神经网络基础

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本堂课大纲

- 全连接神经网络
  - 激活函数
  - 万能逼近定理
- 神经网络中的模块
- 神经网络的训练
  - 初始化
  - 反向传播
  - 凸优化

利用非线性模型的监督学习

- 监督学习

训练数据：$(x_1, y_1), (x_2, y_2), \cdots\cdots, (x_n, y_n)$

线性模型：$f(x) = x^T w$

$f(x) = \Psi(x)^T w$

非线性模型：$f(x; \theta)$

优化均方误差函数：

$$J(\theta) = \frac{1}{n}\sum_{j=1}^{n} J^{(i)}(\theta) \qquad J^{(i)}(\theta) = \frac{1}{2}(f(x_i; \theta) - y_i)^2$$

神经网络

- 全连接神经网络

$$y = f(x;\theta): R^{n_0} \to R^{n_L}$$

$$f(x;\theta) = f_L \circ f_{L-1} \circ \cdots\cdots \circ f_1(x)$$

$$f_i(z) = h^{(i)}\left(W^{(i)}z + b^{(i)}\right): R^{n_{i-1}} \to R^{n_i}$$

矩阵：$W^{(i)} \in R^{n_i \times n_{i-1}}$

向量：$b^{(i)} \in R^{n_i}$

对每个元素作用的(非线性)激活函数：$h^{(i)}$

激活函数

- 激活函数

对每个元素作用的(非线性）激活函数：h

$$h(z) = [\sigma(z_1), \sigma(z_2), \cdots\cdots \sigma(z_n)]^T$$

RELU: $\sigma(z) = \max\{0, z\}$

Sigmoid: $\sigma(z) = \frac{1}{1+e^{-z}}$

Tanh: $\sigma(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$

Leaky RELU: $\sigma(z) = \max\{z, \gamma z\} (\gamma \in (0,1))$

GELU: $\sigma(z) = \frac{z}{2}[1 + \mathrm{erf}(\frac{z}{\sqrt{2}})]$

SoftPlus: $\sigma(z) = \frac{1}{\beta}\log(1 + e^{\beta z}), \beta > 0$

激活函数

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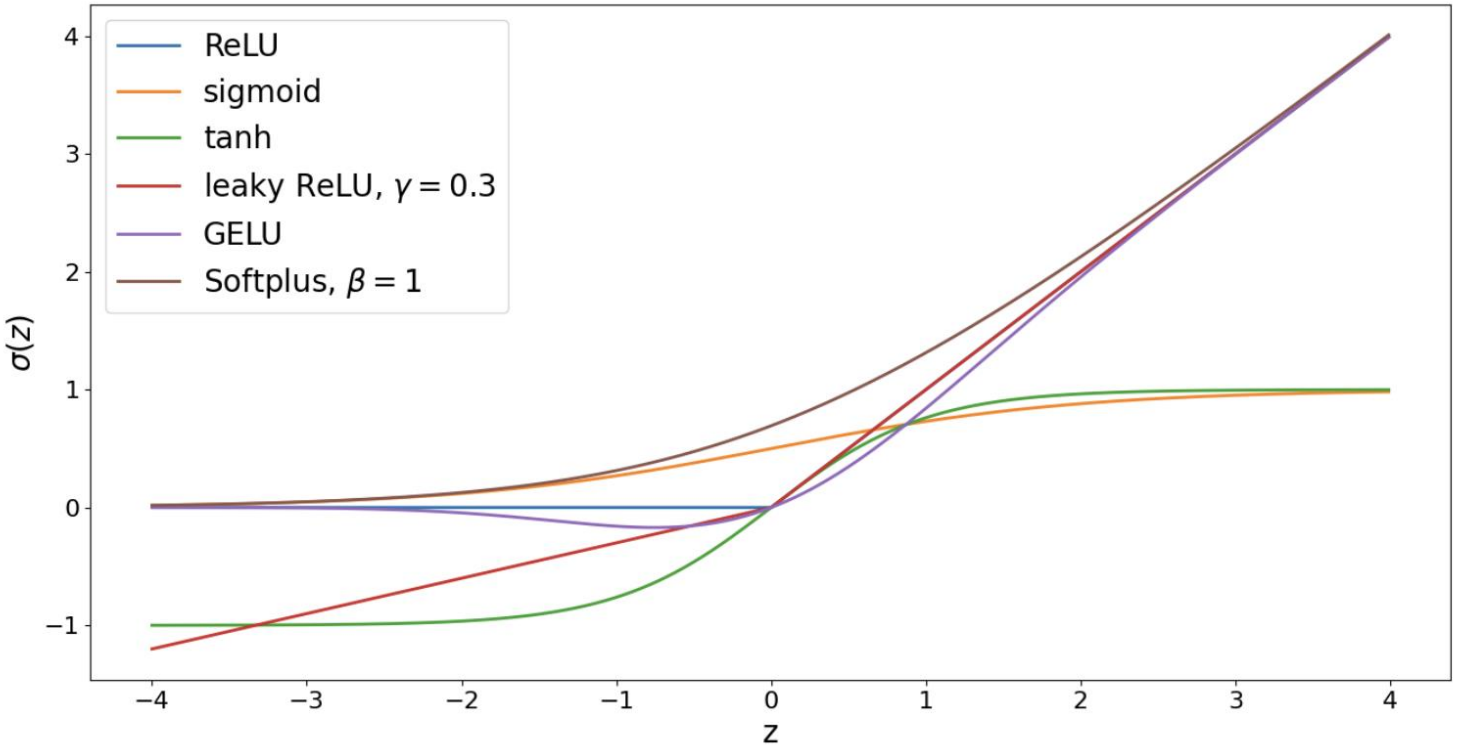
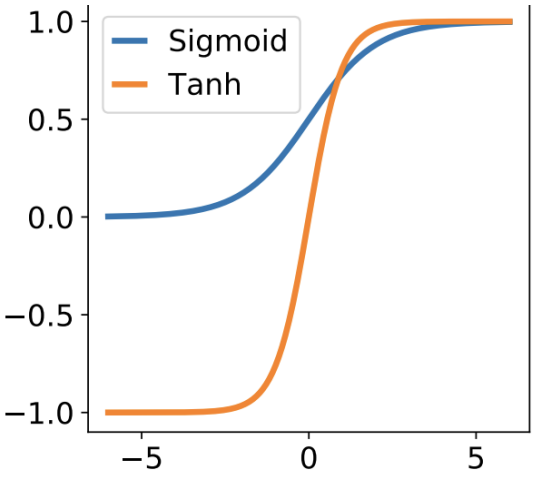
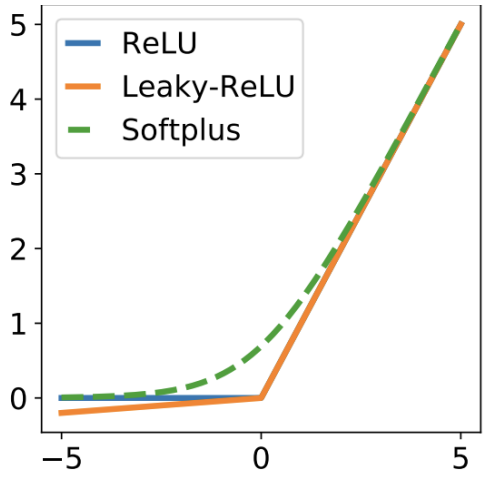
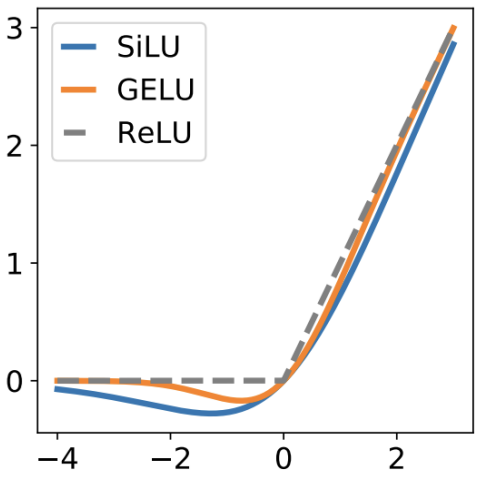


激活函数

- 激活函数饱和(saturating)
  - 饱和(saturating)
  - 导数消失







激活函数

- 激活函数

对每个元素作用的(非线性）激活函数：h

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神经网络

- 全连接神经网络(multi-layer perceptron)

