机器学习 Machine learning

第十章 神经网络与深度学习(4) Neural Network and Deep Learning

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第十章 神经网络与深度学习

- 10.1 概述
- 10.2 多层感知机
- 10.3 卷积网络
- 10.4 Recurrent 网络
- 10.5 前沿概述

深度学习、生成对抗学习、强化学习、知识图谱

中国科学院大学网络安全学院 2021 年研究生秋季课程

深层结构

神经网络 + 深层结构 + 优化 + 计算资源 + 人工智能应用

基本的深度神经网络结构

- Feedforward neural network, also called Multilayer Perceptron (MLP).
- Recurrent neural network.

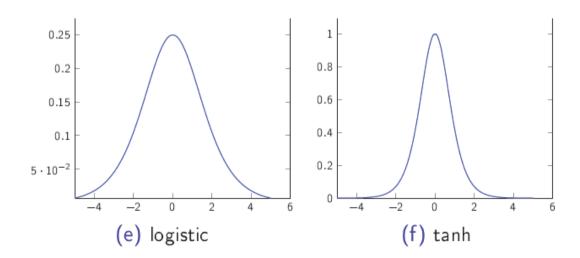
梯度消失

$$\delta^{(l)} = f'_{l}(\mathbf{z}^{(l)}) \odot ((W^{(l+1)})^{\top} \delta^{(l+1)},$$

When we use sigmoid function, such as logistic $\sigma(x)$ and tanh,

$$\sigma'(x) = \sigma(x)(1 - \sigma(x)) \in [0, 0.25]$$

$$\tanh'(x) = 1 - (\tanh(x))^2 \in [0, 1].$$



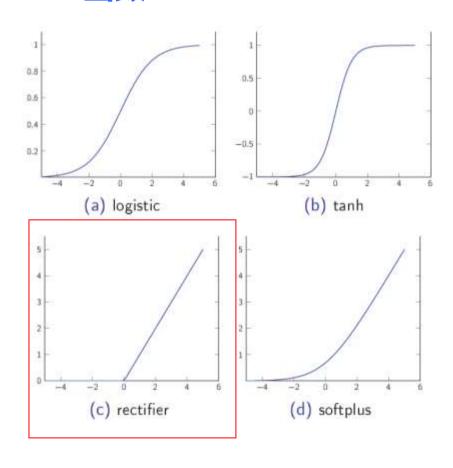
梯度消失

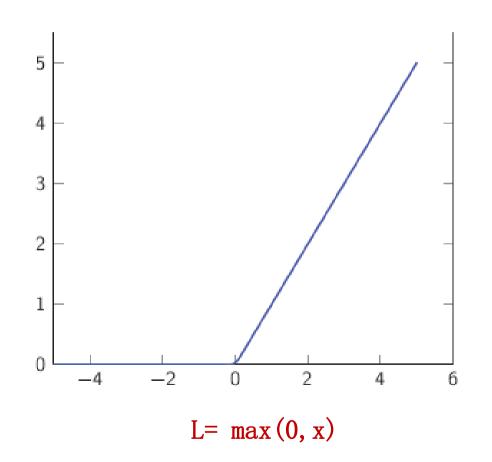
解决梯度消失

- 前馈网络:
 - 自编码、ReLU 激活函数
- Recurrent 网络:
 - 二次优化、非线性逐次状态估计、ReLU 激活函数

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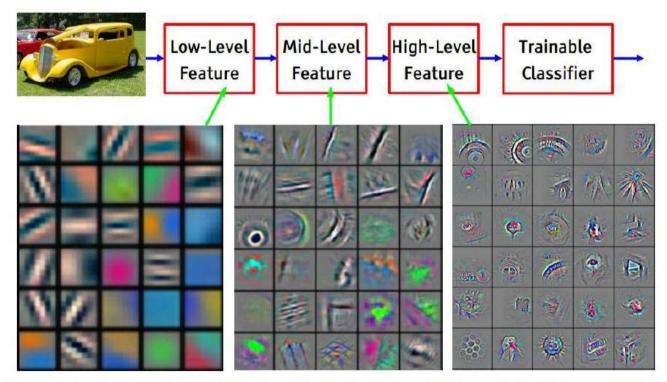
ReLU 函数





视觉识别

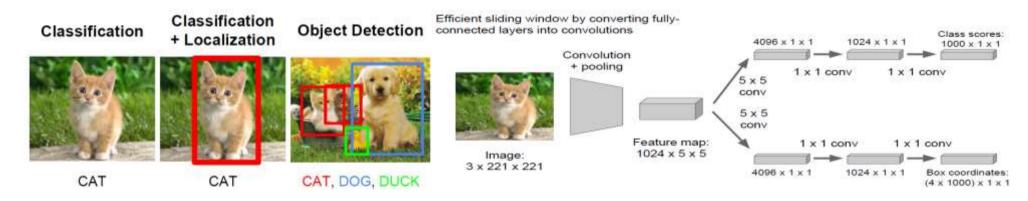
Image Feature and Recognition



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

视觉识别

Image Detection

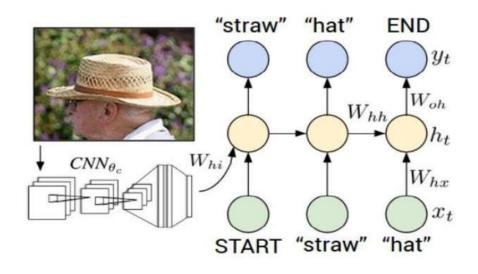


Idea #1: Localization as Regression

Idea #2: Sliding Window

视觉识别

Image Captioning





视觉识别

Attention for Captioning



A woman is throwing a frisbee in a park.



A dog is standing on a hardwood floor.



A stop sign is on a road with a mountain in the background.



A little <u>girl</u> sitting on a bed with a teddy bear.



A group of <u>people</u> sitting on a boat in the water.

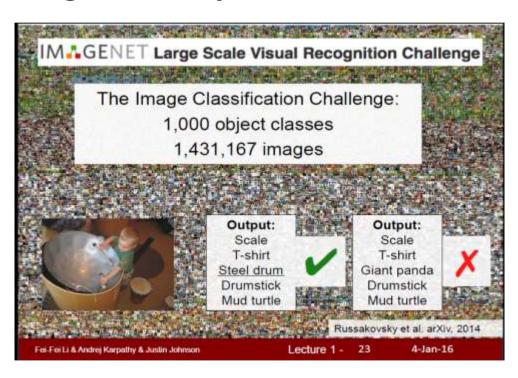


A giraffe standing in a forest with trees in the background.

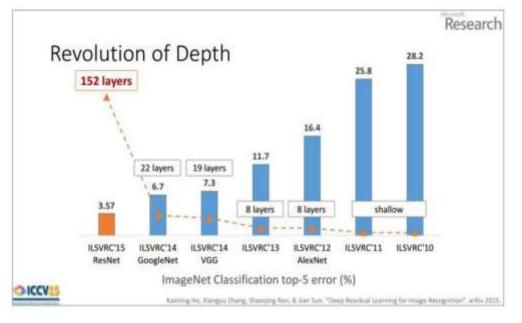
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

视觉识别

ImageNet Completion



网络结构 : CNN+全连接



Case Study: AlexNet

[Krizhevsky et al. 2012]

Full (simplified) AlexNet architecture:

[227x227x3] INPUT

[55x55x96] CONV1: 96 11x11 filters at stride 4, pad 0

[27x27x96] MAX POOL1: 3x3 filters at stride 2

[27x27x96] NORM1: Normalization layer

[27x27x256] CONV2: 256 5x5 filters at stride 1, pad 2

[13x13x256] MAX POOL2: 3x3 filters at stride 2

[13x13x256] NORM2: Normalization layer

[13x13x384] CONV3: 384 3x3 filters at stride 1, pad 1

[13x13x384] CONV4: 384 3x3 filters at stride 1, pad 1

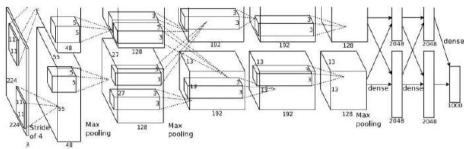
[13x13x256] CONV5: 256 3x3 filters at stride 1, pad 1

