## Advanced concepts in deep learning



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### Sequential models

#### Up to now ...

- Fully connected neural nets, parameters learning and training tricks
- Convolutional neural networks (ConvNets)
- Generative models
- Sequential models: dealing with "ordered sets"
- 2 main state-of-the-art deep architectures
  - Recurrent Neural Networks (RNNs)
  - Attention models & transfomers

# Outline

## I. Recurrent Neural Networks (RNNs)

- a) Vanilla RNNs
- b) RNN training
- c) RNN architectures
- d) Applications

### II. Attention models & transfomers

- Manipulating sequences of " ordered tokens", *i.e.*, atomic elements
  - Ex tokens: characters/word in NLP

"Hello I love you" > "Hello", "I", "love", "you"

- Pixels/patches in images (how to define an order?)
- Features a time t for time series, video: sequences of frames / feature embeddings with CNNs



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- Input sequence  $\{x_t\}_{t \in \{1; T\}}$ ,  $x_t \in \mathbb{R}^d$
- Internal RNN state  $\{h_t\}_{t \in \{1; T\}}$ ,  $h_t \in \mathbb{R}^{I}$
- RNN Cell:  $h_t = \phi_t(x_t, h_{t-1})$ 
  - Loop,  $h_t$  depends on current  $x_t$  and previous state  $h_{t-1}$ 
    - $h_t$ : memory of the network  $\Leftrightarrow$  history up to time t
  - In RNNs, function  $\phi_t = \phi$  shared across time



- RNN Cell:  $h_t = \phi(x_t, h_{t-1})$ 
  - $\phi$ : linear projection of  $x_t$  and  $h_{t-1}$ , *i.e.* fully connected layers
  - $h_t = f(Ux_t + Wh_{t-1} + b_h)$ 
    - U matrix size  $I \times d$ , W matrix size  $I \times I$  (b vector size I)
    - $f \leftarrow tanh$  non-linearity



• **Depending on the task:** prediction at each time step

 $y_t = f'(Vh_t + b_y)$  e.g.,  $f' \leftarrow \text{soft-max if } y_t \leftrightarrow \text{class probabilities}$ 



• Depending on the task: prediction at the last time step

 $y_t = f'(Vh_t + b_y)$  e.g.,  $f' \leftarrow \text{soft-max if } y_t \leftrightarrow \text{class probabilities}$ 



### RNNs expressiveness

- <u>Recap</u>: Feed-forward neural networks are universal function approximators
- Expressibility of the mapping between  $\{x_t\}_{t \in \{1; T\}}$  and  $\{y_t\}_{t \in \{1; T\}}$ ?
  - RNNs are universal program approximators [2]
    - Can approximate any any computable function, *i.e.* Turing machine
  - RNNs can approximate any measurable sequence to sequence mapping



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#### RNNs expressiveness: examples

• Computing sum



• Determining if sum of 1<sup>st</sup> dimension values > than sum of 2<sup>nd</sup> dimension



Toy ex: grammatical analysis, 'deep' => adj

• Input x<sub>t</sub>: character, one-hot encoding

• Output y<sub>t</sub>: grammatical class

'verb' = 
$$[1,0,0,...,0]$$
  
'noun' =  $[0,1,0,...,0]$   
'adj' =  $[0,0,1,...,0]$   $\in \mathbb{R}^M$ 



### Ex: grammatical analysis, 'deep' => adj



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### RNN training: formulation

- Comparing output prediction  $\{y_t\}_{t \in \{1; T\}}$  with supervision  $\{y_t^*\}$ 
  - Task-dependent, *e.g.* only  $\{y_T^*\}$  in many-to-one



### RNN training: formulation

- Loss function at time t:  $\mathcal{L}_t(y_t, y_t^*)$ , e.g. cross-entropy (classification)
- Total loss function  $\mathcal{L}(\{y_t\}, \{y_t^*\}) = \sum_{t=1}^{\prime} \mathcal{L}_t(y_t, y_t^*)$



### Back-Propagation Through Time (BPTT)

• Similar to standard back-prop, with time (sequence) ~ depth



#### Truncated BPTT

- Issue for large T => storage, + vanishing gradients issues (next)
- Truncated BPTT => BPTT on local temporal windows



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#### **BPTT:** Gradient Computation

