

PyTorch

冯哲*

西安电子科技大学计算机学院

2019年2月

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*电子邮件: 1194585271@qq.com

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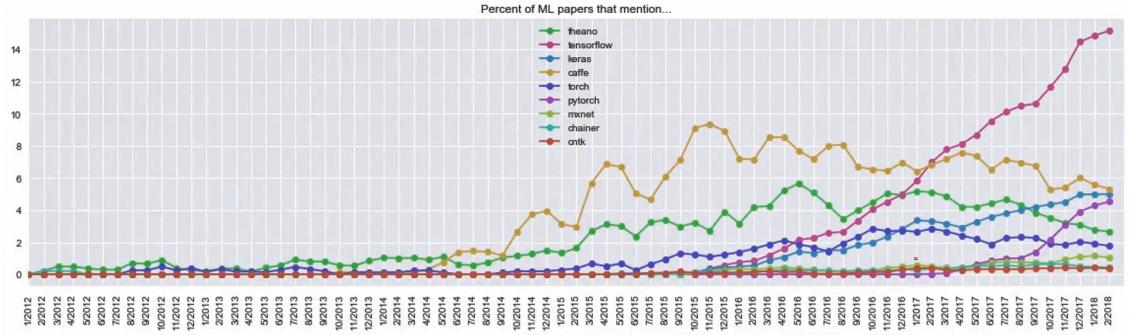
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1 PyTorch 简介

1.1 主流深度学习框架



1.2 两类深度学习框架的优缺点

1. 动态图(PyTorch)

计算图的进行与代码的运行时同时进行的。

2. 静态图(TensorFlow) 【* TensorFlow 2.0 动态图优先】

- 自建命名体系
- 自建时序控制
- 难以介入

1.3 使用深度学习框架的优点

- GPU 加速 (cuda)
- 自动求导
- 常用网络层的API

1.4 PyTorch 的特点

1. 支持 GPU

2. 动态神经网络

3. Python 优先

4. 命令式体验

5. 轻松扩展

2 安装环境准备

1. 操作系统选择 (Windows Linux MacOS) 均可
2. Python 开发环境安装 (Anaconda)
3. PyTorch 安装
 - (a) 安装 Nvidia Cuda
 - (b) 安装 CuDNN
 - (c) 安装 GPU 版本的 PyTorch
 - (d) 测试

配置环境: windows10,NVIDIA GEFORCE GTX 950M

具体安装过程:

1. 更新 nvidia 驱动
2. CUDA10 安装 (采用网络安装)
3. cuDNN7 安装 (解压配置系统变量)
4. Pytorch 安装 (阿里源 conda 安装)
5. 测试

3 初见深度学习

1. 梯度下降算法 (Gradient Decent) 深度学习的精髓。
2. 线性回归的损失函数 $Loss = (w^T x + b - y)^2$ 。
3. 利用梯度下降进行最小化损失函数迭代工作 (平均梯度信息)。
4. 引入手写字体识别问题 (MNIST)。
线性嵌套非线性映射 ReLu。

4 PyTorch 张量操作

4.1 基本数据类型

1. Python PyTorch 数据类型对比

python	PyTorch
Int	IntTensor of size()
float	FloatTensor of size()
Int array	IntTensor of size [d1, d2 ,...]
Float array	FloatTensor of size [d1, d2, ...]
string	--

2. PyTorch 是面向数值计算的 GPU 加速库，没有内建对 str 类型的支持。

- (a) one-hot $[0, 1, 0, 0, \dots]$
- (b) Embedding(常用的编码语言[NLP])
 - i. word2vec
 - ii. glove

3. PyTorch 内建的数据类型

Data type	dtype	CPU tensor	GPU tensor
32-bit floating point	<code>torch.float32</code> or <code>torch.float</code>	<code>torch.FloatTensor</code>	<code>torch.cuda.FloatTensor</code>
64-bit floating point	<code>torch.float64</code> or <code>torch.double</code>	<code>torch.DoubleTensor</code>	<code>torch.cuda.DoubleTensor</code>
16-bit floating point	<code>torch.float16</code> or <code>torch.half</code>	<code>torch.HalfTensor</code>	<code>torch.cuda.HalfTensor</code>
8-bit integer (unsigned)	<code>torch.uint8</code>	<code>torch.ByteTensor</code>	<code>torch.cuda.ByteTensor</code>
8-bit integer (signed)	<code>torch.int8</code>	<code>torch.CharTensor</code>	<code>torch.cuda.CharTensor</code>
16-bit integer (signed)	<code>torch.int16</code> or <code>torch.short</code>	<code>torch.ShortTensor</code>	<code>torch.cuda.ShortTensor</code>
32-bit integer (signed)	<code>torch.int32</code> or <code>torch.int</code>	<code>torch.IntTensor</code>	<code>torch.cuda.IntTensor</code>
64-bit integer (signed)	<code>torch.int64</code> or <code>torch.long</code>	<code>torch.LongTensor</code>	<code>torch.cuda.LongTensor</code>

4. PyTorch 基本数据类型

(a) 标量 (0维)

一维长度为1的张量确实也可以表示张量

为了语义更清晰，在版本PyTorch0.3之后，两个概念从形式上加以区分，并增加了长度为零的 tensor。

(b) 张量 (1维) Bias or Linear input (单张图片输入)

(c) 张量 (2维) Linear input batch (多张图片输入)

(d) 张量 (3维) RNN input Batch (循环神经网络批量输入)

[word,sentence,feature]

(e) 张量 (4维) CNN input Batch (卷积神经网络批量输入)

[batch,channel,height,width] 'r','g','b'三原色通道

5. 区分 dim size shape tensor

(a) dim :表示的是 rank。

(b) size (shape) :表示的是多少行，多少列，……。

(c) tensor :表示具体的数据。

4.2 创建 Tensor

1. import from numpy

```
torch.from_numpy()
```

2. import from list

```
torch.tensor() #data
    torch.tensor([1., 2.])
    torch.Tensor() #data or shape(size) == torch.FloatTensor()
        torch.Tensor([1., 2.]) #No use as far as possible
        torch.Tensor(2, 3)
```

3. uninitialized (未初始化的(有隐患极大与极小))

使用未初始化的数据一定要覆盖，否则可能会出现非常大或者非常小的数据。

导致出现 torch.nan or torch.inf 的 bug。

```
torch.empty() #shape
    torch.Tensor()
    torch.IntTensor()
    torch.FloatTensor()
```

4. set defalt type (设置默认的 tensor 数据类型)

```
In [61]: torch.tensor([1.2, 3]).type()
Out[61]: torch.DoubleTensor

In [62]: torch.set_default_tensor_type(torch.FloatTensor)

In [63]: torch.tensor([1.2, 3]).type()
Out[63]: torch.FloatTensor
```

5. 随机初始化 (rand/rand_like, randint)

```
rand()           input : shape [0,1]
randint(min,max,[shape]) [min,max)
rand_like()      input : tensor
randn()          input : shape      data ~ N(0,1)
torch.normal(mean=torch.full([10], 0), std=torch.arange(1, 0, -0.1))
```

6. 初始化为同一个数 (也可以是标量)

```
torch.full([shape],number)
```

7. 生成递增递减序列

```
arange/range    int
torch.arange(0, 10)      #[0, 10)
torch.arange(0, 10, 2)
torch.arange(10, 0, -1)
torch.range(0, 10)      #[0, 10] no use as far as possible

linspace/logspace float
torch.linspace(0, 10, steps=4) #four numbers
torch.logspace(-1, 0, steps=10) #10^n
```

8. ones/zeros/eyes

```
torch.ones()      #shape
torch.zeros()     #shape
torch.eye()       #shape      no more parameters
torch.*_like()   #tensor
```

9. randperm

生成随机种子功能类似于 `rondom.shuffle` 随机打散进行二元对应。

```
In : torch.randperm(10)
Out: tensor([0, 1, 4, 8, 2, 9, 5, 6, 3, 7])
```

4.3 索引和切片

1. indexing

```
a = torch.rand(10,3,28,28)
a[0].shape #第0张照片
a[0,0].shape #第0张照片的第0个通道
a[0,0,0].shape #第0张照片的第0个通道的第0行像素 dim为1
a[0,0,0,0] #第0张照片的第0个通道的第0行的第0个像素 dim为0
```

2. select first/last N/by step

```
a[:2].shape #取前两张图片
a[-2:].shape #取后两张图片

a[:2,:1].shape #取前两张图片的第一个通道
a[-2:,-2: ].shape #取后两张图片的后两个通道

a[:, :, 0:28:2, 0:28:2].shape #取全部图片的全部通道的长宽均间隔采样
```

3. select by specific index

```
a[2][1][18][26] #取第2张图片的第1通道的第18行26列的像素值, 标量
a.index_select(dim,tensor) #第一个参数表示维度, 第二个是tensor值
a.index_select(0,torch.tensor([0, 3, 3])) #选择第0第3第3张图片
a.index_select(1,torch.tensor([0,2])) #选择四张图片的第0和第2的通道
a.index_select(2,torch.arange(0,8)) #选择四张图片每个通道的前8所有列的像素
```

4. 符号 ... (选取足够多的维度可推测而省略:号)

```
a[...].shape
a[:3,...].shape
a[:,1,...].shape
a[...,:10].shape
a[0,...,:2].shape #间隔采样 ::
```

5. select by mask (依据掩码的位置信息索引)

```
x = torch.randn(3,3)
mask = x.ge(0.5) #>=0.5 的位置信息
torch.masked_select(x,mask) #得到所有>=0.5的tensor值
```

6. select by flatten index (打平索引)

```
src = torch.tensor([[1,2,3], [4,5,6]])
torch.take(src, torch.tensor([0,2,5])).shape #torch.Size([3])
torch.index_select() 类似torch.take 但是未打平
```

4.4 Tensor 维度变换

Tensor 常用API

1. View/reshape (不增加数据和减少数据)

```
a = torch.rand(4, 1, 28, 28)
a.shape #torch.Size([4, 1, 28, 28])
a.view(4,28, 28) #torch.Size([4, 28, 28])
a.reshape(4, 28*28).shape #torch.Size([4, 784]) 全链接层
a.reshape(4*28, 28)
存在问题，丢失维度逻辑信息，数据污染
b = a.reshape(4, 28*28)
b.reshape(4,1,28,28)
```

2. Squeeze(删减维度)/unsqueeze(增加维度)

Pos. Idx	0	1	2	3
	4	3	28	28
Neg. Idx	-4	-3	-2	-1

#unsqueeze 维度增加

```
尽量不要用负数 (不增加数据和减少数据) 插入范围 [-a.dim-1, a.dim+1)
a.shape #torch.Size([4, 1, 28, 28])
a.unsqueeze(0).shape #[1, 4, 1, 28, 28] 0维度前面插入一个维度
a.unsqueeze(-1).shape #[4, 1, 28, 28, 1] 在最后一个维度后面插入一个维度
a.unsqueeze(4).shape #[4, 1, 28, 28, 1]
a.unsqueeze(-5).shape #[1, 4, 1, 28, 28]
```

维度增加例子

```
a = torch.tensor([1.125, 2.258])
a,      #tensor([1.1250, 2.2580])
a.shape, #torch.Size([2])
a.unsqueeze(1), #tensor([[1.1250], [2.2580]])
a.unsqueeze(1).shape #torch.Size([2, 1])
a.unsqueeze(0), #tensor([[1.1250, 2.2580]])
a.shape, ##torch.Size([1, 2])
```

为了实现 `a+b` 先维度增加 `unsqueeze`, 在相关维度扩展后相加

```
b = torch.rand(32)
a = torch.rand(4, 32, 16, 16)
b = b.unsqueeze(1).unsqueeze(2).unsqueeze(0)
b.shape #torch.Size([1, 32, 1, 1])
```

`#squeeze` 压缩/挤压

```
a = torch.rand(1, 32, 1, 1)
a.squeeze().shape #torch.Size([32]) 尽可能多的删减维度
a.squeeze(0).shape #torch.Size([32, 1, 1])
a.squeeze(-2).shape #torch.Size([1, 32, 1])
a.squeeze(1).shape #torch.Size([1, 32, 1, 1]) 维度不变
```

3. Transpose (单次交换) /`t`/permute (多次交换) (维度交换)

```
a = torch.randn(3, 4)
a.t() 只能适用于二维转置
```

```
a = torch.randn(4, 3, 28, 28) 记录维度信息否则污染数据
b = a.transpose(1, 3).reshape(4, 3*28*28).reshape(4, 3, 28, 28) 数据污染
c = a.transpose(1, 3).reshape(4, 3*28*28).reshape(4, 28, 28, 3)
    .transpose(1, 3)
torch.all(torch.eq(a, b)) #tensor(0, dtype=torch.uint8)
torch.all(torch.eq(a, c)) #tensor(1, dtype=torch.uint8)
```

`transpose` 只能做单次交换 但 `permute` 可以做多次交换

```
a = torch.randn(4, 3, 28, 32) 目标 (4, 28, 32, 3)
a.transpose(1, 3).transpose(1, 2).shape #torch.Size([4, 28, 32, 3])
a.permute(0, 2, 3, 1).shape #torch.Size([4, 28, 32, 3])
```

4. Expend/repeat (维度扩展)

Expand: broadcasting 推荐使用, 内存无关, 节约内存。

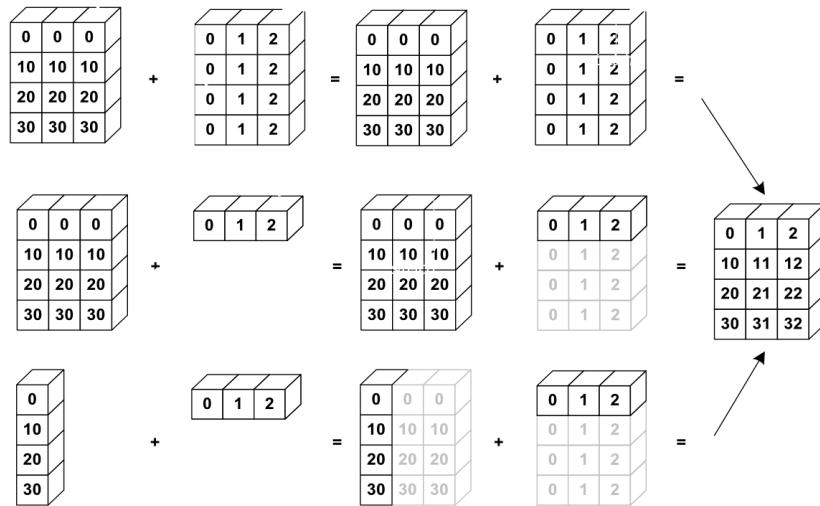
Repeat: memory copied 内存相关。

```
#rexpand 表示扩展到的维度
b = torch.rand(1, 32, 1, 1) 维度元素才可expand, repeat没有此条限制
b.expand(4, 32, 16, 16).shape #torch.Size([4, 32, 16, 16])
b.expand(-1, 32, 16, 16).shape #torch.Size([1, 32, 16, 16])
b.expand(-1, 32, -1, -4).shape #torch.Size([1, 32, 1, -4]) -4 bug 无意义
#repeat 表示复制次数
b.repeat(4, 1, 16, 16).shape #torch.Size([4, 32, 16, 16])
b.repeat(4, 2, 16, 16).shape #torch.Size([4, 64, 16, 16])
```

5 张量高阶操作

5.1 Broadcast

Broadcast (expand+withoutcopying) [广播机制]



关键步骤:

1. Insert 1 dim ahead (unsqueeze)
2. Expand dims with size 1 to same size
3. Feature maps: [4, 32, 14, 14]
4. Bias: [32, 1, 1] \Rightarrow [1, 32, 1, 1] \Rightarrow [4, 32, 14, 14]

存在意义:

1. for actual demanding(实际需求)

- $[class, students, scores]$
- Add bias for every student: $+5score$
- $[4, 32, 8] + [4, 32, 8]$
- $[4, 32, 8] + [5.0]$

2. memory consumption(节约内存)

- $[4, 32, 8] \Rightarrow 1024$
- $[5.0] \Rightarrow 1$

使用环境: match from last dim

1. If current dim=1, expand to same
2. If either has no dim, insert one dim and expand to same
3. otherwise, NOT broadcasting-able

具体案例:

1. Situation 1

- [4, 32, 14, 14]
- [1, 32, 1, 1] => [4, 32, 14, 14]

