PyTorch

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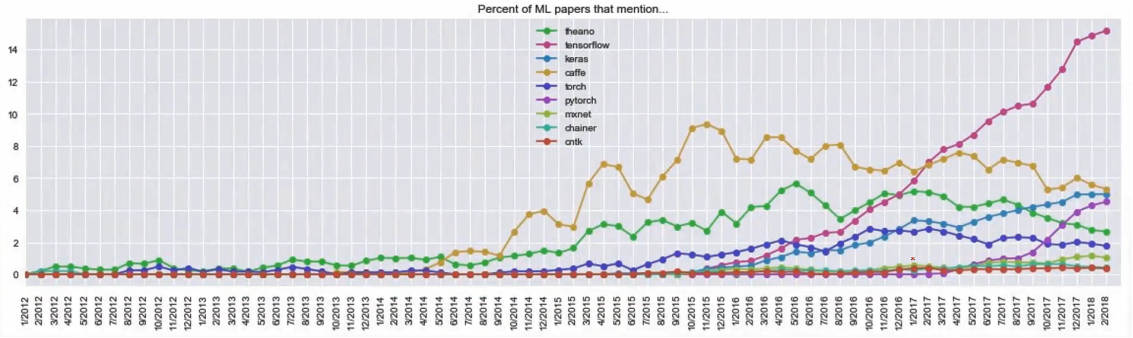
1 PyTorch 简介

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】
   (a) 自建命名体系
   (b) 自建时序控制
   (c) 难以介入

1.3 使用深度学习框架的优点

1. GPU 加速 (cuda)
2. 自动求导
3. 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 $[0, 1, 0, 0, \cdots]$

   (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	`torch.float32` or `torch.float`	`torch.FloatTensor`	`torch.cuda.FloatTensor`
64-bit floating point	`torch.float64` or `torch.double`	`torch.DoubleTensor`	`torch.cuda.DoubleTensor`
16-bit floating point	`torch.float16` or `torch.half`	`torch.HalfTensor`	`torch.cuda.HalfTensor`
8-bit integer (unsigned)	`torch.uint8`	`torch.ByteTensor`	`torch.cuda.ByteTensor`
8-bit integer (signed)	`torch.int8`	`torch.CharTensor`	`torch.cuda.CharTensor`
16-bit integer (signed)	`torch.int16` or `torch.short`	`torch.ShortTensor`	`torch.cuda.ShortTensor`
32-bit integer (signed)	`torch.int32` or `torch.int`	`torch.IntTensor`	`torch.cuda.IntTensor`
64-bit integer (signed)	`torch.int64` or `torch.long`	`torch.LongTensor`	`torch.cuda.LongTensor`

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.non 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 unqueeze，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。

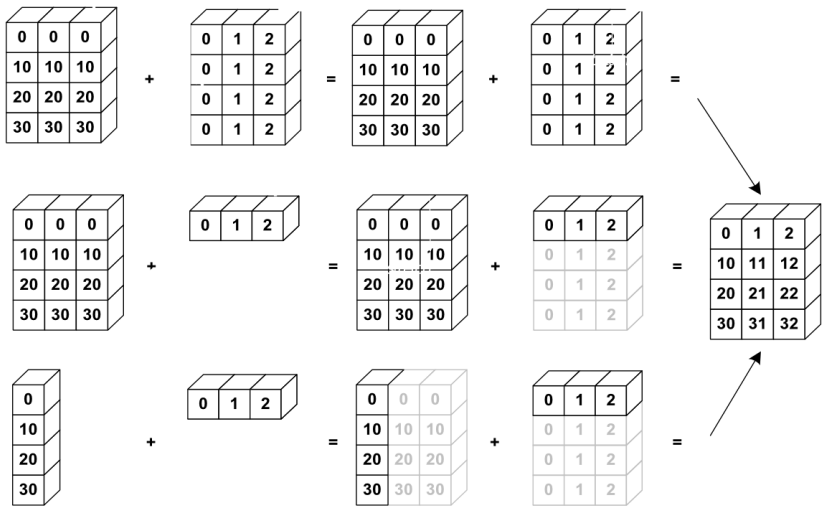
   Repeat： memory copied 内存相关。

```
#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] => [1, 32, 1, 1] => [4, 32, 14, 14]

存在意义:

1. for actual demanding(实际需求)
   - $[class, students, scores]$
   - $Addbias for every students: +5score$
   - $[4, 32, 8] + [4, 32, 8]$
   - $[4, 32, 8] + [5.0]$
2. memory consumption(节约内存)
   - $[4, 32, 8] => 1024$
   - $[5.0] => 1$

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 splite)

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

$$||x||_1 = \sum_{i=1}^{n} |a_i|$$

$$||x||_e = \sqrt{\sum_{i=1}^{n} x_i^2}$$

$$||x||_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{\frac{1}{p}}$$

matrix norm

$$||A||_1 = \max_{i \le j \le n} \sum_{i=1}^{n} |a_{ij}|$$

$$||A||_e = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2}$$

$$||A||_p = \left(\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2\right)^{\frac{1}{p}}$$

```
a = torch.full([8], 1)
b = a.reshape(2, 4)
c = b.reshape(2, 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 braodcast，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
```

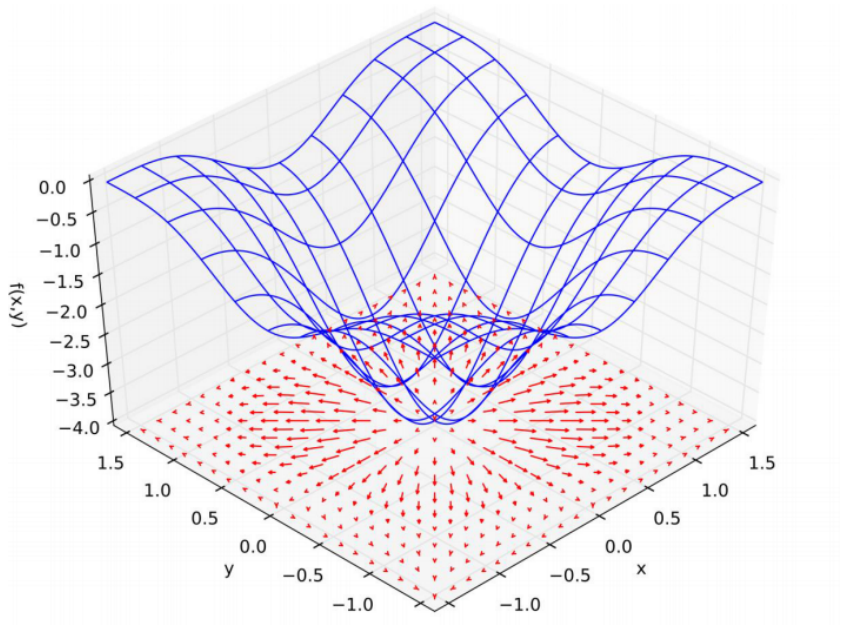
6 随机梯度下降

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

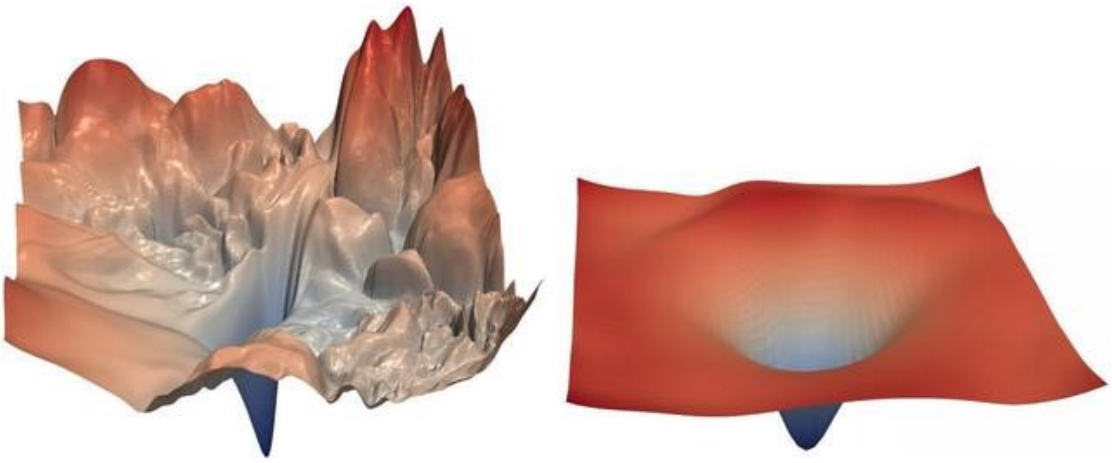
$$\theta_{t+1} = \theta_t - \alpha_t \nabla f(\theta_t)$$

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. 初始化状态
2. 学习率
3. 动量（逃离局部极小值）
4. ···

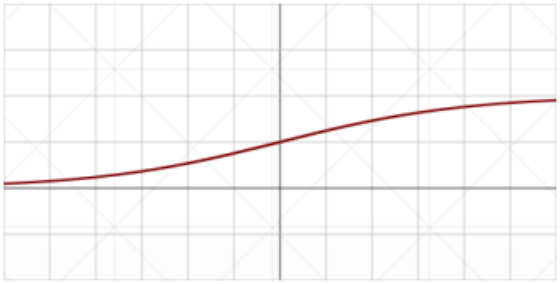
6.2 常见函数的梯度

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	$a^x lna$ e^x
对数函数	$log_a(x)$ lnx	$1/(xlna)$ 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）。

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



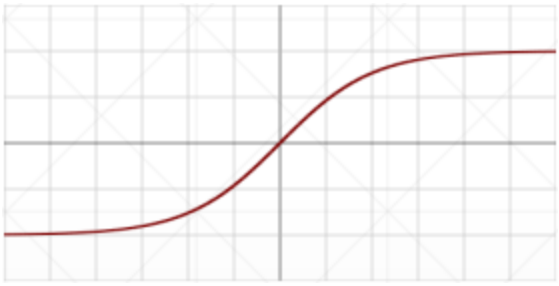
求导:

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