  在最后一层f_L，激活函数的选择由函数最终输出的约束条件所决定

  -多类分类问题：$h^{(L)}(x) = \frac{e^{x_j}}{\sum_{j=1}^{R^{n_L}} e^{x_j}}$

  -正输出问题：$h^{(L)}(x) = e^x$

  -回归问题：没有激活函数$h^{(L)}(x) = x$

- 回顾：回归问题

  $f(x;\theta) = W^{(L)}\phi_{\theta'}(x) + b^{(L)}$

  $\phi_{\theta'}(x)$: 特征

  同时学习权重和特征

万能逼近定理

通用逼近器

$\mathcal{X}$是一个紧致集。函数族 F 被称为是通用逼近器，如果F在有均匀度量的函数空间$C(\mathcal{X})$中稠密。这等价于说对于任意的 $f \in C(\mathcal{X})$和任意的 $\epsilon > 0$，存在 $\hat{f} \in F$使得

$$\sup_x |f(x) - \hat{f}(x)| < \epsilon$$

Weierstrass逼近定理

假设 $f(x)$ 是定义在实数区间$\mathcal{X} = [a, b]$上的实值连续函数。对于任意的 $\epsilon > 0$ ，存在一个多项式 $p(x)$ ，使得对于所有 $[a, b]$区间内的 x ，都有 $|f(x) - p(x)| < \epsilon$。

万能逼近定理

万能逼近定理（ Cybenko 1989, Hoira 1990 ）

设 $\sigma: R \to R$是一个非常数、有界且连续的函数。令 I_d 表示 d-维单位超立方体 $[0,1]^d$。实数值连续函数在 I_d上的空间记为 $C(I_d)$。那么，给定任何 $\epsilon > 0$和任何连续函数 $f \in C(I_d)$。存在宽度为 D 的两层神经网络，

$$F(x) = W^{(2)}\sigma\left(W^{(1)}x + b^{(1)}\right) + b^{(2)}$$

作为函数 f的近似满足

$$\forall x \in I_d \text{，} |F(x) - f(x)| < \epsilon \text{。}$$

万能逼近定理

- 维数灾难（Curse of dimensionality）

对于L-Lipschitz连续函数，两层的神经网络

$$F(x) = W^{(2)}\sigma\left(W^{(1)}x + b^{(1)}\right) + b^{(2)}$$

对$f \in C(I_d)$近似，达到ϵ的L_∞误差估计，宽度需要为

$$D \sim \left(\frac{L}{\epsilon}\right)^d$$

对于线性函数，线性回归能很好近似
对于C^∞光滑的函数，核岭回归能达到指数收敛

对于什么函数类，神经网络近似能克服维数灾难？

万能逼近定理

逼近定理（ Jones , 1992, Barron 1993 ）

考虑cos激活函数。给定全空间的实值函数 f，它的Fourier变换

$$\hat{f}(w) = \frac{1}{(2\pi)^d} \int_{R^d} f(x) e^{-iw^T x} dx$$

满足

$$C_f = \int_{R^d} |f(w)| dw < \infty$$

给定任意概率密度函数ρ，那么存在宽度为D的两层神经网络 $F(x)$，作为函数 f的近似满足

$$\|F(x) - f(x)\|^2_{L_2(\rho)} \leq \frac{C_f^2}{D}$$

万能逼近定理

万能逼近定理（ Jones , 1992, Barron 1993 ）

考虑sigmoid激活函数。给定紧集Ω上的函数 f，考虑它的全空间L_1延拓f_e ，以及相应的Fourier变换

$$\hat{f}_e(w) = \frac{1}{(2\pi)^d}\int_{R^d} f_e(x)e^{-iw^T x}dx$$

满足

$$C_f = \inf_{f_e}\int_{R^d}(1+\|w\|)|f_e(w)|dw < \infty$$

其中$\|w\| = \sup_{x\in\Omega}|w^T x|$。给定任意概率密度函数$\rho$，那么存在宽度为$D$的两层神经网络 $F(x)$ ， 作为函数 f的近似满足

$$\|F(x) - f(x)\|^2_{L_2(\rho)} \leq \frac{C_f^2}{D}$$

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神经网络中的模块

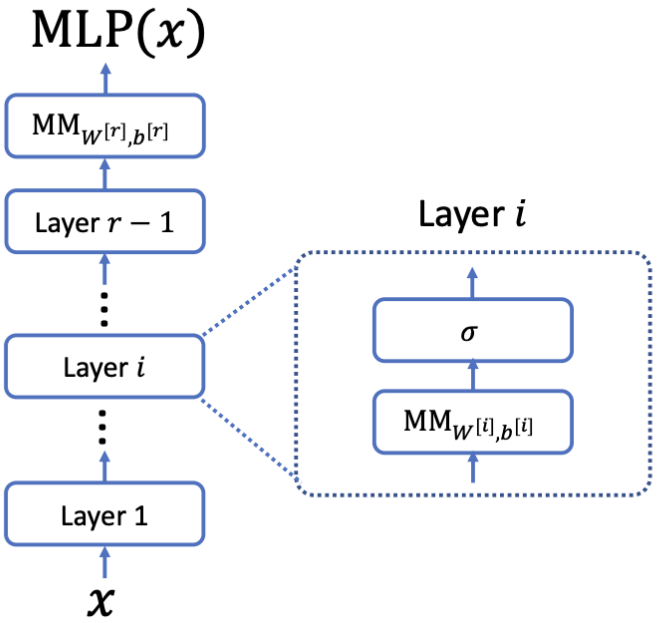
- 矩阵乘法模块：

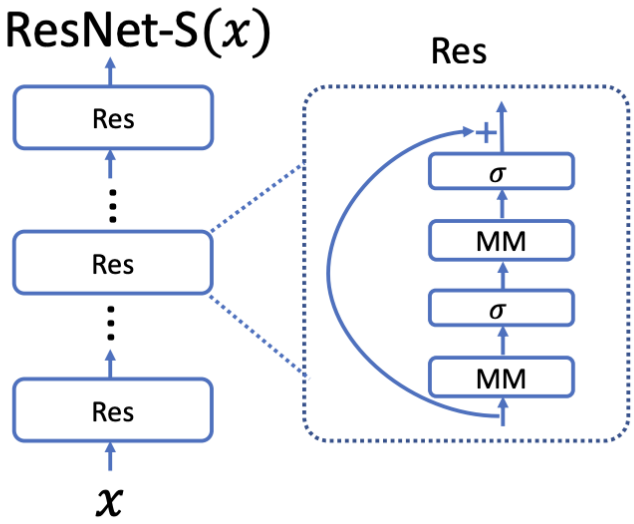
$$MM(z) = Wz + b$$

- 残差连接模块：

$$Res(z) = z + \sigma(MM(\sigma(MM(z))))$$

ODE解释





神经网络中的模块

- 归一化(Layer normalization)层：

$$LN\text{-}S(z) = \begin{bmatrix} \frac{z_1 - \hat{\mu}}{\hat{\sigma}} \\ \frac{z_2 - \hat{\mu}}{\hat{\sigma}} \\ \vdots \\ \frac{z_m - \hat{\mu}}{\hat{\sigma}} \end{bmatrix} \quad \hat{\mu} = \frac{\sum_{i=1}^{m} z_i}{m} \quad \hat{\sigma} = \sqrt{\frac{\sum_{i=1}^{m} (z_i - \hat{\mu})^2}{m}}$$

