Recurrent Neural Networks

CISC 7026: Introduction to Deep Learning

University of Macau

Prof. Qingbiao Li GNN lecture 28 October

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November 4 holiday, no lecture

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Makeup lecture Saturday October 26, 13:00 16:00

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Updated assignment 5 is on Moodle, due in 2 weeks

Agenda

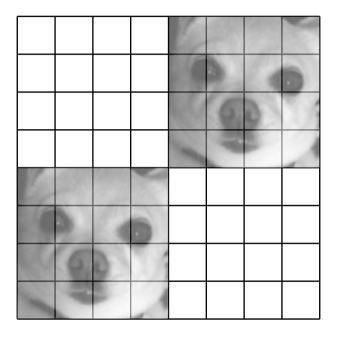
- 1. Review
- 2. Sequence Modeling
- 3. Composite Memory
- 4. Linear Recurrence
- 5. Scans
- 6. Output Modeling
- 7. Recurrent Loss Functions
- 8. Backpropagation through Time
- 9. Recurrent Neural Networks
- 10. Coding

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In perceptrons, each neuron in a layer is independent

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These images are equivalent to a neural network



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It is a miracle that our neural networks could classify clothing!

A **signal** represents information as a function of time, space or some other variable

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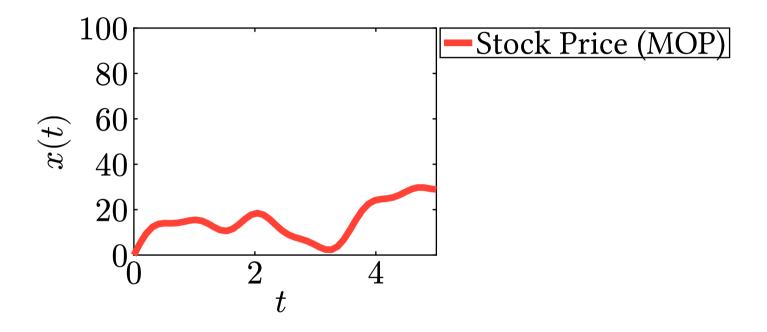
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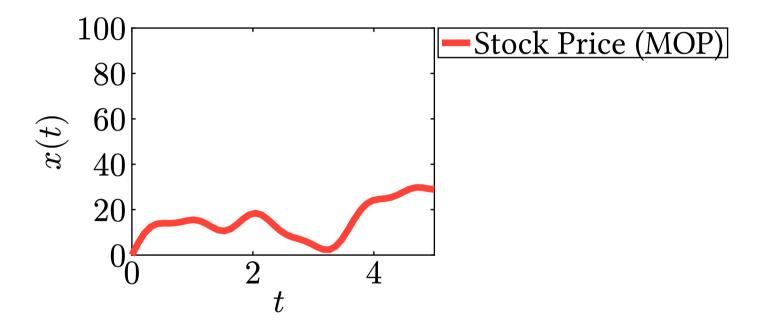
In **signal processing**, we analyze the meaning of signals

$$x(t) = \text{stock price}$$

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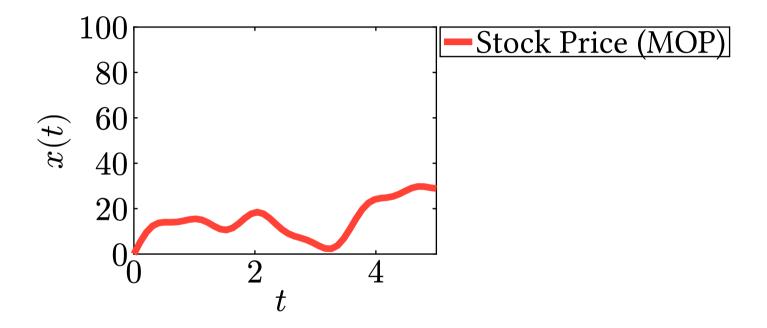


$$x(t) = \text{stock price}$$



There is an underlying structure to x(t)

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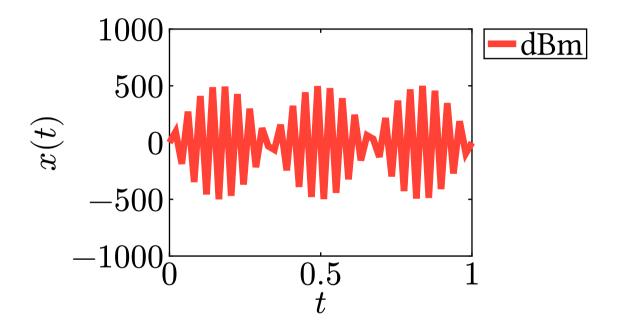


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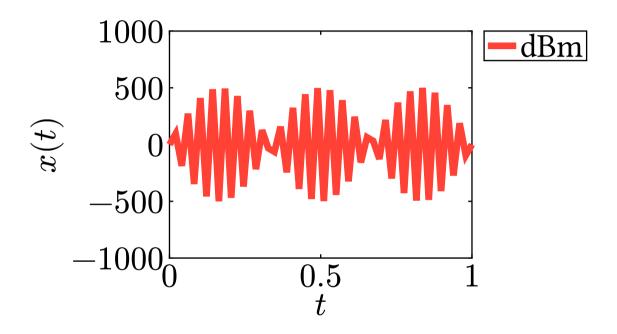
Structure: Tomorrow's stock price will be close to today's stock price