[6x6x256] MAX POOL3: 3x3 filters at stride 2

[4096] FC6: 4096 neurons

[4096] FC7: 4096 neurons

[1000] FC8: 1000 neurons (class scores)



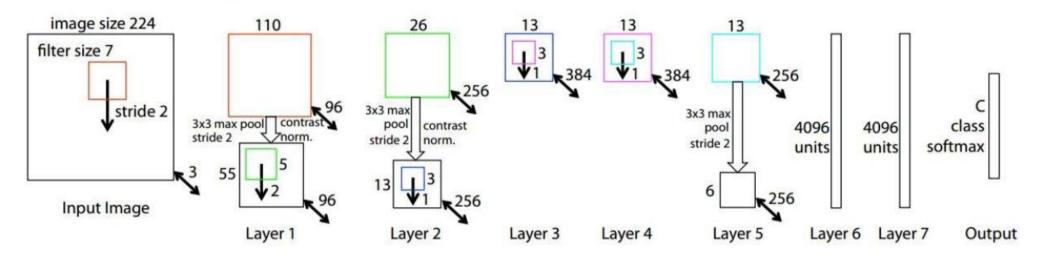
Details/Retrospectives:

- first use of ReLU
- used Norm layers (not common anymore)
- heavy data augmentation
- dropout 0.5
- batch size 128
- SGD Momentum 0.9
- Learning rate 1e-2, reduced by 10 manually when val accuracy plateaus
- L2 weight decay 5e-4
- 7 CNN ensemble: 18.2% -> 15.4%

2012 ILSVRC winner (top 5 error of 16% compared to runner-up with 26% error) 共有 8 层,其中前 5 层卷积层,后边 3 层全连接层 最后的一层的输出是具有 1000 个输出的 softmax

Case Study: ZFNet

[Zeiler and Fergus, 2013]



AlexNet but:

CONV1: change from (11x11 stride 4) to (7x7 stride 2)

CONV3,4,5: instead of 384, 384, 256 filters use 512, 1024, 512

ImageNet top 5 error: 15.4% -> 14.8%

Case Study: VGGNet

[Simonyan and Zisserman, 2014]

Only 3x3 CONV stride 1, pad 1 and 2x2 MAX POOL stride 2

```
(not counting biases)
INPUT: [224x224x3]
                       memory: 224*224*3=150K params: 0
                                                                                        ConvNet Configuration
CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*3)*64 = 1,728
                                                                                                              D
CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*64)*64 = 36,864
                                                                                        13 weight
                                                                                                  16 weight
                                                                                                            16 weight
                                                                                          layers
                                                                                                   layers
                                                                                                             layers
POOL2: [112x112x64] memory: 112*112*64=800K params: 0
                                                                                        put (224 \times 224 RGB imag
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*64)*128 = 73,728
                                                                                                            conv3-64
                                                                                         conv3-64
                                                                                                  conv3-64
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*128)*128 = 147.456
                                                                                         conv3-64
                                                                                                  conv3-64
                                                                                                            conv3-64
POOL2: [56x56x128] memory: 56*56*128=400K params: 0
                                                                                              maxpool
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*128)*256 = 294,912
                                                                                        conv3-128
                                                                                                 conv3-128
                                                                                                           conv3-128
                                                                                        conv3-128
                                                                                                 conv3-128
                                                                                                           conv3-128
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
                                                                                        conv3-256
                                                                                                  conv3-256
                                                                                                           conv3-256
POOL2: [28x28x256] memory: 28*28*256=200K params: 0
                                                                                        conv3-256
                                                                                                  conv3-256
                                                                                                           conv3-256
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*256)*512 = 1,179,648
                                                                                                  conv1-256
                                                                                                           conv3-256
                                                                                                                     co
                                                                                                                     co
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*512)*512 = 2,359,296
                                                                                             maxpoo
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*512)*512 = 2,359,296
                                                                                                           conv3-512
                                                                                        conv3-512
                                                                                                  conv3-512
POOL2: [14x14x512] memory: 14*14*512=100K params: 0
                                                                                        conv3-512
                                                                                                  conv3-512
                                                                                                           conv3-512
                                                                                                  conv1-512
                                                                                                           conv3-512
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
                                                                                                                     co
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
                                                                                             maxpool
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
                                                                                        conv3-512
                                                                                                 conv3-512
                                                                                                           conv3-512
POOL2: [7x7x512] memory: 7*7*512=25K params: 0
                                                                                                  conv3-512
                                                                                                           conv3-512
                                                                                                  conv1-512
                                                                                                           conv3-512
                                                                                                                     co
FC: [1x1x4096] memory: 4096 params: 7*7*512*4096 = 102,760,448
FC: [1x1x4096] memory: 4096 params: 4096*4096 = 16,777,216
                                                                                              maxpool
FC: [1x1x1000] memory: 1000 params: 4096*1000 = 4,096,000
                                                                                             FC-4096
                                                                                             FC-4096
TOTAL memory: 24M * 4 bytes ~= 93MB / image (only forward! ~*2 for bwd)
                                                                                              FC-1000
                                                                                              soft-max
TOTAL params: 138M parameters
```

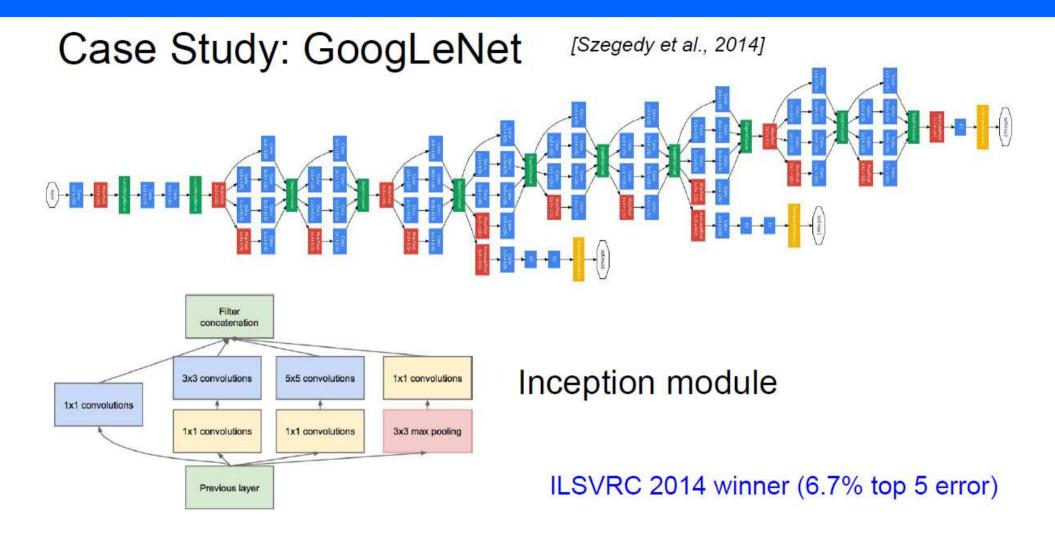
Case Study: VGGNet

[Simonyan and Zisserman, 2014]

Only 3x3 CONV stride 1, pad 1 and 2x2 MAX POOL stride 2

```
(not counting biases)
INPUT: [224x224x3]
                     memory: 224*224*3=150K params: 0
CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*3)*64 = 1,728
                                                                                         Note:
CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*64)*64 = 36,864
POOL2: [112x112x64] memory: 112*112*64=800K params: 0
                                                                                         Most memory is in
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*64)*128 = 73.728
                                                                                         early CONV
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*128)*128 = 147,456
POOL2: [56x56x128] memory: 56*56*128=400K params: 0
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*128)*256 = 294,912
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
POOL2: [28x28x256] memory: 28*28*256=200K params: 0
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*256)*512 = 1,179,648
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*512)*512 = 2,359,296
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*512)*512 = 2,359,296
POOL2: [14x14x512] memory: 14*14*512=100K params: 0
                                                                                         Most params are
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
                                                                                         in late FC
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
POOL2: [7x7x512] memory: 7*7*512=25K params: 0
FC: [1x1x4096] memory: 4096 params: 7*7*512*4096 = 102,760,448
FC: [1x1x4096] memory: 4096 params: 4096*4096 = 16,777,216
FC: [1x1x1000] memory: 1000 params: 4096*1000 = 4.096.000
TOTAL memory: 24M * 4 bytes ~= 93MB / image (only forward! ~*2 for bwd)
TOTAL params: 138M parameters
```