$$LN(z) = \beta + \gamma LN\text{-}S(z)$$

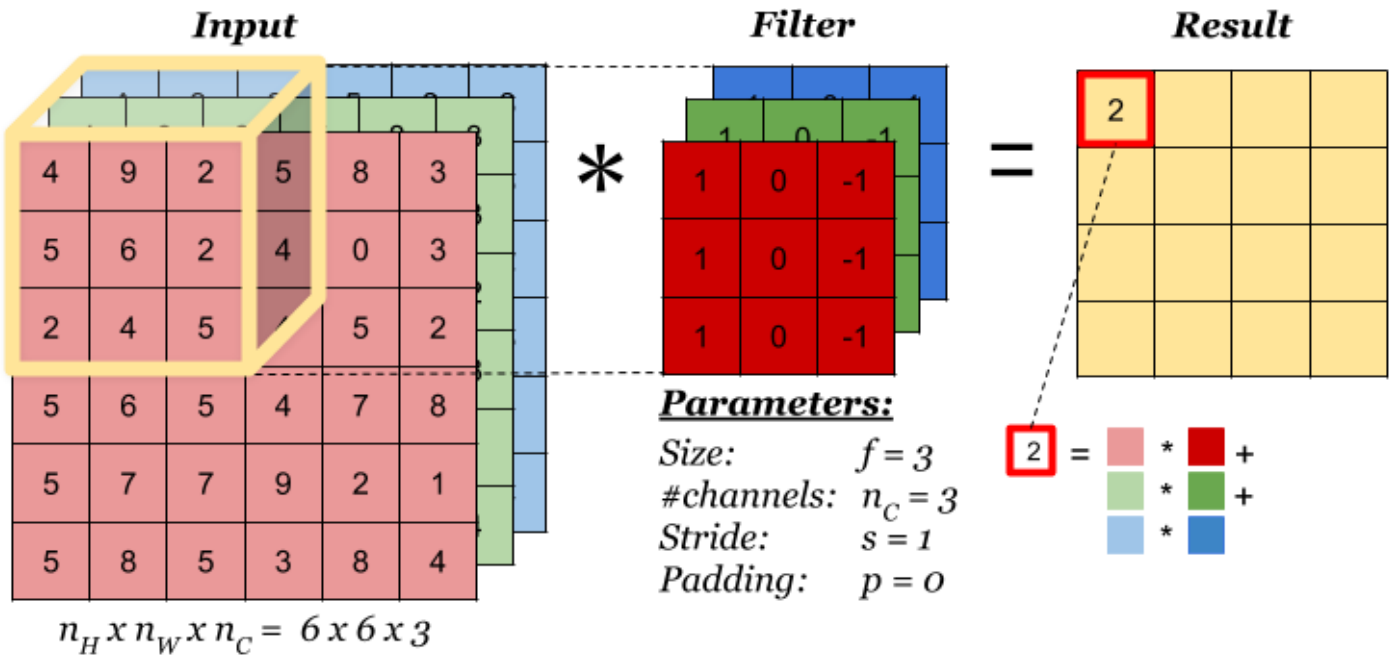
- 尺度不变性(scaling-invariant):

$$LN\left(MM_{\alpha W,\alpha b}(z)\right) = LN\left(MM_{W,b}(z)\right)$$

- 前归一化层、后归一化层（在激活函数之后）

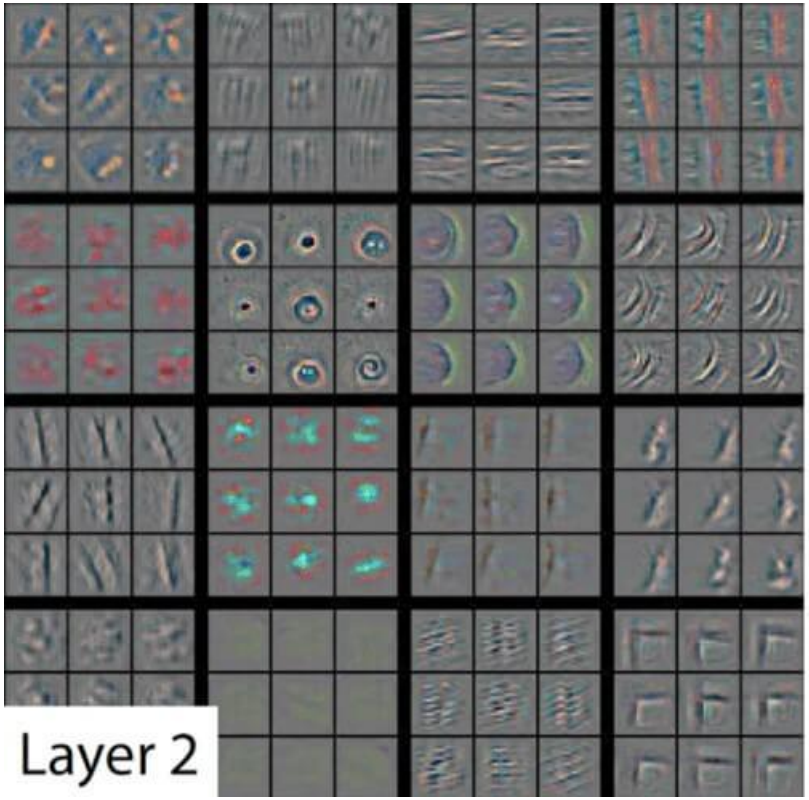
神经网络中的模块

- 卷积模块



神经网络中的模块

- 卷积模块



神经网络中的模块

- 注意力机制(Attention)

编码器状态（encoder states）$x_1, x_2, \cdots, x_n \in R^c$
解码器状态（decoder states）$h \in R^o$

投影：

$$f = < x_1, h > x_1 + < x_1, h > x_2 + \cdots + < x_n, h > x_n$$

计算编码器状态 和解码状态的相关性:

$$\text{score}(h, x_i)$$

注意力权重：

$$a_i = \frac{\exp\big(\text{score}(h, x_i)\big)}{\sum_{i=1}^{n} \exp\big(\text{score}(h, x_i)\big)}$$

输出：$f = a_1 x_1 + a_2 x_2 + \cdots + a_n x_n$

神经网络中的模块

- 自注意力机制(Attention)

编码器状态（encoder states）$x_1, x_2, \cdots, x_n \in R^c$

查询 (query): $q_i = W^q x_i \ (W^q \in R^{m \times c})$
键 (key): $k_i = W^k x_i \ (W^k \in R^{m \times c})$
值 (value): $v_i = W^v x_i \ (W^v \in R^{m \times c})$

相关性(alignment\score):

$$e_{ij} = \frac{q_i \cdot k_j}{\sqrt{d}} \qquad a_{ij} = \frac{\exp(e_{ij})}{\sum_{j'=1}^{n} \exp(e_{ij'})}$$

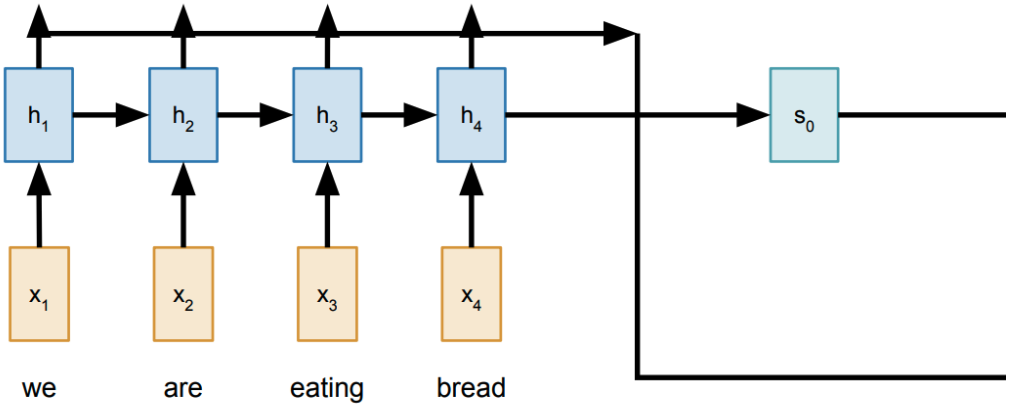
输出：

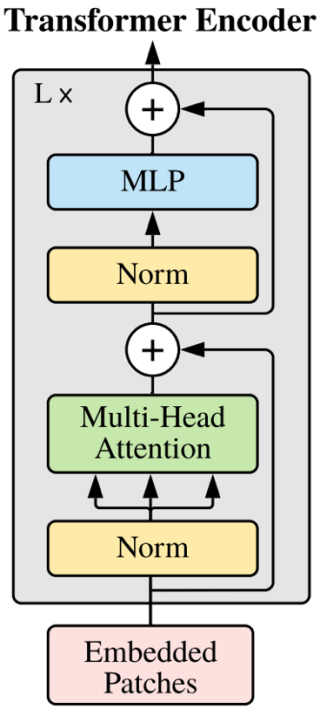
$$\text{Attention}(q, k, v)_i = \sum_{j=1}^{n} a_{ij} v_j$$