```
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

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



求导:

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

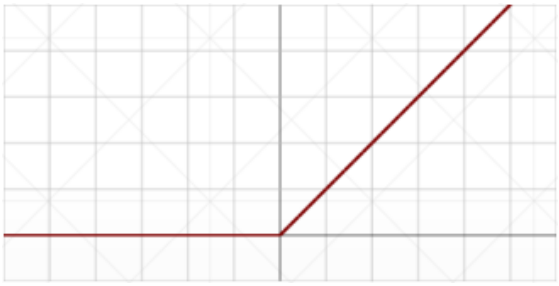
```
z = torch.linspace(-2, 2, 5)
z   #tensor([-2., -1., 0., 1., 2.])
torch.tanh(z) #tensor([-0.9640, -0.7616, 0.0000, 0.7616, 0.9640])
```

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)

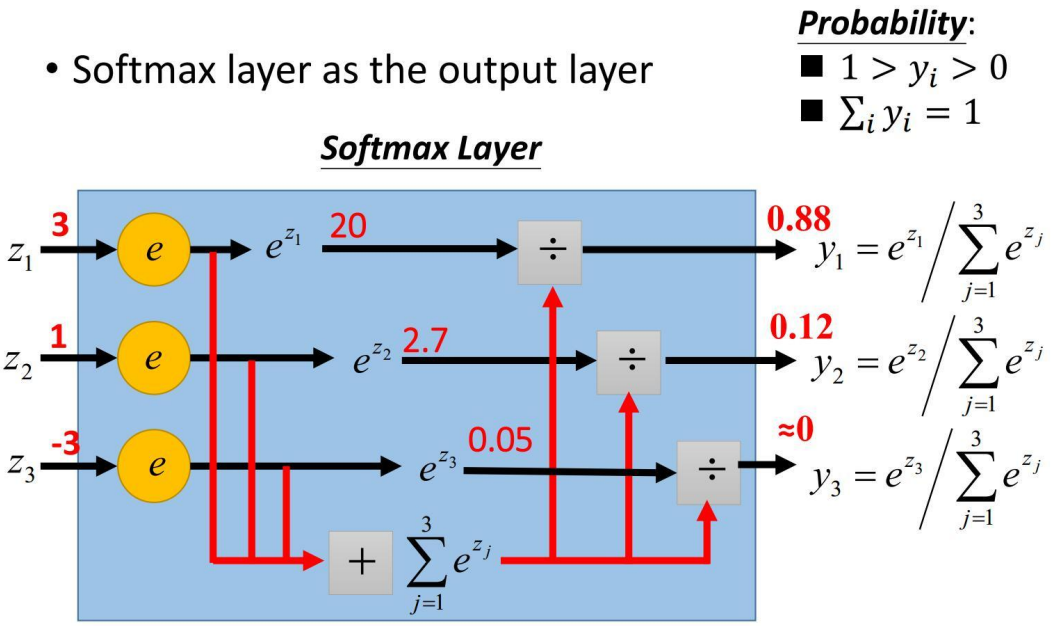
- $loss = \sum \big(y - (w * x + b)\big)^2$
  $loss = norm\big(y - (w * x + b)\big)^2$
- $\frac{\nabla loss}{\nabla \theta} = 2 \sum \big(y - f_\theta(x)\big) * \frac{\nabla f_\theta(x)}{\nabla \theta}$
- Gradient API:

```
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：

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

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

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

$i == j$

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

$i \neq j$

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

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：

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

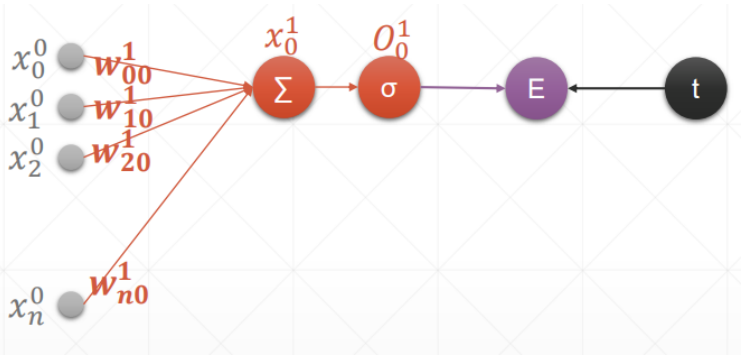
得到公式：

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

```
from torch.nn import functional as F
a = torch.rand(3, requires_grad=True)
p = F.softmax(a, dim=0)
a   #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



$$E = \frac{1}{2}(O_0^1 - t)^2$$

$$\frac{\partial E}{\partial w_{j0}} = (O_0^1 - t)\frac{\partial O_0^1}{\partial w_{j0}} = (O_0^1 - t)\frac{\partial \sigma(x_0^1)}{\partial w_{j0}}$$

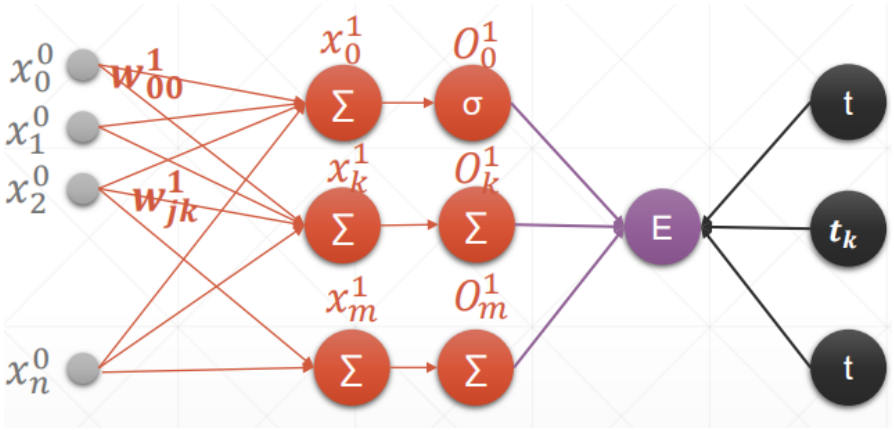
$$\frac{\partial E}{\partial w_{j0}} = (O_0^1 - t)\sigma(x_0^1)(1 - \sigma(x_0^1))\frac{\partial x_0^1}{\partial w_{j0}}$$