Chapter 10 Neural Network and Deep Learning (4)



type	patch size/ stride	output size	depth	#1×1	#3×3 reduce	#3×3	#5×5 reduce	#5×5	pool proj	params	ops
convolution	7×7/2	112×112×64	1							2.7K	34M
max pool	3×3/2	56×56×64	0								
convolution	3×3/1	56×56×192	2		64	192				112K	360M
max pool	3×3/2	28×28×192	0								
inception (3a)		28×28×256	2	64	96	128	16	32	32	159K	128M
inception (3b)		28×28×480	2	128	128	192	32	96	64	380K	304M
max pool	3×3/2	14×14×480	0								
inception (4a)		14×14×512	2	192	96	208	16	48	64	364K	73M
inception (4b)		14×14×512	2	160	112	224	24	64	64	437K	88M
inception (4c)		14×14×512	2	128	128	256	24	64	64	463K	100M
inception (4d)		14×14×528	2	112	144	288	32	64	64	580K	119M
inception (4e)		14×14×832	2	256	160	320	32	128	128	840K	170M
max pool	3×3/2	7×7×832	0								
inception (5a)		7×7×832	2	256	160	320	32	128	128	1072K	54M
inception (5b)		7×7×1024	2	384	192	384	48	128	128	1388K	71M
avg pool	7×7/1	1×1×1024	0								
dropout (40%)		1×1×1024	0								
linear		1×1×1000	1							1000K	1M
softmax		1×1×1000	0								

Fun features:

Only 5 million params!
 (Removes FC layers completely)

Compared to AlexNet:

- 12X less params
- 2x more compute
- 6.67% (vs. 16.4%)

Case Study: ResNet

[He et al., 2015]

ILSVRC 2015 winner (3.6% top 5 error)

Research

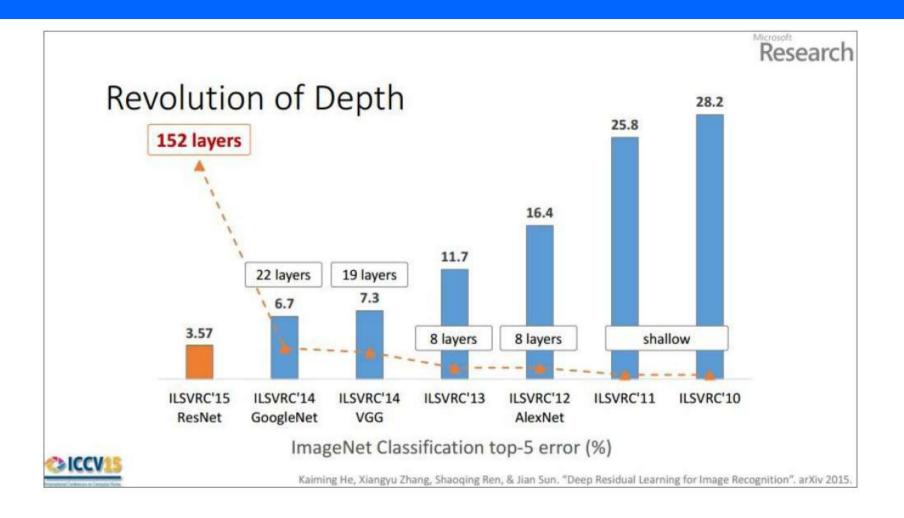
MSRA @ ILSVRC & COCO 2015 Competitions

- 1st places in all five main tracks
 - ImageNet Classification: "Ultra-deep" (quote Yann) 152-layer nets
 - ImageNet Detection: 16% better than 2nd
 - ImageNet Localization: 27% better than 2nd
 - COCO Detection: 11% better than 2nd
 - COCO Segmentation: 12% better than 2nd

V15

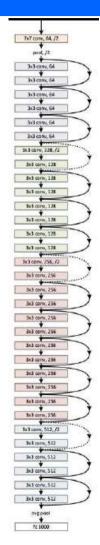
*improvements are relative numbers

Kalming He, Xiangyu Zhang, Shaoping Ren, & Jian Sun, "Deen Residual Learning for Image Recognition", arXiv 2015.



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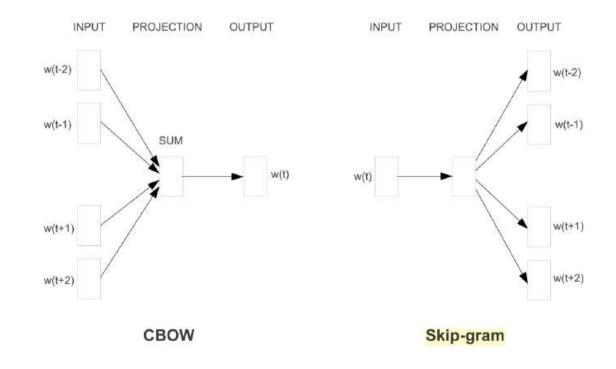
layer name	output size	18-layer	34-layer	50-layer	101-layer	152-layer							
conv1	112×112	7×7, 64, stride 2											
conv2_x	56×56	3×3 max pool, stride 2											
		$\left[\begin{array}{c}3\times3,64\\3\times3,64\end{array}\right]\times2$	$\left[\begin{array}{c}3\times3,64\\3\times3,64\end{array}\right]\times3$	$\begin{bmatrix} 1 \times 1, 64 \\ 3 \times 3, 64 \\ 1 \times 1, 256 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 64 \\ 3 \times 3, 64 \\ 1 \times 1, 256 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 64 \\ 3 \times 3, 64 \\ 1 \times 1, 256 \end{bmatrix} \times 3$							
conv3_x	28×28	$\left[\begin{array}{c} 3\times3, 128\\ 3\times3, 128 \end{array}\right] \times 2$	$\left[\begin{array}{c} 3\times3, 128\\ 3\times3, 128 \end{array}\right] \times 4$	$\begin{bmatrix} 1 \times 1, 128 \\ 3 \times 3, 128 \\ 1 \times 1, 512 \end{bmatrix} \times 4$	$\begin{bmatrix} 1 \times 1, 128 \\ 3 \times 3, 128 \\ 1 \times 1, 512 \end{bmatrix} \times 4$	$\begin{bmatrix} 1 \times 1, 128 \\ 3 \times 3, 128 \\ 1 \times 1, 512 \end{bmatrix} \times 8$							
conv4_x	14×14	$\left[\begin{array}{c} 3\times3,256\\ 3\times3,256 \end{array}\right]\times2$	$\left[\begin{array}{c} 3 \times 3, 256 \\ 3 \times 3, 256 \end{array}\right] \times 6$	$\begin{bmatrix} 1 \times 1, 256 \\ 3 \times 3, 256 \\ 1 \times 1, 1024 \end{bmatrix} \times 6$	$\begin{bmatrix} 1 \times 1, 256 \\ 3 \times 3, 256 \\ 1 \times 1, 1024 \end{bmatrix} \times 23$	$\begin{bmatrix} 1 \times 1, 256 \\ 3 \times 3, 256 \\ 1 \times 1, 1024 \end{bmatrix} \times 36$							
conv5_x	7×7	$\left[\begin{array}{c} 3\times3,512\\ 3\times3,512 \end{array}\right]\times2$	$\left[\begin{array}{c}3\times3,512\\3\times3,512\end{array}\right]\times3$	$\begin{bmatrix} 1 \times 1, 512 \\ 3 \times 3, 512 \\ 1 \times 1, 2048 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 512 \\ 3 \times 3, 512 \\ 1 \times 1, 2048 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 512 \\ 3 \times 3, 512 \\ 1 \times 1, 2048 \end{bmatrix} \times 3$							
	1×1		ave	softmax	-								
FLOPs		1.8×10^{9}	3.6×10^{9}	3.8×10^{9}	7.6×10^9	11.3×10^9							



