

There are minor variants on this architecture that are sometimes used.

GRUs: Example

Example:

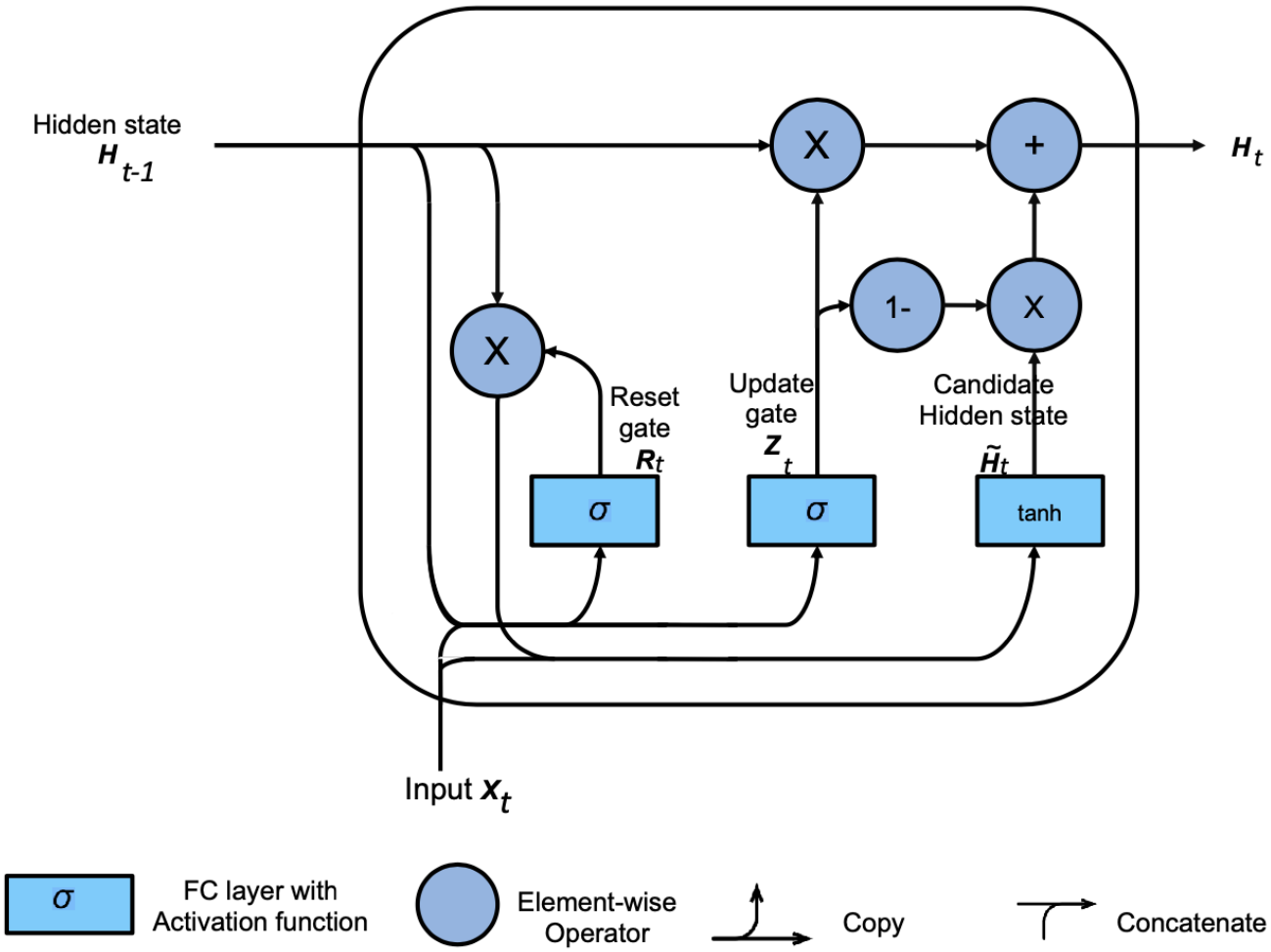
`The leaves, as the weather turned cold in New Haven, fell silently from the trees in November.`

We want to keep `leaves` in memory. It's the subject of the sentence, and plural — syntax

It also has a "foliage" meaning that is relevant when we predict the words `trees` and `November` — semantics

Let's step through on the blackboard how the GRU handles this.