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

$$\frac{\partial E}{\partial w_{j0}} = (O_0^1 - t)O_0^1(1 - O_0^1)x_j^0$$

```
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

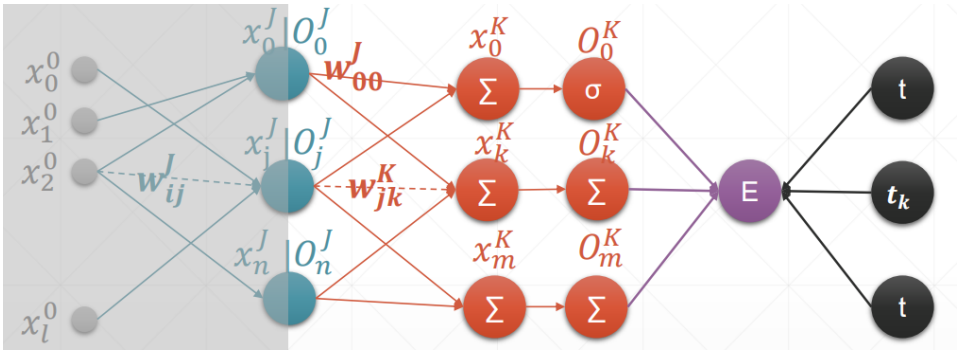
Rules	Function	Derivative
Multiplication by constant	cf	cf′
Power Rule	x^n	nx^{n-1}
Sum Rule	f + g	f′ + g′
Difference Rule	f - g	f′ − g′
Product Rule	fg	f g′ + f′ g
Quotient Rule	f/g	$(f' g - g' f)/g^2$
Reciprocal Rule	1/f	$-f'/f^2$
Chain Rule (as "Composition of Functions")	f ∘ g	(f′ ∘ g) × g′
Chain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

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:

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

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

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

那么再求第J层的权值偏微分:

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial}{\partial w_{ij}} \frac{1}{2} \sum_{k \in K} (O_k - t_k)^2$$

$$\frac{\partial E}{\partial w_{ij}} = \sum_{k \in K} (O_k - t_k) \frac{\partial}{w_{ij}} O_k = \sum_{k \in K} (O_k - t_k) \frac{\partial}{w_{ij}} \sigma(x_k)$$

$$\frac{\partial E}{\partial w_{ij}} = \sum_{k \in K} (O_k - t_k)\sigma(x_k)(1 - \sigma(x_k)) \frac{\partial x_k}{\partial w_{ij}}$$

$$= \sum_{k \in K} (O_k - t_k)\sigma(x_k)(1 - \sigma(x_k)) \frac{\partial x_k}{\partial O_j} \cdot \frac{\partial O_j}{\partial w_{ij}}$$

$$= \sum_{k \in K} (O_k - t_k)O_k(1 - O_k)w_{jk}^K \frac{\partial O_j}{\partial w_{ij}} = \frac{\partial O_j}{\partial w_{ij}} \sum_{k \in K} (O_k - t_k)O_k(1 - O_k)w_{jk}^K$$

$$= O_j(1 - O_j) \frac{\partial x_j}{\partial w_{ij}} \sum_{k \in K} (O_k - t_k)O_k(1 - O_k)w_{jk}^K$$

$$= O_j(1 - O_j)O_i \sum_{k \in K} (O_k - t_k)O_k(1 - O_k)w_{jk}^K$$

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,

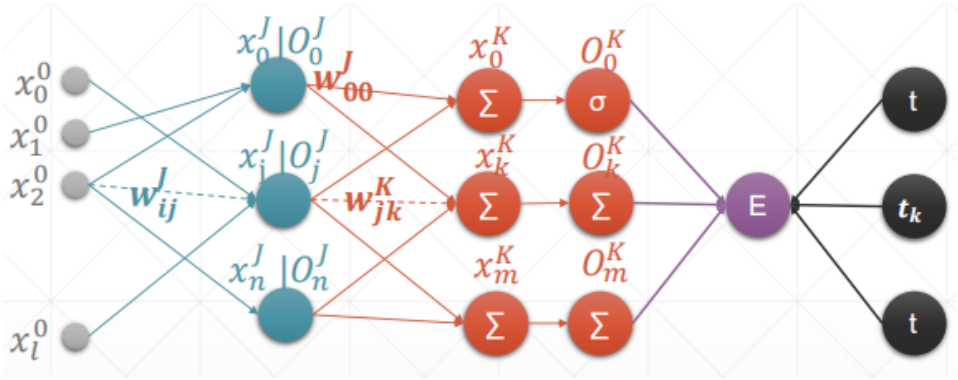
$$\delta_k = O_k(1 - O_k)(O_k - t_k)$$

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:

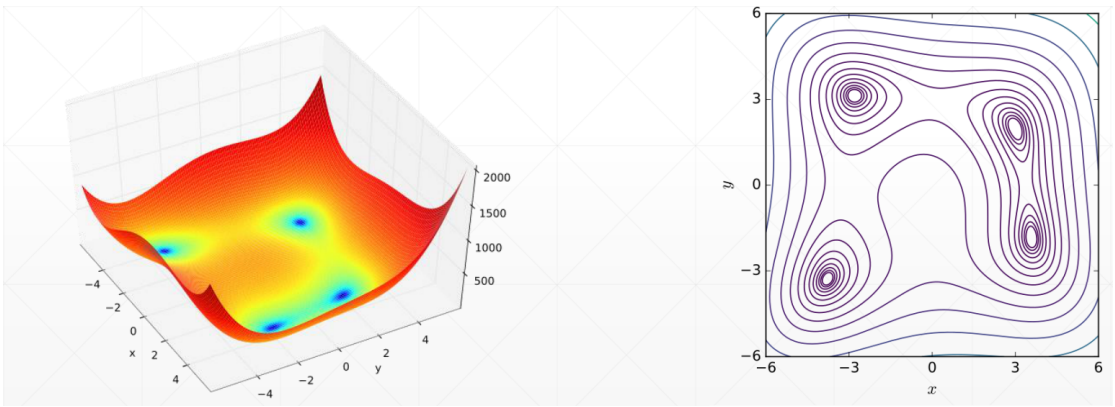
$$O^J \; -->\; O^K \; -->\; E$$

反向传播:

$$\delta^K \; -->\; \frac{\partial E}{\partial w^K} \; -->\; \delta^J \; -->\; \frac{\partial E}{\partial w^J} \; -->\; \delta^L \; -->\; \frac{\partial E}{\partial w^L}$$

7.5 2D 函数优化实例

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



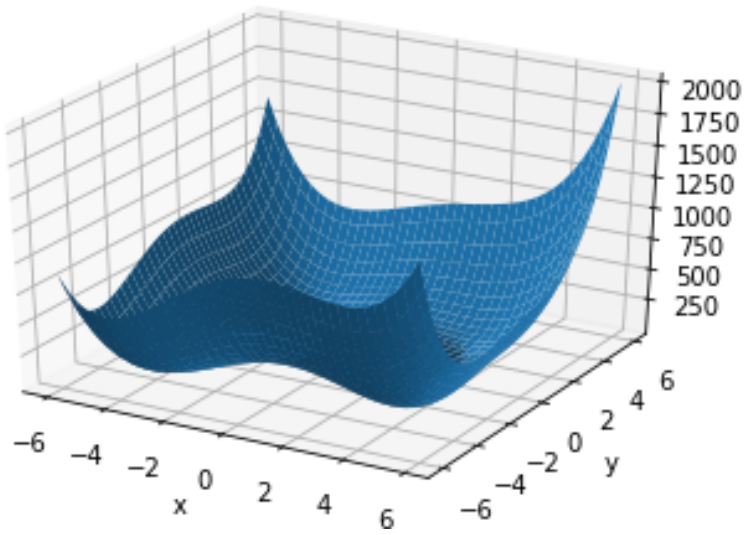
minma:

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

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。
   - acc.= $\frac{I(pred_i==y_i)}{len(Y)}$
   - 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

$$entropy = -\sum_i P(i)logP(i)$$

8.2.2 Cross Entropy

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

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

$$p = q, \quad Cross\ entropy = entropy$$

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

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。

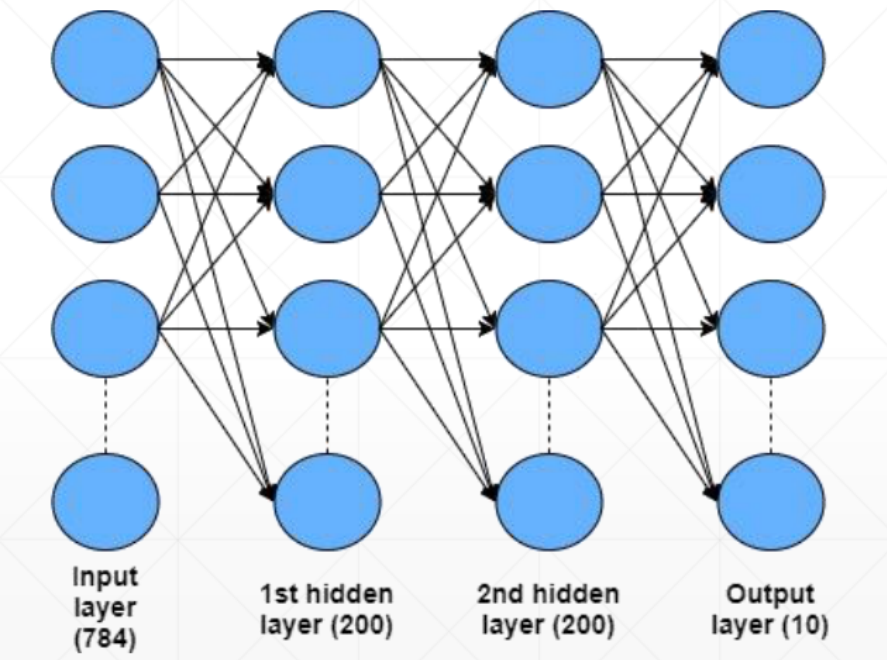
小结:

$$logit --> softmax --> cross\ entropy$$

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 = criteon(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 += criteon(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

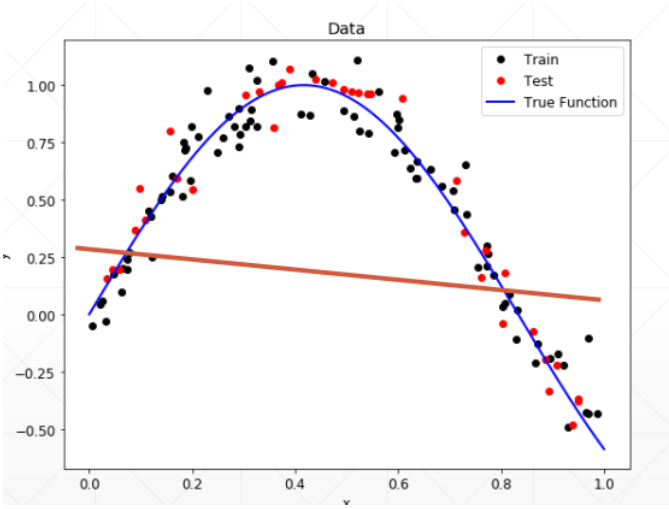
```
python -m visdom.server
```

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

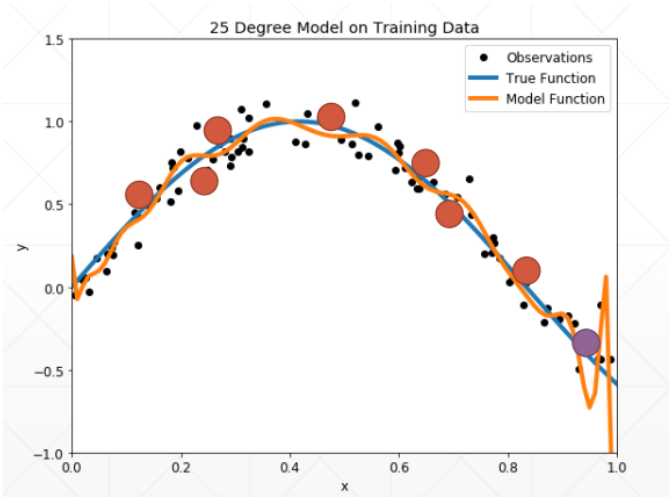
9.1 过拟合与欠拟合

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。

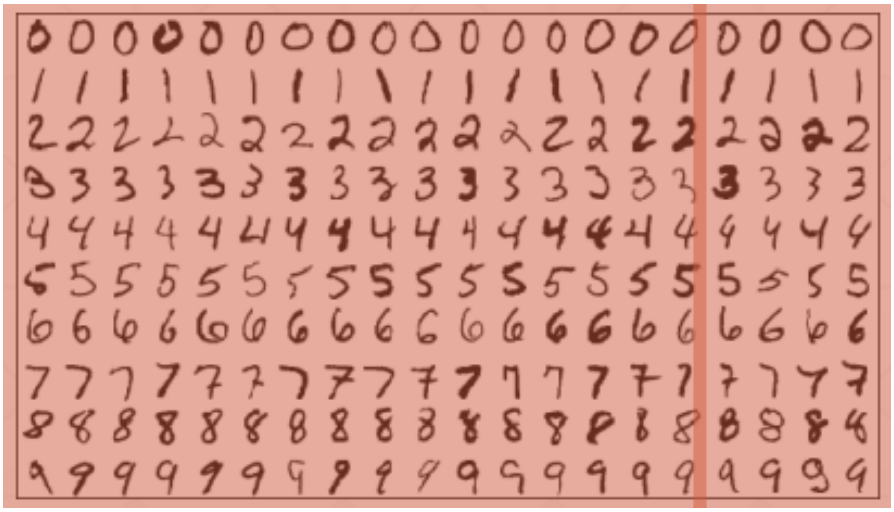
检测过拟合-交叉验证

防止过拟合-正则化

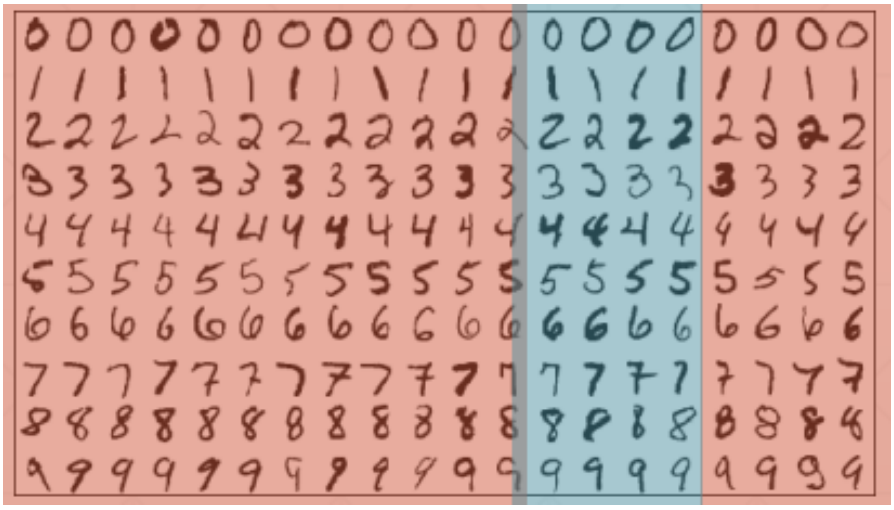
9.2 交叉验证

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。

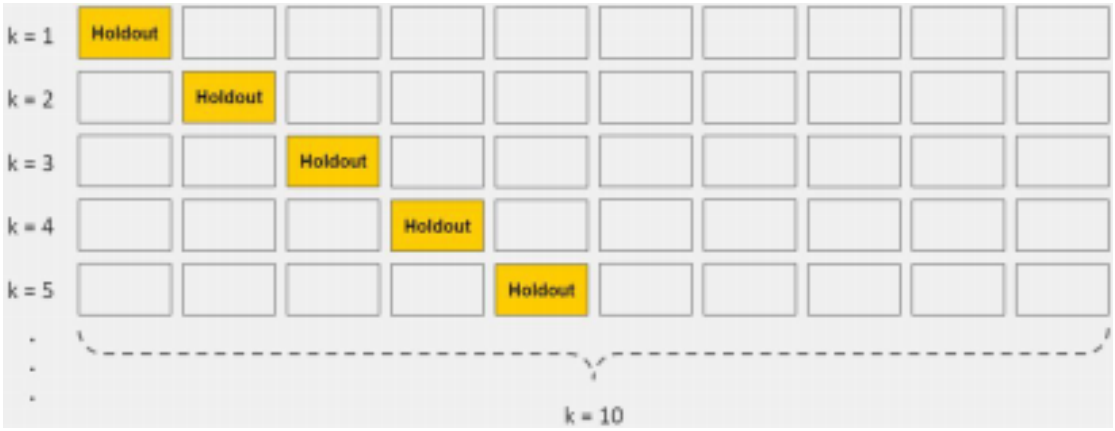


将数据划分成三类，客户用保密的测试集来测试模型效果，防止作弊。