2. Situation 2

- [4, 32, 14, 14]
- [14, 14] => [1, 1, 14, 14] => [4, 32, 14, 14]

3. Situation 3

- [4, 32, 14, 14]
- [2, 32, 14, 14] => error

```
a = torch.rand(1,3)
b = torch.rand(3,1)
(a+b).shape #torch.Size([3, 3])
a = torch.rand(4, 32, 14, 14)
b = torch.rand(1, 32, 1, 1)
(a+b).shape #torch.Size([4, 32, 14, 14])
a = torch.rand(4, 32, 14, 14)
b = torch.rand(14, 14)
(a+b).shape #torch.Size([4, 32, 14, 14])
a = torch.rand(4, 32, 14, 14)
b = torch.rand(2, 32, 14, 14)
(a+b).shape error
(a+b[0]).shape #torch.Size([4, 32, 14, 14]) 手动指定
a = torch.rand(2, 3, 6, 6)
b = torch.rand(1, 3, 6, 1) 给每一个通道的每一行加上相同的像素值
(a+b).shape
```

5.2 Tensor 分割与合并

Tensor 分割与合并(Merge or split)

1. Cat 合并，不增加维度，cat维度可以不同。

```
a = torch.rand(4, 32, 8) #[classes, students, scores]
b = torch.rand(5, 32, 8)
torch.cat([a, b], dim=0).shape #torch.Size([9, 32, 8])
```

2. Stack 合并，创建新的维度，旧维度必须一致。

```
a = torch.rand(32, 8) #[students, scores]
b = torch.rand(32, 8)
c = torch.rand(32, 8)
torch.stack([a, b, c], dim=0).shape #torch.Size([3, 32, 8])
```

3. Split 根据长度来拆分。

```
a = torch.rand(4, 32, 8) #[classes, students, scores]
aa, bb, cc = a.split([1, 2, 1], dim=0)
aaa, bbb = a.split(2, dim=0)
aa.shape #torch.Size([1, 32, 8])
bb.shape #torch.Size([2, 32, 8])
cc.shape #torch.Size([1, 32, 8])
aaa.shape #torch.Size([2, 32, 8])
bbb.shape #torch.Size([2, 32, 8])
```

4. Chunk 根据数量来拆分。

```
a = torch.rand(6, 32, 8) #[classes, students, scores]
aa, bb = a.chunk(2, dim=0)
cc, dd, ee = a.split(2, dim=0)
aa.shape #torch.Size([3, 32, 8])
bb.shape #torch.Size([3, 32, 8])
cc.shape #torch.Size([2, 32, 8])
dd.shape #torch.Size([2, 32, 8])
ee.shape #torch.Size([2, 32, 8])
```

5.3 Tensor 运算

tensor 矩阵的基本运算

1. Add-minus/multiply/divide

```
a = torch.rand(4,3)
b = torch.rand(3)
torch.all(torch.eq(a+b, torch.add(a,b))) #tensor(1, dtype=torch.uint8)
a-b #torch.sub
a*b #torch.mul
a/b #torch.div
a//b 地板除
```

2. Matmul

最后两维做矩阵乘运算，其他符合broadcast机制

```
a = torch.rand(4,3)
b = torch.rand(3,8)
torch.mm(a, b) #only for 2d
(a @ b).shape #torch.matmul torch.Size([4, 8])
```

3. Pow

```
a**2 #torch.pow
```

4. Sqrt/rsqrt/exp/log

平方根/平方根的倒数/自然常数幂/自然常数底

```
a.sqrt() #a**0.5
a.rsqrt()
torch.exp(a) #e**a
```

5. Round 近似运算

```
a = torch.tensor(3.14) #tensor(3.14)
a.floor(), a.ceil(), a.round() #tensor(3.) tensor(4.) tensor(3.)
a.trunc() #tensor(3.)
a.frac() #tensor(0.1400)
```

6. clamp 数字裁剪

使用环境 '梯度裁剪'

梯度弥散 (梯度非常小 $< 0.*$)， 梯度爆炸 (梯度非常大 $> *00$)

打印梯度的 L2 范数观察 (W.grad.norm(2))

```
grad = torch.rand(3,4)*15
grad.min() #min number
grad.max() #max number
grad.median() #medoan number
grad.clamp(10) #min number is 10
grad.clamp(0, 10) #all numbers is [0,10]
```

5.4 Tensor 统计

1. norm

表示范数，不同于 normalize (正则化)

vector norm

$$\begin{aligned} \|x\|_1 &= \sum_{i=1}^n |a_i| \\ \|x\|_e &= \sqrt{\sum_{i=1}^n x_i^2} \\ \|x\|_p &= \left(\sum_{i=1}^n |x_i|^p \right)^{\frac{1}{p}} \end{aligned}$$

matrix norm

$$\begin{aligned} \|A\|_1 &= \max_{i \leq j \leq n} \sum_{i=1}^n |a_{ij}| \\ \|A\|_e &= \sqrt{\sum_{i=1}^n \sum_{j=1}^n a_{ij}^2} \\ \|A\|_p &= \left(\sum_{i=1}^n \sum_{j=1}^n a_{ij}^2 \right)^{\frac{1}{p}} \end{aligned}$$

```
a = torch.full([8], 1)
b = a.reshape(2, 4)
c = b.reshape(2, 2)
a  #tensor([1., 1., 1., 1., 1., 1., 1., 1.])
b  #tensor([[1., 1., 1., 1.], [1., 1., 1., 1.]])
a.norm(1), b.norm(1), c.norm(1) #tensor(8.)
a.norm(2), b.norm(2), c.norm(2) #tensor(2.8284)
#two parameters norm, dimension
a.norm(1, dim=0) #tensor(8.)
b.norm(1, dim=1) #tensor([4., 4.])
c.norm(2, dim=2) #tensor([[1.4142, 1.4142], [1.4142, 1.4142]])
```

2. max, min, mean, sum, prod(累乘)

```
a = torch.arange(8).reshape(2,4).float()  
a.min() #tensor(0.)  
a.max() #tensor(7.)  
a.mean() #tensor(3.5)  
a.mean(1) #tensor([1.5000, 5.5000])  
a.sum() #tensor(28.)  
a.prod() #tensor(0.)
```

3. argmin, argmax (参数 dim, keepdim)

```
a = torch.randn(4, 10) 4张照片 0-9 10个概率值  
a.argmin() a.argmax() 无参数默认打平  
a.argmax(1) 返回每张照片概率最大的数字  
a.argmax(1, keepdim=True) 返回每张照片概率最大的数字并保持维度信息  
a.max(1) 返回每张照片最大的概率及数字
```

4. Kthvalue, topk(比 max 返回更多的数据)

```
a = torch.randn(4, 10) 4张照片 0-9 10个概率值  
a.topk(2, dim=1, largest=True)) largest = False 表示最小的 k 个  
a.kthvalue(10, dim=1) 返回第10小的概率及位置
```

5. compare (比较操作)

>, <, >=, <=, !=, ==
torch.eq() 可 broadcast, 返回 0/1 同型
torch.equal() 比较每一值, 都相等返回 True

5.5 Tensor 高阶操作

1. where (GPU 离散复制)

```
torch.where(condition, x, y) --> Tensor 满足条件取 x, 否则取 y  
其功能可由for 逻辑功能实现, 但运行在CPU, 难以高度并行  
condition 必须是与 x, y 同型的1/0型 x, y可 broadcast  
a = torch.rand(2, 2)  
b = torch.ones(2, 2)  
c = torch.zeros(2, 2)  
torch.where(a>0.5, b, c)
```

2. Gather (GPU 收集查表操作)

```
torch.gather(input, dim, index, out=None) --> Tensor 查表操作  
out[i][j][k] = input[index[i][j][k]][j][k] dim=0  
out[i][j][k] = input[i][index[i][j][k]][k] dim=1  
out[i][j][k] = input[i][j][index[i][j][k]] dim=2
```

Gather 查表用来索引全局标签

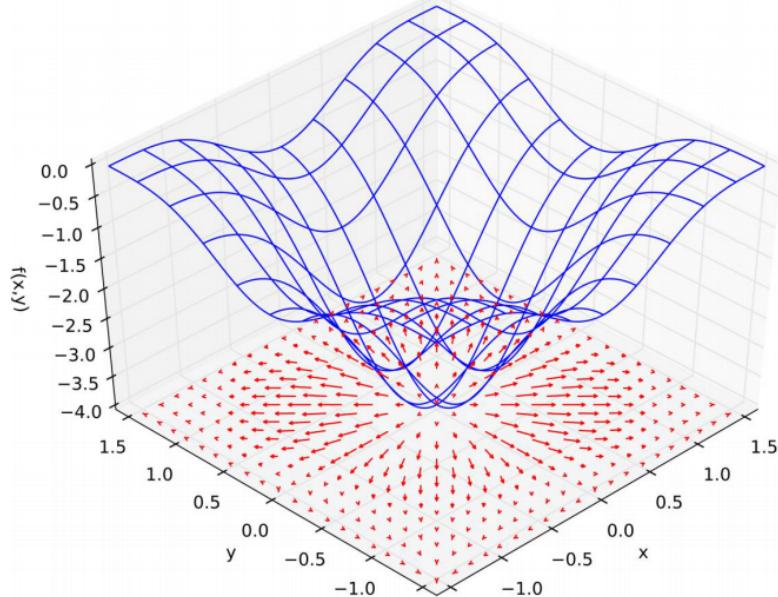
```
prob = torch.rand(4, 10) 四张图片十个概率值  
idx = prob.topk(3, dim=1)[1]  
label = torch.arange(10)+100  
torch.gather(label.expand(4, 10), dim=1, index=idx)  
共四张图片每张查概率最大的三个标签
```

6 随机梯度下降

6.1 梯度

1. 导数 (标量)
2. 偏微分 (函数延某个方向的变换量 标量)
3. 梯度 (函数变化量最大的方向 向量)

梯度的意义：模为变换率大小，矢量方向。



如何求取最小值：梯度下降

$$\theta_{t+1} = \theta_t - \alpha_t \nabla f(\theta_t)$$

Function :

$$J(\theta_1, \theta_2) = \theta_1^2 + \theta_2^2$$

Object :

$$\min_{\theta_1, \theta_2} J(\theta_1, \theta_2)$$

Update rules :

$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1, \theta_2)$$

$$\theta_2 := \theta_2 - \alpha \frac{d}{d\theta_2} J(\theta_1, \theta_2)$$

Derivatives :

$$\frac{d}{d\theta_1} J(\theta_1, \theta_2) = 2\theta_1$$

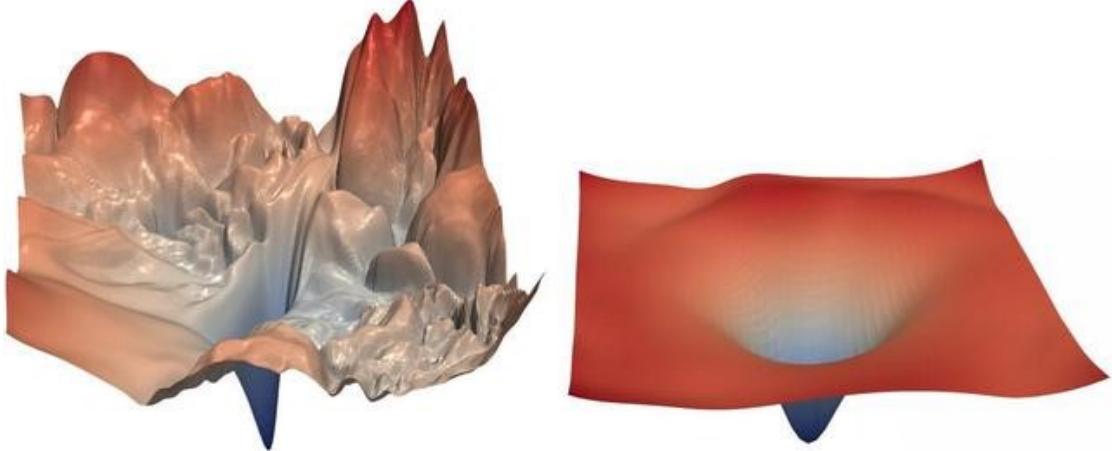
$$\frac{d}{d\theta_2} J(\theta_1, \theta_2) = 2\theta_2$$

影响优化器优化精度的两个重要因素：

1. 局部极小值
2. 鞍点

凸函数才会有全局最小值，通常情况下存在局部极小值。

(ResNet-56 论文-2018 何凯明)



影响优化器搜索过程效果的因素：

1. 初始状态
2. 学习率
3. 动量（逃离局部极小值）
4. ...

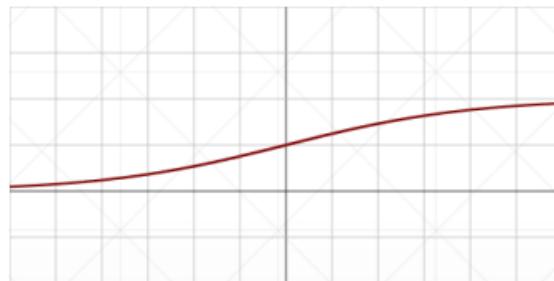
6.2 常见函数的梯度

函数类型	函数	导数
常函数	c	0
线性函数	ax	a
二次函数	ax^2	$2ax$
幂函数	x^a	ax^{a-1}
指数函数	a^x e^x	$a^x \ln a$ e^x
对数函数	$\log_a(x)$ $\ln x$	$1/(x \ln a)$ $1/x$
三角函数	$\sin(x)$ $\cos(x)$ $\tan(x)$	$\cos(x)$ $-\sin(x)$ $\sec(x)$

6.3 激活函数

1. Sigmoid/Logistic 会伴随严重的梯度弥散现象（长时间梯度的不到更新）。

$$f(x) = \sigma(x) = \frac{1}{1 + e^{-x}} \quad [0, 1]$$



求导：

$$\begin{aligned} \frac{d}{dx} \sigma(x) &= \frac{d}{dx} \left(\frac{1}{1 + e^{-x}} \right) = \frac{e^{-x}}{(1 + e^{-x})^2} \\ &= \frac{e^{-x} + 1 - 1}{(1 + e^{-x})^2} = \sigma(1 - \sigma) \end{aligned}$$

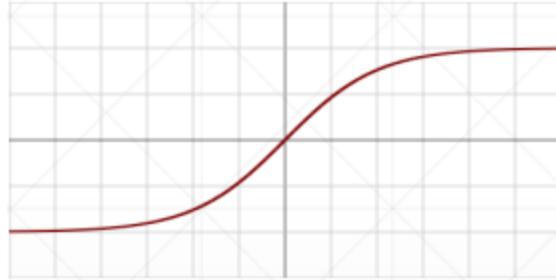
```

z = torch.linspace(-100, 100, 5)
z  #tensor([-100., -50.,  0.,  50., 100.])
torch.sigmoid(z) #tensor([0.00e+00, 1.92e-22, 5.00e-01, 1.00e+00, 1.00e+00])

```

2. tanh 常用于循环神经网络

$$f(x) = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\text{sigmoid}(2x) - 1 \quad [-1, 1]$$



求导:

$$\frac{d}{dx} \tanh(x) = 1 - \tanh^2(x)$$

```
z = torch.linspace(-2, 2, 5)
z  #tensor([-2., -1., 0., 1., 2.])
torch.tanh(z) #tensor([-0.9640, -0.7616, 0.0000, 0.7616, 0.9640])
```

2. ReLu Rectified Linear Unit 整形的线性单元 (最常用的激活函数)

$$f(x) = \begin{cases} 0 & x < 0 \\ x & \geq 0 \end{cases}$$

求导:

$$f(x) = \begin{cases} 0 & x < 0 \\ 1 & x \geq 0 \end{cases}$$



```
z = torch.linspace(-2, 2, 5)
z  #tensor([-2., -1., 0., 1., 2.])
torch.relu(z) #tensor([0., 0., 0., 1., 2.])
```

6.4 Loss 损失函数的梯度

典型的损失函数:

1. Mean Squared Error(均方误差)
2. Cross Entropy Loss(交叉熵损失)

- 可用于二分类
- 可扩展为多分类
- 常与 softmax 函数搭配使用

1. Mean Squared Error(均方误差)

- $loss = \sum (y - (w * x + b))^2$
 $loss = \text{norm}(y - (w * x + b))^2$
- $\frac{\nabla loss}{\nabla \theta} = 2 \sum (y - f_\theta(x)) * \frac{\nabla f_\theta(x)}{\nabla \theta}$
- Gradient API:

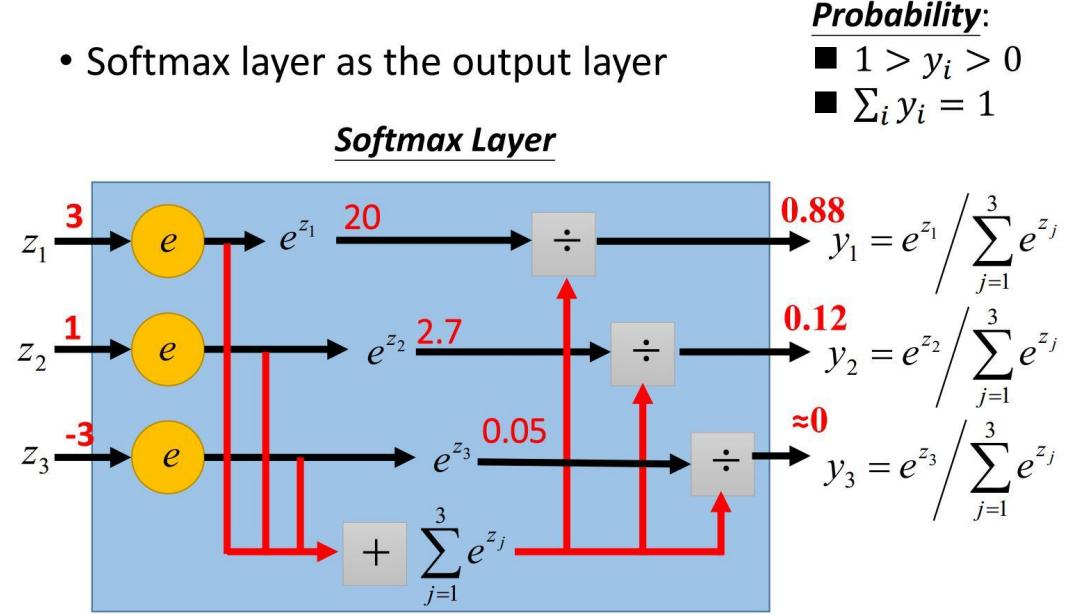
```
1.torch.autograd.grad(loss, [w1, w2, ...])
    [w1 grad, w2 grad, ...]
2.loss.backward()
    w1.grad
    w2.grad
    ...

#Mean Square Error (MSE)
x = torch.ones(1)
y = torch.ones(1)
w = torch.full([1], 2, requires_grad=True)
mse = F.mse_loss(y,w*x)      #(y-w*x)
mse  #tensor(1., grad_fn=<MeanBackward1>)
#1.auto.grad (requires_grad)
torch.autograd.grad(mse, w) #(tensor([2.]),)
#2.backward
mse = F.mse_loss(y,w*x)      #(y-w*x)
mse.backward()
w.grad  #tensor([2.])
```

2. Cross Entropy Loss(交叉熵损失)

3. Softmax

$$p_i = \frac{e^{a_i}}{\sum_{k=1}^N e^{a_k}}$$



1. 转移成概率值

2. 拉大值之间的差距

Softmax 求导:

$$\frac{\partial p_i}{\partial a_j} = \frac{\partial \frac{e^{a_i}}{\sum_{k=1}^N e^{a_k}}}{\partial e^{a_j}}$$

$$f(x) = \frac{g(x)}{h(x)}, \quad f'(x) = \frac{g'(x)h(x) - h'(x)g(x)}{h^2(x)}$$

$$g(x) = e^{a_i}, \quad h(x) = \sum_{k=1}^N e^{a_k}$$

$$i == j$$

$$i \neq j$$

$$\begin{aligned} \frac{\partial \frac{e^{a_i}}{\sum_{k=1}^N e^{a_k}}}{\partial e^{a_j}} &= \frac{e^{a_i} \sum_{k=1}^N e^{a_k} - e^{a_j} e^{a_i}}{\left(\sum_{k=1}^N e^{a_k}\right)^2} \\ &= \frac{e^{a_i} \left(\sum_{k=1}^N e^{a_k} - e^{a_j}\right)}{\left(\sum_{k=1}^N e^{a_k}\right)^2} \\ &= p_i (1 - p_j) \end{aligned}$$

$$\begin{aligned} \frac{\partial \frac{e^{a_i}}{\sum_{k=1}^N e^{a_k}}}{\partial e^{a_j}} &= \frac{0 - e^{a_j} e^{a_i}}{\left(\sum_{k=1}^N e^{a_k}\right)^2} \\ &= -\frac{e^{a_i}}{\sum_{k=1}^N e^{a_k}} \frac{e^{a_j}}{\sum_{k=1}^N e^{a_k}} \\ &= -p_i p_j \end{aligned}$$

总结:

$$\frac{\partial p_i}{\partial a_j} = \begin{cases} p_i(1 - p_i) & i == j \\ -p_i p_j & i \neq j \end{cases}$$

利用:

$$\delta_{ij} = \begin{cases} 1 & i == j \\ 0 & i \neq j \end{cases}$$

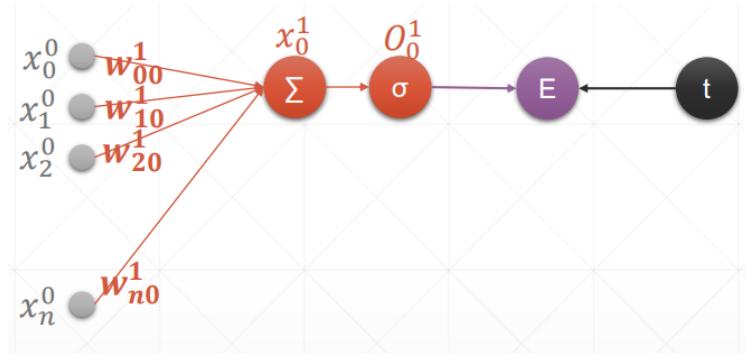
得到公式:

$$\frac{\partial p_i}{\partial a_j} = p_i(\delta_{ij} - p_j)$$

```
from torch.nn import functional as F
a = torch.rand(3, requires_grad=True)
p = F.softmax(a, dim=0)
#tensor([0.4588, 0.0768, 0.0897], requires_grad=True)
p #tensor([0.4212, 0.2875, 0.2912], grad_fn=<SoftmaxBackward>)
torch.autograd.grad(p[0], a, retain_graph=True) #output scalar
#(tensor([ 0.2438, -0.1211, -0.1227]),)
```

7 感知机梯度传播推导

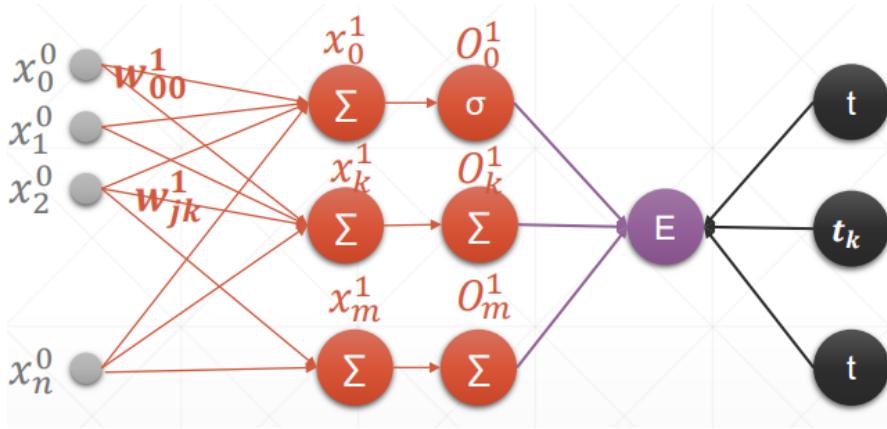
7.1 单一输出感知机



$$\begin{aligned}E &= \frac{1}{2}(O_0^1 - t)^2 \\ \frac{\partial E}{\partial w_{j0}} &= (O_0^1 - t) \frac{\partial O_0^1}{\partial w_{j0}} = (O_0^1 - t) \frac{\partial \sigma(x_0^1)}{\partial w_{j0}} \\ \frac{\partial E}{\partial w_{j0}} &= (O_0^1 - t) \sigma(x_0^1) (1 - \sigma(x_0^1)) \frac{\partial x_0^1}{\partial w_{j0}} \\ \frac{\partial E}{\partial w_{j0}} &= (O_0^1 - t) \sigma(x_0^1) (1 - \sigma(x_0^1)) x_j^0 \\ \frac{\partial E}{\partial w_{j0}} &= (O_0^1 - t) O_0^1 (1 - O_0^1) x_j^0\end{aligned}$$

```
x = torch.randn(1, 10)
w = torch.randn(1, 10, requires_grad=True)
o = torch.sigmoid(x @ w.t())
o.shape    #torch.Size([1, 1])
loss = F.mse_loss(torch.ones(1, 1), o)
loss.shape  #torch.Size([]) scalar
loss.backward()
w.grad    #tensor([[ 2.1023e-04, -4.6425e-04,  2.1561e-04, ...]])
```

7.2 多输出感知机



$$E = \frac{1}{2} \sum_{i=0}^m (O_i^1 - t)^2$$

$$\frac{\partial E}{\partial w_{jk}} = (O_k^1 - t_k) \frac{\partial O_k^1}{\partial w_{jk}} = (O_k^1 - t_k) \frac{\partial \sigma(x_k^1)}{\partial w_{jk}}$$

$$\frac{\partial E}{\partial w_{jk}} = (O_k^1 - t_k) \sigma(x_k^1) (1 - \sigma(x_k^1)) \frac{\partial x_k^1}{\partial w_{jk}}$$

$$\frac{\partial E}{\partial w_{jk}} = (O_k^1 - t_k) \sigma(x_k^1) (1 - \sigma(x_k^1)) x_j^0$$

$$\frac{\partial E}{\partial w_{jk}} = (O_k^1 - t_k) O_k^1 (1 - O_k^1) x_j^0$$

```

x = torch.rand(1, 10)
w = torch.rand(2, 10, requires_grad=True)
o = torch.sigmoid(x@w.t())
o.shape    #torch.Size([1, 2])
loss = F.mse_loss(torch.ones(1,2), o)
loss      #tensor(0.0158, grad_fn=<MeanBackward1>)
loss.backward()
w.grad.shape    #torch.Size([2, 10])

```

7.3 链式法则

7.3.1 求导法则

Rules	Function	Derivative
Multiplication by constant	cf	cf'
Power Rule	x^n	nx^{n-1}
Sum Rule	$f + g$	$f' + g'$
Difference Rule	$f - g$	$f' - g'$
Product Rule	fg	$f g' + f' g$
Quotient Rule	f/g	$(f' g - g' f)/g^2$
Reciprocal Rule	$1/f$	$-f'/f^2$
Chain Rule (as " Composition of Functions ")	$f \circ g$	$(f' \circ g) \times g'$
Chain Rule (using ')	$f(g(x))$	$f'(g(x))g'(x)$
Chain Rule (using $\frac{dy}{dx}$)	$\frac{dy}{dx} = \frac{\partial y}{\partial u} \frac{\partial u}{\partial x}$	

7.3.2 链式法则公式

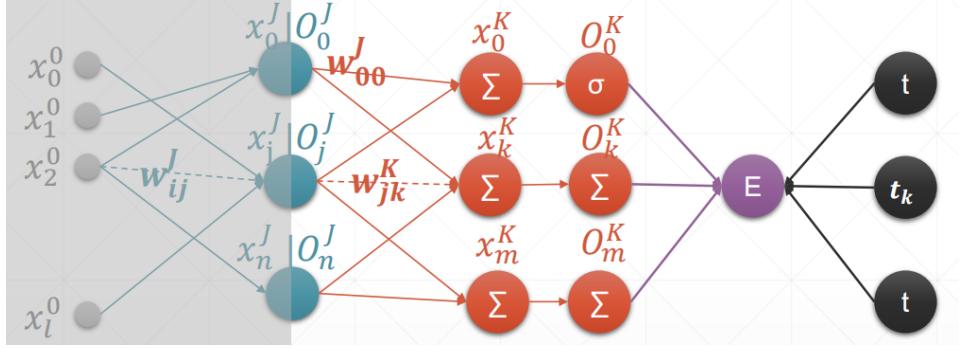
$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u} \frac{\partial u}{\partial x}$$

```

x = torch.tensor(1.)
w1 = torch.tensor(2., requires_grad=True)
b1 = torch.tensor(1.)
w2 = torch.tensor(2., requires_grad=True)
b2 = torch.tensor(1.)
y1 = x*w1 + b1
y2 = y1*w2 + b2
dy2_dy1 = torch.autograd.grad(y2, y1, retain_graph=True)[0]
dy1_dw1 = torch.autograd.grad(y1, w1, retain_graph=True)[0]
dy2_dw1 = torch.autograd.grad(y2, w1, retain_graph=True)[0]
dy2_dw1, dy2_dy1, dy1_dw1  #tensor(2.) tensor(2.) tensor(1.)

```

7.4 MLP 反向传播推导



那么第K层的权值偏微分可知:

$$\frac{\partial E}{\partial w_{jk}^K} = (O_k^K - t_k)O_k^K(1 - O_k^K)O_j^K$$

$$\text{令 } \delta_k^K = (O_k^K - t_k)O_k^K(1 - O_k^K)$$

$$\frac{\partial E}{\partial w_{jk}^K} = \delta_k^K O_j^K$$

那么再求第J层的权值偏微分:

$$\begin{aligned} \frac{\partial E}{\partial w_{ij}} &= \frac{\partial}{\partial w_{ij}} \frac{1}{2} \sum_{k \in K} (O_k - t_k)^2 \\ \frac{\partial E}{\partial w_{ij}} &= \sum_{k \in K} (O_k - t_k) \frac{\partial}{\partial w_{ij}} O_k = \sum_{k \in K} (O_k - t_k) \frac{\partial}{\partial w_{ij}} \sigma(x_k) \\ \frac{\partial E}{\partial w_{ij}} &= \sum_{k \in K} (O_k - t_k) \sigma(x_k)(1 - \sigma(x_k)) \frac{\partial x_k}{\partial w_{ij}} \\ &= \sum_{k \in K} (O_k - t_k) \sigma(x_k)(1 - \sigma(x_k)) \frac{\partial x_k}{\partial O_j} \cdot \frac{\partial O_j}{\partial w_{ij}} \\ &= \sum_{k \in K} (O_k - t_k) O_k (1 - O_k) w_{jk}^K \frac{\partial O_j}{\partial w_{ij}} = \frac{\partial O_j}{\partial w_{ij}} \sum_{k \in K} (O_k - t_k) O_k (1 - O_k) w_{jk}^K \\ &= O_j (1 - O_j) \frac{\partial x_j}{\partial w_{ij}} \sum_{k \in K} (O_k - t_k) O_k (1 - O_k) w_{jk}^K \\ &= O_j (1 - O_j) O_i \sum_{k \in K} (O_k - t_k) O_k (1 - O_k) w_{jk}^K \end{aligned}$$

$$\text{令 } \delta_j^J = O_j (1 - O_j) \sum_{k \in K} \delta_k w_{jk}$$

$$\frac{\partial E}{\partial w_{ij}} = O_i^I \delta_j$$

总结:

对于一个输出层的节点 $k \in K$

$$\frac{\partial E}{\partial w_{jk}} = O_j \delta_k$$

这里,

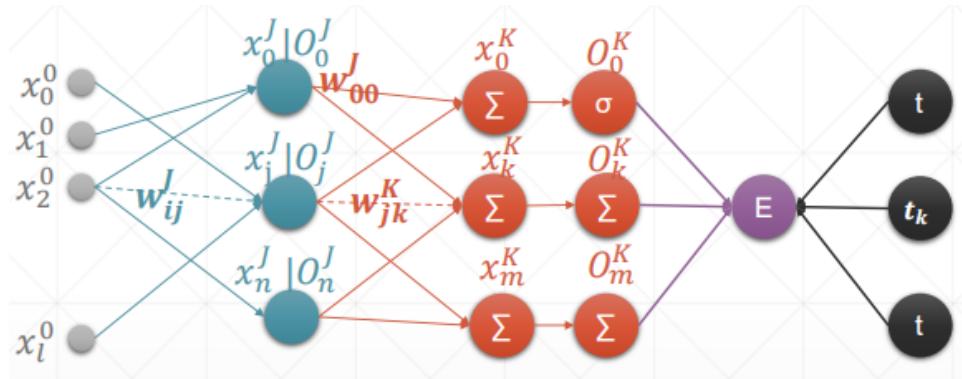
$$\delta_k = O_k(1 - O_k)(O_k - t_k)$$

对于一个隐藏层的节点 $j \in J$

$$\frac{\partial E}{\partial w_{ij}} = O_i \delta_j$$

这里,

$$\delta_j = O_j(1 - O_j) \sum_{k \in K} \delta_k w_{jk}$$



正向传播:

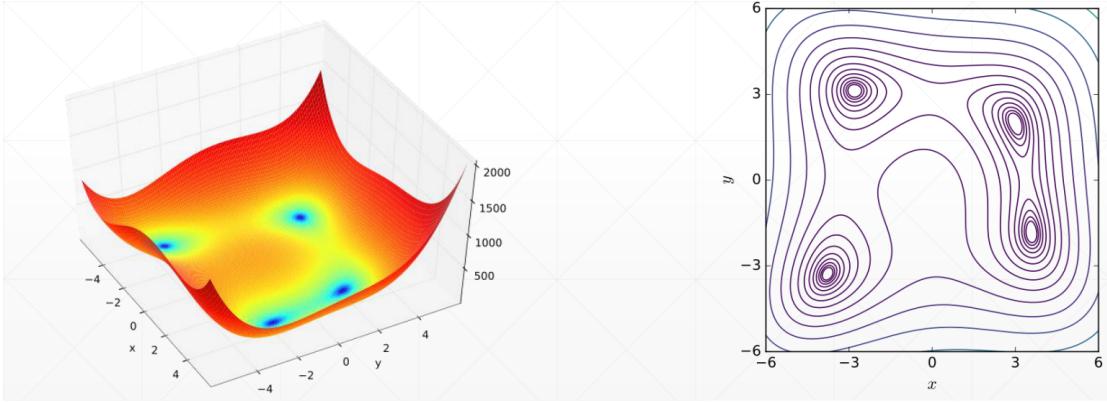
$$O^J \dashrightarrow O^K \dashrightarrow E$$

反向传播:

$$\delta^K \dashrightarrow \frac{\partial E}{\partial w^K} \dashrightarrow \delta^J \dashrightarrow \frac{\partial E}{\partial w^J} \dashrightarrow \delta^L \dashrightarrow \frac{\partial E}{\partial w^L}$$

7.5 2D 函数优化实例

$$f(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$



minma:

- $f(3, 2) = 0$
- $f(-2.805118, 3.131312) = 0$
- $f(-3.779310, -3.283186) = 0$
- $f(3.584428, -1.848126) = 0$

绘图 3d

```
import numpy as np
import matplotlib.pyplot as plt

def himmelblau(x):
    return (x[0]**2+x[1]-11)**2+(x[0]+x[1]**2-7)**2

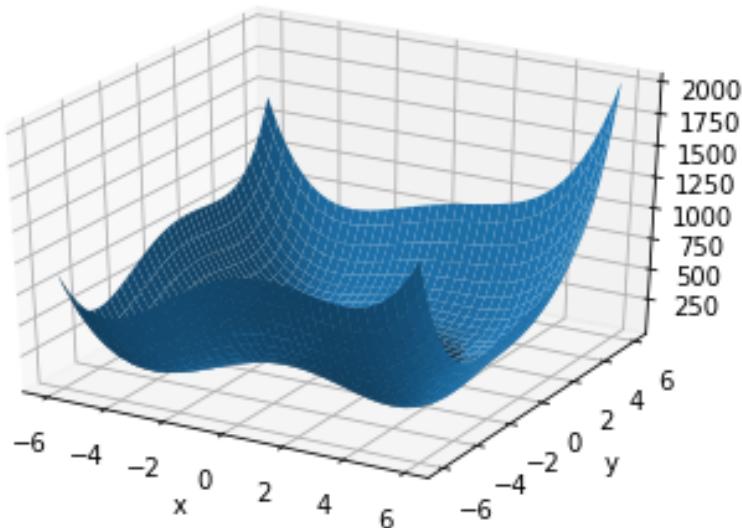
x = np.arange(-6, 6, 0.1)
y = np.arange(-6, 6, 0.1)
print (x,y range:, x.shape, y.shape)
X, Y = np.meshgrid(x, y)
print (X,Y range:, X.shape, Y.shape)
Z = himmelblau([X,Y])

fig = plt.figure(himmelblau)
```

```

ax = fig.gca(projection=3d)
ax.plot_surface(X, Y, Z)
#ax.view_init(60, -30)
ax.set_xlabel(x)
ax.set_ylabel(y)
plt.show()

```



优化

```

import torch
x = torch.tensor([0., 0.], requires_grad=True)
optimizer = torch.optim.Adam([x], lr=1e-3) # 建立梯度更新式 x:=x-grad_x
for step in range(20000):
    pred = himmelblau(x) #得到预测值
    optimizer.zero_grad() #清零梯度值
    pred.backward() #得到 x 的梯度
    optimizer.step() #更新 x 梯度

    if step % 2000 == 0:
        print (step : x = , f(x) = .format(step, x.tolist(), pred.item()))

```

8 多层感知机与分类器

8.1 逻辑回归

1. 对于逻辑回归我们不能直接最大化 accuracy。

- $\text{acc.} = \frac{\sum_{i=1}^n I(\text{pred}_i == y_i)}{n}$
- grad 出现等于零的情况。
- grad 不连续。

2. 为什么叫 regression。

- MSE -- > regression.
- cross entropy -- > classification.

3. 多类:

- 实现多个二分类器。
- softmax。

8.2 交叉熵

8.2.1 Entropy

1. uncertain 不确定度
2. measure of surprise 惊喜程度
3. higher entropy = less info

$$\text{entropy} = - \sum_i P(i) \log P(i)$$

8.2.2 Cross Entropy

$$H(p, q) = \sum p(x) \log q(x)$$

$$H(p, q) = H(p) + D_{KL}(p|q)$$

$$p = q, \quad \text{Cross entropy} = \text{entropy}$$

$$H(P, Q) = -(y \log p + (1 - y) \log(1 - p))$$

对于分类为什么不用MSE:

1. sigmoid+MSE(梯度弥散)。
2. 收敛非常慢。
3. 但是有时可以试试MSE, 求导简单。

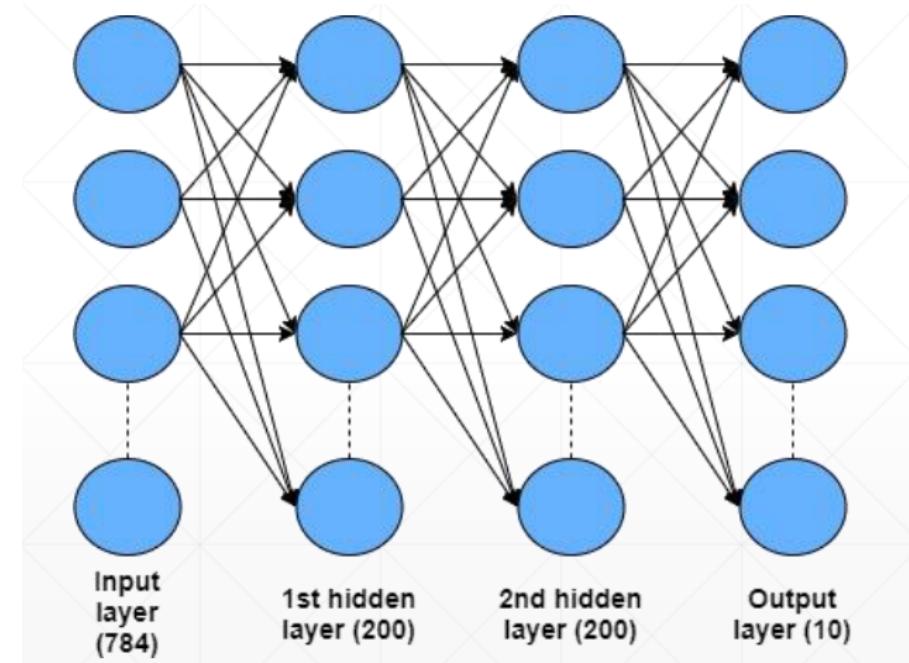
小结:

$$\text{logit} \rightarrow \text{softmax} \rightarrow \text{cross entropy}$$

一般不建议自己单独使用 softmax 与 cross entropy。使用 pytorch 组合的框架。

```
import torch
from torch.nn import functional as F
x = torch.randn(1,784)
w = torch.randn(10,784)
logits = x@w.t()
pred = F.softmax(logits, dim=1)
pred_log = torch.log(pred)
F.nll_loss(pred_log, torch.tensor([1]))
#F.cross_entropy=F.softmax+log+F.nll_loss
F.cross_entropy(logits, torch.tensor([1]))
```

8.3 多分类实战-Mnist



建立网络：

```
w1, b1 = torch.randn(200, 784, requires_grad=True), torch.zeros(200,
    requires_grad=True)
w2, b2 = torch.randn(200, 200, requires_grad=True), torch.zeros(200,
    requires_grad=True)
w3, b3 = torch.randn(10, 200, requires_grad=True), torch.zeros(10,
    requires_grad=True)

#向前传播
def forward(x):
    x = x@w1.t()+b1
    x = F.relu(x)
    x = x@w2.t()+b2
    x = F.relu(x)
    x = x@w3.t()+b3
    x = F.relu(x)
    return x
```

训练：

```
optimizer = optim.SGD([w1, b1, w2, b2, w3, b3], lr=learning_rate)
criteon = nn.CrossEntropyLoss()
```

```

for epoch in range(epochs):

    #训练
    for batch_idx, (data, target) in enumerate(train_loader):
        data = data.reshape(-1, 28*28) #torch.Size([200, 784])

        logits = forward(data) #torch.Size([200, 10])
        loss = criterion(logits, target)

        optimizer.zero_grad() #梯度清零
        loss.backward() #反向回传
#        print(w1.grad.norm(), w2.grad.norm())
        optimizer.step() #更新梯度值

```

通过打印 weight.grad.norm(),得知常常陷入局部极小值。解决这个问题可以利用何凯明的初始化方法。

```

torch.nn.init.kaiming_normal_(w1)
torch.nn.init.kaiming_normal_(w2)
torch.nn.init.kaiming_normal_(w3)

```

8.4 全连接层

在上节中，我们未用 PyTorch 封装的 API 去建立神经网络，这节来使用 PyTorch 封装的 API。

1. 继承 nn.module 类
2. 用 __init__ 来初始化
3. 应用向前传播

```

class MLP(nn.Module):

    def __init__(self):

```

```
super(MLP, self).__init__()

self.model = nn.Sequential(
    nn.Linear(784, 200),
    nn.ReLU(inplace=True),
    nn.Linear(200, 200),
    nn.ReLU(inplace=True),
    nn.Linear(200, 10),
    nn.ReLU(inplace=True),
)

def forward(self, x):
    x = self.model(x)
    return x
```

PyTorch 两种风格的API

1. class-style API (nn.***)
2. function-style API (F.***)

没有遇到上节遇到的初始化问题，参数未暴露给用户，拥有自己的初始化体系，一般来说够用，否则自己必须编写相应的初始化代码。

8.5 激活函数与GPU加速

8.5.1 常用激活函数

1. Sigmoid
2. ReLu
3. tanh
4. Leaky ReLu

5. SELU

6. softplus

8.5.2 一键部署 GPU 加速

```
device = torch.device(cuda)
net = MLP().to(device)
optimizer = optim.SGD(net.parameters(), lr=learning_rate)
criteon = nn.CrossEntropyLoss().to(device)

time1 = time.time()
for epoch in range(epochs):

    for batch_idx, (data, target) in enumerate(train_loader):
        data = data.view(-1, 28*28)
        data, target = data.to(device), target.cuda()

        logits = net(data)
        loss = criteon(logits, target)

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```

8.6 测试与可视化

8.6.1 测试

神经网络的表达能力非常强，容易过拟合，所以要测试。不能单一观测 Loss 的大小判断模型的好坏，还要观测测试集的准确度，确保模型的泛化能力。

```
test_loss = 0
correct = 0
for data, target in test_loader:
```

```
data = data.view(-1, 28 * 28)
data, target = data.to(device), target.cuda()
logits = net(data)
test_loss += criterion(logits, target).item()

pred = logits.argmax(1)
correct += pred.eq(target.data).sum()

test_loss /= len(test_loader.dataset)
```

8.6.2 可视化-Visdom

通过pip install visdom等方式成功安装完之后，开启服务

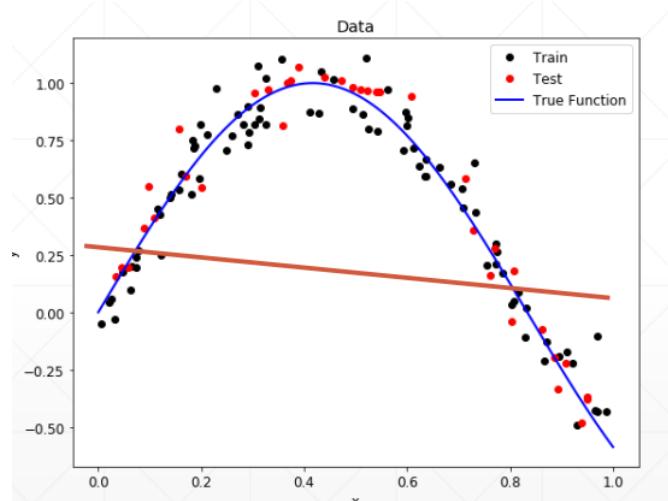
```
python -m visdom.server
```

出现了Mnist图片 viz.images() 全黑故障，估计是由于样本标准化引起的。

9 深度学习的其他技巧

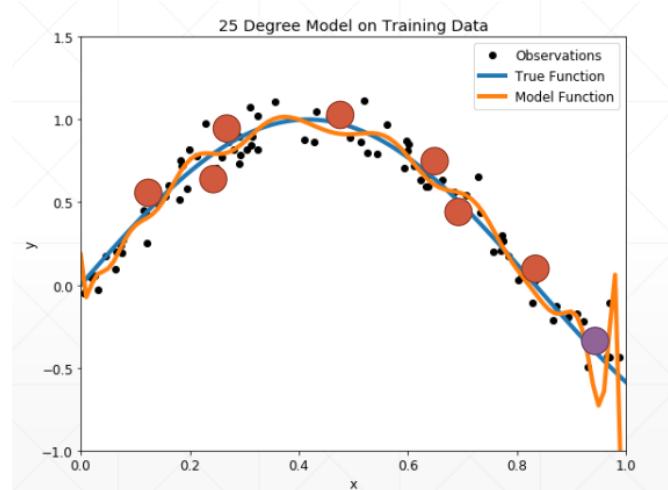
9.1 过拟合与欠拟合

9.1.1 欠拟合



模型简单，表达能力不够，导致欠拟合。

9.1.2 过拟合



现实生活中更多地是过拟合，模型表达能力太强，数据量太少导致的。

那如何检测过拟合状况，当发生了过拟合如何减少过拟合，是要着重考虑和解决的问题。

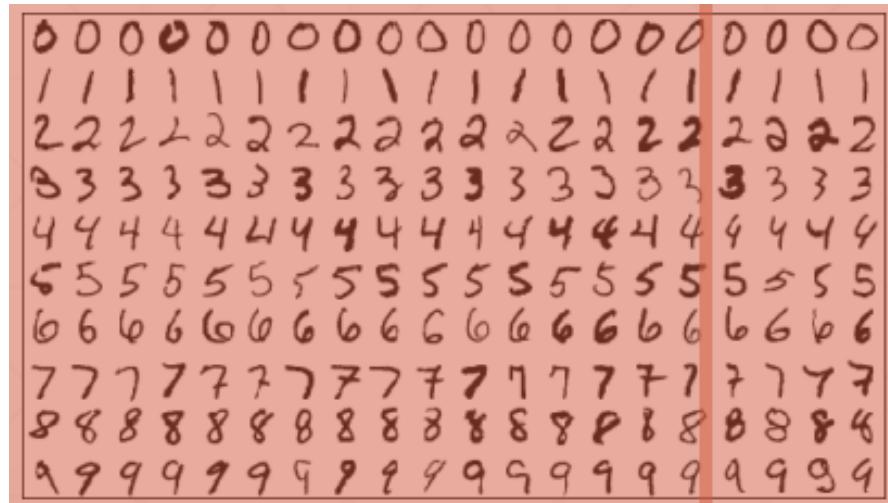
检测过拟合-交叉验证

防止过拟合-正则化

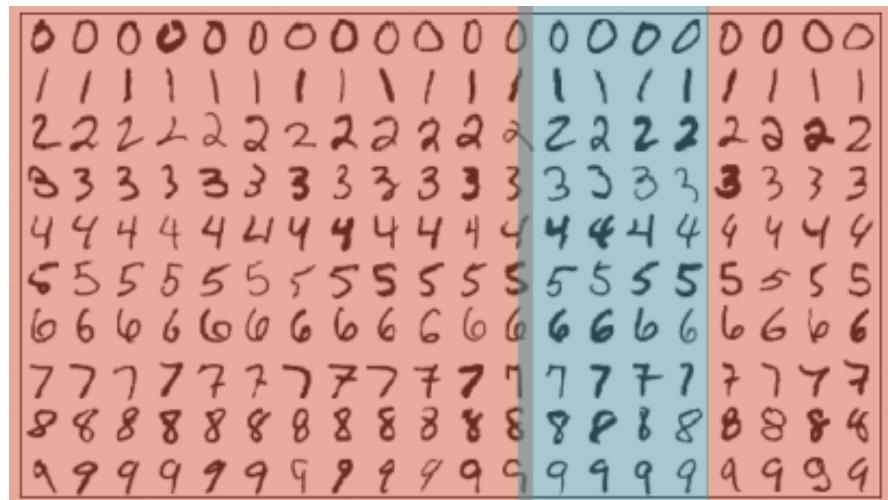
9.2 交叉验证

9.2.1 数据划分

过拟合是模型学习过程中非常重要的一个问题。那么如何检测过拟合也是非常重要的。通过在数据集划分进行训练测试，寻找在过拟合之前的最优参数。



事实上将数据划分成训练集，验证集，测试集。



将数据划分成三类，客户用保密的测试集来测试模型效果，防止作弊。