$$x(t) = audio$$

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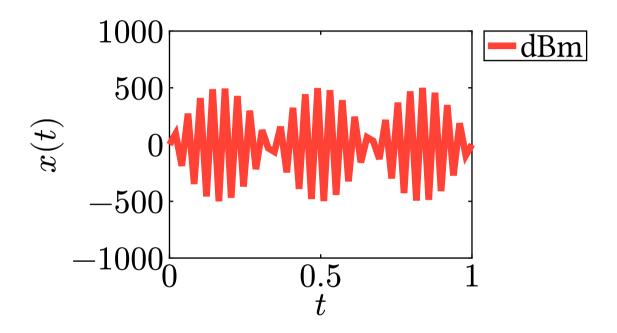


$$x(t) = audio$$



Structure: Nearby waves form syllables

$$x(t) = audio$$

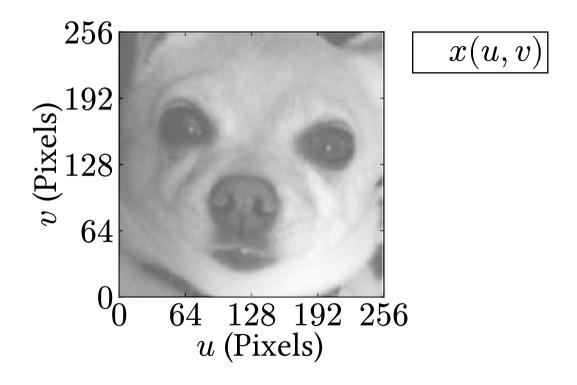


Structure: Nearby waves form syllables

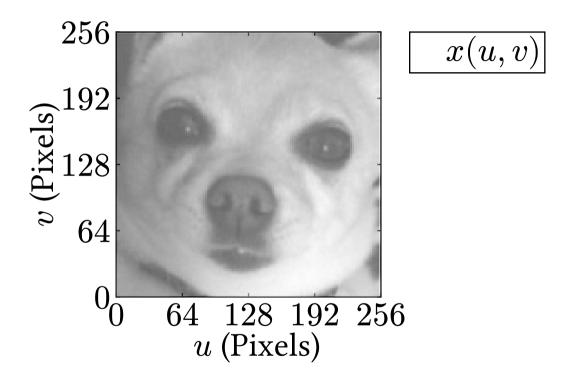
Structure: Nearby syllables combine to create meaning

$$x(u, v) = \text{image}$$

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$$x(u, v) = \text{image}$$



Structure: Repeated components (circles, symmetry, eyes, nostrils, etc)

Two common properties of signals:

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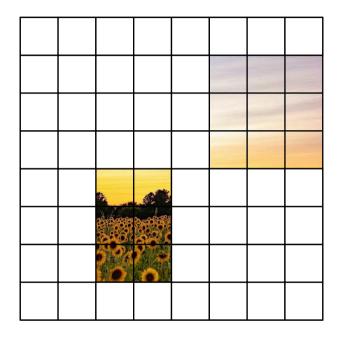
Locality: Information concentrated over small regions of space/time

Two common properties of signals:

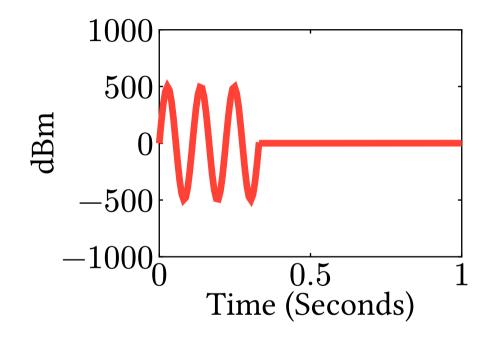
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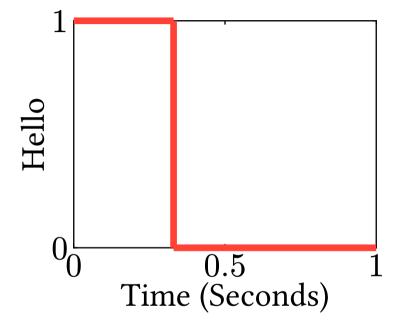
Translation Equivariance: Shift in signal results in shift in output

A more realistic scenario of locality and translation equivariance

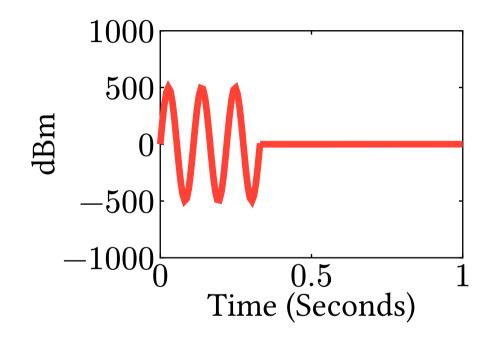


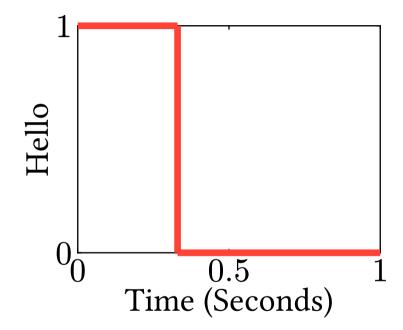
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Convolution is translation equivariant and local

Convolution is the sum of products of a signal x(t) and a **filter** g(t)

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$$x(t)*g(t) = \int_{-\infty}^{\infty} x(t-\tau)g(\tau)d\tau$$