```
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，选择较好的时间戳权值参数。

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

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

```
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

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

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

9.4 动量与学习率衰减

9.4.1 动量

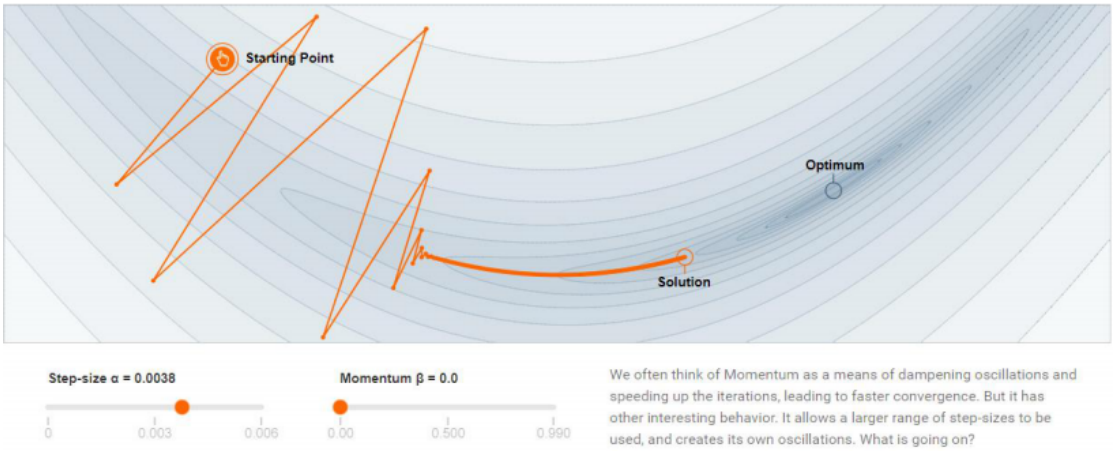
momentum 动量也称惯性

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

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

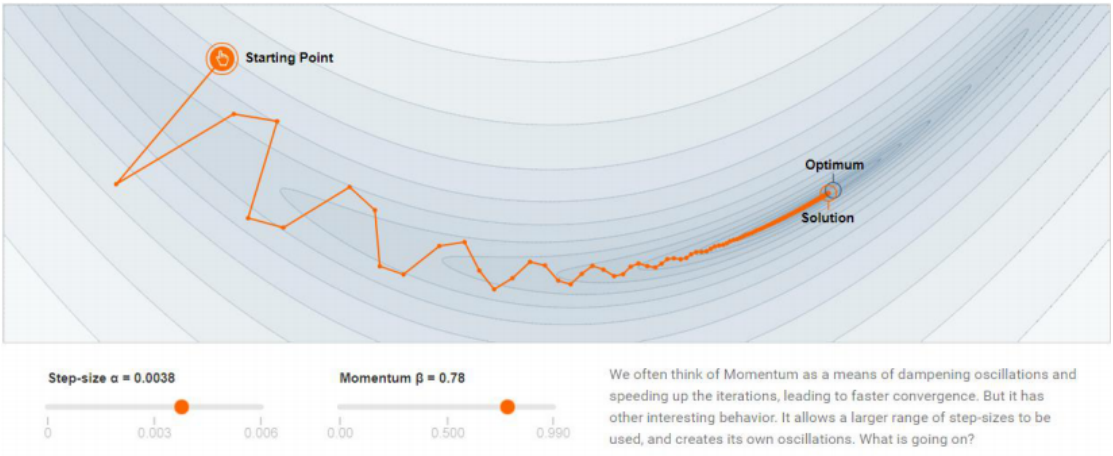
加入动量的迭代式，实际上就是当前的梯度方向加上上一次的惯性的方向。尽快收敛，并且大概率的跳出局部极小值。

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



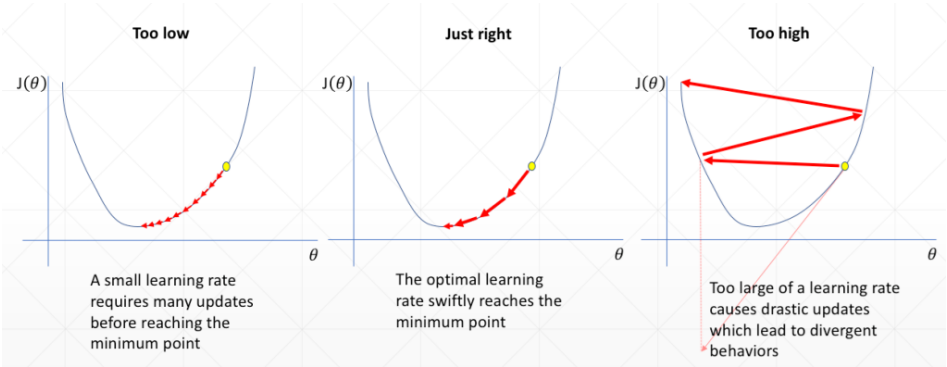
梯度更新效率高，越过了局部极小，步入全局最小。