```
train_db = datasets.MNIST(..../data, train=True, download=True,
                        transform=transforms.Compose([
                            transforms.ToTensor(),
                            transforms.Normalize((0.1307,), (0.3081,))])
)
train_loader = torch.utils.data.DataLoader(
```

```

    train_db,
    batch_size=batch_size, shuffle=True)

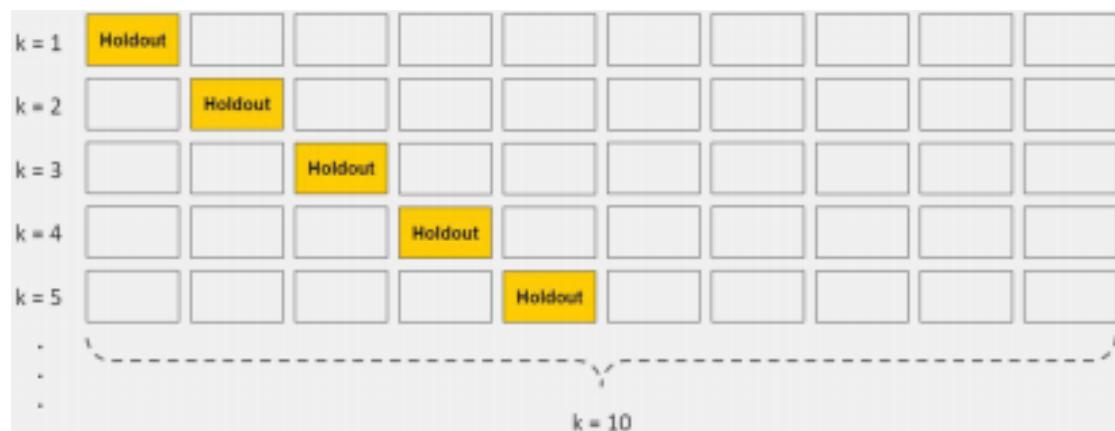
test_db = datasets.MNIST(..../data, train=False, transform=transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize((0.1307,), (0.3081,))

]))
test_loader = torch.utils.data.DataLoader(test_db,
    batch_size=batch_size, shuffle=True)

print(train:, len(train_db), test:, len(test_db))
train_db, val_db = torch.utils.data.random_split(train_db, [50000, 10000])
print(db1:, len(train_db), db2:, len(val_db))
train_loader = torch.utils.data.DataLoader(
    train_db,
    batch_size=batch_size, shuffle=True)
val_loader = torch.utils.data.DataLoader(
    val_db,
    batch_size=batch_size, shuffle=True)

```

9.2.2 K-fold交叉验证



将训练集划分成十份，每次将其中九份用于训练，一份用于验证，选择较好的时间截权值参数。

9.3 正则化

9.3.1 奥卡姆剃刀原理

能使用简单模型参数量解决的模型问题不要使用复杂模型的参数量。

More things should not be used than are necessary

9.3.2 防止过拟合的方法

1. 数据扩充
2. 限制模型的复杂度
 - 浅层网络
 - 添加正则化项
3. Dropout
4. Data argument(数据增强)
5. Early Stop

9.3.3 正则化

Regularization == Weight Decay

1. L1范数

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^m [y_i \log \hat{y}_i + (1 - y_i) \log (1 - \hat{y}_i)] + \lambda \sum_{i=1}^n |\theta_i|$$

```
regularizatin_loss = 0
for param in model.parameters():
    regularization_loss += torch.sum(torch.abs(param))

classify_loss = criteon(logits, target)
loss = classify_loss + 0.01 + regularization_loss

optimizer.zero_grad()
loss.backward()
optimizer.step()
```

2. L2范数

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^m [y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i) + \frac{1}{2} \lambda \|W\|^2]$$

```
net = MLP().to(device)
optimizer = optim.SGD(net.parameters(), lr=learning_rate,
                      weight_decay=0.01)
criterion = nn.CrossEntropyLoss().to(device)
```

9.4 动量与学习率衰减

9.4.1 动量

momentum 动量也称惯性

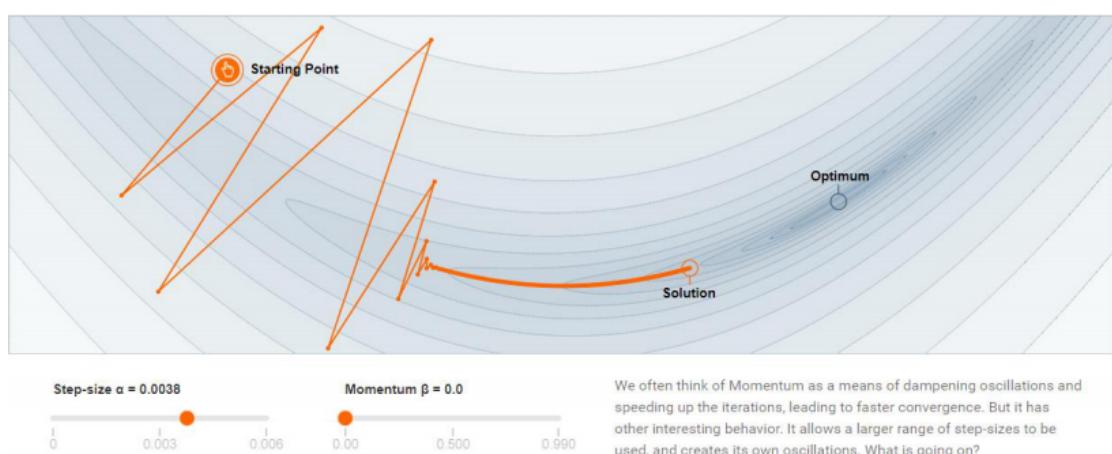
$$w^{k+1} = w^k - \alpha \nabla f(w^k)$$

$$z^{k+1} = \beta z^k + \nabla f(w^k)$$

$$w^{k+1} = w^k - \alpha z^{k+1}$$

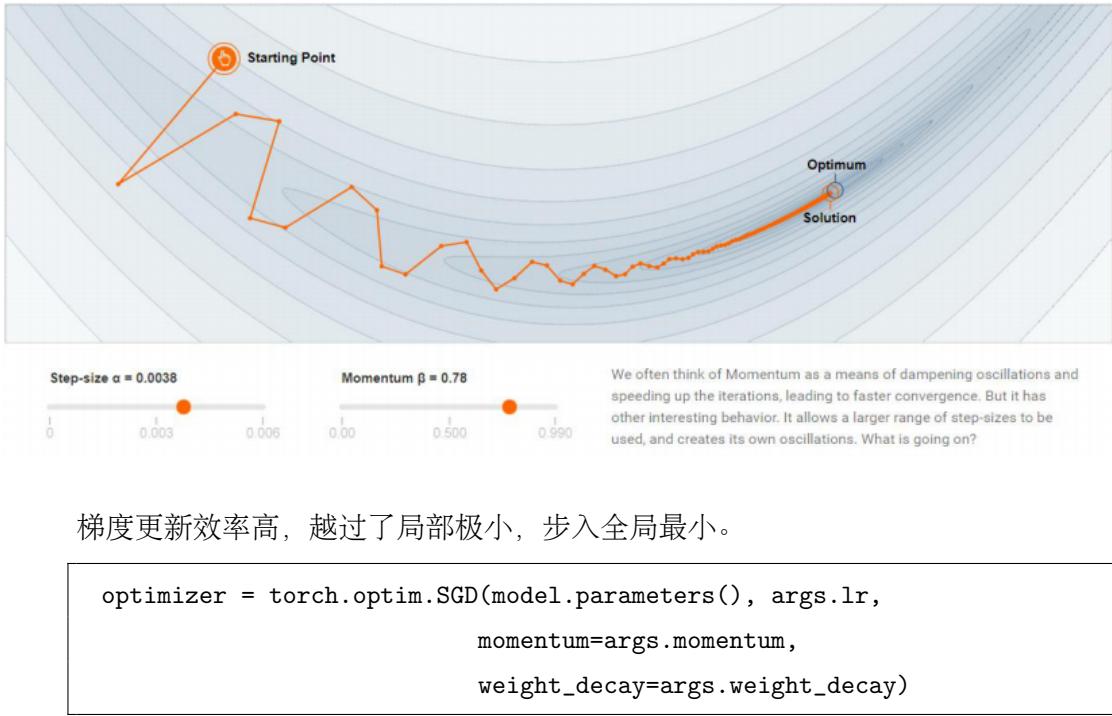
加入动量的迭代式，实际上就是当前的梯度方向加上上一次的惯性的方向。尽快收敛，并且大概率的跳出局部极小值。

1. 没加动量的例子



梯度更新刁钻，迭代效率低，容易陷入局部极小。

2. 引入动量的例子



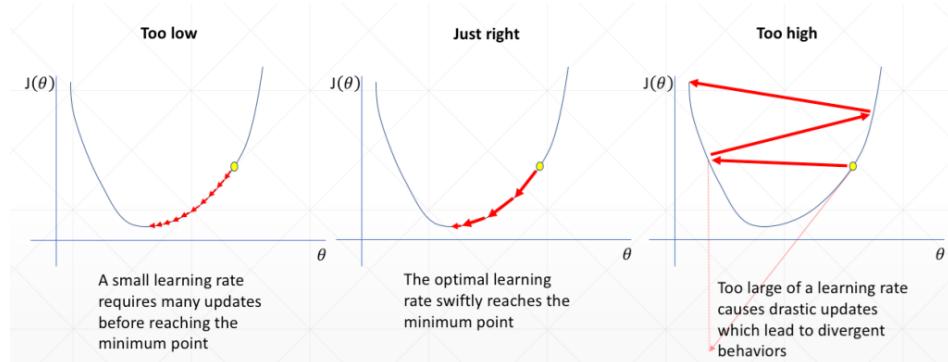
梯度更新效率高，越过了局部极小，步入全局最小。

```
optimizer = torch.optim.SGD(model.parameters(), args.lr,
                            momentum=args.momentum,
                            weight_decay=args.weight_decay)
```

PyTorch 中 Adam 优化器已经内置了 momentum 机制，所以不需要变量维护；但是 SGD 却没有。

9.4.2 学习率衰减

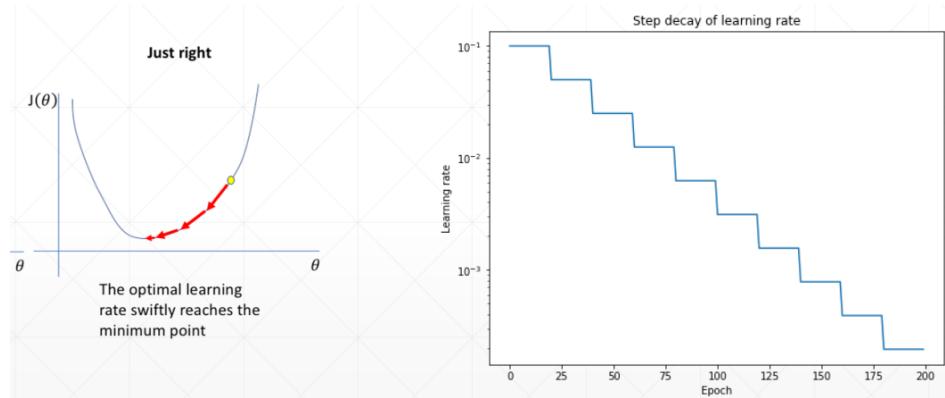
learning rate decay



Learning Rate 设置过大，导致摇摆，得不到较好的效果。

Learning Rate 设置过小，更新迭代次数过多。

学习率衰减，刚开始选择大一点的学习率，也不会较大影响，前期还能较快更新。



PyTorch 设置学习率衰减

1. 方法一遇平原衰减

```
optimizer = torch.optim.SGD(model.parameters(), args.lr,
                            momentum=args.momentum,
                            weight_decay=args.weight_decay)
schedule = ReduceLROnPlateau(optimizer, min) # 学习率衰减监听

for epoch in xrange(args.start_epoch, args.epochs):
    train(train_loader, model, criterion, optimizer, epoch)
    result_avg, loss_val = validate(val_model, criterion, epoch)
    schedule.step(loss_val)
```

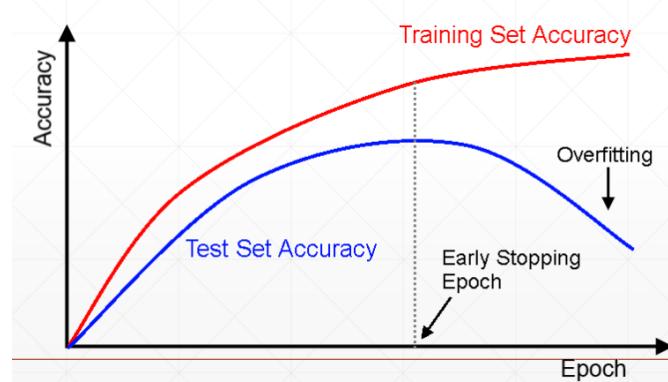
2. 方法二定时衰减

```
# Assuming optimizer uses lr = 0.05 for all groups
#lr = 0.05          if epoch < 30
#lr = 0.005         if 30 <= epoch <= 60
#lr = 0.0005        if 60 <= epoch <= 90
# ...
scheduler = StepLR(optimizer, step_size=30, gamma=0.1)
for epoch in range(100)
    schedule.step()
    train(...)
    validate(...)
```

9.5 提前停止更新与Dropout

9.5.1 提前停止更新

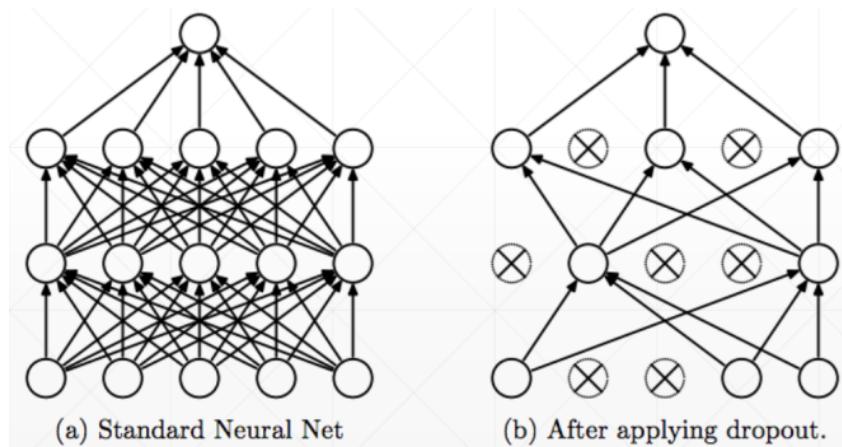
提前停止更新是为了模型学习过拟合。



9.5.2 Dropout

dropout 也是防止过拟合常用的小技巧。

1. Learning less to learn better
2. Each connection has $\rho = 0, 1$ to lose