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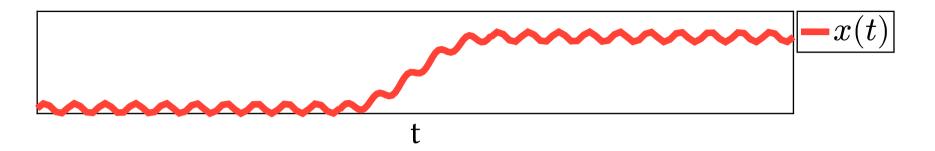
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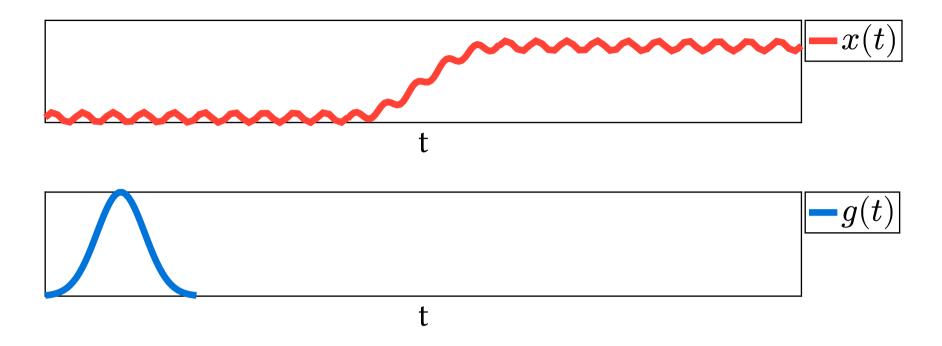
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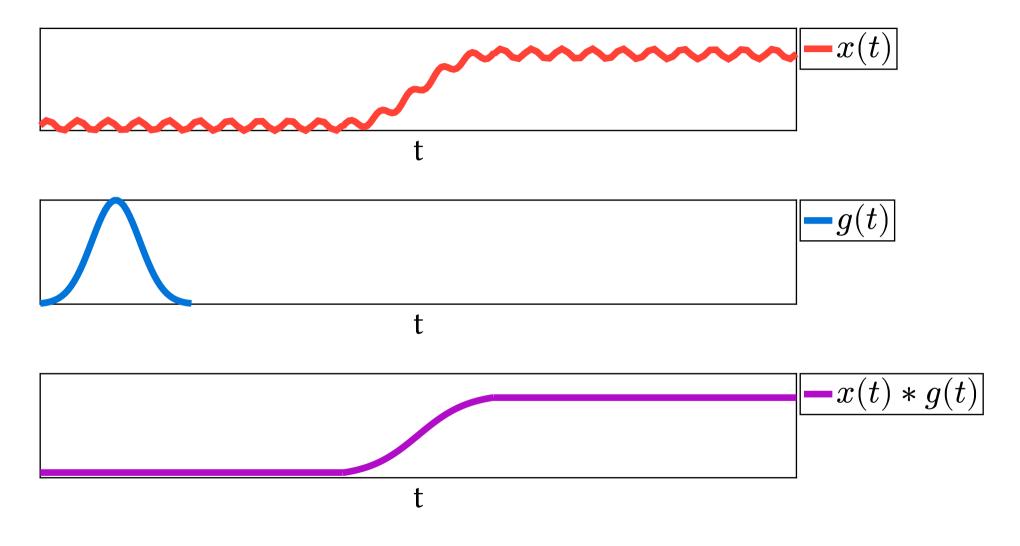
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We slide the filter g(t) across the signal x(t)







$$\begin{bmatrix} x(t) \\ g(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 1 & & \\ & & & \end{bmatrix}$$

$$\begin{bmatrix} x(t) \\ g(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} \mathbf{1} & \mathbf{2} & 3 & 4 & 5 \\ \mathbf{2} & \mathbf{1} & & \\ \mathbf{4} & & & \end{bmatrix}$$

$$\begin{bmatrix} x(t) \\ g(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ & 2 & 1 & \\ 4 & 7 & & \end{bmatrix}$$

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To make a convolution layer, we make the filter with trainable parameters

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We can write both a perceptron and convolution in vector form

$$f(x(t), oldsymbol{ heta}) = \sigma \left(egin{array}{c|c} oldsymbol{ heta}^{ op} & 1 \ x(0.1) \ x(0.2) \ dots \end{array}
ight)$$

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A convolution layer applies a "mini" perceptron to every few timesteps

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A convolution layer applies a "mini" perceptron to every few timesteps.

The output size depends on the signal length

$$z(t) = f(x(t), \boldsymbol{\theta}) = \left[\sigma\left(\boldsymbol{\theta}^{\intercal}\begin{bmatrix}1\\x(0.1)\\x(0.2)\end{bmatrix}\right) \ \sigma\left(\boldsymbol{\theta}^{\intercal}\begin{bmatrix}1\\x(0.2)\\x(0.3)\end{bmatrix}\right) \ \dots\right]^{\intercal}$$

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$$\mathrm{SumPool}(z(t)) = \sigma \left(\boldsymbol{\theta}^\top \begin{bmatrix} 1 \\ x(0.1) \\ x(0.2) \end{bmatrix}\right) + \sigma \left(\boldsymbol{\theta}^\top \begin{bmatrix} 1 \\ x(0.2) \\ x(0.3) \end{bmatrix}\right) + \dots$$

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$$\operatorname{MeanPool}(z(t)) = \frac{1}{T-k+1} \ \operatorname{SumPool}(z(t)); \quad \operatorname{MaxPool}(z(t)) = \max(z(t))$$

Our examples considered:

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• 1 dimensional variable t

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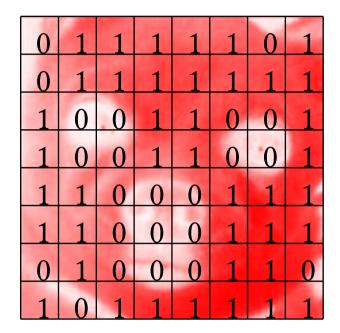
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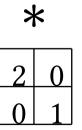
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- Arbitrary signals

The idea is exactly the same



0	1	1	1	1	1	0	1
0	1	1	1	1	1	1	1
1	0	0	1	1	0	0	1
1	0	0	1	1	0		1
1	1	0	0	0	1	1	1
1	1	0	0	0	1	1	1
0	1	0	0	0	1	1	0
1	0	1	1	1	1	1	1

0	1	1	1	1	1	0	1
0	1	1	1	1	1	1	1
1	0	0	1	1	0	0	1
1	0	0	1	1	0	0	1
1	1	0	0	0	1	1	1
1	1	0	0	0	1	1	1
0	1	0	0	0	1	1	0
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+

$$\begin{array}{c|c} 1 & 1 \\ 0 & 1 \end{array}$$

+

 $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$

One last thing, **stride** allows you to "skip" cells during convolution

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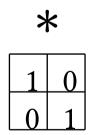
This can decrease the size of image without pooling

One last thing, **stride** allows you to "skip" cells during convolution

This can decrease the size of image without pooling

Padding adds zero pixels to the image to increase the output size

0	1	1	1	1	1	0	1
0	1	1	1	1	1	1	1
1	0	0	1	1	0	0	1
1	0	0	1	1	0	0	1
1	1	0	0	0	1	1	1
1	1	0	0	0	1	1	1
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We call these models **recurrent models**

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So what is the difference between convolution and recurrent models?

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Let us examine some real life signals, and see if these properties hold

Example 1: You like dinosaurs as a child, you grow up and study dinosaurs for work

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Question: Is this local?

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Question: Is this local?

Answer: No, two related events separated by 20 years

Example 2: Your parent changes your diaper

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Question: Translation equivariant?

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No! Ok if you are a baby, different meaning if you are an adult!

Example 3: You hear a gunshot then see runners



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Answer: No! (1) gunshot, (2) see runners, enjoy the race. (1) see

runners, (2) hear gunshot, you start running too!

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Question: Translation equivariant?

Answer: No! (1) gunshot, (2) see runners, enjoy the race. (1) see runners, (2) hear gunshot, you start running too!

Question: Any other examples?

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Can we design a neural network based on human perceptions of time?

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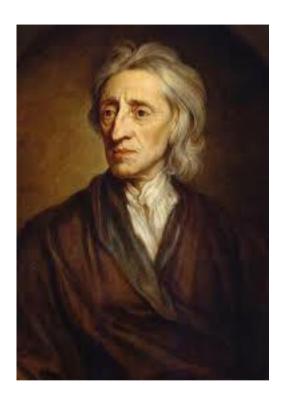
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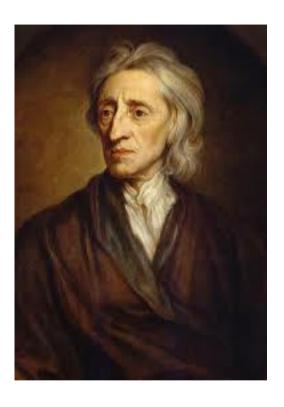
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Humans process temporal data by storing and recalling memories

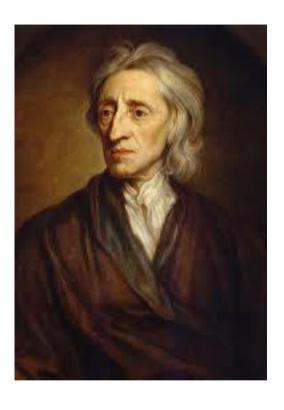


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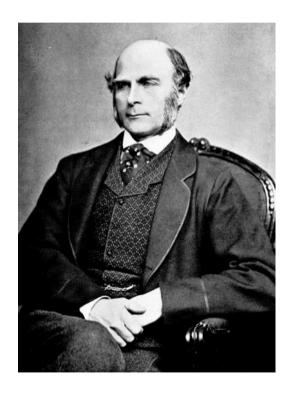
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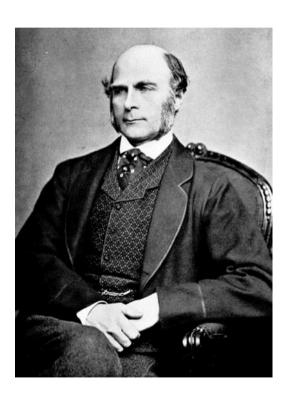
Without the ability to reason over memories, we would only react to stimuli like bacteria

So how do we model memory in humans?

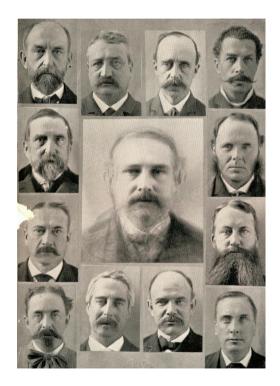
Francis Galton (1822-1911) photo composite memory



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Composite photo of members of a party



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Composite photography/memory uses a weighted sum

$$f(oldsymbol{x}, oldsymbol{ heta}) = \sum_{i=1}^T oldsymbol{ heta}^ op \overline{oldsymbol{x}}_i$$

$$f(\boldsymbol{x},\boldsymbol{\theta}) = \sum_{i=1}^T \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_i$$

$$f(\boldsymbol{x},\boldsymbol{\theta}) = \sum_{i=1}^T \boldsymbol{\theta}^{\top} \overline{\boldsymbol{x}}_i$$

What if we see a new face?