神经网络中的模块

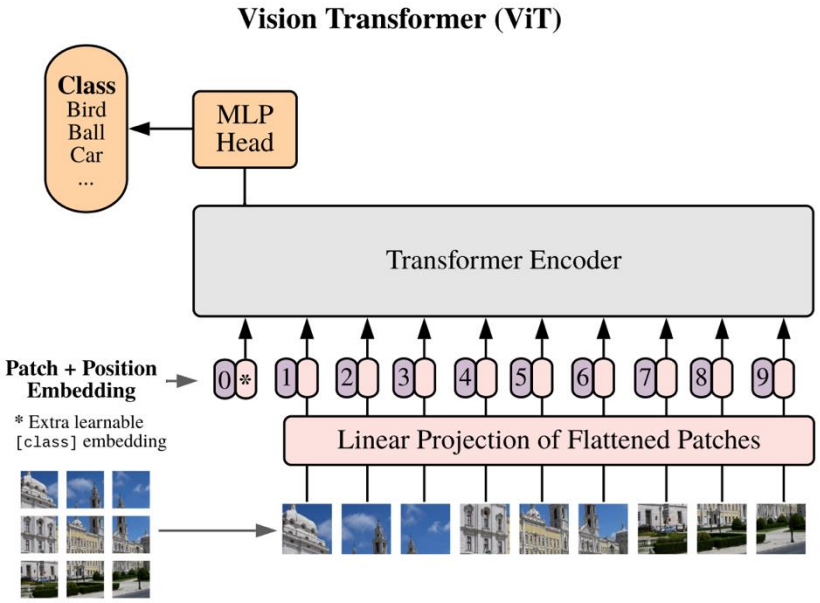
- 自注意力机制(Attention)

自然语言处理





图像处理



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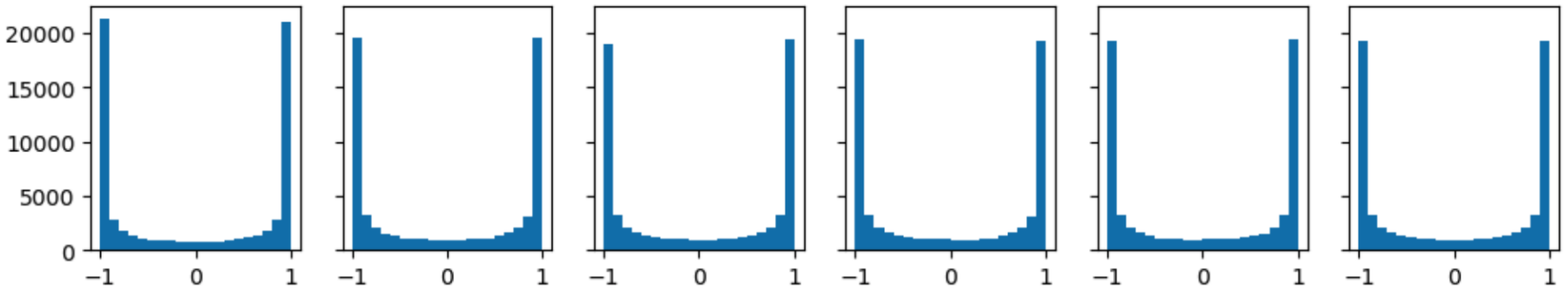
- 神经网络的训练
  - 初始化
  - 反向传播
  - 凸优化

初始化

- 例子

```
dims = [4096] * 7
hs = []
x = np.random.randn(16,dims[0])

for n_in, n_out in zip(dims[:-1], dims[1:]):
    W = 0.05*np.random.randn(n_in, n_out)
    x = np.tanh(x.dot(W))
    hs.append(x)
```



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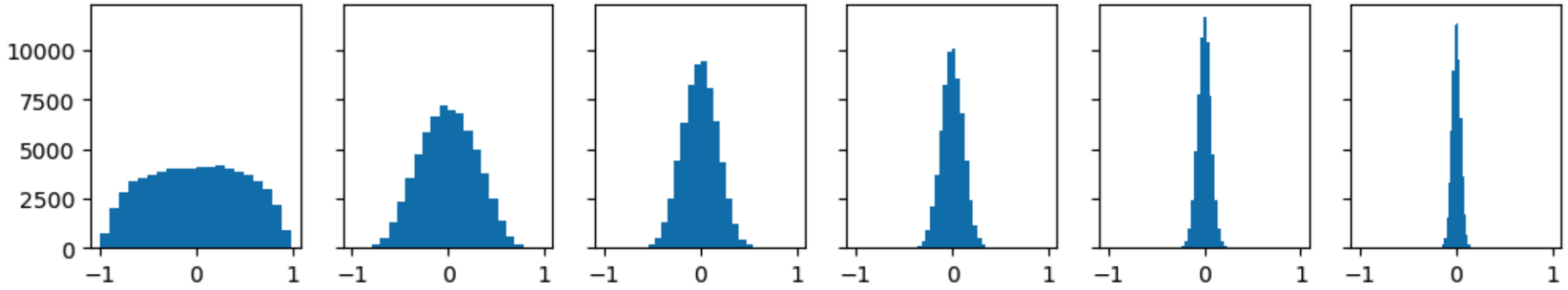


初始化

- Xavier初始化

考虑 $y = Wz$，假设 $W_{i,j} \sim \mathcal{N}(0, w^2)$

$$\mathrm{Cov}[y_i] = n_{in} w^2 \times \mathrm{Cov}\,[z_i] \Longrightarrow w = \frac{1}{\sqrt{n_{in}}}$$

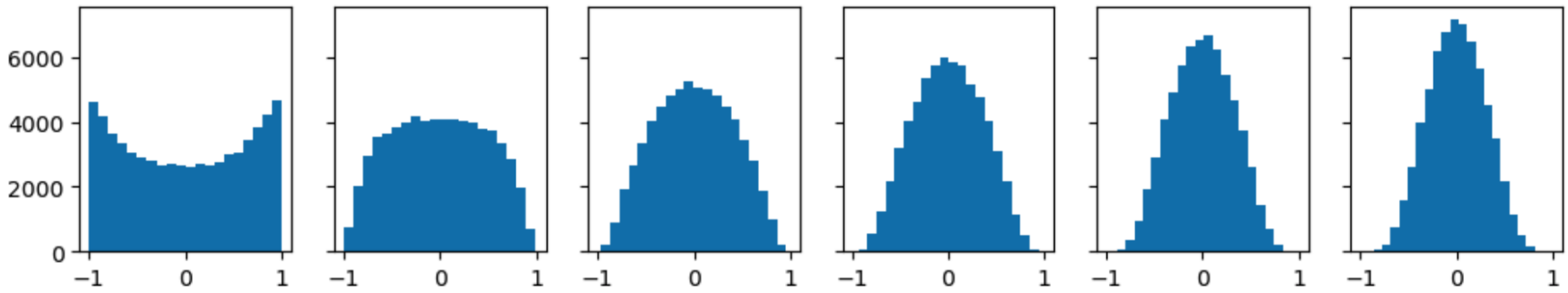
如果激活函数为ReLU，考虑 $y = \sigma(Wz)$，假设 $W_{i,j} \sim \mathcal{N}(0, w^2)$

$$\mathrm{Cov}[y_i] = \frac{1}{2} n_{in} w^2 \times \mathrm{Cov}[z_i] \Longrightarrow w = \frac{1}{\sqrt{\frac{n_{in}}{2}}}$$