```
net_dropped = torch.nn.Sequential(  
    torch.nn.Linear(784, 200),  
    torch.nn.Dropout(0.5), #dropout 50% of the neuron  
    torch.nn.ReLU(),  
    torch.nn.Linear(200, 200),  
    torch.nn.Dropout(0.5), #dropout 50% of the neuron  
    torch.nn.ReLU(),
```

```
    torch.nn.Linear(200, 10)
)
```

在训练时，我们把部分连接断掉；但是在测试或者验证时，必须把状态切换回来。

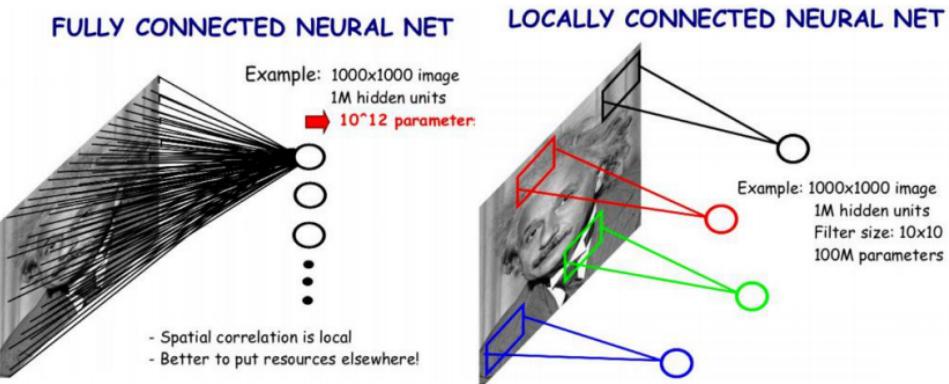
```
for epoch in range(epochs):

    # train
    net_dropped.train()
    for batch_idx, (data, target) in enumerate(train_loader):
        ...

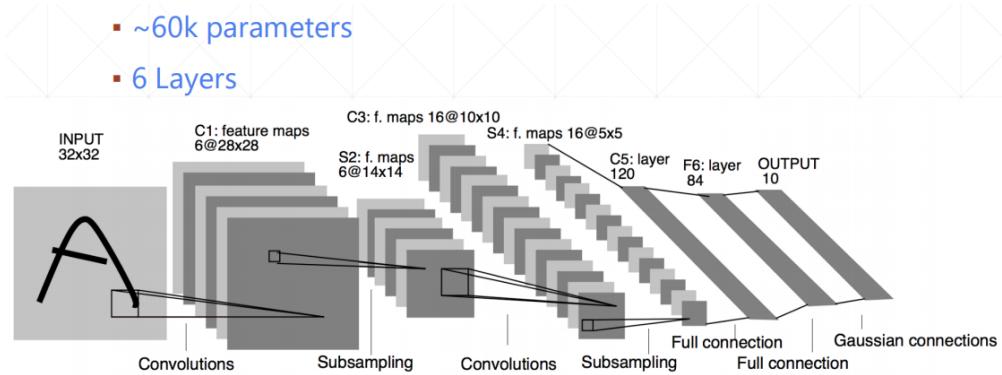
    net_dropped.eval()
    test_loss = 0
    correct = 0
    for data, target in test_loader:
        ...
```

10 卷积神经网络

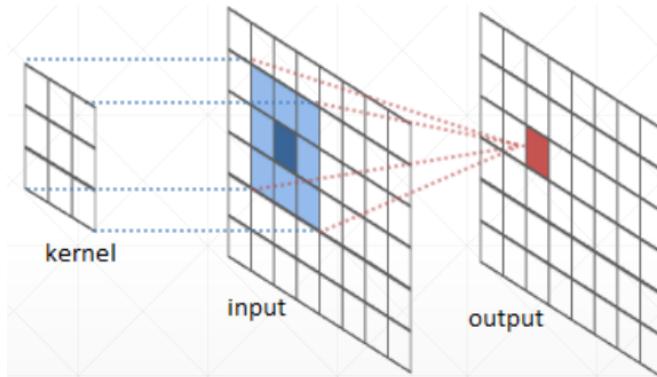
10.1 卷积



卷积实则是一种特征映射，解决了在线性全连接层下的参数维度过大的问题。同时卷积也来源于人类视觉局部性的感受区域。参数共享是卷积神经网络的一个重要特征，也极大地减少了参数维度。

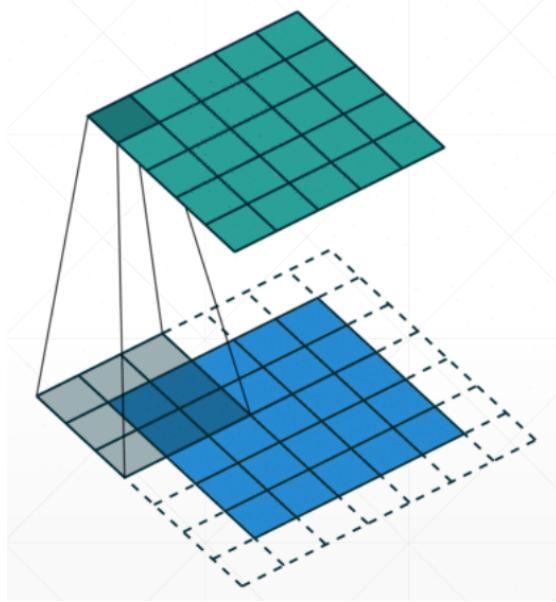


卷积一次来源于信号处理上两个函数之间的卷积运算，操作可视化后类似。



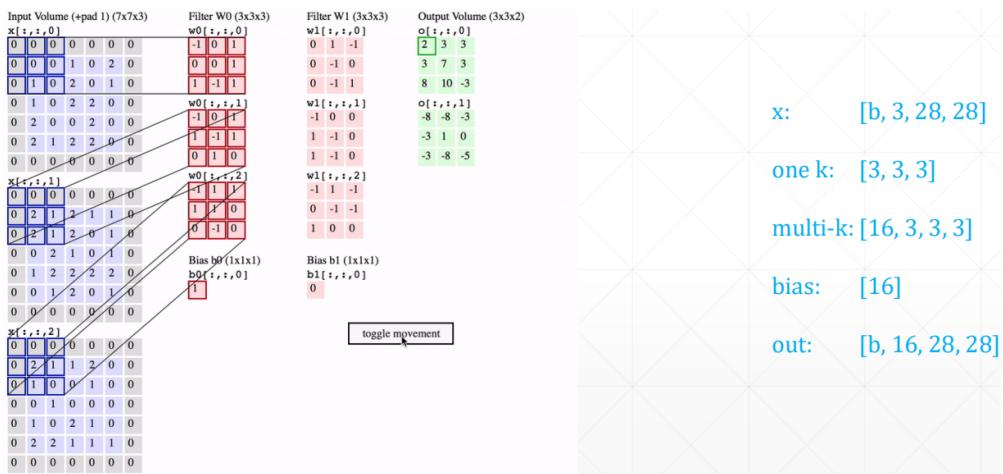
10.2 卷积神经网络

10.2.1 notation

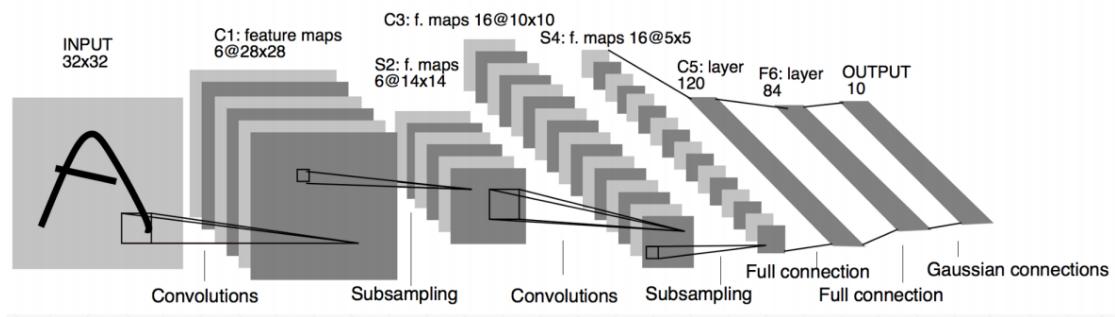


1. Input_channels
2. Kernel_channels: 2ch
3. Kernel_size
4. Stride 步幅。
5. Padding 填充。

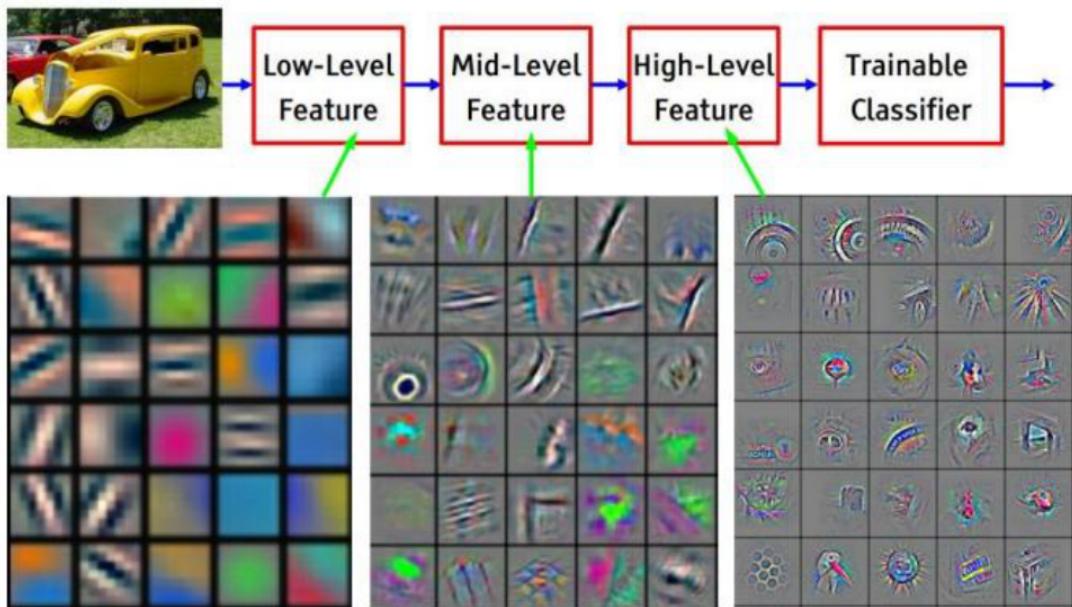
10.2.2 Multi-Kernel



10.2.3 LeNet-5



10.2.4 卷积层的作用效果



从图片来看卷积层的作用效果，浅层次的卷积越能捕捉图片细节特征，往后就可以捕捉图片的局部特征。

10.2.5 nn.Conv2d

```
#Class API    in_channels, out_channels(number of kernel)
layer = nn.Conv2d(2, 16, kernel_size=3, stride=1, padding=0)
x = torch.rand(1, 2, 28, 28)
out = layer.forward(x)
out.shape # torch.Size([1, 16, 26, 26])
out_ = layer(x) #python provide magic to call __call__
out_.shape # torch.Size([1, 16, 26, 26])
layer.weight.shape # torch.Size([16, 2, 3, 3])
layer.bias.shape #torch.Size([16])
```

10.2.6 F.conv2d

```
#Functional API
x = torch.rand(1, 3, 28, 28)
w = torch.rand(16, 3, 5, 5)
b = torch.rand(16)
out = F.conv2d(x, w, b, stride=1, padding=1)
out.shape #torch.Size([16, 3, 26, 26])
```

10.3 池化层

10.3.1 pooling

pooling is also called down sample.

池化层为了缩减数据维度。

pooling 策略:

1. Max Pooling.
2. Avg Pooling.

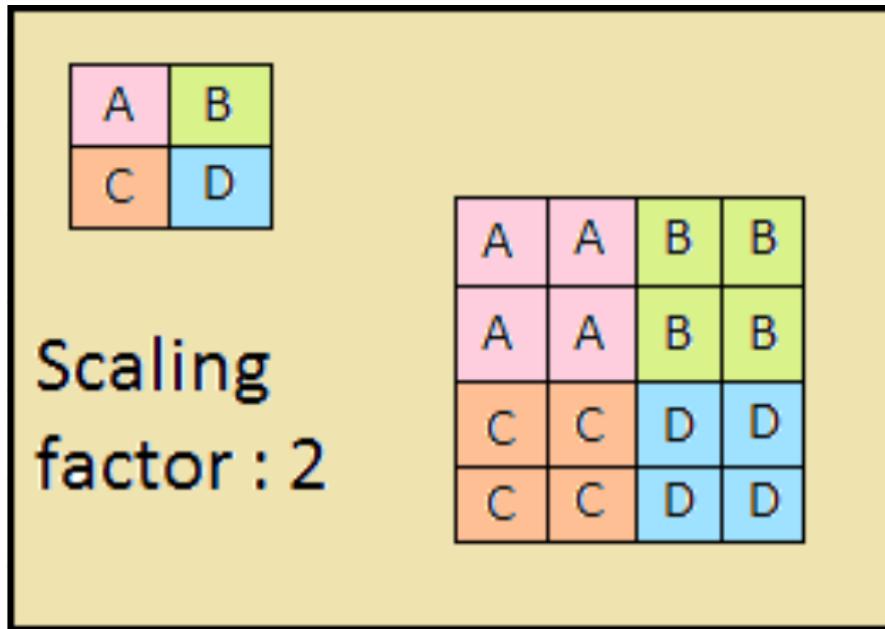
```
layer = nn.Conv2d(2, 16, kernel_size=3, stride=1, padding=1)
x = torch.rand(1, 2, 28, 28)
out = layer(x) #python provide magic to call __call__
out.shape # torch.Size([1, 16, 28, 28])

# Class API
layerPooling = nn.AvgPool2d(2, stride=4)
outPClassAPI = layerPooling(out)
outPClassAPI.shape # torch.Size([1, 16, 7, 7])

# Functional API
outPFuncAPI = F.max_pool2d(out, 2, stride=4)
outPFuncAPI.shape # torch.Size([1, 16, 7, 7])
```

10.3.2 upsample

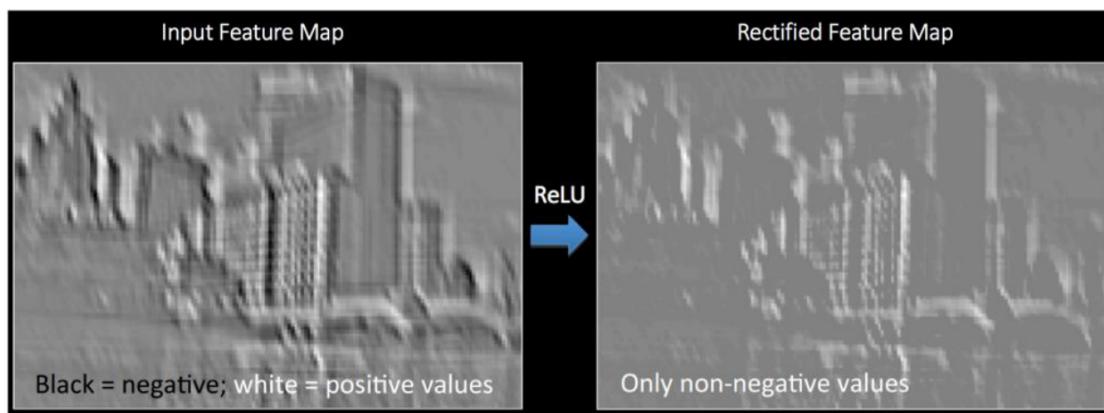
upsample 可以看做是图片的放大。