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We repeat the same process for each new face

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We repeat the same process for each new face

We can rewrite f as a **recurrent function**

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$$\textcolor{red}{\boldsymbol{h_1}} = f(\boldsymbol{0}, \boldsymbol{x}_1, \boldsymbol{\theta}) = \boldsymbol{0} + \boldsymbol{\theta}^{\top} \overline{\boldsymbol{x}}_1$$

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Question: What is the meaning of *h* in humans?

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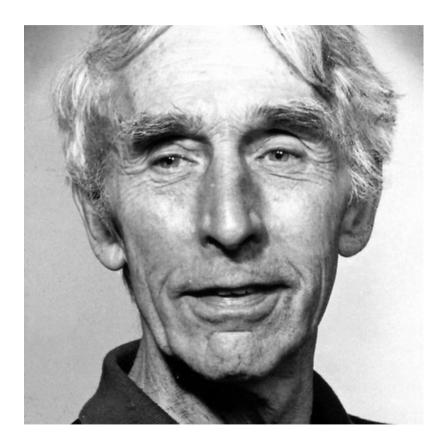
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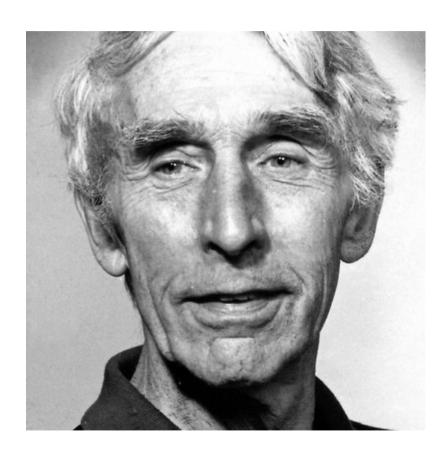
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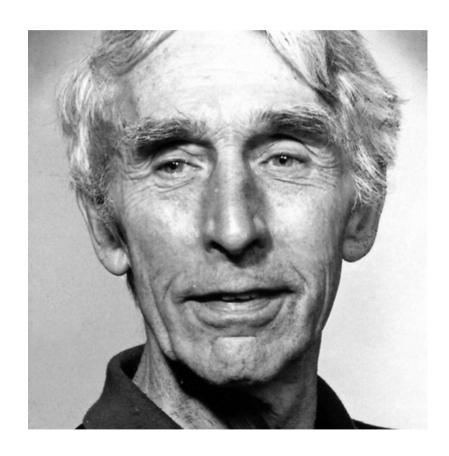
Humans cannot remember everything!

We forget old information



$$f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\gamma} \boldsymbol{h} + \boldsymbol{\theta}^{\top} \overline{\boldsymbol{x}}; \quad 0 < \gamma < 1$$

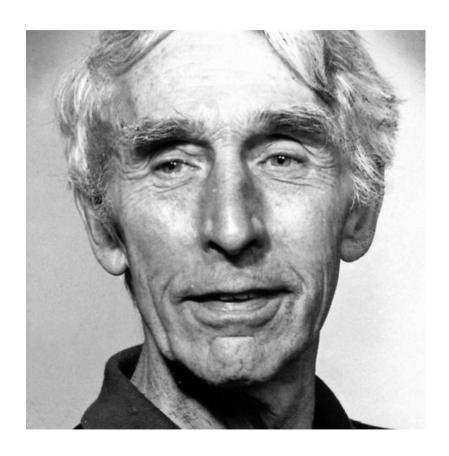




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Key Idea:
$$\lim_{T\to\infty} \gamma^T = 0$$

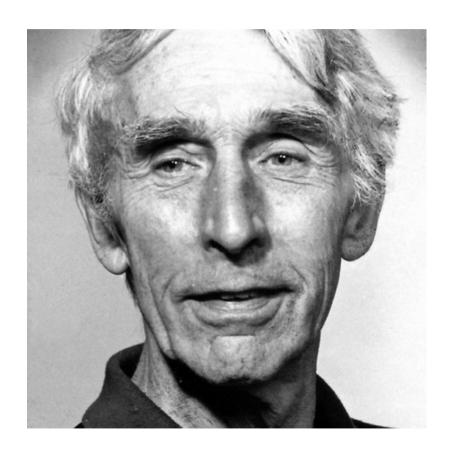
Murdock (1982)



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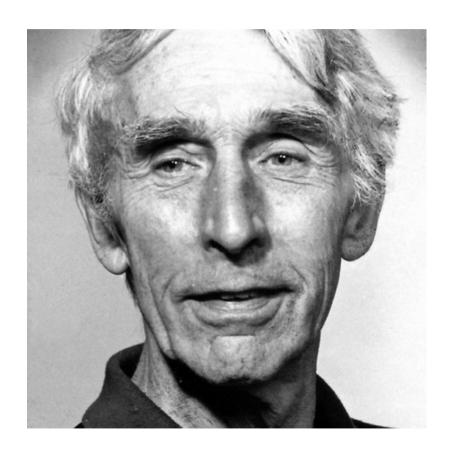


