Basic RL.6

Judy Tutorial

Softmax (Multiclass Logistic) Regression

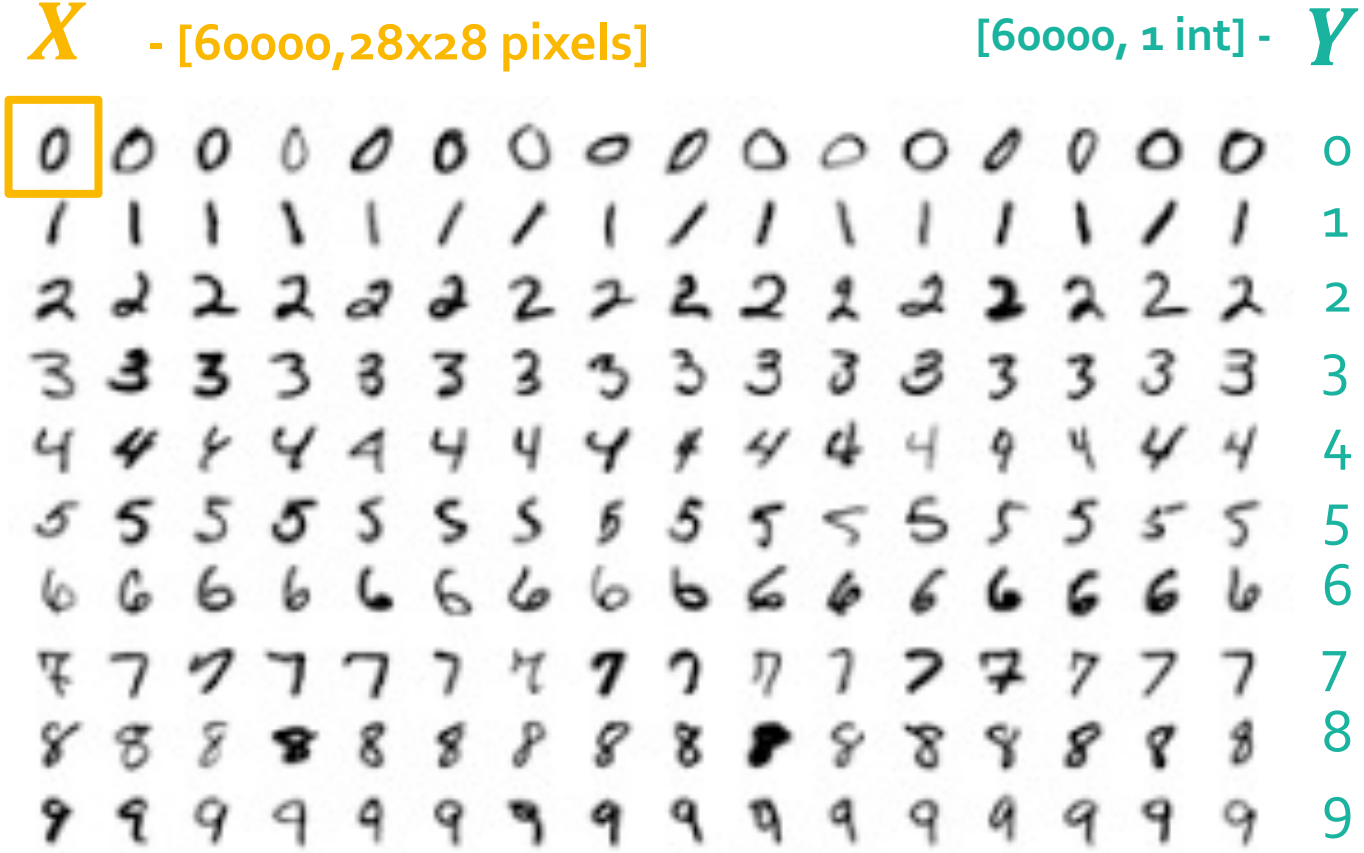
&

Neural Networks

MNIST dataset

[LeCun 1998]