```
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

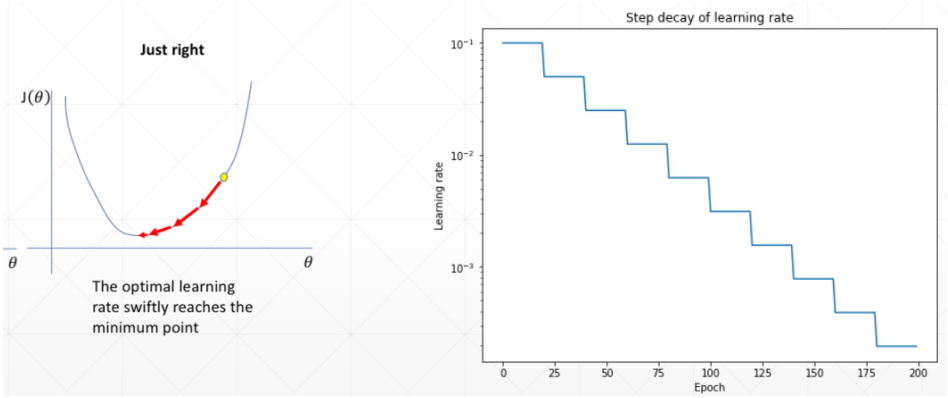
learning rate decay



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

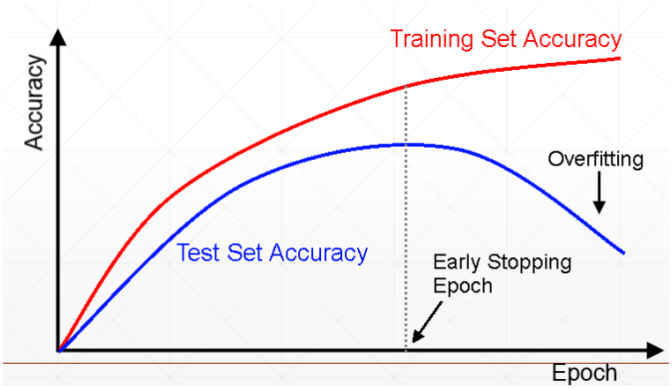
2. 方法二定时衰减

```
#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

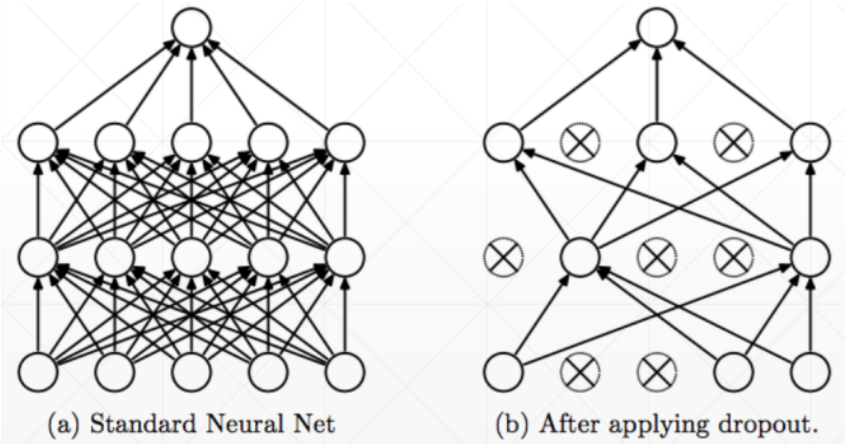
提前停止更新是为了模型学习过拟合。



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 ρ= 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(),
```

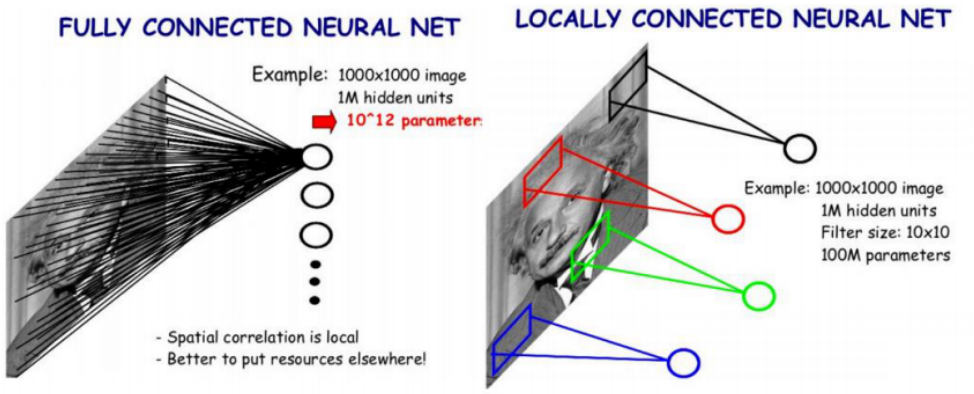
```
    torch.nn.Linear(200, 10)
)
```

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。

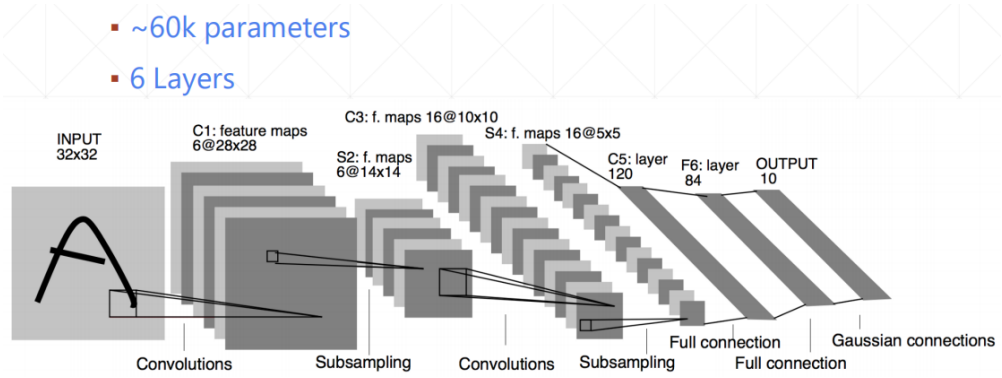
```
for epoch for range(epochs):

    # 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

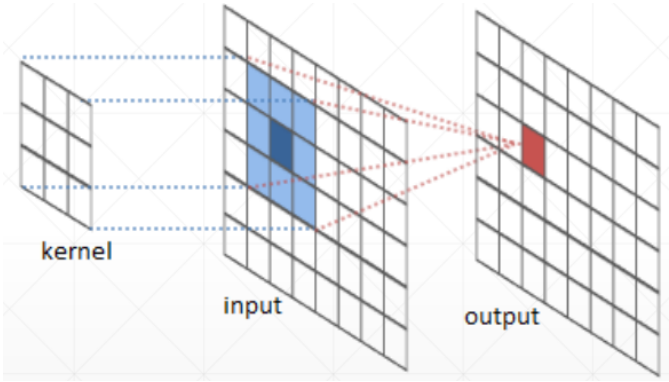
10.1 卷积



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。

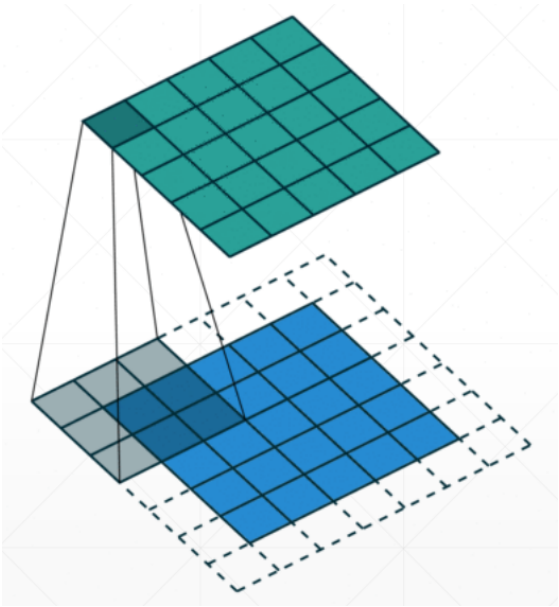


卷积一次来源于信号处理上两个函数之间的卷积运算，操作可视化后类似。



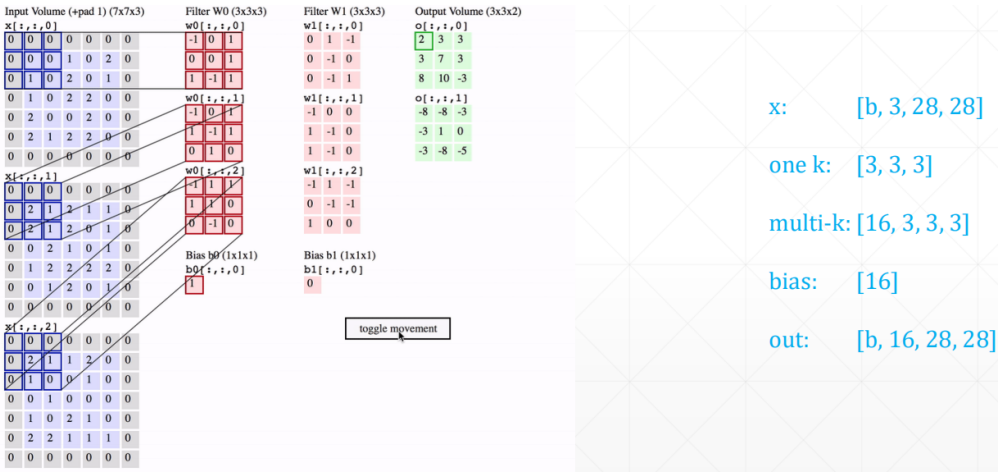
10.2 卷积神经网络

10.2.1 notation

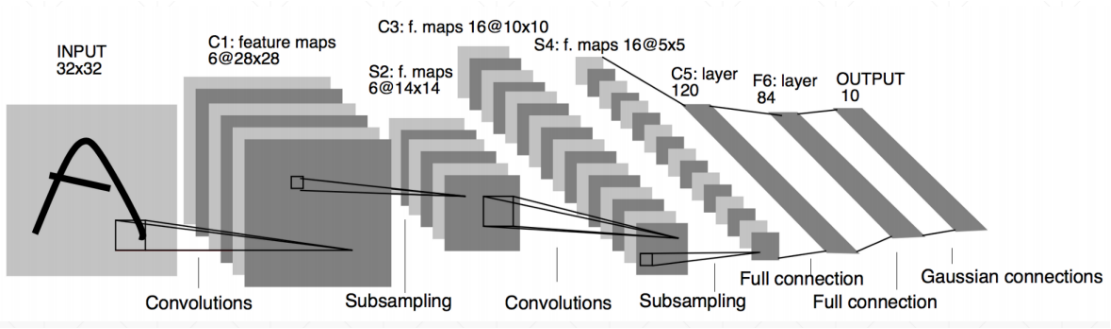


1. Input_channels
2. Kernel_channels: 2ch
3. Kernel_size
4. Stride 步幅。
5. Padding 填充。

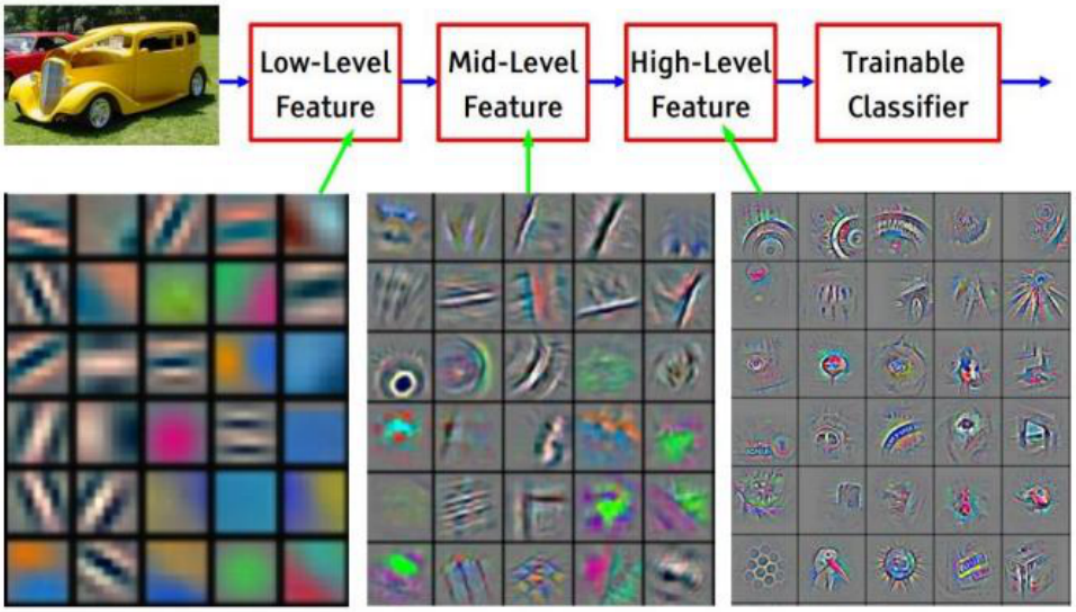
10.2.2 Multi-Kernel



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。

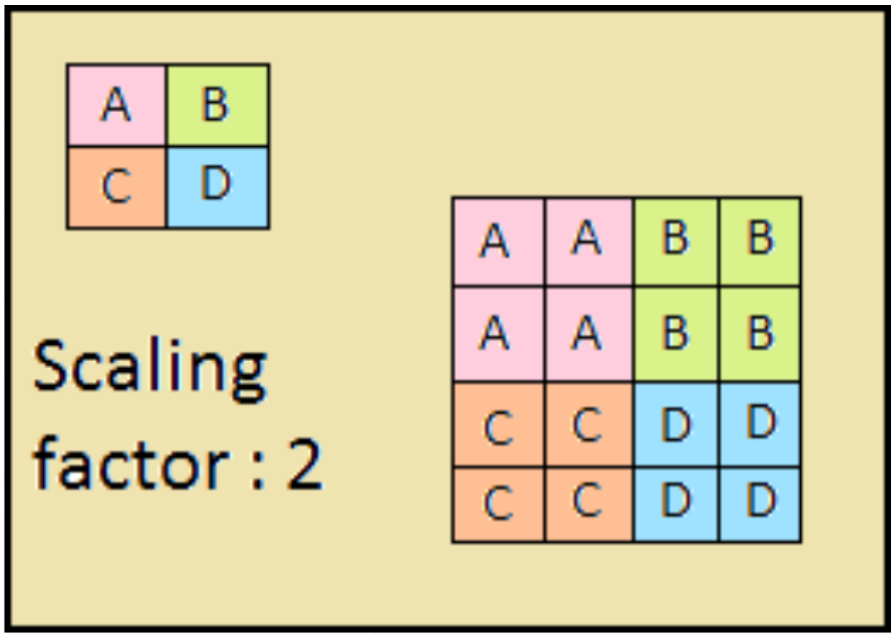
pooling 策略:

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])
```