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Let
$$\gamma = 0.9$$

$$0.9 \cdot 0.9 \cdot h = 0.81h$$



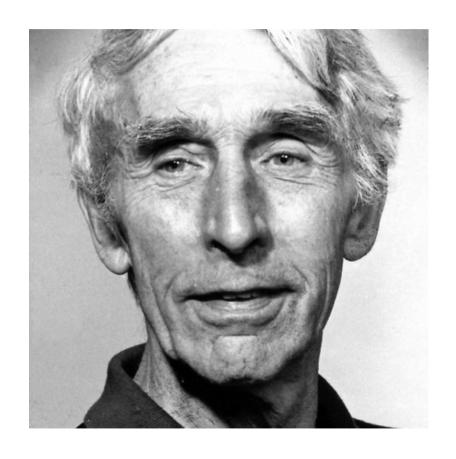
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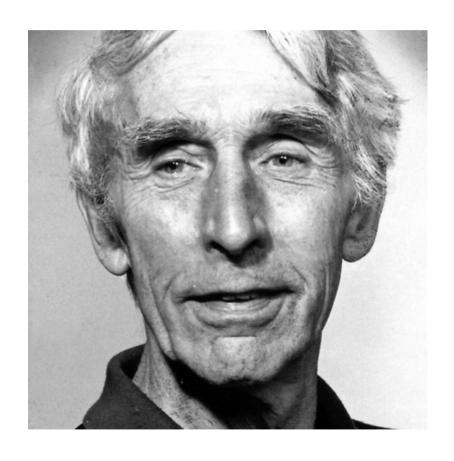
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Let us work out how forgetting works

$$f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = \gamma \boldsymbol{h} + \boldsymbol{\theta}^{\top} \overline{\boldsymbol{x}}; \quad 0 < \gamma < 1$$

$$f(m{h}, m{x}, m{ heta}) = \gamma m{h} + m{ heta}^ op \overline{m{x}}; \quad 0 < \gamma < 1$$
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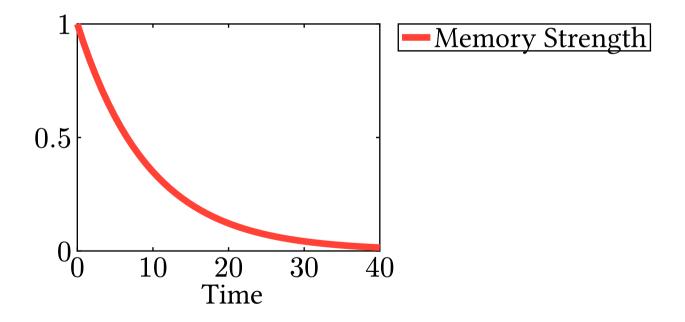
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As T increases, we add new information $oldsymbol{x}_T$

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We can learn the parameters γ , θ using gradient descent

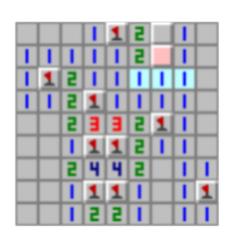
Morad et al., *Reinforcement Learning with Fast and Forgetful Memory*. Neural Information Processing Systems. (2024).

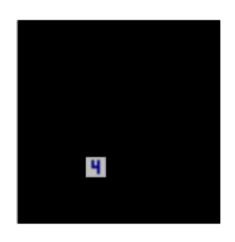
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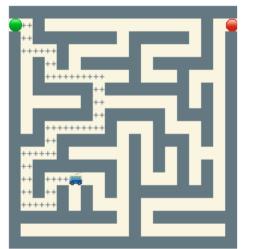
$$oldsymbol{H}_T = oldsymbol{\gamma} oldsymbol{H}_{T-1} + g(oldsymbol{x}_T)$$

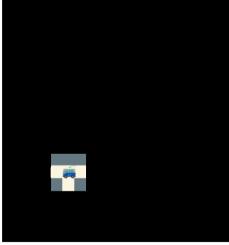
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https://www.youtube.com/watch?v=0ey63XPB-4U&t=85s

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$$f: H \times X \times \Theta \mapsto H, \quad \operatorname{scan}(f): H \times X^T \times \Theta \mapsto H^T$$

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$$\mathrm{scan}(f) \left(\boldsymbol{h}_0, \begin{bmatrix} \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix}, \boldsymbol{\theta} \right) = \begin{bmatrix} f(h_0, x_1, \boldsymbol{\theta}) \\ f(h_1, x_2, \boldsymbol{\theta}) \\ \vdots \\ f(h_{T-1}, x_T, \boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} f(h_0, x_1) \\ f(f(h_0, x_1), x_2) \\ \vdots \\ f(...f(h_0, x_1)..., x_T) \end{bmatrix}$$

```
import jax
import jax.numpy as jnp
T, d \times d = 10, 2, 4
xs, h0 = jnp.ones((T, d x)), jnp.zeros((d h,))
theta = [jnp.ones((d h,)), jnp.ones((d x, d h))] # (b, W)
def f(h, x):
    b, W = theta
    result = h + (W.T @ x + b)
    return result, result # return one, return all
hT, hs = jax.lax.scan(f, init=h0, xs=xs) # Scan f over x
```

torch does NOT have built-in scans, and is very slow compared to jax

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We will write our own scan

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We will write our own scan

```
def scan(f, h, xs):
    # h shape is (d h,)
    \# xs shape is (T, d x)
    hs = []
    for x in xs:
        h = f(h, x, theta)
        hs.append(h)
    # output shape is (T, d h)
    return torch.stack(hs)
```

```
import torch
T, d \times d + 10, 2, 4
xs, h0 = torch.ones((T, d x)), torch.zeros((d h,))
theta = (torch.ones((d h,)), torch.ones((d x, d h)))
def f(h, x):
    b, W = theta
    result = h + (W.T @ x + b)
    return result # h
hs = scan(f, h0, xs)
```

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Question: Does $f(h, x, \theta) = \gamma h + \theta^{\top} \overline{x}$ obey the associative property?