Multiple Labels
$y \in \{0,1,2,\ldots,9\}$



Hypothesis function

$$h_k(\boldsymbol{\theta}) = g(\boldsymbol{\theta}_k^{\mathrm{T}} X)$$

inputs

parameters

Activation function

$$g(z_k) = \frac{e^{z_k}}{\sum_{l=1}^{K} e^{z_l}}$$

softmax

Objective function

$$J(\boldsymbol{\theta}) = -\frac{1}{N} \sum_{i=1}^{N} \sum_{l=1}^{K} y_l^{(i)} \log h_l(\theta)^{(i)}$$

Cross entropy loss

Hypothesis function

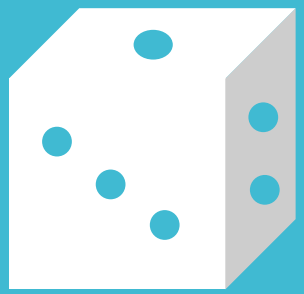
$$h(\boldsymbol{\theta}) = \begin{bmatrix} g(\boldsymbol{\theta}_{k=1}^{\mathrm{T}} X) \\ g(\boldsymbol{\theta}_{k=2}^{\mathrm{T}} X) \\ g(\boldsymbol{\theta}_{k=3}^{\mathrm{T}} X) \\ \vdots \\ \cdot \\ \cdot \\ g(\boldsymbol{\theta}_{k=K}^{\mathrm{T}} X) \end{bmatrix} = \begin{bmatrix} \dfrac{\exp \boldsymbol{\theta}_{k=1}^{\mathrm{T}} X}{\sum_{l=1}^{K} \exp \boldsymbol{\theta}_{l}^{\mathrm{T}} X} \\ \dfrac{\exp \boldsymbol{\theta}_{k=2}^{\mathrm{T}} X}{\sum_{l=1}^{K} \exp \boldsymbol{\theta}_{l}^{\mathrm{T}} X} \\ \dfrac{\exp \boldsymbol{\theta}_{k=3}^{\mathrm{T}} X}{\sum_{l=1}^{K} \exp \boldsymbol{\theta}_{l}^{\mathrm{T}} X} \\ \vdots \\ \cdot \\ \cdot \\ \dfrac{\exp \boldsymbol{\theta}_{k=K}^{\mathrm{T}} X}{\sum_{l=1}^{K} \exp \boldsymbol{\theta}_{l}^{\mathrm{T}} X} \end{bmatrix}$$

Objective function

$$J(\boldsymbol{\theta}) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{l=1}^{K} y_l^{(i)} \log h_l(\boldsymbol{\theta})^{(i)}$$

Negative **Log**-**Likelihood** of
Multinomial distribution

Multinomial Distribution



Wiki:

- the Multinomial distribution gives the probability of any particular combination of numbers of successes for the various categories

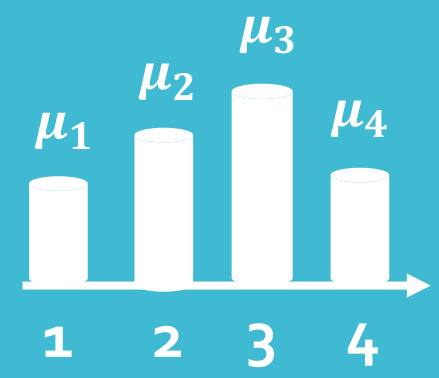
Example:

- Repeat rolling a dice for many times
- Suppose we roll a dice 5 times, what's the probability of the appearances of two 3s and three 4s?
- $p(34344|\boldsymbol{\mu}) = \frac{5!}{2!3!}\left(\frac{1}{6}\right)^2\left(\frac{1}{6}\right)^3$

Parameter vector for dice probability

where $\mu_k = \frac{1}{6}, K = 6$

Multinomial Distribution



$\mu_4 = 1 - \mu_1 - \mu_2 - \mu_3$

- x_k- the number of repeatition of a specific outcome when conducting some events
- μ_k- the probability of each event