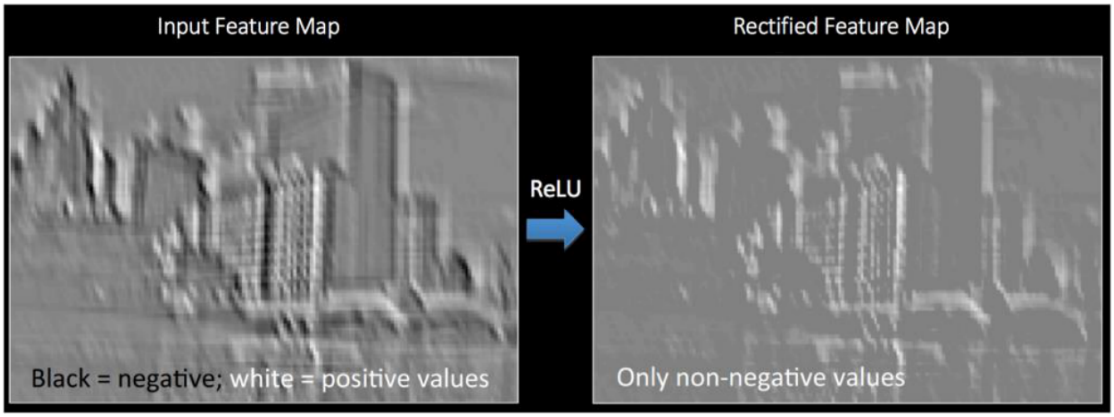
10.3.2 upsample

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



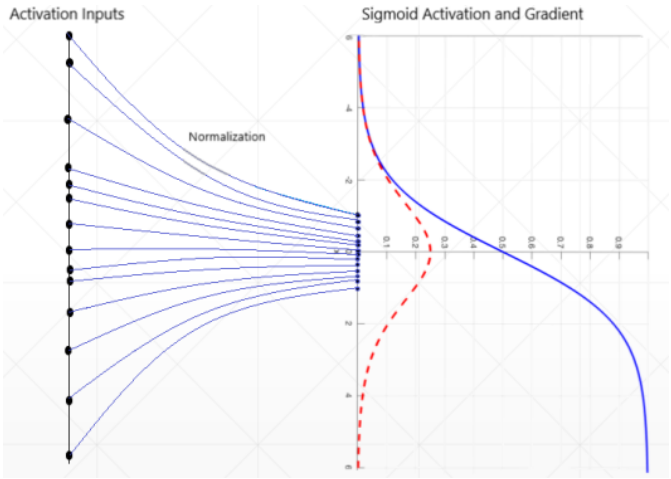

```
layer = nn.Conv2d(2, 16, kernel_size=3, stride=1, padding=1)
x = torch.rand(1, 2, 28, 28)
```

```
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。

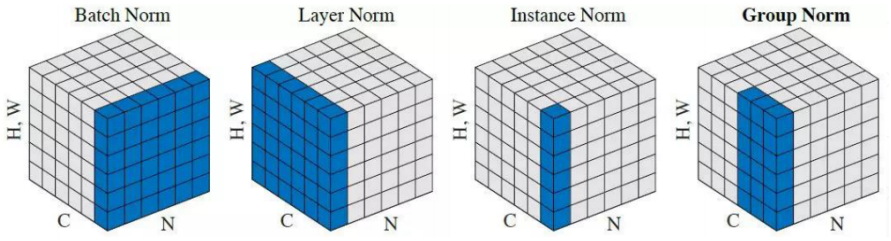
1. image Normlization

```
normlize = 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 Normlization

常见的 Norm 类型。



可以看出来 Batch Normlization 只保留 channel 的统计数据 mean 以及 varience.

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

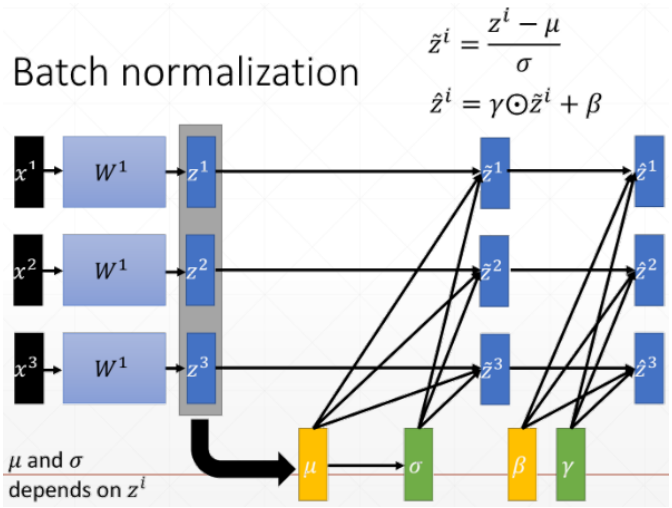
$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma^2_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

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



Batch Normlization 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

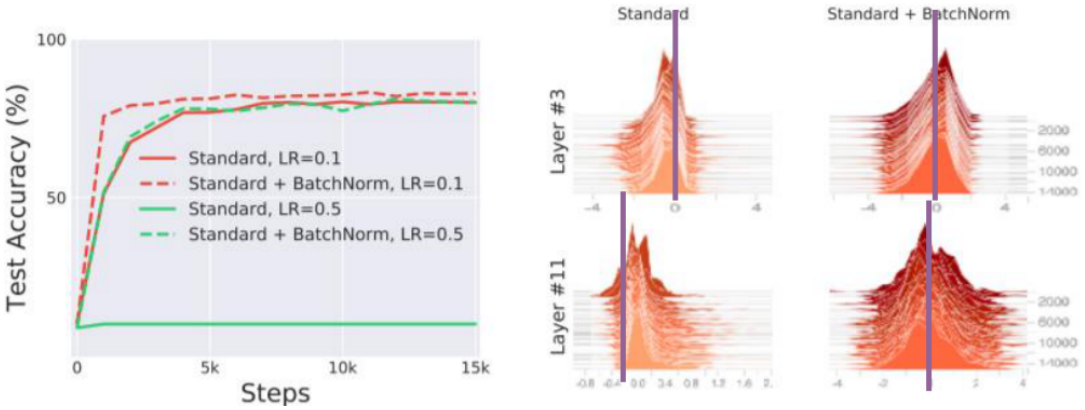
```
vars(layer)
# affine: True,   otherwise weight=1, bias=0 not update
# training: True,   not test mode
```