初始化

- 例子

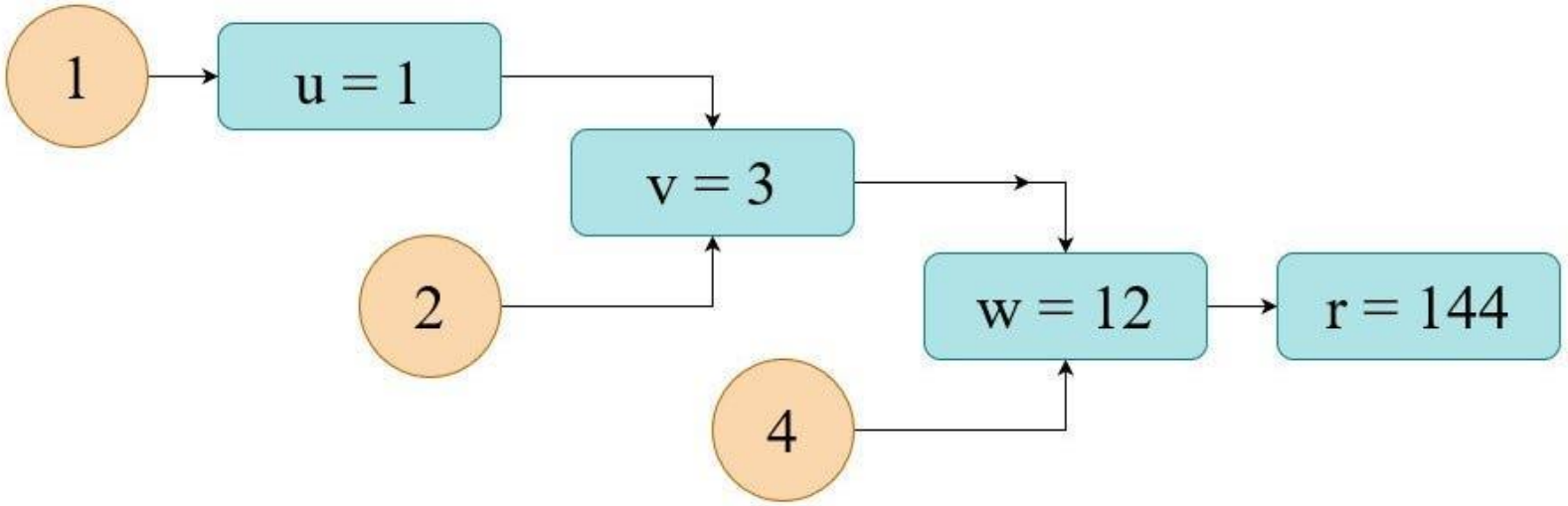
```
dims = [4096] * 7
hs = []
x = np.random.randn(16,dims[0])
for n_in, n_out in zip(dims[:-1], dims[1:]):
    W = np.random.randn(n_in, n_out) / np.sqrt(n_in)
    x = np.tanh(x.dot(W))
    hs.append(x)
```



反向传播

- 链式法则

$$r(x,y,z) = z^2(x^2+y)^2$$
$$u = x^2$$
$$v = u + y$$
$$w = zu$$
$$r = w^2$$
$$(x,y,z) = (1,2,4)$$



反向传播

- 链式法则

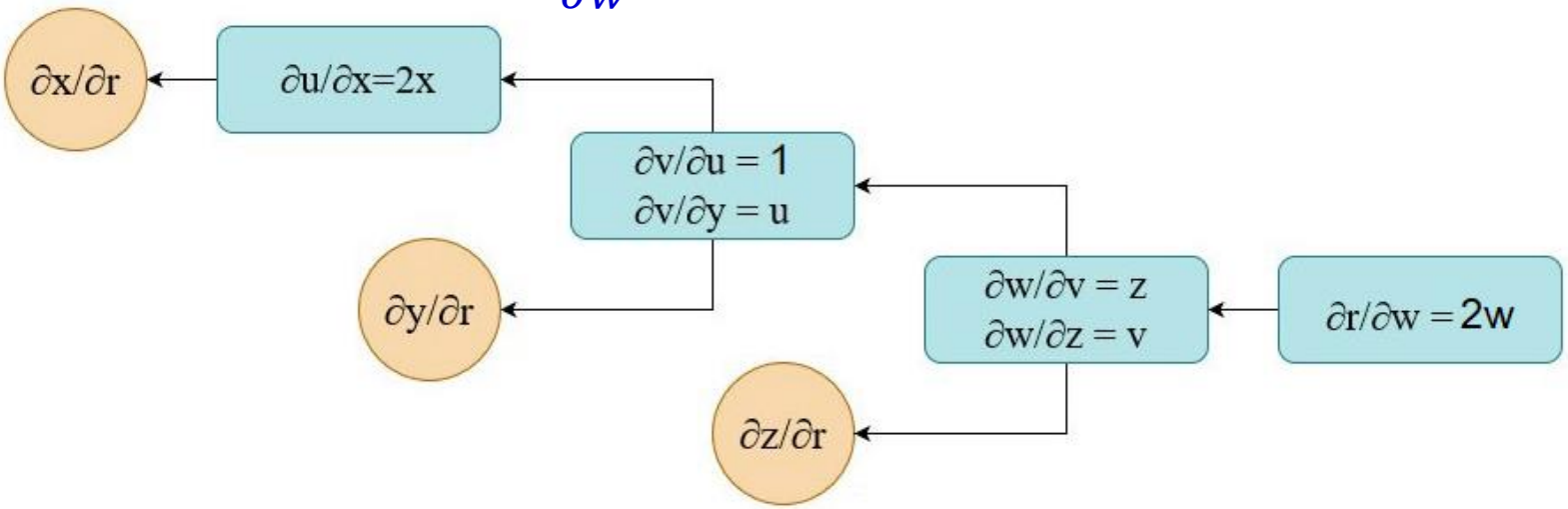
$$r(x,y,z) = z^2(x^2+y)^2$$

$$u = x^2 \qquad \frac{\partial u}{\partial x} = 2x$$

$$v = u + y \qquad \frac{\partial v}{\partial u} = 1 \qquad \frac{\partial v}{\partial y} = 1$$

$$w = zu \qquad \frac{\partial w}{\partial u} = z \qquad \frac{\partial w}{\partial z} = u$$

$$r = w^2 \qquad \frac{\partial r}{\partial w} = 2w$$



反向传播

- 链式法则

$$f(x;\theta) = f_L \circ f_{L-1} \circ \cdots\cdots \circ f_1(x)$$

我们神经网络中的操作(加减乘除激活函数等)，以及它们的导数或偏导数，都可以在 $O(1)$ 时间内计算出来。如果$f(x;\theta)$的复杂度为 $O(N)$，那么计算 $\nabla_\theta f(x;\theta)$ 的复杂度也为 $O(N)$ 。

非凸优化

- 监督学习

  极小化均方误差函数：

$$J(\theta) = \frac{1}{n}\sum_{j=1}^{n} J^{(i)}(\theta) \qquad J^{(i)}(\theta) = \frac{1}{2}(f(x_i;\theta) - y_i)^2$$

- 最速度梯度下降法

$$\theta := \theta - \alpha \nabla_\theta J(\theta)$$

$$:= \theta - \alpha \sum_{\mathrm{i}=1}^{\mathrm{n}} \nabla_\theta J^{(i)}(\theta)$$

初始化

- 随机梯度下降法

均匀地（无放回）从$\{1,2\cdots n\}$中选取B个实例$j_1, j_2, \cdots, j_B$

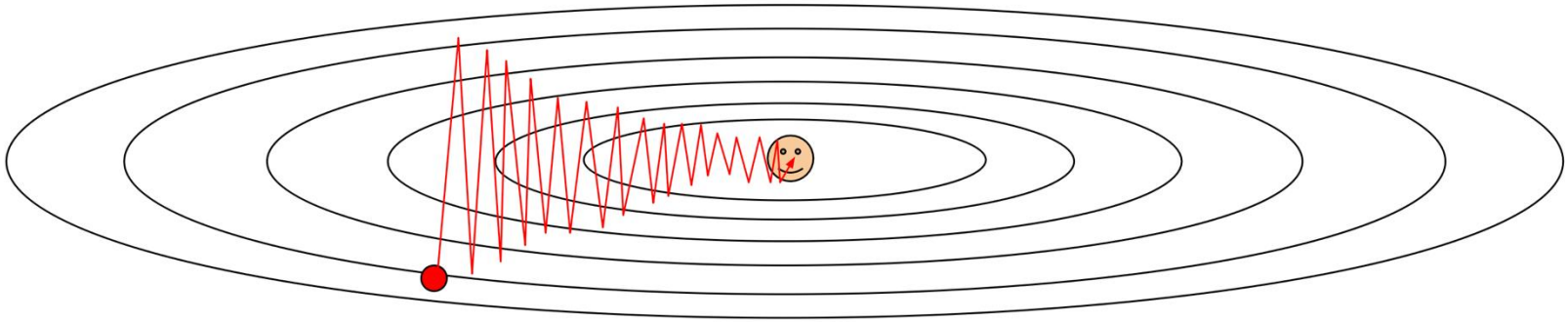
$$\theta := \theta - \alpha \frac{n}{|B|} \sum_{k=1}^{B} \nabla_\theta J^{(j_k)}(\theta)$$

每次把$\{1,2\cdots n\}$分为k组$B_1, B_2 \cdots B_k$

$$\theta := \theta - \alpha \sum_{i \in B_j} \nabla_\theta J^{(i)}(\theta) \quad j = 1,2,\cdots k$$