- **<u>BPTT</u>**: computing gradient  $\frac{\partial \mathcal{L}_t}{\partial W}$ ,  $\frac{\partial \mathcal{L}_t}{\partial U}$ ,  $\frac{\partial \mathcal{L}_t}{\partial V}$  (+biases)
- Unfolded RNN: same spirit as back-prop with fully connected networks (chain rule)
  - **BUT:** shared parameters W, U, V across time



#### **BPTT:** Gradient Computation

- Shared parameters W, U, V across time
  ⇒ gradients depend on the whole past history
- Ex: for W:  $\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{k=1}^t \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$



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#### **BPTT:** Gradient Computation

• 
$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{k=1}^t \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial h_t} \left[ \frac{\partial h_t}{\partial h_k} \right] \frac{\partial h_k}{\partial W}$$

• Chain rule (again): 
$$\frac{\partial h_t}{\partial h_k} = \prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}}$$

• 
$$h_t = f(Ux_t + Wh_{t-1} + b_h)$$
, e.g. f tanh

• Jacobian matrix 
$$\frac{\partial h_j}{\partial h_{j-1}} = W^T diag[f'(h_{j-1})]$$

$$\Rightarrow \text{Analyzing} \left\| \frac{\partial h_t}{\partial h_k} \right\| = \left\| \prod_{j=k+1}^t W^T \operatorname{diag}[f'(h_{j-1})] \right\|$$

**BPTT: Exploding and Vanishing Gradients** 

$$\left\|\frac{\partial \mathsf{h}_{t}}{\partial \mathsf{h}_{k}}\right\| = \left\|\prod_{j=k+1}^{t} \mathsf{W}^{\mathsf{T}} diag[f'(\mathsf{h}_{j-1})]\right\| \le (\beta_{w}\beta_{h})^{t-k}$$

- β<sub>h</sub> for activation (tanh=1, sigmoid=0.25), β<sub>w</sub> for W (largest eigenvalue)
  β<sub>h</sub> · β<sub>w</sub> > 1 ⇒ exploding gradients
  - $\beta_h \cdot \beta_w > 1 \rightarrow$  exploding gradients •  $\beta_v \cdot \beta_w < 1 \rightarrow$  vanishing gradients
  - $\beta_h \cdot \beta_w < 1 \Rightarrow$  vanishing gradients
- True for any deep networks, exacerbated for RNNs



### Exploding and Vanishing Gradients: challenges & solutions

#### Main challenge: modeling long-range dependencies

Solution for exploding

- Regularization, e.g.,  $||W||_2$
- Simple common strategy: gradient clipping

 $\Rightarrow$  Exploding gradients relatively easy to detect and fix

Solution for vanishing

- Use Truncated BPTT, but smaller range dependencies
- Using ReLU activation instead of tanh/sigmoid
- Specific architectures/models, e.g. GRU/LSTM

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### Long Short-Term Memory (LSTM) [3]

• Recap: Vanilla RNN cell



Long Short-Term Memory (LSTM) [Hochreiter and Schmidhuber, 1997]



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## Long Short-Term Memory (LSTM)



Only elementwise multiplication and addition, no matrix multiply by W
 <u>Key property</u>: Uninterrupted gradient flow!



## Long Short-Term Memory (LSTM)

• Only elementwise multiplication and addition, no matrix multiply by W

Key property: Uninterrupted gradient flow!



**Sounds familiar?** 

Similar to ResNets!



### Gated Recurrent Unit [4]

- LSTM popular variant: Gated Recurrent Unit (GRU) [Cho et al., 2014]
  - Combines forget and input gates into a single "update gate"
  - Merges the cell state and hidden state



$$z_t = \sigma \left( W_z \cdot [h_{t-1}, x_t] \right)$$
$$r_t = \sigma \left( W_r \cdot [h_{t-1}, x_t] \right)$$
$$\tilde{h}_t = \tanh \left( W \cdot [r_t * h_{t-1}, x_t] \right)$$
$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

• Simpler than LSTM, generally slightly inferior performances

[4] K. Cho, B. van Merrienboer, C. Gulcehre, D. Bahdanau, F. Bougares, H. Schwenk, and Y. Bengio. Learning phrase representations using rnn encoder-decoder for statistical machine translation. EMNLP 2014.

### Deep RNNs

- Stacking RNN/ LSTM layers  $\Rightarrow$  learning more complex features
- Deep LSTM: very powerful, especially when stacked and made even deeper and if you have lots and lots of data



### **Bi-directionnal RNNs**

For classification, incorporate information from words both preceding and following



 $h = [\vec{h}; \vec{h}]$  now represents (summarizes) the past and future around a single token.