Batch Normlization 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 varience .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



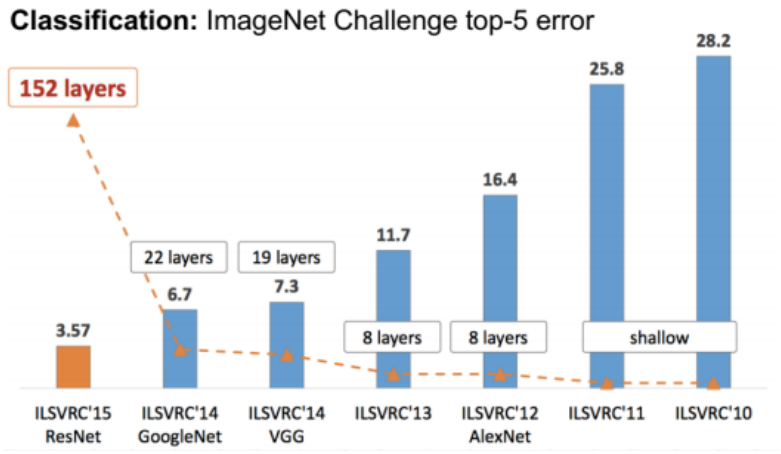
10.4.4 使用优势

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

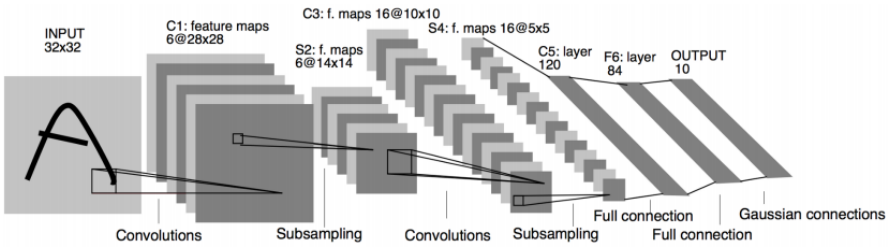
10.5 经典的卷积神经网络

10.5.1 ImageNet dataset 224x224



10.5.2 LeNet-5

Yann LeCun 深度学习三驾马车之一



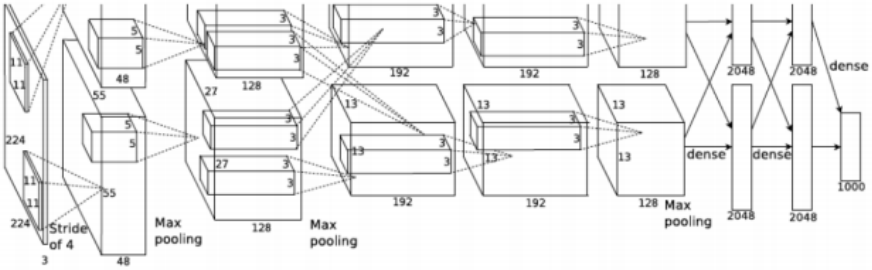
上世纪80年代产物，用于手写字体识别，精度优秀。

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

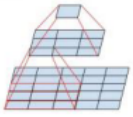
VGGNet: ILSVRC 2014 2nd place

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
input (224 × 224 RGB image)					
conv3-64	conv3-64 **LRN**	conv3-64 **conv3-64**	conv3-64 conv3-64	conv3-64 conv3-64	conv3-64 conv3-64
maxpool					
conv3-128	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 **conv1-256**	conv3-256 conv3-256 **conv3-256**	conv3-256 conv3-256 conv3-256 **conv3-256**
maxpool					
conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512 **conv1-512**	conv3-512 conv3-512 **conv3-512**	conv3-512 conv3-512 conv3-512 **conv3-512**
maxpool					
conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512 **conv1-512**	conv3-512 conv3-512 **conv3-512**	conv3-512 conv3-512 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)



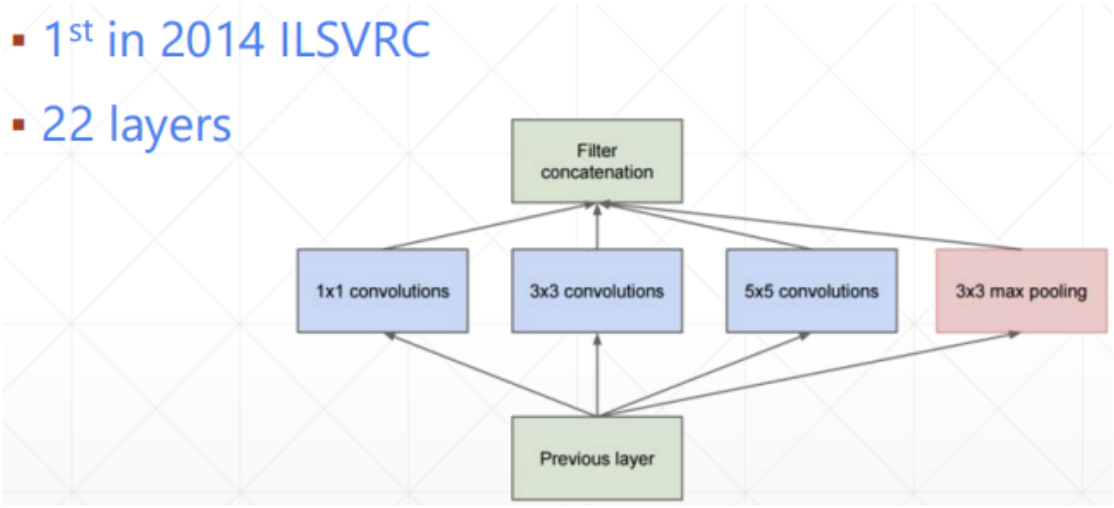
- One 7x7 conv layer with C feature maps needs $49C^2$ weights, three 3x3 conv layers need only $27C^2$ weights
- Experimented with 1x1 convolutions

K. Simonyan and A. Zisserman,
Very Deep Convolutional Networks for Large-Scale Image Recognition, ICLR 2015

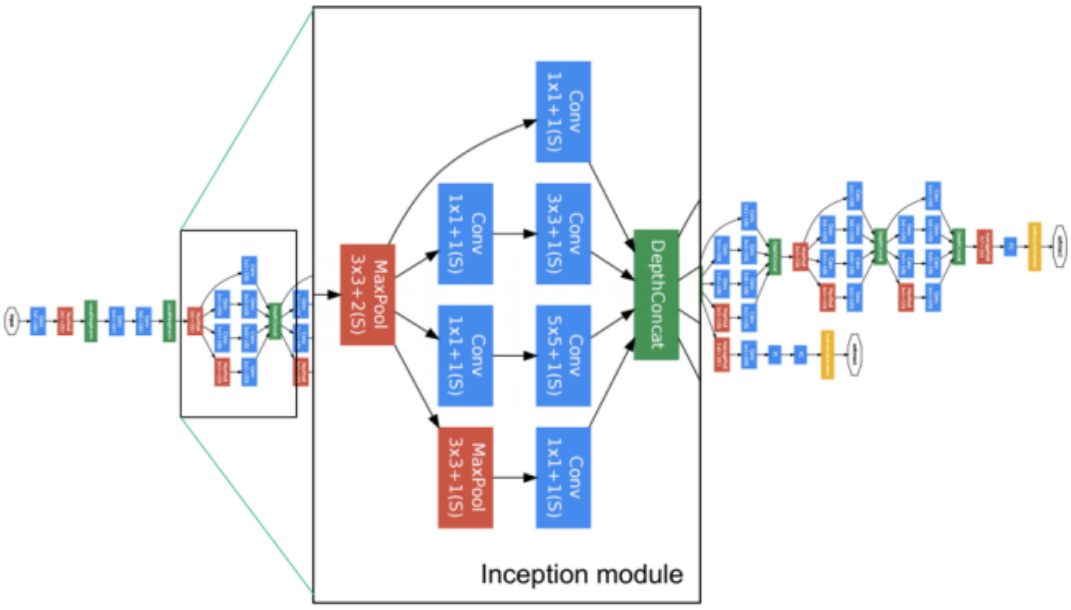
1x1 convolution

1. less computation 2. c_in => c_out

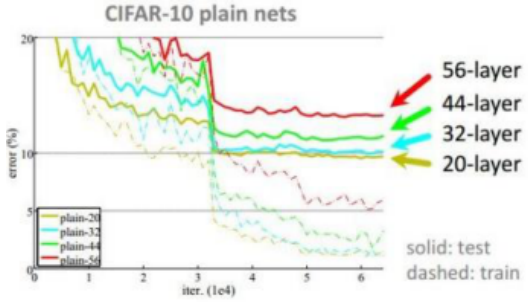
10.5.5 GoogLeNet

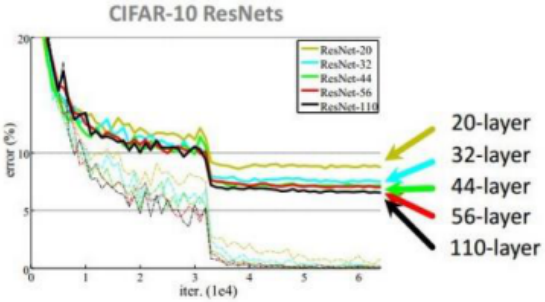


综合不同 size's kernel 的感受野。



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**



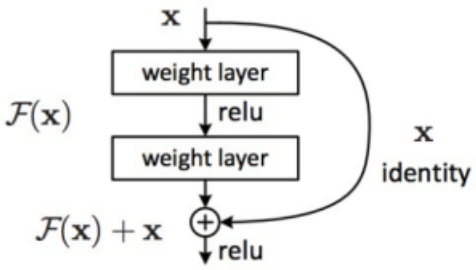


10.6 ResNet

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

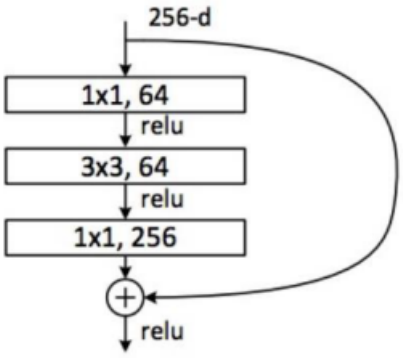


Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun,
Deep Residual Learning for Image Recognition, CVPR 2016 (Best Paper)