#events

$$Mult(x_1, x_2, \dots, x_K | \boldsymbol{\mu}, N) = C_N^{x_1 x_2 \dots x_K} \prod_{k=1}^{K} \mu_k^{x_k}$$

distribution parameter vector

- $0 \le \mu_k \le 1, \sum_{k=1}^{K} \mu_k = 1$
- $\sum_{k=1}^{K} x_k = N$
- $C_N^{x_1 x_2 \dots x_K} = \frac{N!}{x_1! x_2! \dots x_K!}$

$$Mult(x_1, x_2, \dots, x_K|\boldsymbol{\mu}) \propto \prod_{k=1}^{K} \mu_k^{x_k}$$

Multinomial Likelihood

$$y_l^{(i)} = 1_{y=k} = \begin{cases} 1, \text{if } y = k \\ 0, \text{if } y \neq k \end{cases}$$

#data

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^{N} \prod_{l=1}^{K} h_l(\boldsymbol{\theta})^{(i)} y_l^{(i)}$$

One hot classification label

$$g(\boldsymbol{\theta}_k^T \boldsymbol{X})$$

$$0 \leq h_k(\boldsymbol{\theta}) \leq 1$$
$$\sum_l^K h_l(\boldsymbol{\theta}) = 1$$

MLE for Softmax Regression

$$\max_{\theta} \log \mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{N} \sum_{l=1}^{K} y_l^{(i)} \log h_l(\boldsymbol{\theta})^{(i)}$$

$$\min_{\theta} J(\boldsymbol{\theta}) = -\frac{1}{N} \sum_{i=1}^{N} \sum_{l=1}^{K} y_l^{(i)} \log h_l(\boldsymbol{\theta})^{(i)}$$

Cross entropy loss

Objective function

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{l=1}^{K} y_l^{(i)} \log h_l(\boldsymbol{\theta})^{(i)}$$

Batch Gradient

$$\nabla_{\theta_j} J(\theta_j) = \nabla_{\theta_j} -\frac{1}{N}\sum_{i=1}^{N}\sum_{l=1}^{K} y_l^{(i)} \log h_l(\boldsymbol{\theta})^{(i)}$$

$$= -\frac{1}{N}\sum_{i=1}^{N}\sum_{l=1}^{K} \frac{y_l^{(i)}}{h_l(\theta_j)^{(i)}} \nabla_{\theta_j} h(\theta_j)^{(i)}$$

Element-wise

$$= \frac{1}{N}\sum_{i=1}^{N}\sum_{l=1}^{K} \left[h(\theta_j)^{(i)} - y_l^{(i)}\right] x^{(i)}$$

Matrix-wise

$$= \frac{1}{N}\boldsymbol{X}[\boldsymbol{h}(\boldsymbol{\theta}) - \boldsymbol{Y}]^T$$

same as linear/logistic regression related to Exponential Family and Generalized Linear Model

Gradient Descent

$$\boldsymbol{\theta_{t+1}} \leftarrow \boldsymbol{\theta_t} - \alpha \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

Batch

Mini Batch

&

Stochastic Gradient Descent

Require a batch/entire dataset

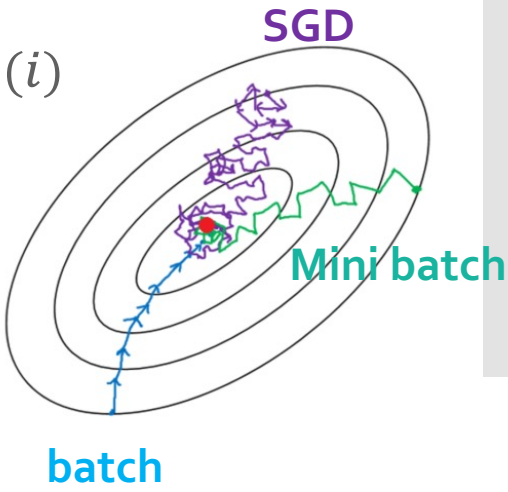
$$\nabla_{\theta_j} J(\theta_j) = \frac{1}{N} \sum_{i=1}^{N} \left[h(\theta_j)^{(i)} - y^{(i)} \right] x^{(i)}$$