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### **RNN** applications

- RNN: mapping input sequence  $\{x_t\}_{t \in \{1; T\}}$  into  $\{y_t\}_{t \in \{1; T\}}$
- Different tasks ⇔ different mappings



Language models, Image captioning Sentiment classification, Visual Question Answering (VQA)

Translation, char

nn

### Medical Visual Question answering (MVQA) [5]



#### Image Captioning: medical report generation [6]



[6] From G. Liu, T.M. Harry Hsu, M. McDermott, W. Boag, W.H. Weng, P. Szolovits, M. Ghassemi. Clinically Accurate Chest X-Ray Report Generation. ArxiV, 2019.

**Clinical Coherent Reward** 

#### Video classification $Y_{t-1}$ $Y_{t-2}$

- ConvLSTM [Shi et. al. 2015]
  - generic module for video classification
  - Many-to-many mapping



Phase 2



ConvLSTM

Cell

 $X_{t-2}$ 

 $H_{t-2}$ 

ConvLSTM

Cell

 $X_{t-1}$ 

H<sub>t-1</sub>





Yt

ConvLSTM

Cell

 $X_t$ 

[7] G. Yengera, D. Mutter, J. Marescaux, N. Padoy. Less is More: Surgical Phase Recognition with Less Annotations through Self-Supervised Pre-training of CNN-LSTM Networks. ArXiv, 2019.

Preparation

Phase 1

Calot Triangle Clipping & Cutting Dissection

Phase 3

Gallbladder Dissection

Gallbladder Cleaning Packaging & Coagulation Gallbladder Extraction

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# Outline

I. Recurrent Neural Networks (RNNs)II. Attention models & transformers

### a) Context

- b) Transformer block
- c) Medical image segmention
## Transformers everywhere since 2017

### NLP: BERT, GPT-3/4, Chat-GPT, etc

Vision since '21: Vision Image Transformer (ViT)

explain quantum theory to a child in the style of snoop dogg

Yo, little homie, let me break it down for you Quantum theory, it's a crazy thing, it's true See, the world is made up of tiny, tiny particles That are always moving, and changing, and actin' wild

These particles, they don't always behave like we think Sometimes they're waves, and sometimes they're points, it's a trip They can be in two places at once, and they can be in two states It's a mind-blowing concept, but that's the quantum fate

So don't be scared, little homie, it's all good Quantum theory, it's just the way the world works, it's understood It's a wild ride, but it's a cool one too Quantum theory, it's the way the world does what it do.





## Transformer in medical image analysis

### Used in various contexts and tasks

- Image classification, detection, e.g. COVID, Semantic segmentation
- Image Registration
- Image Generation
- Im-2-im translation



Zhang L, Wen Y. Mia-cov19d: A transformer-based framework for covid19 classification in chest cts. arXiv, 2021.

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### Used in various contexts and tasks

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Chen J, Du Y, He Y, et al. Transmorph: Transformer for unsupervised medical image registration. Medical Image Analysis, 2022.

## Transformer in medical image analysis

### Used in various contexts and tasks

- Image classification, detection, e.g. COVID, semantic segmentation
- Image Registration
- Image Generation
- Im-2-im translation



Korkmaz Y, Dar SU, Yurt M, et al. Unsupervised MRI reconstruction via zero-shot learned adversarial transformers. IEEE TMI, VOL. 41, NO. 7, JULY 2022

## Focus on this talk

• Paper on transformer every day...





• By no means exhaustive literature review



Intelligent Medicine 3 (2023) 59-78

Review

Transformers in medical image analysis

Check for updates

Kelei He<sup>1,2,#</sup>, Chen Gan<sup>2,#</sup>, Zhuoyuan Li<sup>1,2,#</sup>, Islem Rekik<sup>3,4,#</sup>, Zihao Yin<sup>2</sup>, Wen Ji<sup>2</sup>, Yang Gao<sup>2,5</sup>, Qian Wang<sup>6,\*</sup>, Junfeng Zhang<sup>1,2,\*</sup>, Dinggang Shen<sup>6,7,8,\*</sup>

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## From sequence to set

- A sequence of elements → a set of tokens, no order
  - Token: primitives, elementary elements of data
    - Text: token are e.g. words
    - Image: token are e.g. patches