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 x 256 x 3 x 3 ~ 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 x 64 x 1 x 1 ~ 16K
  64 x 64 x 3 x 3 ~ 36K
  64 x 256 x 1 x 1 ~ 16K
  Total: ~70K

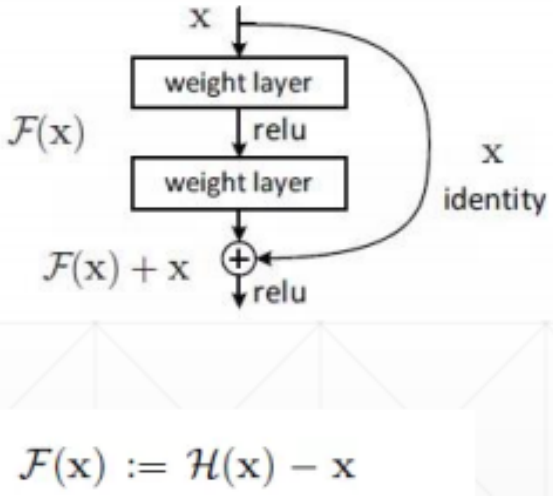
Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun,
Deep Residual Learning for Image Recognition, CVPR 2016 (Best Paper)

新的 Unit 单元，shape 不能变。将短路权利交给网络。

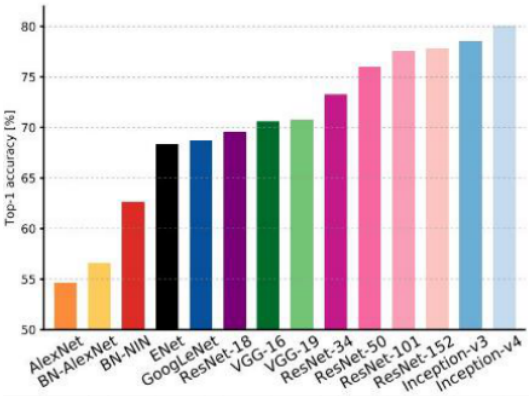
MSRA @ ILSVRC & COCO 2015 Competitions

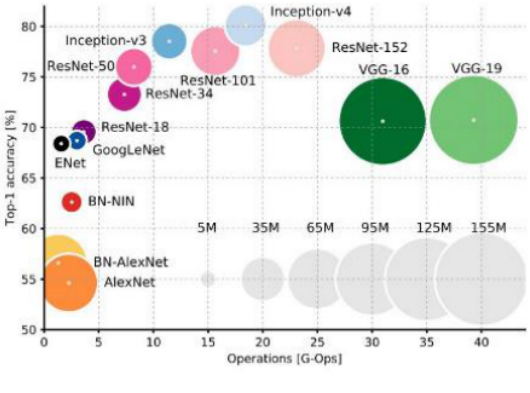
- **1st places in all five main tracks**
  - ImageNet Classification: "*Ultra-deep*" (quote Yann) 152-layer nets
  - ImageNet Detection: 16% better than 2nd
  - ImageNet Localization: 27% better than 2nd
  - COCO Detection: 11% better than 2nd
  - COCO Segmentation: 12% better than 2nd

为什么叫残差(Residual)?

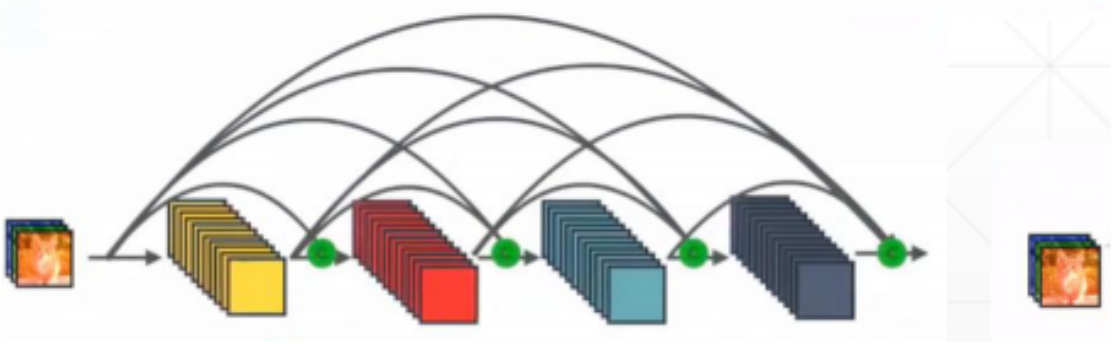


层数性能比较:





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

- 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.

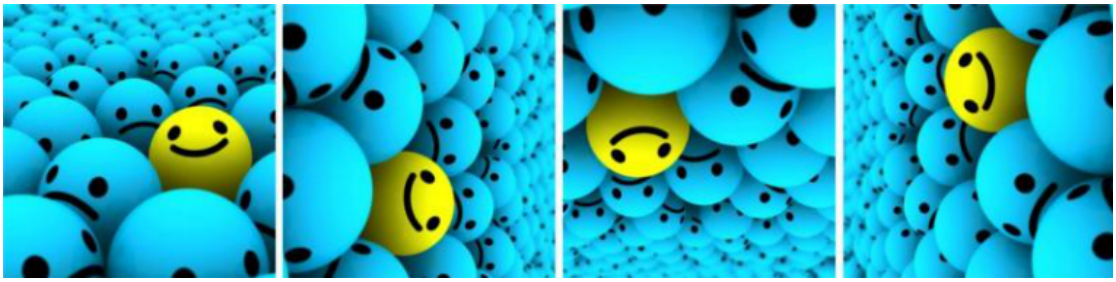
Data Argumentation

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

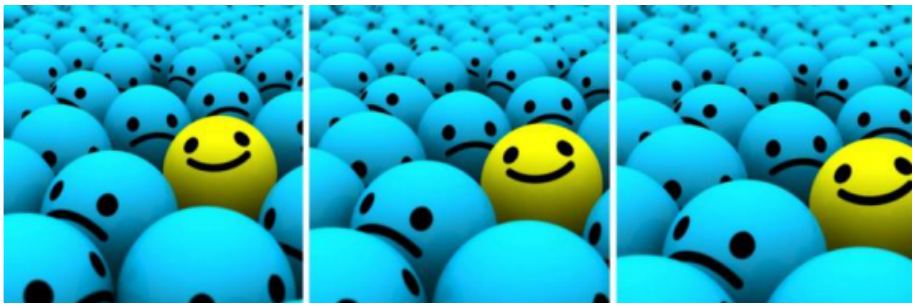
```
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST(../data, train=True, download=True,
                   transform=transforms.Compose([
                       transforms.RandomHorizontalFlip(),
                       transforms.RandomVerticalFlip(),
                   ])),
```

10.9.2 Rotation



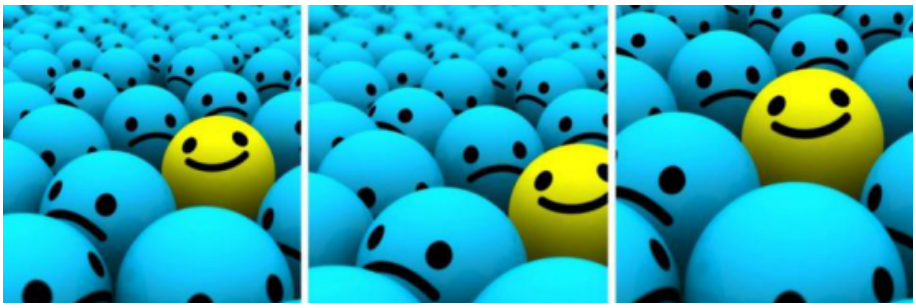
```
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST(../data, train=True, download=True,
                   transform=transforms.Compose([
                       transforms.RandomRotation(15),
                       transforms.RandomRotation([90, 180, 270]),
                   ]))
```

10.9.3 Scale



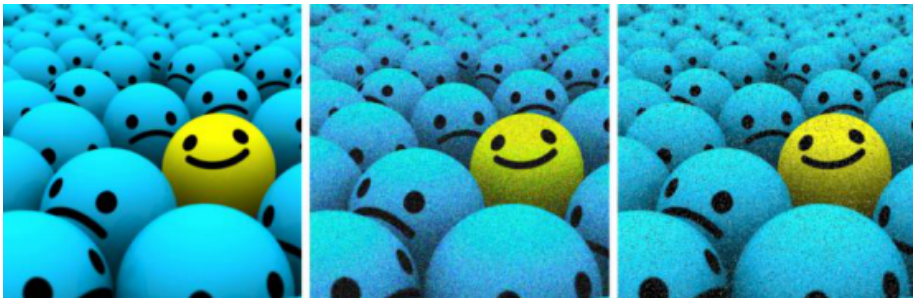
```
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST(../data, train=True, download=True,
                   transform=transforms.Compose([
                       transforms.Resize([32, 32]),
                   ])),
```

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。