自然语言处理

Representation

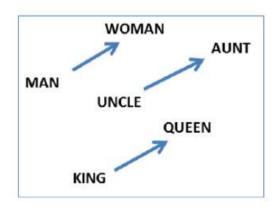
Word2Vector

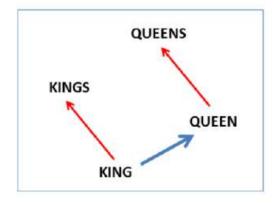


自然语言处理

Representation

Knowledge Embedding

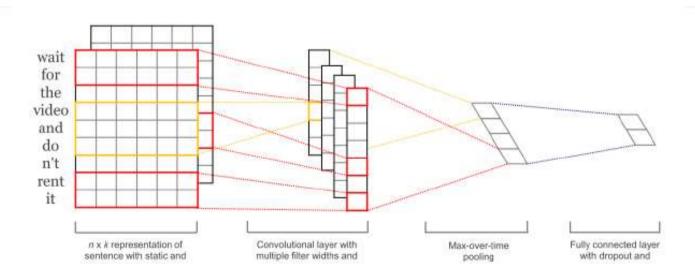




自然语言处理

Representation

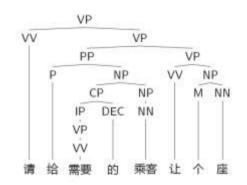
Sentence Modeling

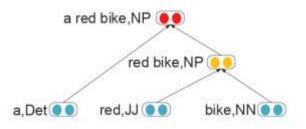


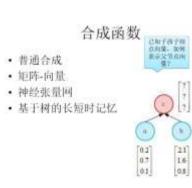
自然语言处理

Representation

Recursive Neural Network(结构的递归神经网络)

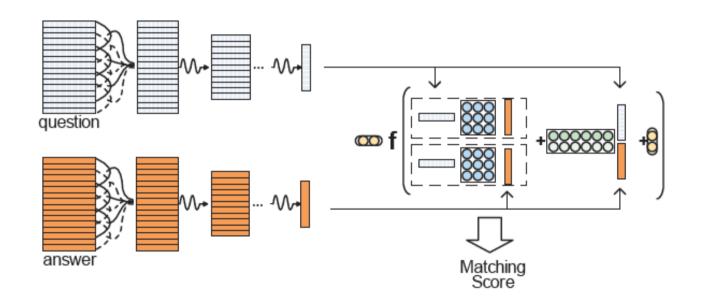






自然语言处理

Question Answering



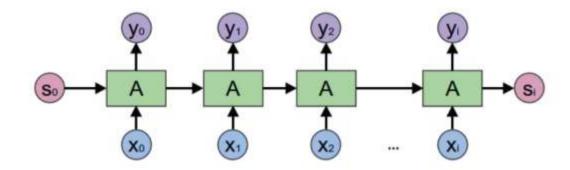
自然语言处理

Sequence to Sequence Modeling

• 输入: 任意长度的序列

• 输出:任意长度的序列

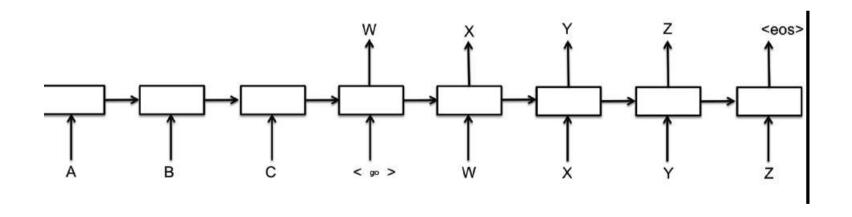
• 应用:语音识别、中文分词、词性标注



自然语言处理

Sequence to Sequence Modeling

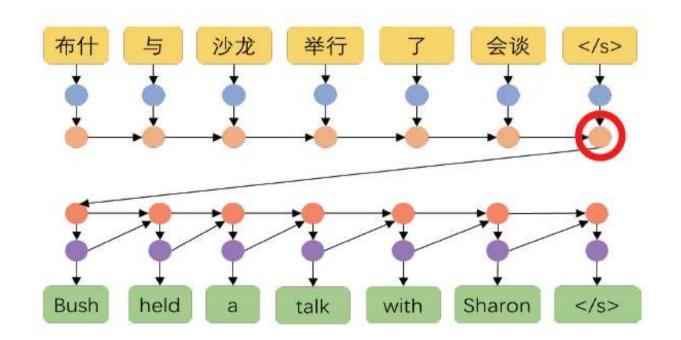
Encoder-Decoder
 自然语言中的典型应用:机器翻译、文档摘要、对话系统、自动问答。



自然语言处理

Sequence to Sequence Modeling

• 机器翻译例子



自然语言处理

Sequence to Sequence Modeling

Attention Model

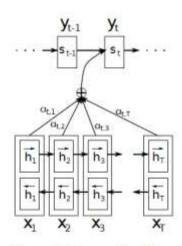


Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence (x_1, x_2, \ldots, x_T) .

$$\begin{split} \alpha_{ij} = & \frac{\exp\left(e_{ij}\right)}{\sum_{k=1}^{T_x} \exp\left(e_{ik}\right)} \\ e_{ij} = & v_a^{\top} \tanh\left(W_a s_{i-1} + U_a h_j\right), \end{split}$$

(Bahdanau, 2014)

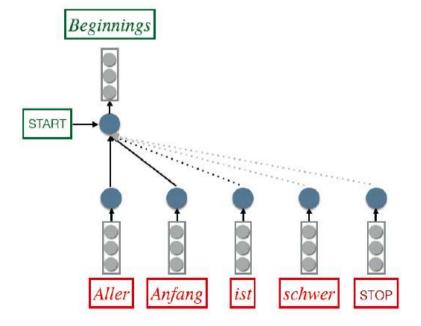
自然语言处理

Sequence to Sequence Modeling

• It seems too much to expect one vector of input c can do everything.

• During decoding, dynamically pay attention to different parts of the

input.



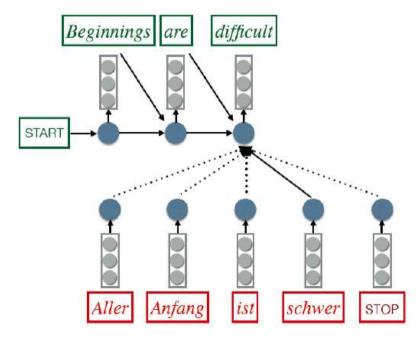
自然语言处理

Sequence to Sequence Modeling

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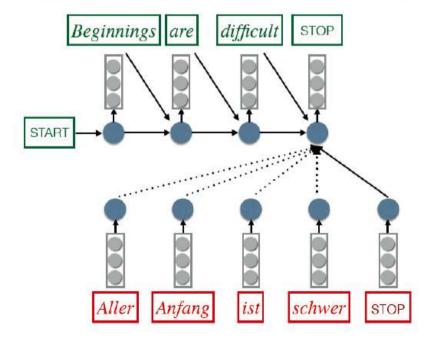
自然语言处理

Sequence to Sequence Modeling

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• During decoding, dynamically pay attention to different parts of the

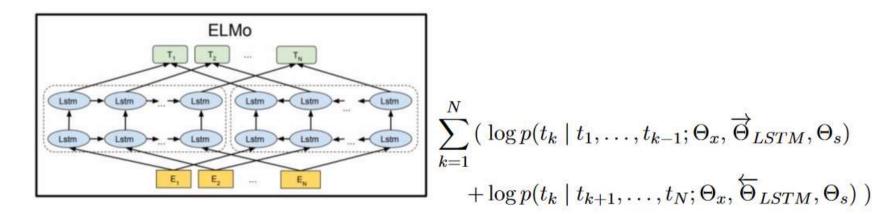
input.