非凸优化

- 最速度梯度下降法

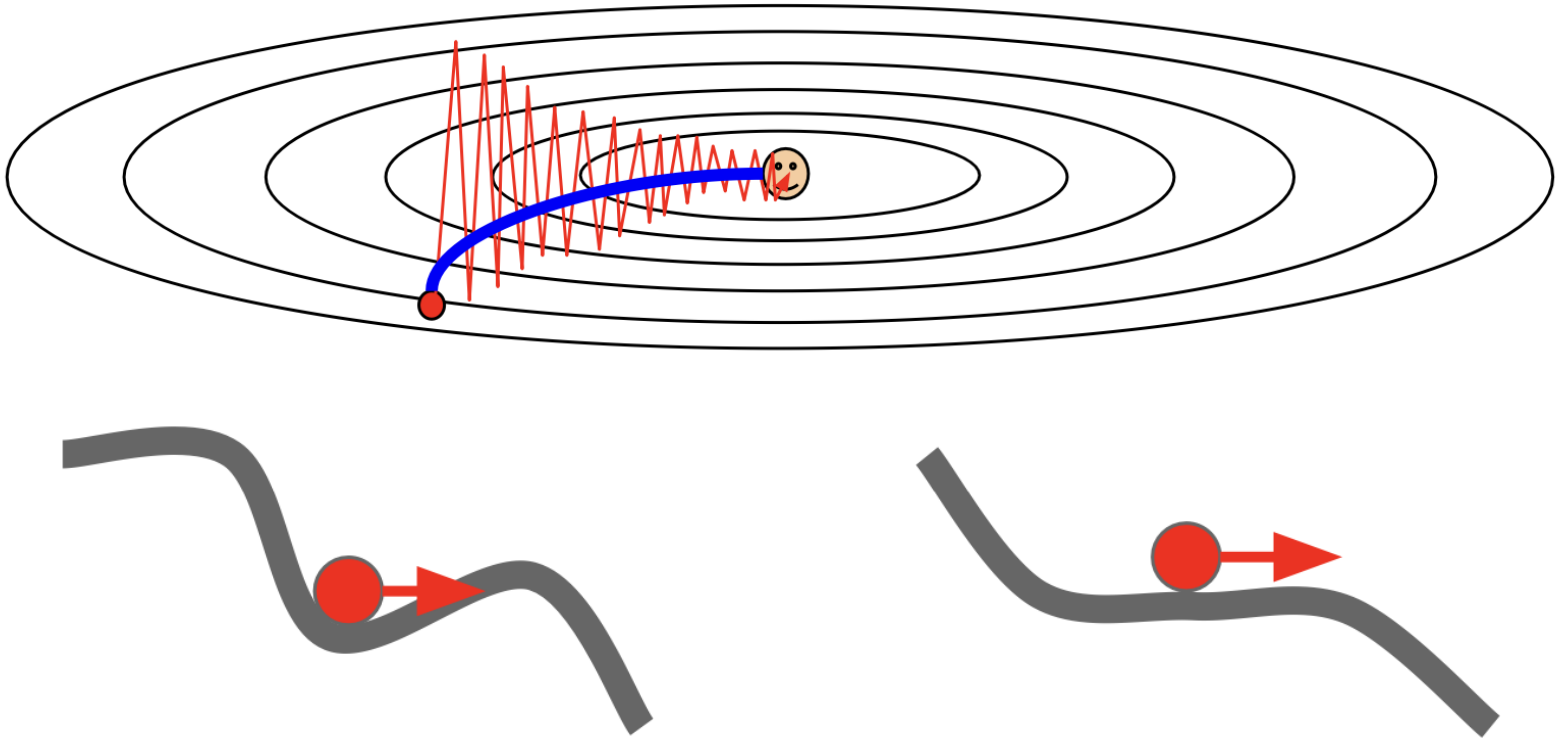


- 损失函数具有高条件数，损失函数在一个方向上变化很快，而在另一个方向上变化很慢，会出现震荡。

- 鞍点和局部极小点

非凸优化

- 动量更新



非凸优化

- 动量更新

Polyak重球法(heavy ball method)

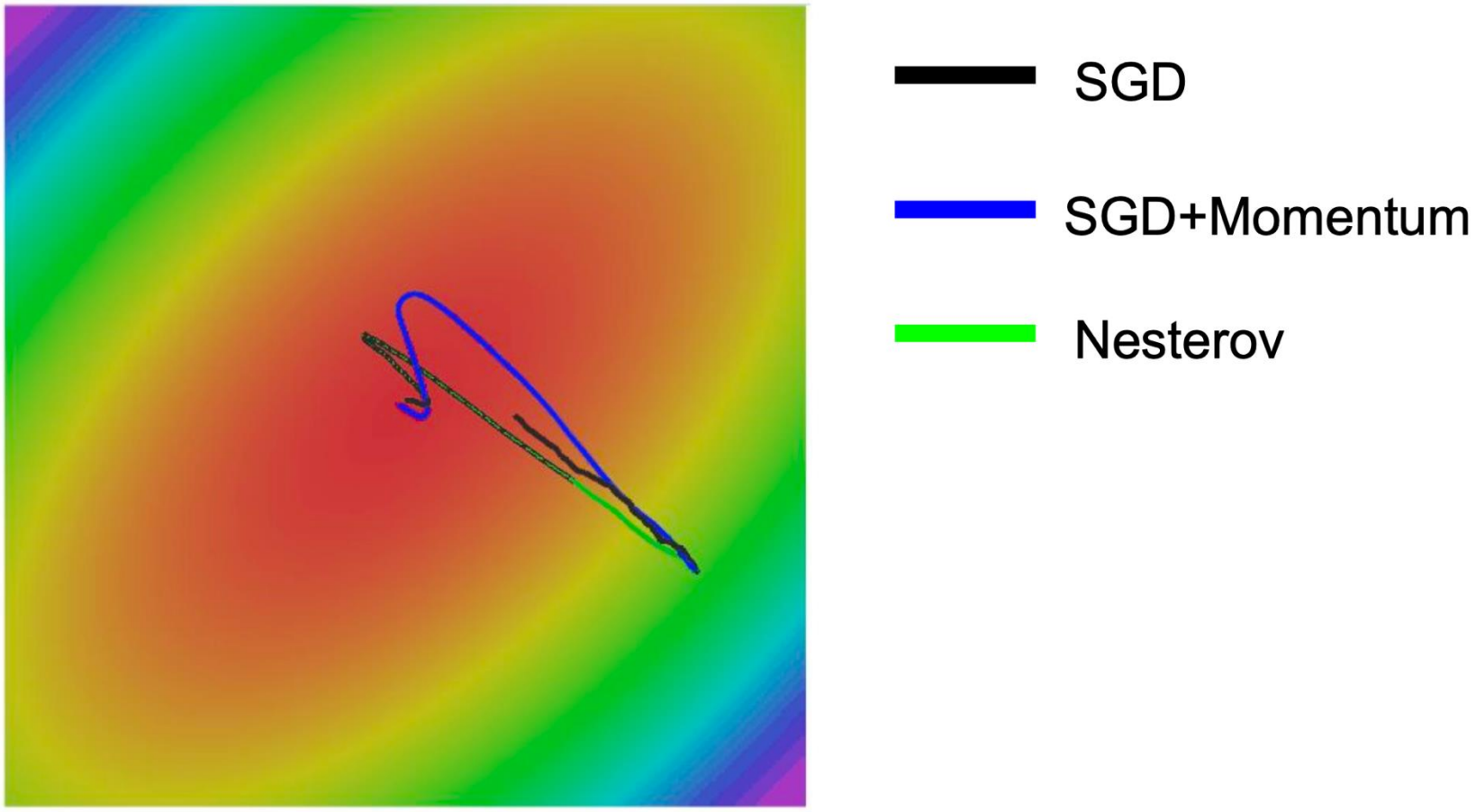
$$y_{k+1} = x_k + \beta(x_k - x_{k-1})$$
$$x_{k+1} = y_k - \alpha\nabla f(x_k)$$

Nesterov 加速梯度下降(accelerated gradient descent)

$$y_{k+1} = x_k + \beta(x_k - x_{k-1})$$
$$x_{k+1} = y_k - \alpha\nabla f(y_k)$$

非凸优化

- 步长选取



非凸优化

- 步长选取

AdaGrad

$$dx_k = \nabla f(x_k)$$
$$\text{grad}_{k+1}^2 = \text{grad}_{k+1}^2 + dx_k \cdot dx_k$$
$$x_{k+1} = y_k - \frac{\alpha}{\sqrt{\text{grad}_{k+1}^2 + 10^{-7}}} dx_k$$