Answer: Yes, linear operations obey the associative property

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There is one more step we must consider, **memory recall**

h stores all memories, but humans only access a few memories at once

Example: I ask you your favorite ice cream flavor

You recall previous times you ate ice cream, but not your phone number

We will model this recall of memories using a function g

Let g define our memory recall function

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$$g: H \times X \times \Theta \mapsto Y$$

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 $oldsymbol{x}$: "What is your favorite ice cream flavor?"

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Now, we will combine f and g

Step 1: Perform scan to find recurrent states

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$$egin{bmatrix} egin{bmatrix} m{h}_1 \ dash m{h}_T \end{bmatrix} = \mathrm{scan}(f) \left(m{h}_0, egin{bmatrix} m{x}_1 \ dash m{x}_T \end{bmatrix}, m{ heta}_f
ight)$$

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Step 2: Perform recall on recurrent states

$$egin{bmatrix} egin{bmatrix} oldsymbol{y}_1 \ dots \ oldsymbol{y}_T \end{bmatrix} = egin{bmatrix} g(oldsymbol{h}_1, oldsymbol{x}_1, oldsymbol{ heta}_g) \ dots \ g(oldsymbol{h}_T, oldsymbol{x}_T, oldsymbol{ heta}_g) \end{bmatrix}$$

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Questions? This is on the homework

To summarize, we defined:

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• Recurrent function f

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To run our model:

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Relax

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Let us examine some example tasks:

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• Clock

Let us examine some example tasks:

- Clock
- Explaining a video

Task: Clock – keep track of time

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Every minute, the minute hand ticks

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Count/remember the ticks to know the time

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$$X \in \{0, 1\}, \quad Y \in \mathbb{R}^2$$

Example input sequence:

 $egin{bmatrix} 1 \ 1 \ dots \ 1 \end{bmatrix}$

Example input sequence:

Desired output sequence

 $\begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$

 $\begin{bmatrix} 0 & 1 \\ 0 & 2 \\ \vdots & \vdots \\ 2 & 13 \end{bmatrix}$

We have a corresponding label y for each input x

Can use square error

Can use square error

First, scan f over the inputs to find h

$$m{h}_{[i],j} = ext{scan}(f) \left(m{h}_0, egin{bmatrix} m{x}_{[i],1} \ dots \ m{x}_{[i],T} \end{bmatrix}, m{ heta}_f
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Onto the next task

Task: Watch a video, then explain it

$$X \in \mathbb{Z}^{3 \times 32 \times 32}$$
, $Y \in \{\text{comedy show, action movie}, ...\}$

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Example input sequence:

Example output:

$$\begin{bmatrix} I_1 \\ I_2 \\ \vdots \\ I_T \end{bmatrix}$$

"dancing dog"

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, $Y \in \{\text{comedy show, action movie}, ...\}$

Example input sequence:

$$egin{array}{c} I_1 \ I_2 \ dots \ I_T \end{array}$$

Example output:

"dancing dog"

Unlike before, we have many inputs but just one output!

We will use the classification loss

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We scan f over the sequence, the compute g for the final timestep

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$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{d_y} y_{[i], j} \log g \left(\boldsymbol{h}_{[i], T}, \boldsymbol{x}_{[i], T}, \boldsymbol{\theta}_g\right)_{j}$$

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We only care about the $m{h}_T$

To summarize, we use standard losses for recurrent loss functions

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Just be careful – we often sum over an additional axis

$$\sum_{i=1}^{n} \sum_{j=1}^{T} \dots$$

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Backpropagation through Time

1. We created the model

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How do we compute gradients for recurrent functions?

First, compute gradient of f

$$f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = \gamma \boldsymbol{h} + \boldsymbol{\theta}^{\top} \overline{\boldsymbol{x}}$$

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Question: What is $\nabla_{\theta} f$?

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$$abla_{m{ heta}} f(m{h}, m{x}, m{ heta}) = \overline{m{x}}^{ op}$$

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Question: What is $\nabla_{\theta} f$?

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = \overline{\boldsymbol{x}}^\top$$

Too easy, now let us find the gradient of scan(f)

$$\operatorname{scan}(f) \left(\boldsymbol{h}_0, \begin{bmatrix} \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix}, \boldsymbol{\theta} \right) = \begin{bmatrix} f(h_0, x_1, \boldsymbol{\theta}) \\ f(h_1, x_2, \boldsymbol{\theta}) \\ \vdots \\ f(h_{T-1}, x_T, \boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} f(h_0, x_1) \\ f(f(h_0, x_1), x_2) \\ \vdots \\ f(\dots f(h_0, x_1) \dots, x_T) \end{bmatrix}$$

Question: What is $\nabla_{\theta} \operatorname{scan}(f)$?

Hint: Chain rule

$$\operatorname{scan}(f) \left(\boldsymbol{h}_0, \begin{bmatrix} \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix}, \boldsymbol{\theta} \right) = \begin{bmatrix} f(h_0, x_1, \boldsymbol{\theta}) \\ f(h_1, x_2, \boldsymbol{\theta}) \\ \vdots \\ f(h_{T-1}, x_T, \boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} f(h_0, x_1) \\ f(f(h_0, x_1), x_2) \\ \vdots \\ f(\dots f(h_0, x_1) \dots, x_T) \end{bmatrix}$$

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Question: Any issues with this?

$$\nabla_{\boldsymbol{\theta}} \operatorname{scan}(f) \left(\boldsymbol{h}_0, \begin{bmatrix} \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix}, \boldsymbol{\theta} \right) = \begin{bmatrix} \nabla_{\boldsymbol{\theta}}[f] \\ \nabla_{\boldsymbol{\theta}}[f] \nabla_{\boldsymbol{\theta}}[f] \\ \nabla_{\boldsymbol{\theta}}[f] \nabla_{\boldsymbol{\theta}}[f] \end{bmatrix}$$

Question: Any issues with this?