自然语言处理

ELMo

• Pre-train bidirectional language models



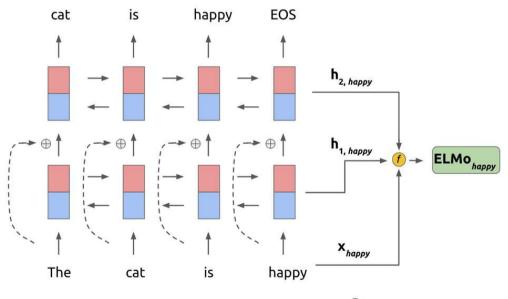
ELMo contextualized word representations

$$R_{k} = \{\mathbf{x}_{k}^{LM}, \overrightarrow{\mathbf{h}}_{k,j}^{LM}, \overleftarrow{\mathbf{h}}_{k,j}^{LM} \mid j = 1, \dots, L\}$$
$$= \{\mathbf{h}_{k,j}^{LM} \mid j = 0, \dots, L\},$$

自然语言处理

ELMo

• ELMo for supervised NLP tasks



$$\mathbf{ELMo}_k^{task} = E(R_k; \Theta^{task}) = \gamma^{task} \sum_{j=0}^{L} s_j^{task} \mathbf{h}_{k,j}^{LM}$$

自然语言处理

Transformer

- Positional Encoding
- Multi-Head Attention

Encoder: Over all words (self-attention)

Decoder: (1) Over previously generated words (self-attention)

(2) Between outputs of encoder and (1)

(not self-attention)

Residual Connection

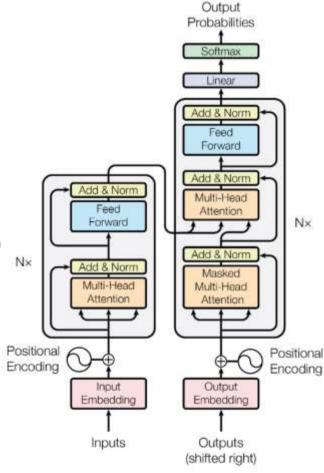
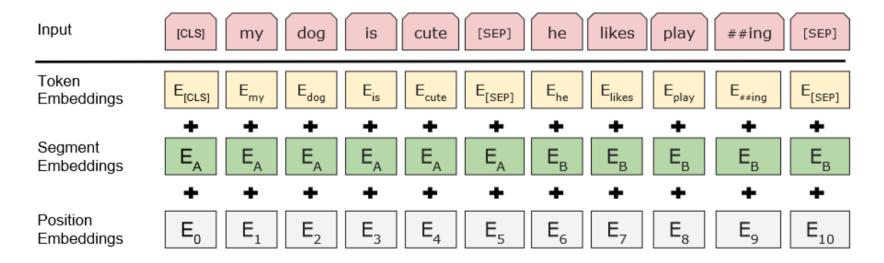


Figure 1: The Transformer - model architecture.

自然语言处理

BERT

- Model Architecture: Transformer Encoder
- Input Embedding:

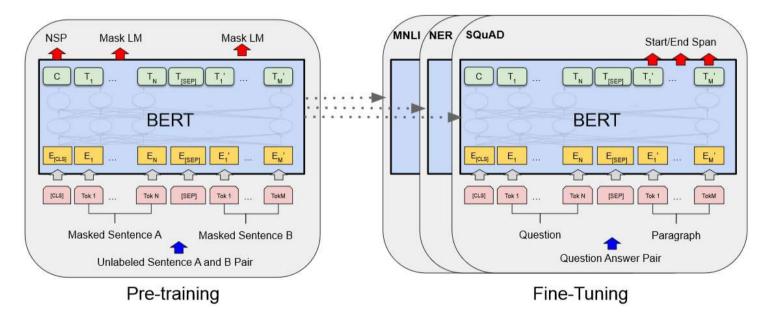


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自然语言处理

BERT

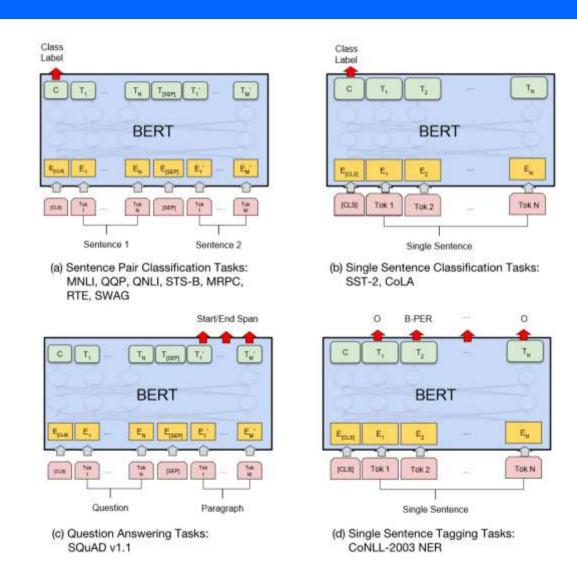
Pre-training BERT (Masked LM Task & Next Sentence Prediction Task)



自然语言处理

BERT

Fine-tuning BERT on different tasks



深度学习平台

Caffe

http://caffe.berkeleyvision.org

- From U.C. Berkeley
- Written in C++
- Has Python and MATLAB bindings
- Good for training or finetuning feedforward models

Torch

http://torch.ch

- From NYU + IDIAP
- Written in C and Lua
- Used a lot a Facebook, DeepMind

深度学习平台

Theano

http://deeplearning.net/software/theano/

- From Yoshua Bengio's group at University of Montreal 蒙特利尔(加拿大)
- Embracing computation graphs, symbolic computation
- High-level wrappers: Keras, Lasagne

TensorFlow

https://www.tensorflow.org

- From Google
- Very similar to Theano all about computation graphs
- Easy visualizations (TensorBoard)
- Multi-GPU and multi-node training

第十章 神经网络与深度学习

- 10.1 概述
- 10.2 多层感知机
- 10.3 卷积网络
- 10.4 Recurrent 网络
- 10.5 前沿概述

深度学习、生成对抗学习、强化学习、知识图谱

生成对抗模型原理

生成器 (Generator)

尽可能去学习真实样本的分布,迷惑鉴别器。

鉴别器 (Discriminator)

尽可能的正确判断输入数据是来自真实数据还是来自生成器。

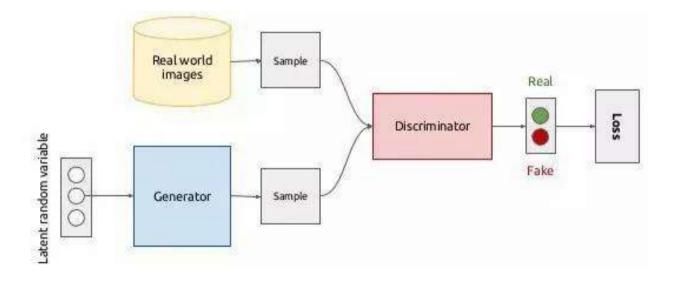
损失函数

$$\min_{G} \max_{D} V(D, G) = \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})} [\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})} [\log (1 - D(G(\boldsymbol{z})))]$$

训练过程

$$\min_{G} \max_{D} V(D,G) = \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log (1 - D(G(\boldsymbol{z})))]$$

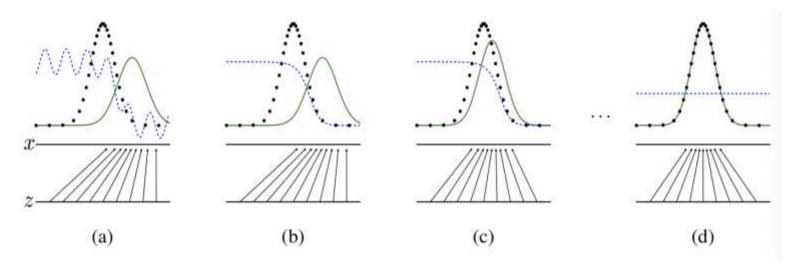
生成器与鉴别器交替训练,互相提升各自的生成能力和鉴别能力,最终寻找二者之间的一个纳什均衡。