RMSProp

$$dx_k = \nabla f(x_k)$$
$$\text{grad}_{k+1}^2 = \beta \text{grad}_{k+1}^2 + (1-\beta) dx_k \cdot dx_k$$
$$x_{k+1} = y_k - \frac{\alpha}{\sqrt{\text{grad}_{k+1}^2 + 10^{-7}}} dx_k$$

非凸优化

- 步长选取

AdaGrad

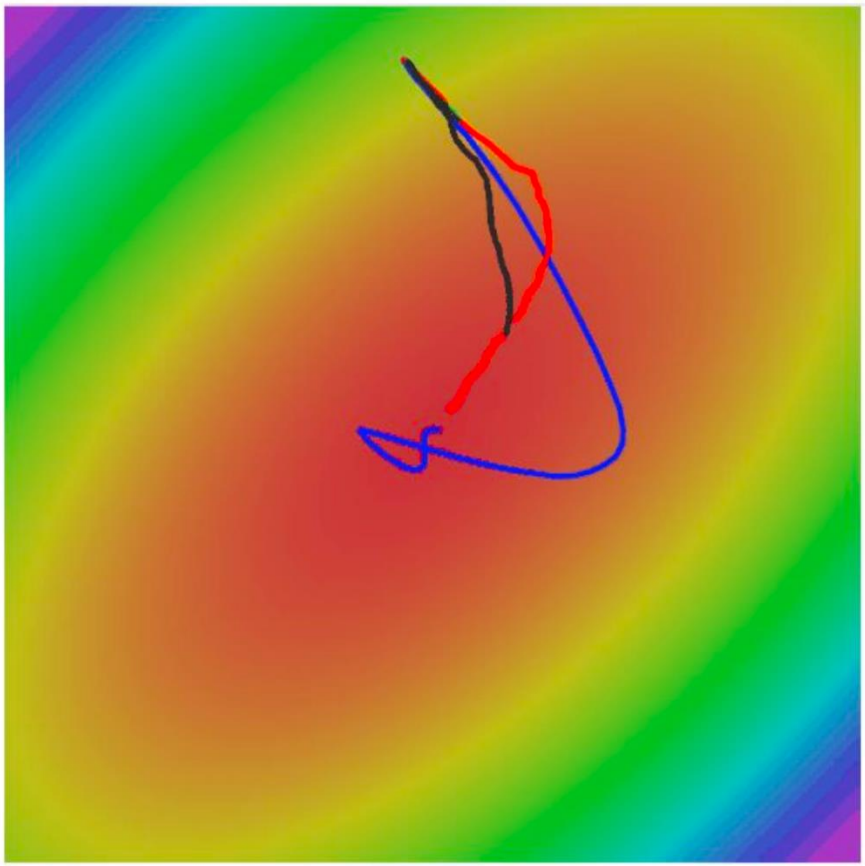
$$dx_k = \nabla f(x_k)$$
$$s_{k+1}^2 = s_k^2 + dx_k \cdot dx_k$$
$$x_{k+1} = x_k - \frac{\alpha}{\sqrt{s_{k+1}^2 + 10^{-7}}} dx_k$$

RMSProp

$$dx_k = \nabla f(x_k)$$
$$s_{k+1}^2 = \beta s_k^2 + (1-\beta) dx_k \cdot dx_k$$
$$x_{k+1} = x_k - \frac{\alpha}{\sqrt{s_{k+1}^2 + 10^{-7}}} dx_k$$

非凸优化

- 步长选取



自适应矩估计(Adaptive Moment Estimation,Adam)

$$dx_k = \nabla f(x_k)$$
$$v_{k+1} = \beta_1 v_k + (1-\beta_1) dx_k$$
$$s_{k+1} = \beta_2 s_k + (1-\beta_2) dx_k \cdot dx_k$$

偏差矫正：

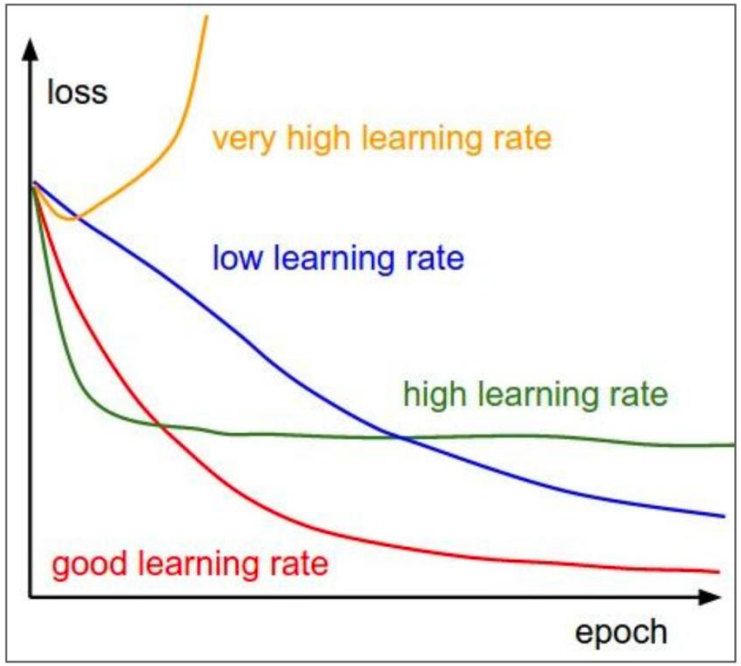
$$\hat{v}_{k+1} = \frac{v_{k+1}}{1-\beta_1^{k+1}} \qquad \hat{s}_{k+1} = \frac{s_{k+1}}{1-\beta_2^{k+1}}$$

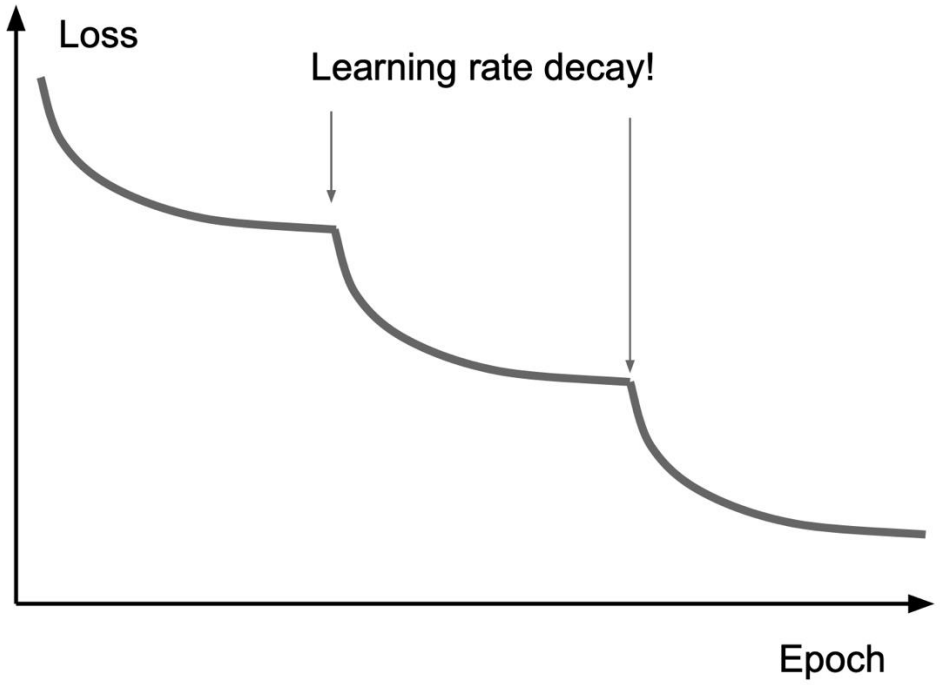
$$x_{k+1} = x_k - \frac{\alpha}{\sqrt{\hat{s}_{k+1} + 10^{-7}}} \hat{v}_{k+1}$$