Sample random mini batch from the entire dataset

$$\nabla_{\theta_j} J(\theta_j) = \frac{1}{N_{mini}} \sum_{i=1}^{N_{mini}} \left[h(\theta_j)^{(i)} - y^{(i)} \right] x^{(i)}$$

Require only one data point

$$\nabla_{\theta_j} J(\theta_j) = \left[h(\theta_j)^{(i)} - y^{(i)} \right] x^{(i)}$$



Feedforward Neural Networks

(MultiLayer Perceptron)

$$f(X) = f^{[M]} \dots (f^{[3]}(f^{[2]}(f^{[1]}(X))))$$

Mth layer

Third layer

Second layer

First layer

$$h(\boldsymbol{\theta}) = g(\boldsymbol{\theta}^T X)$$

$$h(\boldsymbol{W}, \boldsymbol{b}) = g(X\boldsymbol{W} + \boldsymbol{b})$$

inputs

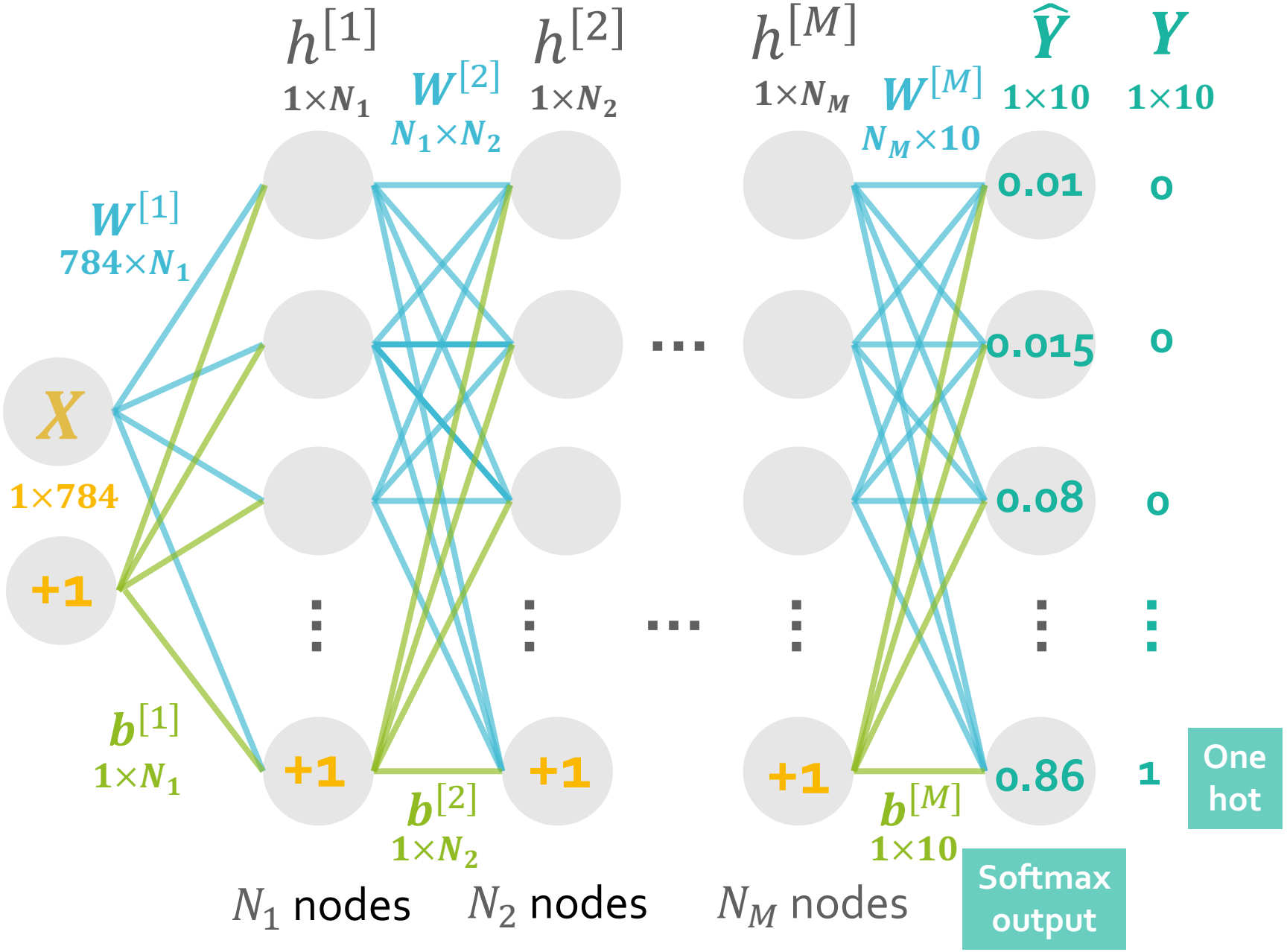
parameters