训练过程

蓝色鉴别器输出的分布,黑色真实数据分布,绿色生成器输出分布

- (a) 初始化状态
- (b) 固定 G, 训练 D: 导致真实样本聚集区域 D 的输出大, 生成器输出集中区域 D 的输出小。
- (c) 固定 D, 训练 G; 导致 G 的输出集中区域向 D 值高的区域稍微移动。
- (d) 最终的纳什均衡状态。



算法流程

Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used k=1, the least expensive option, in our experiments.

for number of training iterations do

for k steps do

- Sample minibatch of m noise samples $\{z^{(1)}, \ldots, z^{(m)}\}$ from noise prior $p_q(z)$.
- Sample minibatch of m examples $\{x^{(1)}, \dots, x^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x}).$
- Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^m \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right) \right].$$

end for

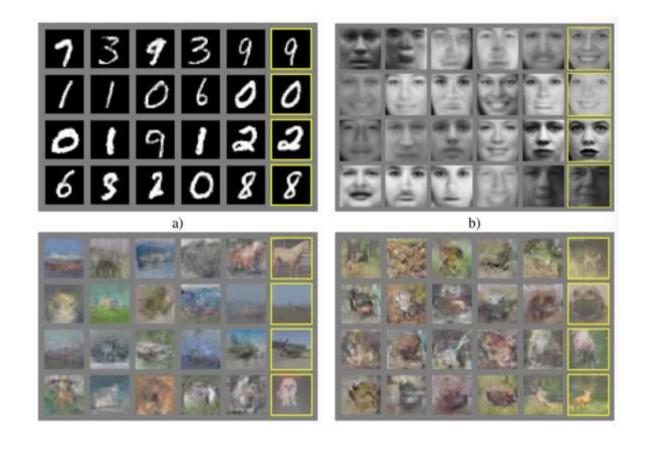
- Sample minibatch of m noise samples $\{z^{(1)}, \ldots, z^{(m)}\}$ from noise prior $p_a(z)$.
- Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log \left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right) \right).$$

end for

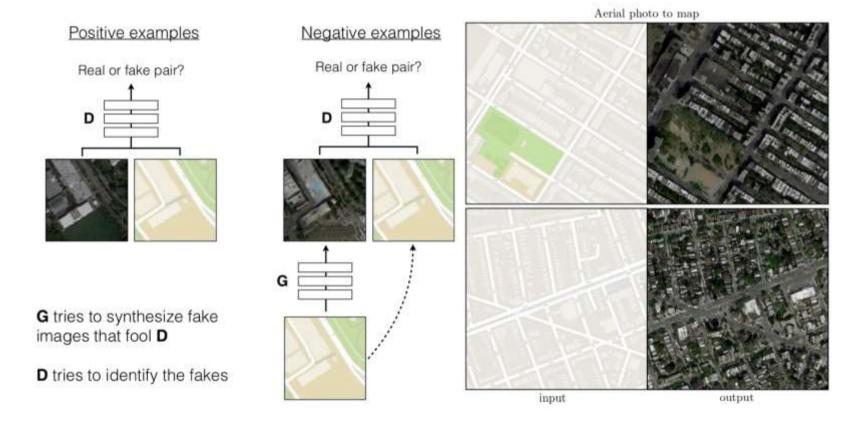
The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

生成效果



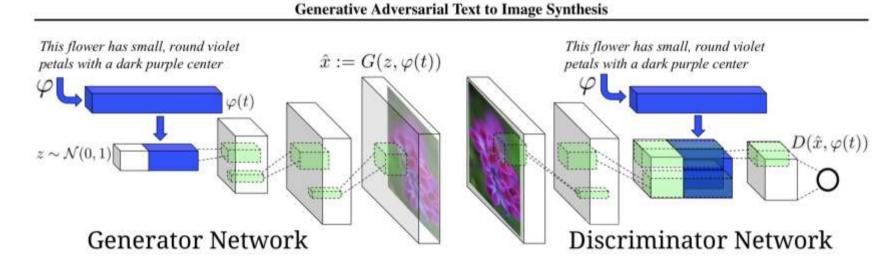
GAN 应用

• Image to Image



GAN 应用

Text to Image



GAN 应用

• Text to Image



GAN 应用

• Super-Resolution

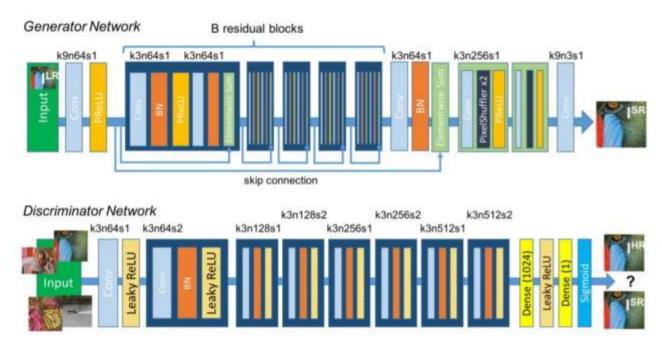


Figure 4: Architecture of Generator and Discriminator Network with corresponding kernel size (k), number of feature maps (n) and stride (s) indicated for each convolutional layer.

GAN 应用

• Super-Resolution

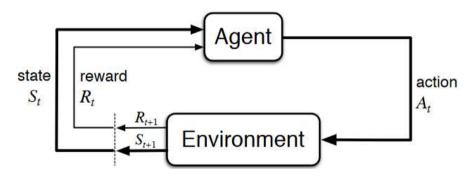


Figure 2: From left to right: bicubic interpolation, deep residual network optimized for MSE, deep residual generative adversarial network optimized for a loss more sensitive to human perception, original HR image. Corresponding PSNR and SSIM are shown in brackets. [4× upscaling]

马尔科夫决策过程

智能体环境交互

智能体的目标是最大化将来的期望累积奖励 (expected return)



Episodes:

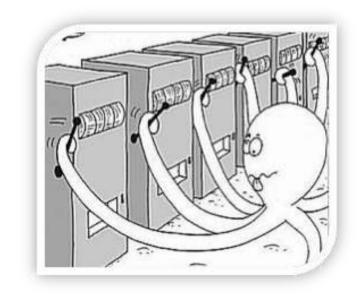
$$S_1$$
, a_1 , R_2 , S_2 , a_2 , R_3 , S_3 , a_3 , R_4 , ...

折扣回报(discounted return):

$$G_t \doteq R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \cdots = \sum_{k=0}^{\infty} \gamma^k R_{t+k+1}$$

多臂老虎机

问题: 一台赌博机有多个摇臂,每个摇臂摇出的奖励(reward)大小不确定,玩家希望摇固定次数的臂所获得的期望累积奖励最大.