What if $\nabla_{\theta} f$ is $\ll 1$ or $\gg 1$?

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Until now, f was a linear function

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If we make f a neural network, then we have a **recurrent neural network** (RNN)

The simplest recurrent neural network is the **Elman Network**

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$$f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}_1^{ op} \boldsymbol{h} + \boldsymbol{\theta}_2^{ op} \overline{\boldsymbol{x}})$$

The simplest recurrent neural network is the **Elman Network**

$$f(m{h},m{x},m{ heta}) = \sigma(m{ heta}_1^ opm{h} + m{ heta}_2^ opar{m{x}})$$
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1!

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 \boldsymbol{h} grows large and causes exploding gradients, σ should be sigmoid!

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Question: Anything missing from our linear model?

Answer: Forgetting!

Add forgetting

$$f(m{h},m{x},m{ heta}) = \sigmaig(m{ heta}_1^ opm{h}\odotm{f}_{ ext{forget}}(m{h},m{x},m{ heta}) + m{ heta}_2^ opar{m{x}}ig)$$

Add forgetting

$$egin{aligned} f(m{h},m{x},m{ heta}) &= \sigmaig(m{ heta}_1^ opm{h}\odotm{f}_{ ext{forget}}(m{h},m{x},m{ heta}) + m{ heta}_2^ opar{m{x}}ig) \ f_{ ext{forget}}(m{h},m{x},m{ heta}) &= \sigmaig(m{ heta}_1^ opar{m{x}} + m{ heta}_2^ opm{h}ig) \end{aligned}$$

Add forgetting

$$f(\boldsymbol{h},\boldsymbol{x},\boldsymbol{\theta}) = \sigma\big(\boldsymbol{\theta}_1^{\top}\boldsymbol{h} \odot f_{\text{forget}}(\boldsymbol{h},\boldsymbol{x},\boldsymbol{\theta}) + \boldsymbol{\theta}_2^{\top}\overline{\boldsymbol{x}}\big)$$

$$f_{ ext{forget}}(m{h},m{x},m{ heta}) = \sigma(m{ heta}_1^ opm{\overline{x}} + m{ heta}_2^ opm{h})$$

Question: σ is sigmoid. What is range/codomain of f_{forget} ?

Add forgetting

$$f(\boldsymbol{h},\boldsymbol{x},\boldsymbol{\theta}) = \sigma\big(\boldsymbol{\theta}_1^{\top}\boldsymbol{h}\odot f_{\mathrm{forget}}(\boldsymbol{h},\boldsymbol{x},\boldsymbol{\theta}) + \boldsymbol{\theta}_2^{\top}\overline{\boldsymbol{x}}\big)$$

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Question: σ is sigmoid. What is range/codomain of f_{forget} ?

Answer: [0,1]

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Question: σ is sigmoid. What is range/codomain of f_{forget} ?

Answer: [0, 1]

When $f_{\text{forget}} < 1$, we forget some of our memories!

Add forgetting

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Through gradient descent, neural network learns which memories to forget

Minimal gated unit (MGU) is a modern RNN

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Minimal gated unit (MGU) is a modern RNN

MGU defines two helper functions

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Left term forgets old, right term replaces forgotten memories

There are even more complicated models

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• Long Short-Term Memory (LSTM)

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MGU is simpler and performs similarly to LSTM and GRU

Recall the gradient for the linear recurrence

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$$\nabla_{\boldsymbol{\theta}} \operatorname{scan}(f) \left(\boldsymbol{h}_0, \begin{bmatrix} \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix}, \boldsymbol{\theta} \right) = \begin{bmatrix} \nabla_{\boldsymbol{\theta}}[f] \\ \nabla_{\boldsymbol{\theta}}[f] \nabla_{\boldsymbol{\theta}}[f] \\ \nabla_{\boldsymbol{\theta}}[f] \nabla_{\boldsymbol{\theta}}[f] \end{bmatrix}$$

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Elman network f:

$$f(m{h}, m{x}, m{ heta}) = \sigma(m{ heta}_1^ op m{h} + m{ heta}_2^ op \overline{m{x}})$$

Question: What is the gradient for scan(f) of Elman network?

$$f(m{h},m{x},m{ heta}) = \sigma(m{ heta}_1^{ op}m{h} + m{ heta}_2^{ op}\overline{m{x}})$$

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Answer: Vanishing gradient

$$\nabla[\sigma] \cdot \nabla[\sigma] \cdot \dots = 0$$

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Question: What can we do?

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Question: What can we do?

All RNNs suffer from either exploding gradient (ReLU) or vanishing gradient (sigmoid). Active area of research!

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- 3. Composite Memory
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- 9. Recurrent Neural Networks
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Coding

Jax RNN https://colab.research.google.com/drive/147z7FNGyERV8oQ_4 gZmxDVdeoNt0hKta#scrollTo=TUMonlJ1u8Va

Homework https://colab.research.google.com/drive/1CNaDxx1yJ4-phyMvgbxECL8ydZYBGQGt?usp=sharing