$$h^{[1]}(\boldsymbol{W}^{[1]}, \boldsymbol{b}^{[1]}) = g^{[1]}(X\boldsymbol{W}^{[1]} + \boldsymbol{b}^{[1]})$$

$$h^{[2]}(\boldsymbol{W}^{[2]}, \boldsymbol{b}^{[2]}) = g^{[2]}(h^{[1]}\boldsymbol{W}^{[2]} + \boldsymbol{b}^{[2]})$$

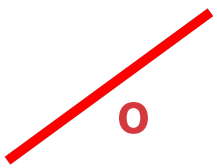
$$h^{[3]}(\boldsymbol{W}^{[3]}, \boldsymbol{b}^{[3]}) = g^{[3]}(h^{[2]}\boldsymbol{W}^{[3]} + \boldsymbol{b}^{[3]})$$

$$\vdots$$


$h^{[1]}$
$1\times N_1$
$h^{[2]}$
$1\times N_2$
$h^{[M]}$
$1\times N_M$
$\hat{Y}$
1×10
Y
1×10
$W^{[1]}$
$784\times N_1$
$W^{[2]}$
$N_1\times N_2$
$W^{[M]}$
$N_M\times 10$
X
1×784
+1
+1
+1
+1
$b^{[1]}$
$1\times N_1$
$b^{[2]}$
$1\times N_2$
$b^{[M]}$
1×10
0.01
0.015
0.08
0.86
0
0
0
1
One hot
N_1 nodes
N_2 nodes
N_M nodes
Softmax output