参数$\beta_1 = 0.9$，$\beta_2 = 0.999$和α

非凸优化

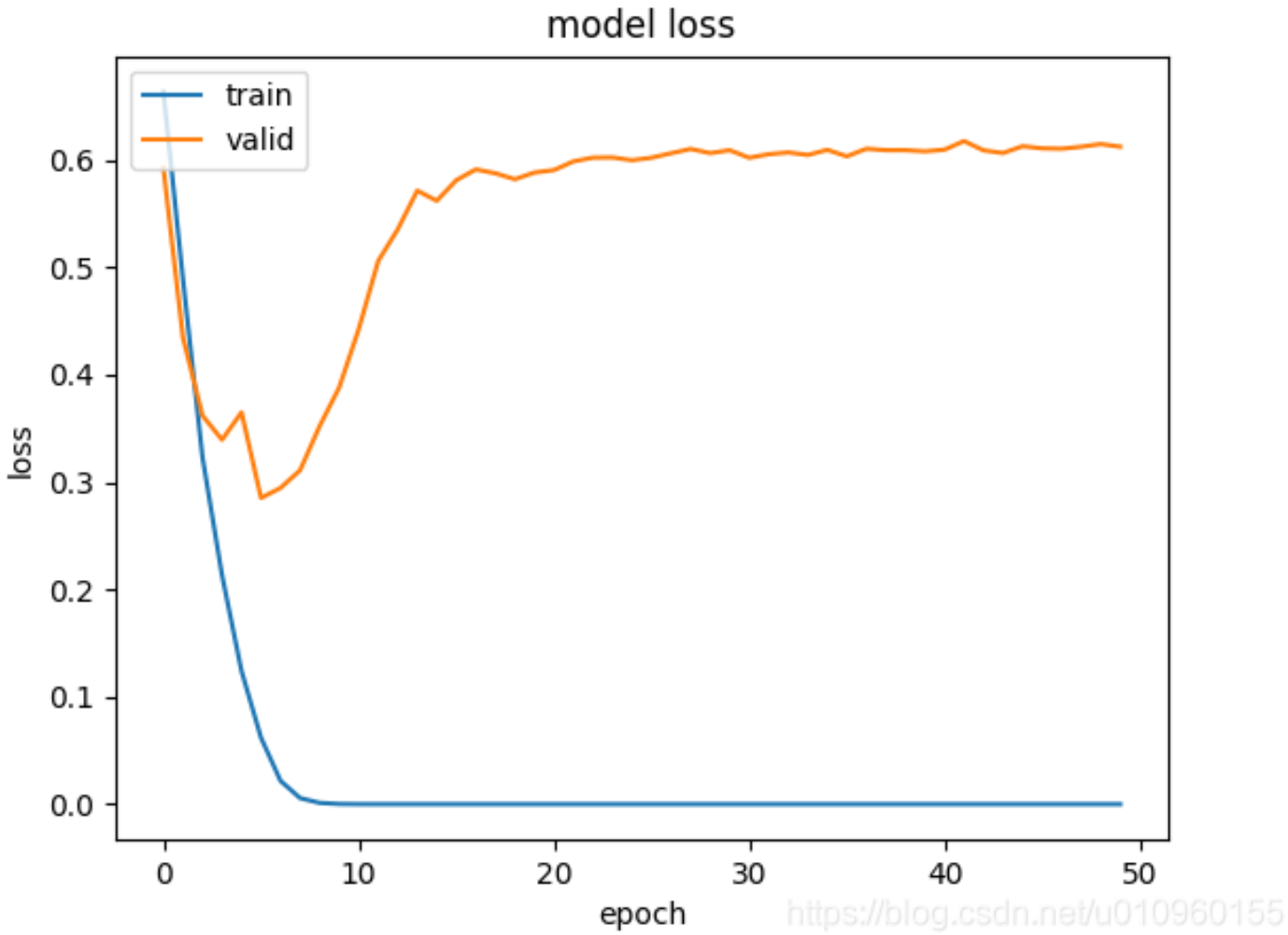
- 学习率选α的取





非凸优化

- 过拟合



非凸优化

- 过拟合：正则化

$$J(\theta) = J(\theta) + \lambda R(\theta)$$

L_2正则化(weight decay)：

$$R(\theta) = \sum \theta_i^2$$

L_1正则化：

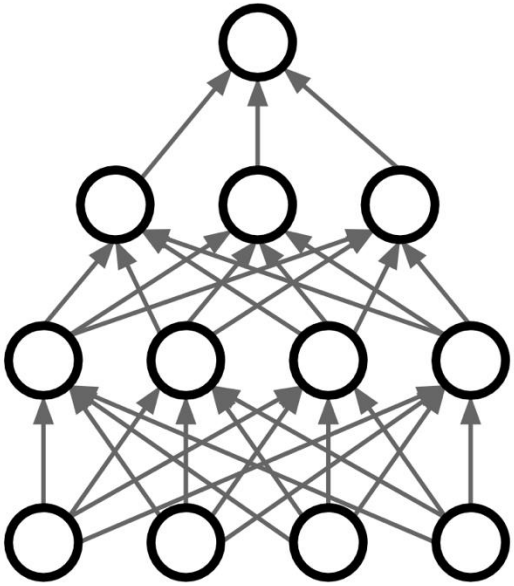
$$R(\theta) = \sum |\theta_i|$$

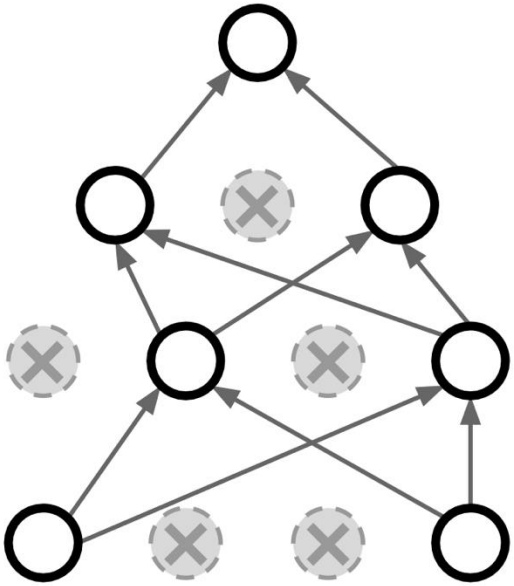
弹性网络(Elastic net)：

$$R(\theta) = \beta \sum \theta_i^2 + \sum |\theta_i|$$

非凸优化

- 过拟合：丢弃法(Dropout)





- 在训练的时候(每一个批次(batch))，以概率$1-p$随机删去该层的一些输出，并把其余输出乘以$1/p$
- 训练了多个模型

非凸优化

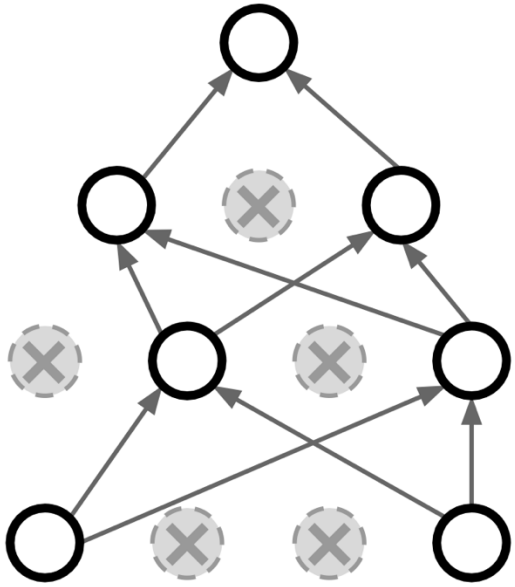
- 过拟合：丢弃法(Dropout)

```
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  out = np.dot(W3, H2) + b3
```



测试时保持不变

参考文献

参考文献

斯坦福CS231课件：
cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

Cybenko, George. "Approximation by superpositions of a sigmoidal function." Mathematics of control, signals and systems 2, no. 4 (1989): 303-314.

Hornik, Kurt. "Approximation capabilities of multilayer feedforward networks." Neural networks 4, no. 2 (1991): 251-257.

Jones, Lee K. "A simple lemma on greedy approximation in Hilbert space and convergence rates for projection pursuit regression and neural network training." The annals of Statistics (1992): 608-613.

Barron, Andrew R. "Universal approximation bounds for superpositions of a sigmoidal function." IEEE Transactions on Information theory 39, no. 3 (1993): 930-945.

维斯康星麦迪逊CS726课件： Lecture 9–10: Accelerated Gradient Descent

神经网络中的模块

- Batch normalization 模块

$$\mathrm{BN}(z) = \frac{z - E[z]}{\sqrt{Var[z] + \epsilon}}$$

$$\mathrm{BN}(z) = \beta + \gamma \odot \mathrm{BN}\text{–}S(z)$$