```
layer = nn.Conv2d(2, 16, kernel_size=3, stride=1, padding=1)
x = torch.rand(1, 2, 28, 28)
out = layer(x) #python provide magic to call __call__
out.shape # torch.Size([1, 16, 28, 28])

out = F.interpolate(out, scale_factor=2, mode=nearest)
out.shape # torch.Size([1, 16, 56, 56])
```

10.3.3 ReLU



```
layer = nn.Conv2d(2, 16, kernel_size=3, stride=1, padding=1)
x = torch.rand(1, 2, 28, 28)
```

```

out = layer(x) #python provide magic to call __call__
out.shape # torch.Size([1, 16, 28, 28])
out.min() # tensor(-1.2756, grad_fn=<MinBackward1>

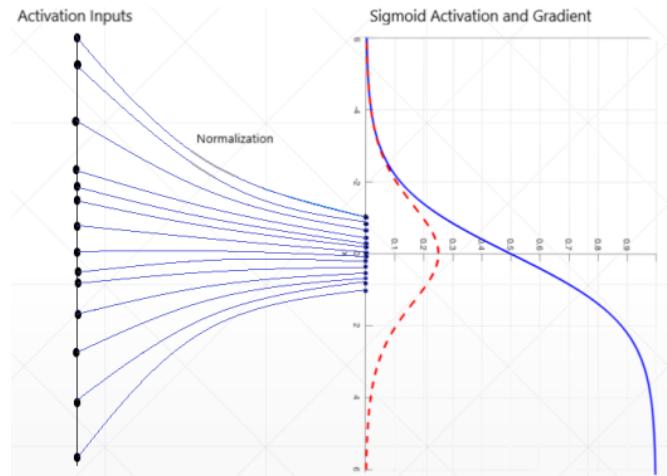
layer = nn.ReLU(inplace=True)
out = layer(out)
out.shape # torch.Size([1, 16, 28, 28])
out.min() tensor(0., grad_fn=<MinBackward1>

```

10.4 Batch Norm

Batch normalization 广泛应用于深度学习,CNN,RNN.

10.4.1 使用原因



通过 BatchNorm 极大地避免使用 Sigmoid 函数时的梯度弥散情况，加快迭代收敛速度。

10.4.2 Feature Scaling

更加利于搜索最优解。

1. image Normalization

```

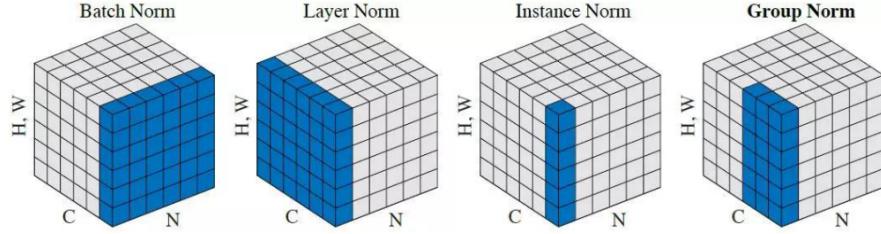
normalize = transforms.Normalize(mean=[0.485, 0.456, 0.406]
                                std=[0.229, 0.224, 0.225]) #RGB

```

将输入的 image 数据,范围在 0-1 之间, 经过标准化, 使其服从 $N(0, 1)$ 分布, 更利用于空间搜索最优解。

2. Batch Normalization

常见的 Norm 类型。



可以看出来 Batch Normalization 只保留 channel 的统计数据 mean 以及 variance.

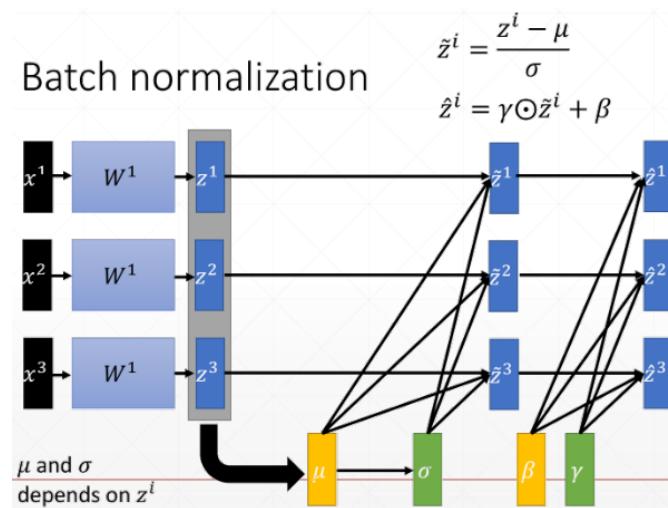
Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\dots m}\}$;

Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\begin{aligned} \mu_{\mathcal{B}} &\leftarrow \frac{1}{m} \sum_{i=1}^m x_i && // \text{mini-batch mean} \\ \sigma_{\mathcal{B}}^2 &\leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 && // \text{mini-batch variance} \\ \hat{x}_i &\leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} && // \text{normalize} \\ y_i &\leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) && // \text{scale and shift} \end{aligned}$$

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.



Batch Normalization 只会平移和缩放数据。

```

x = torch.rand(100, 16, 784)
layer = nn.BatchNorm1d(16)
out = layer(x)
out.shape # torch.Size([100, 16, 784])
layer.running_mean.shape # torch.Size([16])
layer.running_var.shape # torch.Size([16])

```

Class Variables, 查看类变量

```

vars(layer)
# affine: True, otherwise weight=1, bias=0 not update
# training: True, not test mode

```

Batch Normalization 在 training 以及 test 行为不一样。

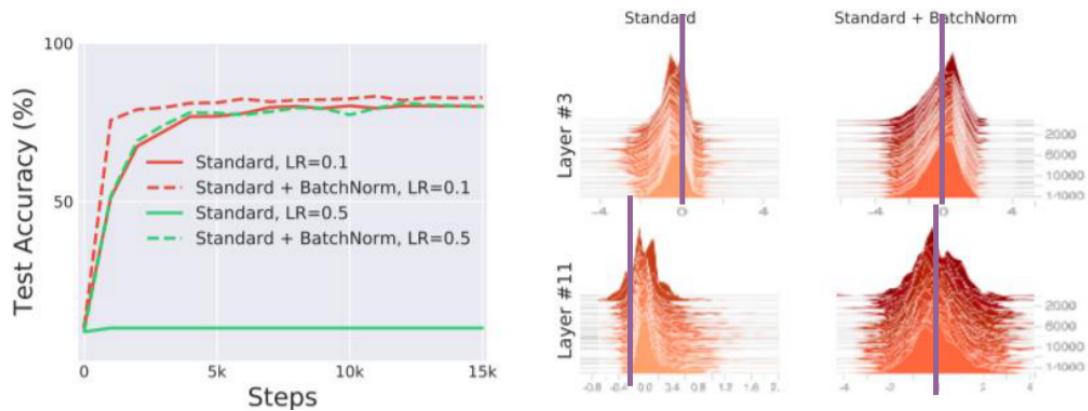
因为在test时，数据没有Batch统计单个数据没有意义，因此只会使用全局的mean以及variance。且weight以及bias是不需要更新的。

```

layer.eval()    # training: False,
hatx = torch.rand(1, 16, 7, 7)
test = layer(hatx)

```

10.4.3 使用效果



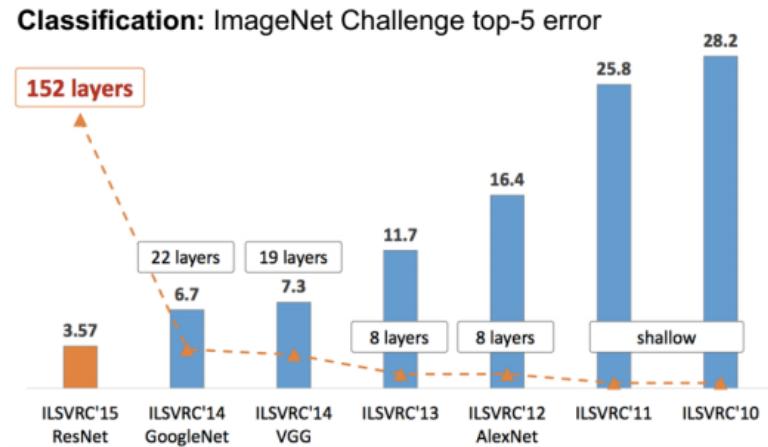
10.4.4 使用优势

1. 加快收敛速度
2. 更好的效果
3. 模型更健壮

- 稳定性
- 学习率过大

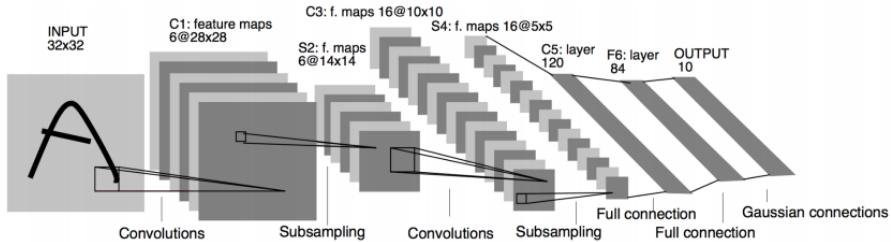
10.5 经典的卷积神经网络

10.5.1 ImageNet dataset 224x224



10.5.2 LeNet-5

Yann LeCun 深度学习三驾马车之一



上世纪80年代产物，用于手写字体识别，精度优秀。

10.5.3 AlexNet

Geoffrey Hinton 深度学习三驾马车之首

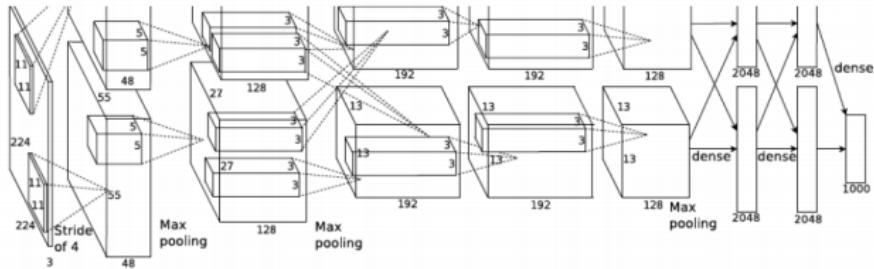
1. GTX 580

- 3GB x 2

2. 11 x 11

3. 8 layers

AlexNet: ILSVRC 2012 winner



- Similar framework to LeNet but:
 - Max pooling, ReLU nonlinearity
 - More data and bigger model (7 hidden layers, 650K units, 60M params)
 - GPU implementation (50x speedup over CPU)
 - Trained on two GPUs for a week
 - Dropout regularization

A. Krizhevsky, I. Sutskever, and G. Hinton,
[ImageNet Classification with Deep Convolutional Neural Networks](#), NIPS 2012

10.5.4 VGGNet

1. 3x3

2. 1x1

3. 11-19 layer

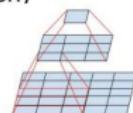
VGGNet: ILSVRC 2014 2nd place

ConvNet Configuration					
A	A-LRN	B	C	D	E
11 weight layers	11 weight layers	13 weight layers	16 weight layers	16 weight layers	19 weight layers
conv3-64	conv3-64	conv3-64	conv3-64	conv3-64	conv3-64
LRN					
		maxpool			
conv3-128	conv3-128	conv3-128	conv3-128	conv3-128	conv3-128
	conv3-128		conv3-128		conv3-128
		maxpool			
conv3-256	conv3-256	conv3-256	conv3-256	conv3-256	conv3-256
conv3-256	conv3-256	conv3-256	conv3-256	conv3-256	conv3-256
		conv1-256		conv3-256	
				conv3-256	
		maxpool			
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
		conv1-512		conv3-512	
				conv3-512	
		maxpool			
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
		conv1-512		conv3-512	
				conv3-512	
		maxpool			
FC-4096					
FC-4096					
FC-1000					
soft-max					

Table 2: Number of parameters (in millions).

Network	A,A-LRN	B	C	D	E
Number of parameters	133	133	134	138	144

- Sequence of deeper networks trained progressively
- Large receptive fields replaced by successive layers of 3x3 convolutions (with ReLU in between)
- One 7x7 conv layer with C feature maps needs $49C^2$ weights, three 3x3 conv layers need only $27C^2$ weights
- Experimented with 1x1 convolutions



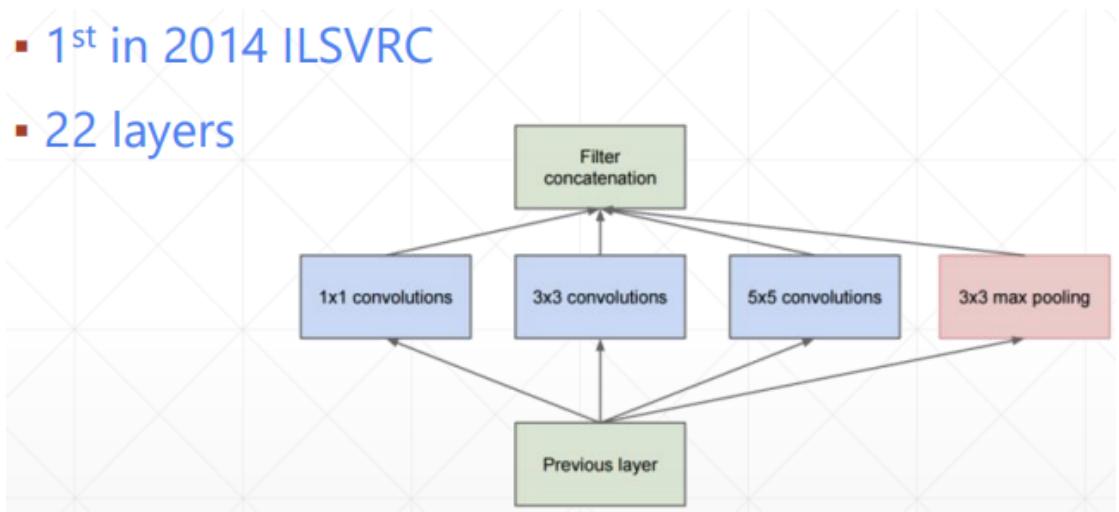
K. Simonyan and A. Zisserman,
[Very Deep Convolutional Networks for Large-Scale Image Recognition](#), ICLR 2015

1x1 convolution

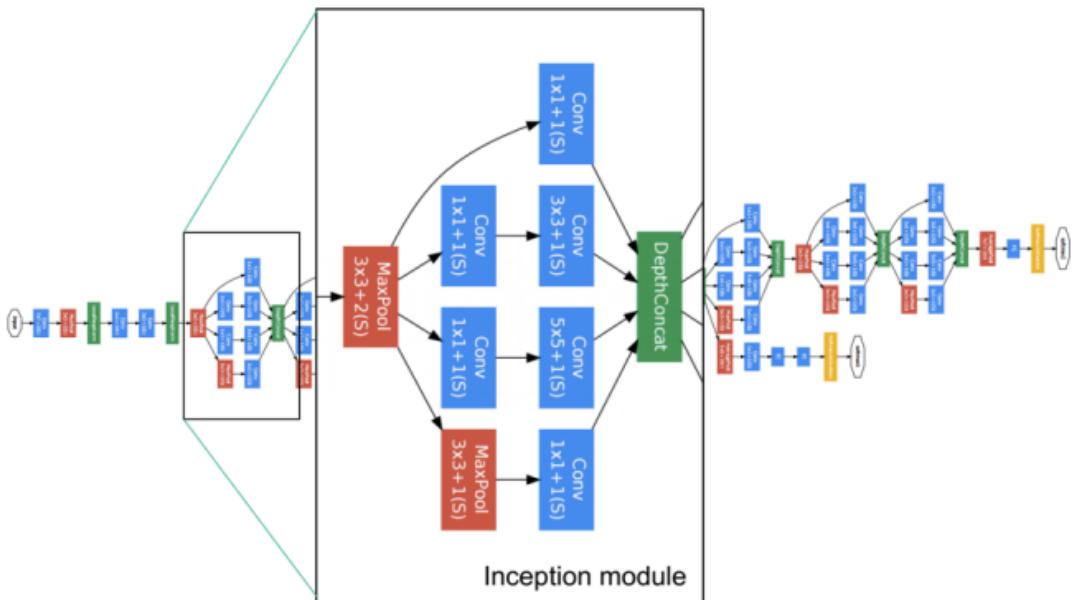
- less computation
- $c_{in} \Rightarrow c_{out}$

10.5.5 GoogLeNet

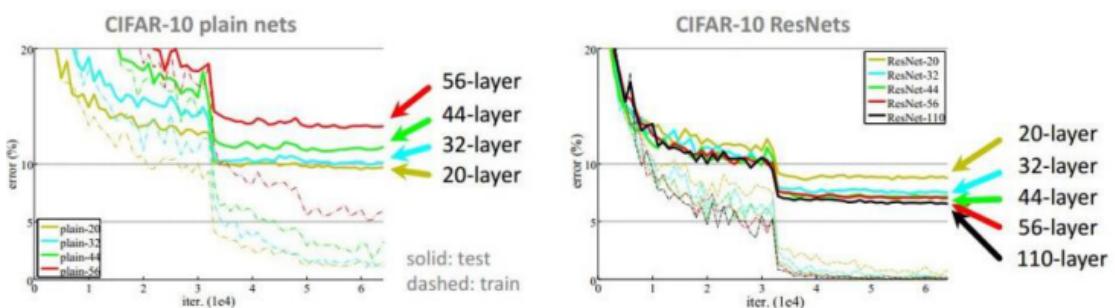
- 1st in 2014 ILSVRC
- 22 layers



综合不同 size's kernel 的感受野。



虽然深度学习随着网络层数的增加精度上有了明显的提升，但也不能无限制的增加网络层数，否则 training 难度增加，精度不升反降。ResNet

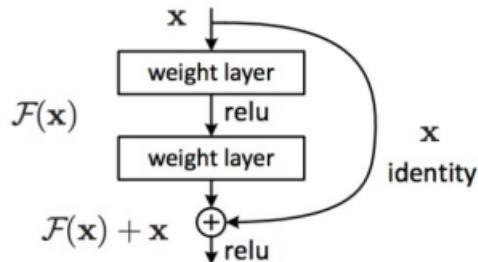


10.6 ResNet

深度残差网络

ResNet

- The residual module
 - Introduce *skip* or *shortcut* connections (existing before in various forms in literature)
 - Make it easy for network layers to represent the identity mapping
 - For some reason, need to skip at least two layers

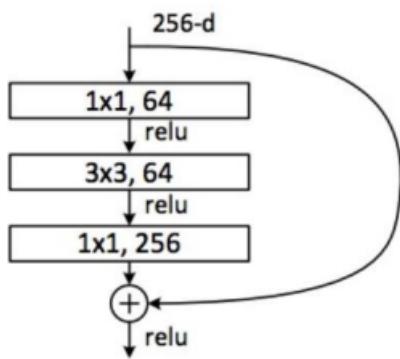


Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun,
[Deep Residual Learning for Image Recognition](#), CVPR 2016 (Best Paper)

提出短路层, 寻找梯度回传的捷径。将新的 Unit 进行叠加形成 ResNet.

ResNet

Deeper residual module
(bottleneck)



- Directly performing 3x3 convolutions with 256 feature maps at input and output:
 $256 \times 256 \times 3 \times 3 \sim 600K$ operations
- Using 1x1 convolutions to reduce 256 to 64 feature maps, followed by 3x3 convolutions, followed by 1x1 convolutions to expand back to 256 maps:
 $256 \times 64 \times 1 \times 1 \sim 16K$
 $64 \times 64 \times 3 \times 3 \sim 36K$
 $64 \times 256 \times 1 \times 1 \sim 16K$
Total: $\sim 70K$

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun,
[Deep Residual Learning for Image Recognition](#), CVPR 2016 (Best Paper)

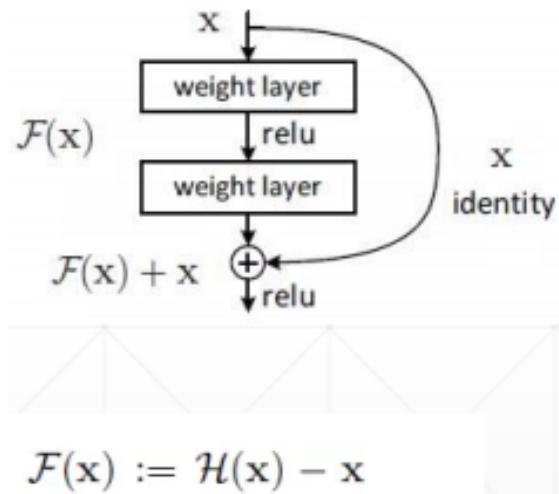
新的 Unit 单元, shape 不能变。将短路权利交给网络。

MSRA @ ILSVRC & COCO 2015 Competitions

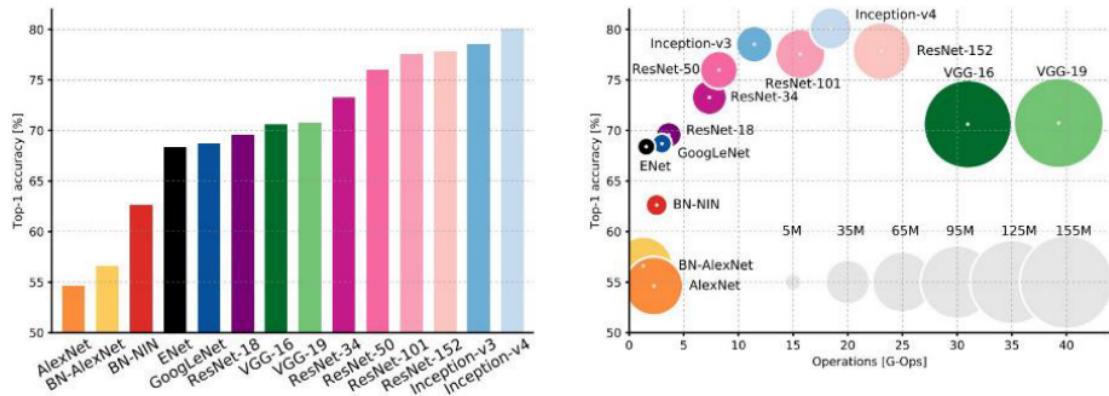
- **1st places in all five main tracks**

- 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

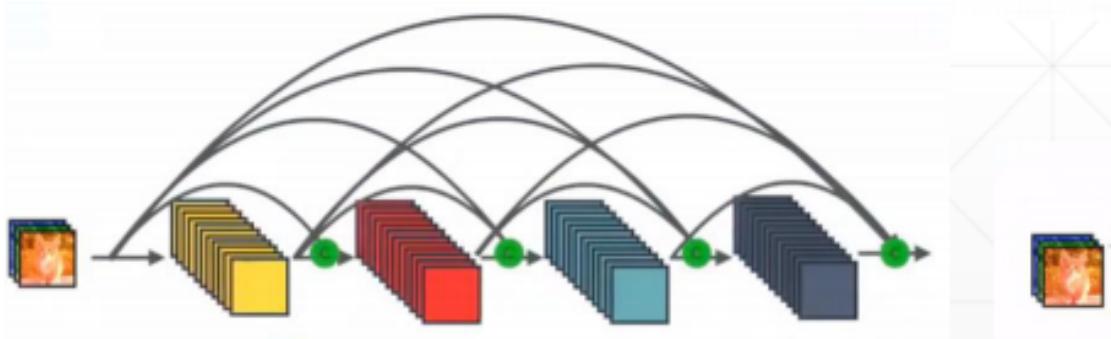
为什么叫残差(Residual)?



层数性能比较:



10.7 DenseNet



10.8 nn.Module

当我们自己定义网络层时，必须继承 `nn.Module` 父类。常用的线性层，卷积层等 PyTorch 官方已经写好。