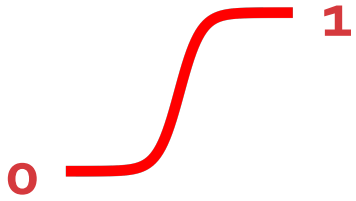
Activation functions

$$g(z) = z$$



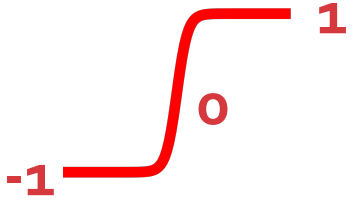
linear

$$g(z) = \frac{1}{1 + e^{-z}}$$



Sigmoid

$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$



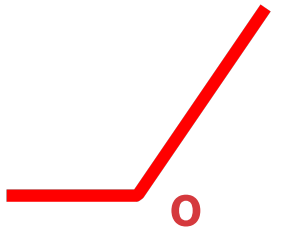
tanh

$$g(z_k) = \frac{e^{z_k}}{\sum_{l=1}^{K} e^{z_l}}$$

A generalized sigmoid

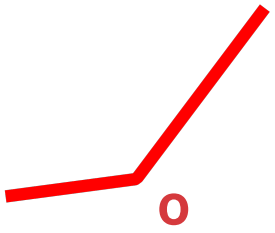
softmax

$$g(z) = \max(z, 0)$$



ReLU

$$g(z) = \max(z, 0.1z)$$



Leaky ReLU

Objective functions

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

MSE

$$-[y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)]$$

Binary Cross entropy

$$\frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

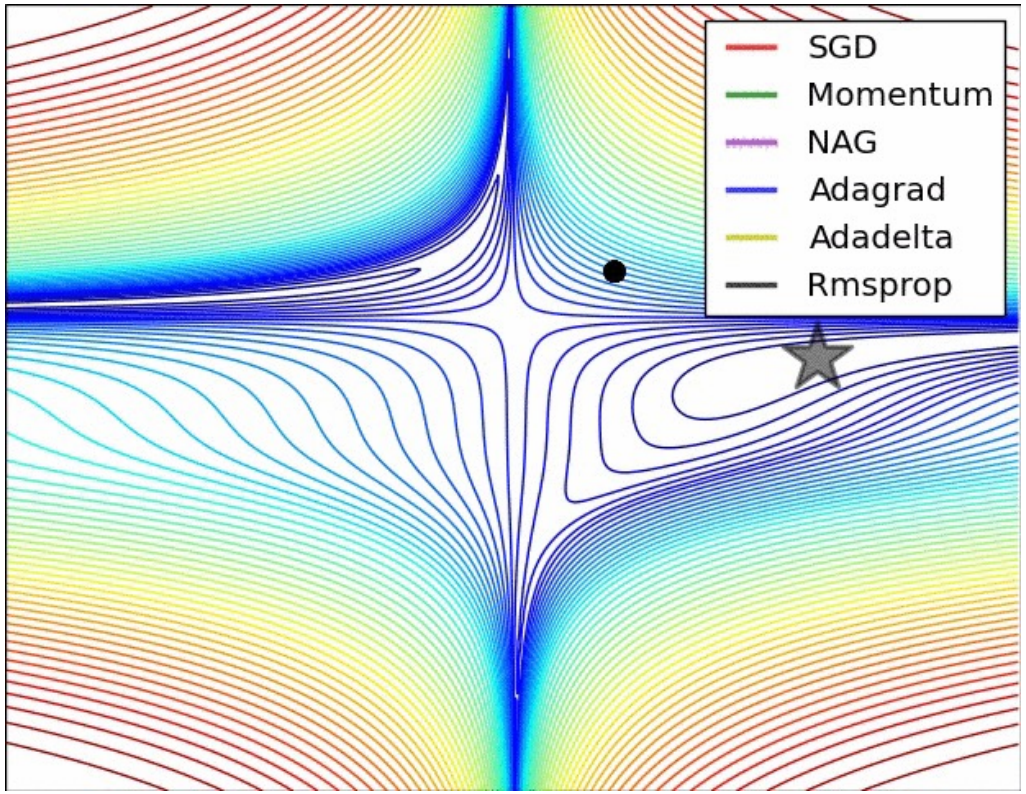
MAE

$$-\frac{1}{N}\sum_{i=1}^{N} y_i \log \hat{y}_i$$

Multiclass Cross entropy

Optimizers

- Batch Gradient
- MiniBatch Gradient
- SGD
- SGD+momentum
- Adam
- Adagrad
- Rmsprop
- ...



https://www.analyticsvidhya.com/blog/2021/10/a-comprehensive-guide-on-deep-learning-optimizers/

Backpropagation – chain rule

$$h^{[1]} = g^{[1]}(XW^{[1]} + b^{[1]})$$
$$h^{[2]} = g^{[2]}(h^{[1]}W^{[2]} + b^{[2]})$$
$$\hat{Y} = g^{[3]}(h^{[2]}W^{[3]} + b^{[3]})$$
$$J = -\sum_{i=1}^{N} y_i \log \hat{y}_i \rightarrow -\log \hat{y}_i$$