Text Tokenization



## Input embedding

- Token: input vector in  $\mathbb{R}^t$ 
  - Word: t = |V|, V vocabulary
  - Image patch:  $t = s^2$ , where s is the patch size
- Input embedding: linear projection  $\mathbb{R}^t \rightarrow \mathbb{R}^d : e_i = x_i W^e$



## Positional encoding

- Sequence  $\rightarrow$  set of token:
  - Permutation invariant
  - Loosing structural information from data
- Recovering structure: **positional encoding (PE)** 
  - Mapping token position t to a vector  $\mathbf{p}_t \in \mathbb{R}^d$
  - Seminal PE: sinusoidal

## Sinusoidal positional encoding

- Unique vector  $\mathbf{p}_t$  for each position t
- $p_t(i) \in [-1;1]$ : natural normalization



d=128, max length of token set = 50

- Models relative position
- Positional similarity: K = PPt

- 0.75

0.50

0.25

0.00

-0.25

-0.50

-0.75



## Positional encoding

- Other possible encoding, can be learned
- Final embedding :



### => Input of transformer!



# Transformer [8] : the encoder

- A stack a N transformer blocks
  - Input a set of embedded tokens
  - Output: a set of re-embedded tokens

[8] Attention Is All You Need. A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, I. Polosukhin. NeurIPS 2017.

## Transformer: self attention

- The most important and specific module in transformers
- Project the input set into 3 sets
  - Query: sought info
  - Key: context elements
  - Value: retrieved





## Self-attention



$$\begin{aligned} X \in \mathbb{R}^{wh \times d}, W_q \in \mathbb{R}^{d \times d}, W_k \in \mathbb{R}^{d \times d}, W_v \in \mathbb{R}^{d \times d} \\ Q = XW_q, K = XW_k, V = XW_v \\ A = Softmax(\frac{QK^T}{\sqrt{d}}) \\ Y = AV \end{aligned}$$

## Self-attention: conclusion



- Each token y<sub>i</sub> in Y: computed a linear combination of v<sub>i</sub>
  - Enables to model **global interactions** between v<sub>i</sub> tokens: full contextual information
  - *≠* ConvNets in vision, interactions limited by the size of the receptive field
  - ≠ RNNs for sequence processing, interactions limited by vanishing gradients
- Self attention: O(N<sup>2</sup>) complexity
  - Expensive (or impossible) for large N

## Multi-headed attention

• High-level idea: multiple self-attention in parallel

- Each head: attend to different parts
- Combine the heads' outputs



[Vaswani et al. 2017]



Wizards of the Coast, Artist: Todd Lockwood



## Multi-headed attention



- Concatenate the heads' outputs
- Use a linear layer: desired output size

## Layer normalization

• Normalization on joint channel and spatial dimensions



• Stabilize training, faster convergence



## Layer normalization

• Normalization on joint channel and spatial dimensions

$$egin{aligned} \mu_n &= rac{1}{K} \sum_{k=1}^K x_{nk} \ \sigma_n^2 &= rac{1}{K} \sum_{k=1}^K \left( x_{nk} - \mu_n 
ight)^2 \ \hat{x}_{nk} &= rac{x_{nk} - \mu_n}{2}, \hat{x}_{nk} \in R \end{aligned}$$







 $\beta$ ,  $\gamma$  learnable parameters

## Layer normalization + residual connections



# LayerNorm(

### **Residual connections**

- Better gradient flow (vanishing gradients)
- Leverage input encoding, *e.g.* PE

## Feed-Forward Network (FFN)

 Position-wise FFN: applied to each token separately and identically

$$FFN(x) = \max(0, xW_1 + b_1)W_2 + b_2$$



# Transformer: conclusion

- Importance of attention: global interactions between tokens
- On the other hand relaxes inductive biases
  - e.g. ConvNets translation equivariant
    - vs transformers permutation equivariant
  - More flexibility to learn adequate mapping
  - Needs more data



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# Vision Image Transformer (ViT) [9]





- Direct application of transformer's encoder for images
- Learned on JFT (300.10<sup>6</sup> images)
- Extra learnable token: used for class prediction
  - "Learned" pooling wrt visual tokens

[9] An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale. A. Dosovitskiy, L. Beyer, A. Kolesnikov, D. Weissenborn, X. Zhai, T. Unterthiner, M. Dehghani, M. Minderer, G. Heigold, S. Gelly, J. Uszkoreit, N. Houlsby. ICLR 2020.