```
class MyLinear(nn.Module):

    def __init__(self, inp, outp):
        super(MyLinear, self).__init__()

        # requires_grad = True
        self.w = nn.Parameter(torch.randn(outp, inp))
        self.b = nn.Parameter(torch.randn(outp))

    def forward(self, x):
        x = x @ self.w.t() + self.b
        return x
```

Magic

1. Every Layer is `nn.Module`
 - `nn.Linear`
 - `nn.BatchNorm2d`
 - `nn.Conv2d`
2. `nn.Module` is nested in `nn.Module`

使用 `nn.Module` 的好处

1. 可以使用大量现成的网络层。

- Linear
- ReLu
- Sigmoid
- Conv2d
- ConvTransposed2d
- Dropout
- etc.

2. Container 容器

- $\text{net}(x)$

```
self.model = nn.Sequential(
    nn.Linear(784, 200),
    nn.LeakyReLU(inplace=True),
    nn.Linear(200, 200),
    nn.LeakyReLU(inplace=True),
    nn.Linear(200, 10),
    nn.LeakyReLU(inplace=True),
)
```

3. 有效管理参数

```
net.parameters() # iterator
net.named_parameters # auto-named weight and bias iterator
```

4. Modules

- modules: all nodes
- children: direct children

```
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()

        self.net = nn.Sequential(BasicNet(),
                               nn.ReLU(),
                               nn.Linear(3, 2))
```

```
def forward(self, x):
    return self.net(x)

modules: net Sequential(
(0): BasicNet(
    (net): Linear(in_features=4, out_features=3, bias=True)
)
(1): ReLU()
(2): Linear(in_features=3, out_features=2, bias=True)
)

modules: net.0 BasicNet(
    (net): Linear(in_features=4, out_features=3, bias=True)
)
modules: net.0.net Linear(in_features=4, out_features=3, bias=True)

modules: net.1 ReLU()
modules: net.2 Linear(in_features=3, out_features=2, bias=True)
```

5. GPU 加速

```
device = torch.device(cuda)
net = Net()
net.to(device)
```

6. 保存与加载中间数据

```
net.load_state_dict(torch.load(ckpt.mdl))
...train...
torch.save(net.state_dict(), ckpt.mdl)
```

7. train&test 状态切换方便。

```
# train
net.train()
...
# test
net.eval()
```

8. 实现我们自己的类。

```
class Flatten(nn.Module):

    def __init__(self):
        super(Flatten, self).__init__()

    def forward(self, input):
        return input.view(input.size(0), -1)

class TestNet(nn.Module):

    def __init__(self):
        super(TestNet, self).__init__()

        self.net = nn.Sequential(nn.Conv2d(1, 16, stride=1, padding=1),
                               nn.MaxPool2d(2, 2),
                               Flatten(),
                               nn.Linear(1*14*14, 10))

    def forward(self, x):
        return self.net(x)
```

9. 自己实现的线性层

```
class MyLinear(nn.Module):

    def __init__(self, inp, outp):
        super(MyLinear, self).__init__()

        # requires_grad = True
        self.w = nn.Parameter(torch.randn(outp, inp))
        self.b = nn.Parameter(torch.randn(outp))

    def forward(self, x):
        x = x @ self.w.t() + self.b
        return x
```

10.9 数据增强

确保深度学习的深度网络有良好的表现，防止过拟合的重要标准就是要使用的是大数据集。

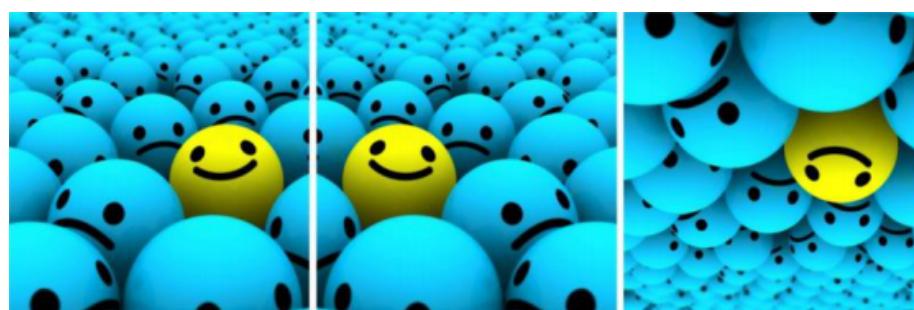
数据量小时训练技巧

1. Small network capacity.
2. Regularization.
3. data argumentation.

Data Argumentation

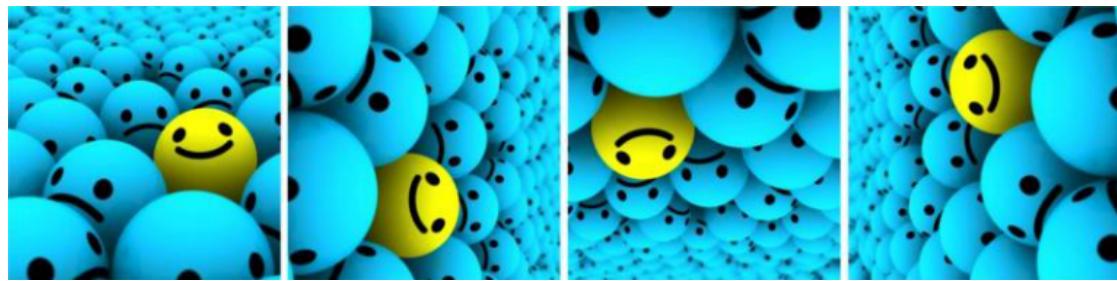
1. Flip 翻转
2. Rotation 旋转
3. scale 缩放
4. Random Move & Crop 平移&缩放
5. GAN 生成对抗网络

10.9.1 Flip



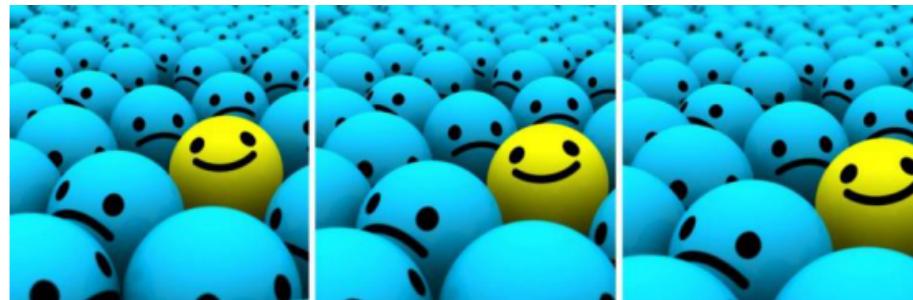
```
train_loader = torch.utils.data.DataLoader(  
    datasets.MNIST(..../data, train=True, download=True,  
        transform=transforms.Compose([  
            transforms.RandomHorizontalFlip(),  
            transforms.RandomVerticalFlip(),  
        ])),
```

10.9.2 Rotation



```
train_loader = torch.utils.data.DataLoader(  
    datasets.MNIST('../data', train=True, download=True,  
        transform=transforms.Compose([  
            transforms.RandomRotation(15),  
            transforms.RandomRotation([90, 180, 270]),  
        ]))
```

10.9.3 Scale



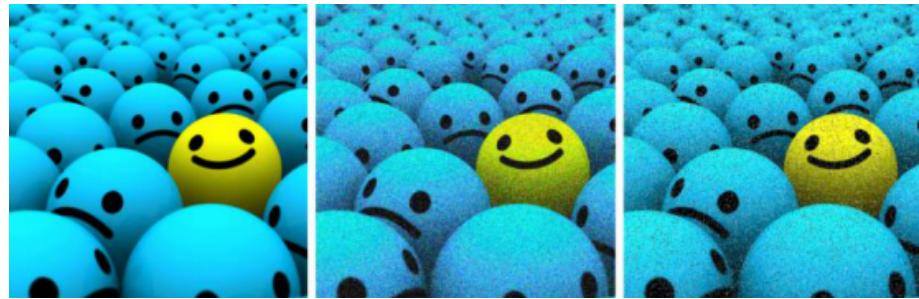
```
train_loader = torch.utils.data.DataLoader(  
    datasets.MNIST('../data', train=True, download=True,  
        transform=transforms.Compose([  
            transforms.Resize([32, 32]),  
        ])),
```

10.9.4 crop part



```
train_loader = torch.utils.data.DataLoader(  
    datasets.MNIST(..../data, train=True, download=True,  
        transform=transforms.Compose([  
            transforms.RandomCrop([28, 28]),  
        ])),
```

10.9.5 noise



pytorch 没有加入高斯白噪点的 API，可人为加上高斯分布图片实现图片的随机噪声。