ReLU

ReLU

softmax

Multiclass Cross entropy

$$\frac{\partial J}{\partial W^{[3]}} = \frac{\partial J}{\partial \hat{Y}} \frac{\partial \hat{Y}}{\partial g^{[3]}} \frac{\partial g^{[3]}}{\partial W^{[3]}} \qquad h^{[2]}$$

$$\frac{\partial J}{\partial W^{[2]}} = \frac{\partial J}{\partial \hat{Y}} \frac{\partial \hat{Y}}{\partial g^{[3]}} \frac{\partial g^{[3]}}{\partial h^{[2]}} \frac{\partial h^{[2]}}{\partial g^{[2]}} \frac{\partial g^{[2]}}{\partial W^{[2]}} \qquad h^{[1]}$$

$$\frac{\partial J}{\partial W^{[1]}} = \frac{\partial J}{\partial \hat{Y}} \frac{\partial \hat{Y}}{\partial g^{[3]}} \frac{\partial g^{[3]}}{\partial h^{[2]}} \frac{\partial h^{[2]}}{\partial g^{[2]}} \frac{\partial g^{[2]}}{\partial h^{[1]}} \frac{\partial h^{[1]}}{\partial g^{[1]}} \frac{\partial g^{[1]}}{\partial W^{[1]}} \qquad X$$

$(\hat{Y} - Y)$ $W^{[3]}$ $0, 1$ $W^{[2]}$ $0, 1$

$$\frac{\partial J}{\partial b^{[3]}} = \frac{\partial J}{\partial \hat{Y}} \frac{\partial \hat{Y}}{\partial g^{[3]}} \frac{\partial g^{[3]}}{\partial b^{[3]}} \qquad 1$$

$$\frac{\partial J}{\partial b^{[2]}} = \frac{\partial J}{\partial \hat{Y}} \frac{\partial \hat{Y}}{\partial g^{[3]}} \frac{\partial g^{[3]}}{\partial h^{[2]}} \frac{\partial h^{[2]}}{\partial g^{[2]}} \frac{\partial g^{[2]}}{\partial b^{[2]}} \qquad 1$$

$$\frac{\partial J}{\partial b^{[1]}} = \frac{\partial J}{\partial \hat{Y}} \frac{\partial \hat{Y}}{\partial g^{[3]}} \frac{\partial g^{[3]}}{\partial h^{[2]}} \frac{\partial h^{[2]}}{\partial g^{[2]}} \frac{\partial g^{[2]}}{\partial h^{[1]}} \frac{\partial h^{[1]}}{\partial g^{[1]}} \frac{\partial g^{[1]}}{\partial b^{[1]}} \qquad 1$$

$(\hat{Y} - Y)$ $W^{[3]}$ $0, 1$ $W^{[2]}$ $0, 1$

Learning Flow

Given a training dataset $(\boldsymbol{X}, \boldsymbol{Y})$

1. Initialize $\boldsymbol{W}, \boldsymbol{b}$
2. Forward: calculate $\boldsymbol{h}^{[1]}, \boldsymbol{h}^{[2]}, \ldots, \widehat{\boldsymbol{Y}}, \boldsymbol{J}$
3. Backward: calculate $\frac{\partial \boldsymbol{J}}{\partial \boldsymbol{W}}, \frac{\partial \boldsymbol{J}}{\partial \boldsymbol{b}}$
4. Optimize: e.g. SGD
5. Verify with test dataset

in python keras

```
x_train,y_train,x_test,y_test=process_data()

model=Sequential()
model.add(Dense(10,input_dim=784,activation='relu'))
model.add(Dense(10,activation='softmax'))
model.compile(optimizer=SGD(lr=0.1),
              loss='categorical_crossentropy',
              metrics=['categorical_accuracy'])
```

Build model

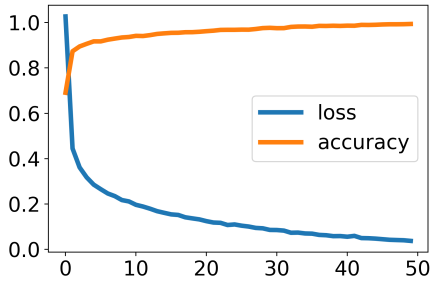
```
traj=model.fit(x_train,
               y_train,
               epochs=50,
               batch_size=32,
               validation_data=(x_test, y_test),
               shuffle=True,verbose=0)
```