GRU Diagram (using slightly different notation)



LSTMs

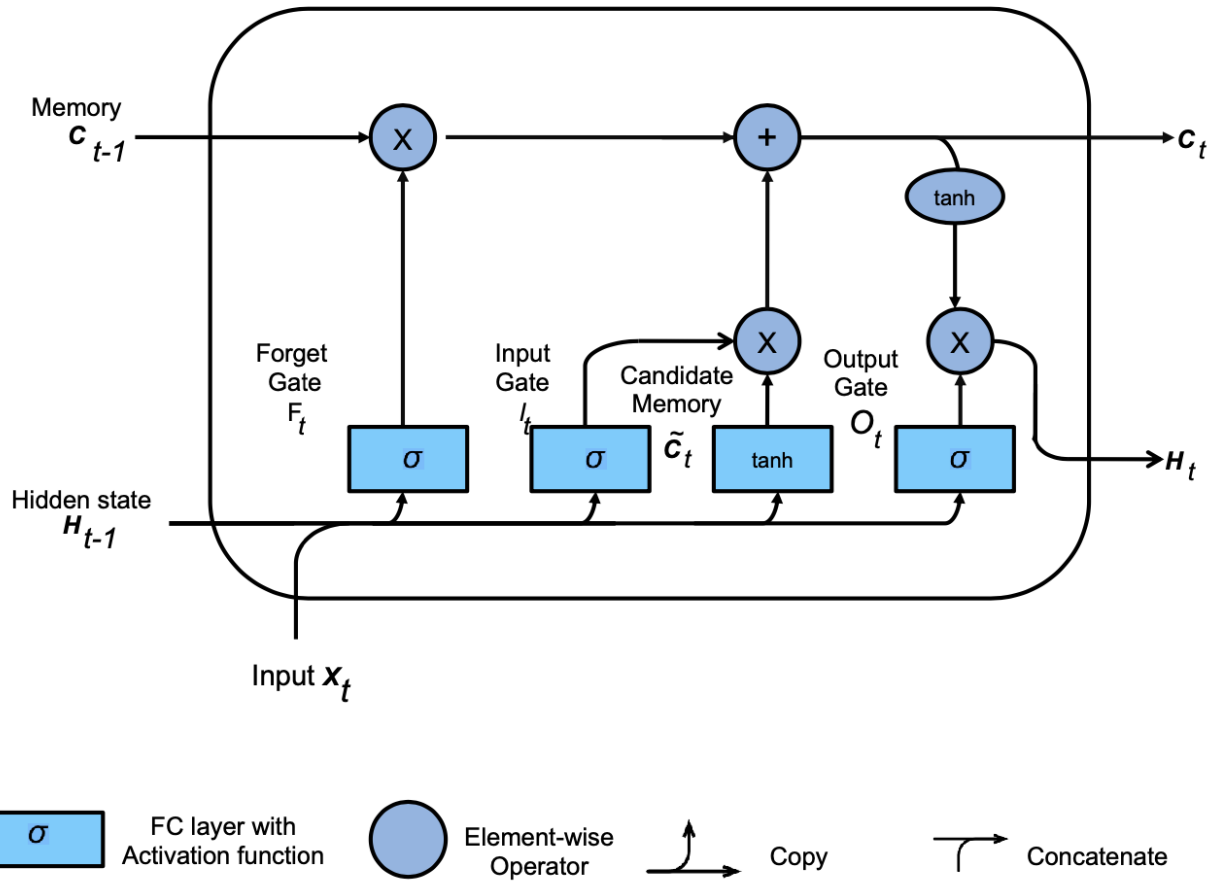
A variant called “Long Short-Term Memory” RNNs has a special context/hidden layer that “includes” or “forgets” information from the past.

$$\text{forget: } F_t = \sigma\left(W_{fh} h_{t-1} + W_{fx} x_t + b_f\right)$$
$$\text{include: } I_t = \sigma\left(W_{ih} h_{t-1} + W_{ix} x_t + b_i\right)$$

“Memory cell” or “context” c_t evolves according to

$$c_t = F_t \odot c_{t-1} + I_t \odot \widetilde{c}_t$$
$$\widetilde{c}_t = \tanh\left(W_{ch} h_{t-1} + W_{cx} x_t + b_c\right)$$

LSTM Diagram (using slightly different notation)



Summary

- Recurrent neural networks are used for sequential data
- LSTMs and GRUs model longer range dependencies through special gates that control what moves in and out of memory
- RNNs are unsupervised, generative models, able to generate realistic looking sequences when sufficiently well trained.