多臂老虎机

形式化定义:行为 A_t 代表第 t 次选择哪个臂,奖励 R_t 代表第 t 次摇臂带来的奖励。采取行为a的期望奖励为:

$$q_*(a) \doteq \mathbb{E}[R_t | A_t = a]$$

假设一共要进行 T 次摇臂,在期望奖励未知的情况下,采取什么样的策略可以获得最大的累计奖励?

$$Q_t(a) \doteq \frac{\text{sum of rewards when } a \text{ taken prior to } t}{\text{number of times } a \text{ taken prior to } t} = \frac{\sum_{i=1}^{t-1} R_i \cdot \mathbb{1}_{A_i = a}}{\sum_{i=1}^{t-1} \mathbb{1}_{A_i = a}}$$

答案:可以使用 Qt(a)对 q*(a)进行估算。

多臂老虎机

贪心策略:

$$A_t \doteq \arg\max_{a} Q_t(a)$$

ε-贪心策略:

$$\pi(a|s) = \left\{ \begin{array}{ll} \epsilon/m + 1 - \epsilon & \text{if } a^* = \mathop{\mathrm{argmax}}\limits_{a \in \mathcal{A}} Q(s, a) \\ \epsilon/m & \text{otherwise} \end{array} \right.$$

深度强化学习

• Alpha-Go

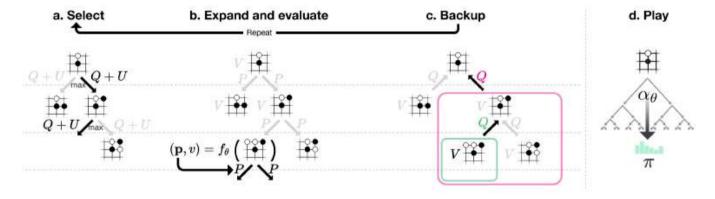


Figure 2: Monte-Carlo tree search in AlphaGo Zero. a Each simulation traverses the tree by selecting the edge with maximum action-value Q, plus an upper confidence bound U that depends on a stored prior probability P and visit count N for that edge (which is incremented once traversed). b The leaf node is expanded and the associated position s is evaluated by the neural network $(P(s,\cdot),V(s))=f_{\theta}(s)$; the vector of P values are stored in the outgoing edges from s. c Action-values Q are updated to track the mean of all evaluations V in the subtree below that action. d Once the search is complete, search probabilities π are returned, proportional to $N^{1/\tau}$, where N is the visit count of each move from the root state and τ is a parameter controlling temperature.

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深度强化学习

• SeqGAN

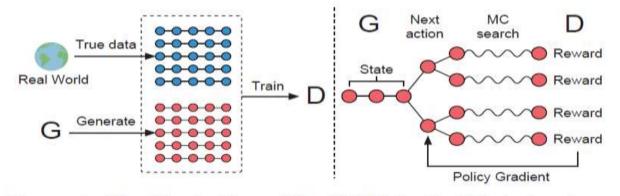


Figure 1: The illustration of SeqGAN. Left: D is trained over the real data and the generated data by G. Right: G is trained by policy gradient where the final reward signal is provided by D and is passed back to the intermediate action value via Monte Carlo search.

深度强化学习

• Visual navigation

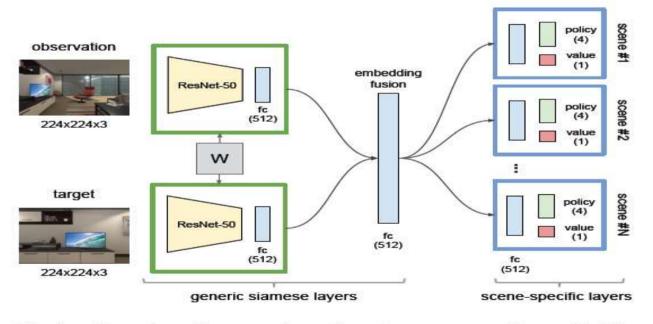


Fig. 4. Network architecture of our deep siamese actor-critic model. The numbers in parentheses show the output dimensions. Layer parameters in the green squares are shared. The ResNet-50 layers (yellow) are pre-trained on ImageNet and fixed during training.

背景

知识图谱的概念最早出现于 Google 公司的知识图谱项目,体现在使用 Google 搜索引擎时,出现于搜索结果右侧的相关知识展示。

截止到 2016 年底, Google 知识图谱中的知识数量已经达到了 600 亿条,关于 1500 个类别的 5.7 亿个实体,以及它们之间的 3.5 万种关系。

实体、关系和事实

实体(entity): 现实世界中可区分、可识别的事物或概念。

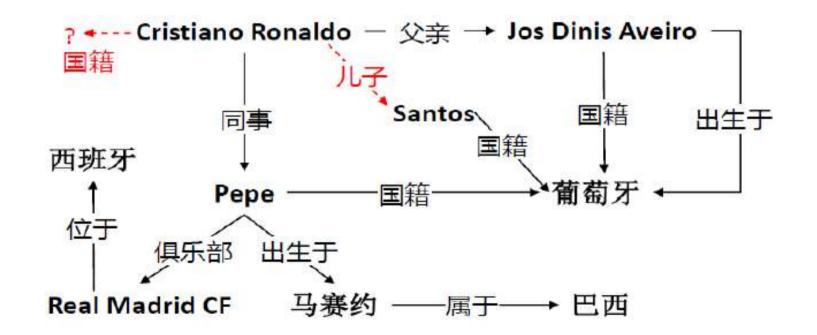
关系(relation):实体和实体之间的语义关联。

事实(fact): (head entity, relation, tail entity) 三元组形式。

狭义知识图谱

狭义知识图谱: 具有图结构的三元组知识库。

节点:实体。 边:事实(由头实体指向尾实体)。 边的类型:关系。



链接预测、三元组分类

知识图谱上的链接预测[Bordes et al., 2013]:

INPUT (HEAD AND LABEL)	PREDICTED TAILS
J. K. Rowling influenced by	G. K. Chesterton, J. R. R. Tolkien, C. S. Lewis, Lloyd Alexander, Terry Pratchett, Roald Dahl, Jorge Luis Borges, Stephen King, Ian Fleming
Anthony LaPaglia performed in	Lantana, Summer of Sam, Happy Feet, The House of Mirth, Unfaithful, Legend of the Guardians, Naked Lunch, X-Men, The Namesake
Camden County adjoins	Burlington County, Atlantic County, Gloucester County, Union County, Essex County, New Jersey, Passaic County, Ocean County, Bucks County
The 40-Year-Old Virgin nominated for	MTV Movie Award for Best Comedic Performance, BFCA Critics' Choice Award for Best Comedy, MTV Movie Award for Best On-Screen Duo, MTV Movie Award for Best Breakthrough Performance, MTV Movie Award for Best Movie, MTV Movie Award for Best Kiss, D. F. Zanuck Producer of the Year Award in Theatrical Motion Pictures, Screen Actors Guild Award for Best Actor - Motion Picture
Costa Rica football team has position	Forward, Defender, Midfielder, Goalkeepers, Pitchers, Infielder, Outfielder, Center, Defenseman
Lil Wayne born in	New Orleans, Atlanta, Austin, St. Louis, Toronto, New York City, Wellington, Dallas, Puerto Rico
WALL-E has the genre	Animations, Computer Animation, Comedy film, Adventure film, Science Fiction, Fantasy, Stop motion, Satire, Drama

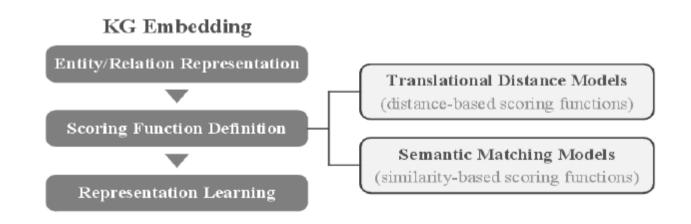
分布式知识表示方法分类[Wang et al., 2017]:

位移距离模型 (translational distance models):

采用基于距离的打分函数来衡量三元组成立的可能性。

语义匹配模型 (semantic matching models):

采用基于相似度的打分函数来衡量三元组成立的可能性。

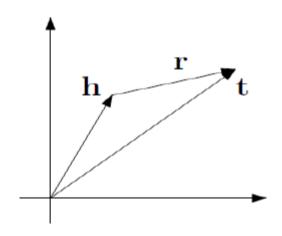


主要的方法

位移距离模型: TransE

TransE [Bordes et al., 2013] 是最具代表性的位移距离模型,其核心思想是实体和关系间的位移假设,即 $\mathbf{h} + \mathbf{r} \approx \mathbf{t}$

China – **Beijing** = **France** – **Paris** = **capital-of**



TransE

实体表示:向量 h, t

关系表示: 向量 r

位移操作: $h+r\approx t$

打分函数: $f(\mathbf{h}, r, t) = \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|_{1/2}$