## Transformer in segmentation

Vanilla idea: use ViT encoder, add a classification layer for each patch (token) => SETR [10]



Figure 3: SETR architecture and its variants adapted from [5]. (a) SETR consists of a standard Transformer. (b) SETR-PUP with a progressive up-sampling design. (c) SETR-MLA with a multi-level feature aggregation.

[10] S. Zheng, J. Lu, H. Zhao, X. Zhu, Z. Luo, Y. Wang, Y. Fu, J. Feng, T. Xiang, P. H. Torr, et al. Rethinking semantic segmentation from a sequence-tosequence perspective with transformers. CVPR 2021.

# Transformer in medical image segmentation

#### **Organ segmentation**

**Ex: Pancreas segmentation** 

field





c) U-Net

### Long-range dependencies: crucial context in segmentation Main challenge of transformers: self attention complexity - O(N<sup>2</sup>)

• Expensive (or impossible) for large N => critical for large 2D images, 3D volumes

# Hybrid conv / transformers architectures

- Trans U-Net [11], U-Transformer [12]: seminal works for using transformers in medical image segmentation
- Adding self-attention on U-Net's bottleneck
  - Inspired from non-local networks [13]



Trans U-Net architecture

[11] TransUNet: Transformers Make Strong Encoders for Medical Image Segmentation. J. Chen et.al. arXiv, Feb 2021.

[12] U-Net Transformer: Self and Cross Attention for Medical Image Segmentation. O. Petit, N. Thome, C. Rambour, L. Soler. arXiv, March 2021.

[13] Non-local Neural Networks. X. Wang, R. Girshick, A. Gupta, K. He. CVPR 2018.

## U-Transformer [12]



a) Ground Truth

b) Attention map

c) U-Net d) U-Transformer

[12] U-Net Transformer: Self and Cross Attention for Medical Image Segmentation. O. Petit, N. Thome, C. Rambour, L. Soler. arXiv, March 2021.

# Full transformers in segmentation

## **Motivation:** breaking self-attention complexity

- Swin-Transformer [14]
  - Multi-resolution transformer
    - Local attention in lower-layers
      - Shifted windows at layers I/I+1
    - Patch merging => larger receptive field



(a) Swin Transformer (ours)



# 3D medical image segmentation

### **<u>Challenge:</u>** input volume size

- •Intractable memory requirements (180Gb for U-Net with image 512x512x256
- •Common strategy: train on 3 crops





- Full context lost
- Even on patch: full context challenging!

# nn-Former [15]

- Global self-attention in bottleneck
- Local self-attention in higher-resolution feature maps
  - ~ 3D Swin-Unet
- No context beyond patch
- No global context in high-resolution maps



[15] nnFormer: Interleaved Transformer for Volumetric Segmentation. H.Y. Zhou, J. Guo, Y. Zhang, L. Yu, L. Wang, Y. Yu. Arxiv, September 2021.

# CoTR: Convolutional NN and Transformer [16]

- **CoTr:** Conv encoder => flattened multi-scale feature
  - Deformable transformer encoder (DeTrans) in multi-res input
  - Several DeTrans layers, sent to conv decoder



[16] CoTr: Efficiently Bridging CNN and Transformer for 3D Medical Image Segmentation. Y. Xie, J. Zhang, C. Shen, Y. Xia. MICCAI 2021

## Global attention in multi-resolution transformers (GLAM) [17]

• GLAM block in any multi-resolution architecture (e.g. Swin, nn-Former)



## GLAM block

- Define learnable global tokens in each window, cf CLS in VIT
  - Window self-attention (W-MSA): attention between visual and global tokens
  - Global attention (G-MSA) between global token
- G-MSA: indirection between all visual tokens
  - Break computational complexity of full attention between visual token
  - But enables full indirect interaction between them



=> full attention even in high-resolution features!

## FINE : Full resolutIoN mEmory transformer [18]

- Extends GLAM for full context modelling in 3D segmentation
  - Global tokens for the full volume



## => (indirect) full interaction between all voxels!

[18] Memory transformers for full context and high-resolution 3D Medical Segmentation. L. Themyr, C. Rambour, N. Thome, T. Collins, A. Hostettler. MLMI workshop, MICCAI 2022.
## FINE results



## Thank you for your attention!

Questions?