语义匹配模型

计算实体和关系在隐式向量空间的语义匹配程度,以此来判断三元组成立的可能性。

简单匹配模型:RESCAL及其变种。

将头实体和尾实体的表示进行组合后再与关系的表示进行匹配,即:

Matching (relation, Composition (head, tail))

复杂匹配模型:深度神经网络。

利用较为复杂的神经网络结构完成实体和关系的语义匹配,即:

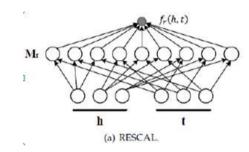
NueralMatching (head, relation, tail)

RESCAL 及其变种

将头尾实体的表示进行组合后再与关系的表示进行匹配。

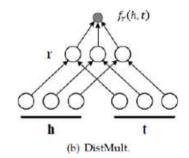
RESCAL [Nickel et al., 2011]

$$[\mathbf{h} \otimes \mathbf{t}]_{ij} = [\mathbf{h}]_i \cdot [\mathbf{t}]_j, \quad f_r(h,t) = \langle \mathbf{M}_r, \mathbf{h} \otimes \mathbf{t} \rangle = \sum_{i=0}^{d-1} \sum_{j=0}^{d-1} [\mathbf{M}_r]_{ij} \cdot [\mathbf{h}]_i \cdot [\mathbf{t}]_j$$



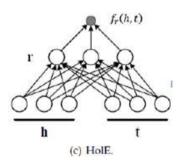
DistMult [Yang et al., 2015]

$$[\mathbf{h} \odot \mathbf{t}]_i = [\mathbf{h}]_i \cdot [\mathbf{t}]_i, \quad f_r(h,t) = \langle \mathbf{r}, \mathbf{h} \odot \mathbf{t} \rangle = \sum_{i=0}^{d-1} [\mathbf{r}]_i \cdot [\mathbf{h}]_i \cdot [\mathbf{t}]_i$$



HolE [Nickel et al., 2016]

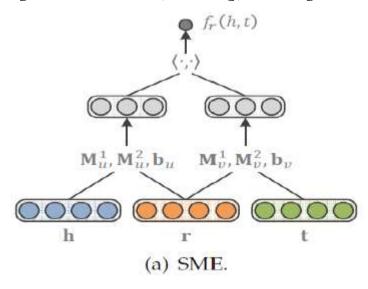
$$[\mathbf{h} \star \mathbf{t}]_i = \sum_{k=0}^{d-1} [\mathbf{h}]_k \cdot [\mathbf{t}]_{(k+i) \bmod d}, \quad f_r(h,t) = \langle \mathbf{r}, \mathbf{h} \star \mathbf{t} \rangle = \sum_{i=0}^{d-1} [\mathbf{r}]_i \sum_{k=0}^{d-1} [\mathbf{h}]_k \cdot [\mathbf{t}]_{(k+i) \bmod d}$$



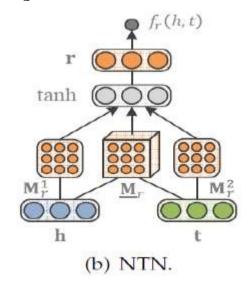
深度神经网络

利用神经网络结构完成实体和关系的语义匹配。

SME[Bordes et al., 2014], NTN[Socher et al., 2013]



$$f_r(h,t) = g_u(\mathbf{h}, \mathbf{r})^{\top} g_v(\mathbf{t}, \mathbf{r}).$$

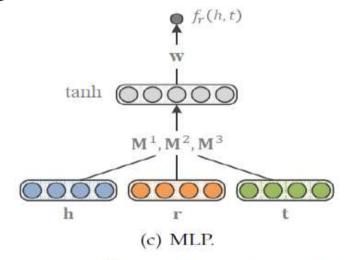


$$f_r(h, t) = \mathbf{r}^{\top} \tanh(\mathbf{h}^{\top} \underline{\mathbf{M}}_r \mathbf{t} + \mathbf{M}_r^1 \mathbf{h} + \mathbf{M}_r^2 \mathbf{t} + \mathbf{b}_r),$$

深度神经网络

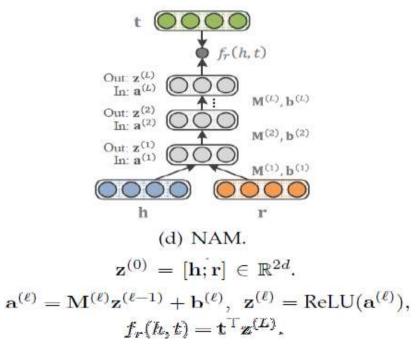
利用神经网络结构完成实体和关系的语义匹配。

MLP[Dong et al., 2014], NAM[Liu et al., 2016]



$$f_r(h,t) = \mathbf{w}^{\mathsf{T}} \tanh(\mathbf{M}^1 \mathbf{h} + \mathbf{M}^2 \mathbf{r} + \mathbf{M}^3 \mathbf{t}).$$

Chapter 10 Neural Network and Deep Learning (4)

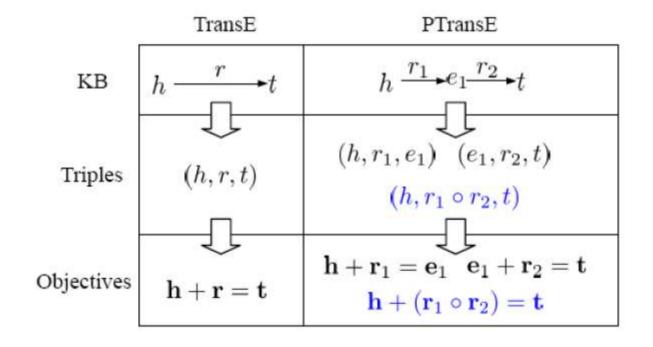


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融合关系路径:PTransE

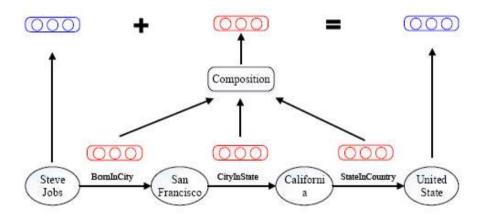
Path-based TransE (PTransE) [Lin et al., 2015a]:

关系路径可被视为远距离实体间的位移操作。



融合关系路径: PTransE

路径表示等于路径上关系表示的语义组合。



Addition : $\mathbf{p} = \mathbf{r}_1 + \ldots + \mathbf{r}_l$.

Multiplication : $\mathbf{p} = \mathbf{r}_1 \cdot \ldots \cdot \mathbf{r}_l$.

Recurrent Neural Network : $c_i = f(W[c_{i-1}; r_i]),$

融合关系路径:PTransE

建模三元组(h, r, t)

$$\mathcal{L}(h, r, t) = \sum_{(h', r, t') \in \mathcal{S}^{-}} \left[\gamma + \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|_{1} - \|\mathbf{h}' + \mathbf{r} - \mathbf{t}'\|_{1} \right]_{+}$$

建模关系路径(h, p, t)

$$\begin{split} E(h,p,t) &= ||\mathbf{p} - (\mathbf{t} - \mathbf{h})|| = ||\mathbf{p} - \mathbf{r}|| = E(p,r), \\ \mathcal{L}(p,r) &= \sum_{(h,r',t) \in \mathcal{S}^-} \left[\gamma + \|\mathbf{p} - \mathbf{r}\|_1 - \|\mathbf{p} - \mathbf{r}'\|_1\right]_+ \end{split}$$

联合学习

$$L(\mathbf{S}) = \sum_{(h,r,t) \in \mathbf{S}} \left[L(h,r,t) + \frac{1}{Z} \sum_{p \in P(h,t)} R(p|h,t) L(p,r) \right].$$

本讲参考文献

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- 2. Stanford Class-CS231n: Convolutional Neural Networks for Visual Recognition.
- 3. 第十一届中国中文信息学会暑期学校,暨中国中文信息学会《前沿技术讲习班》,201607。
- 4. Simon Haykin, Neural Network and Learning Machine. 3rd