Training

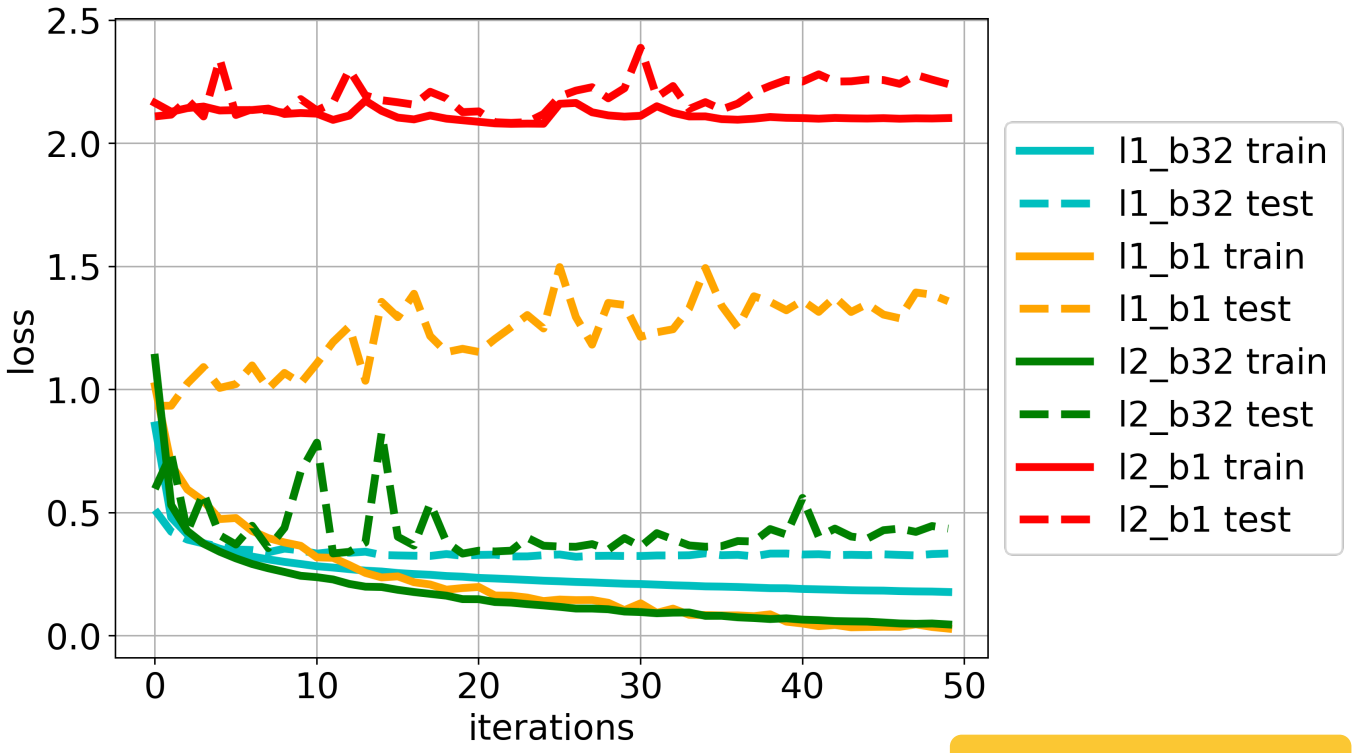
```
plt.plot(traj.history['loss'],linewidth=4,label='loss')
plt.plot(traj.history['categorical_accuracy'],linewidth=4,label='accuracy')
plt.legend()
```

Plot results

x_train: (5000,784)
y_train: (5000,10) - one hot
x_test: (1000,784)
y_test: (1000,10) – one hot



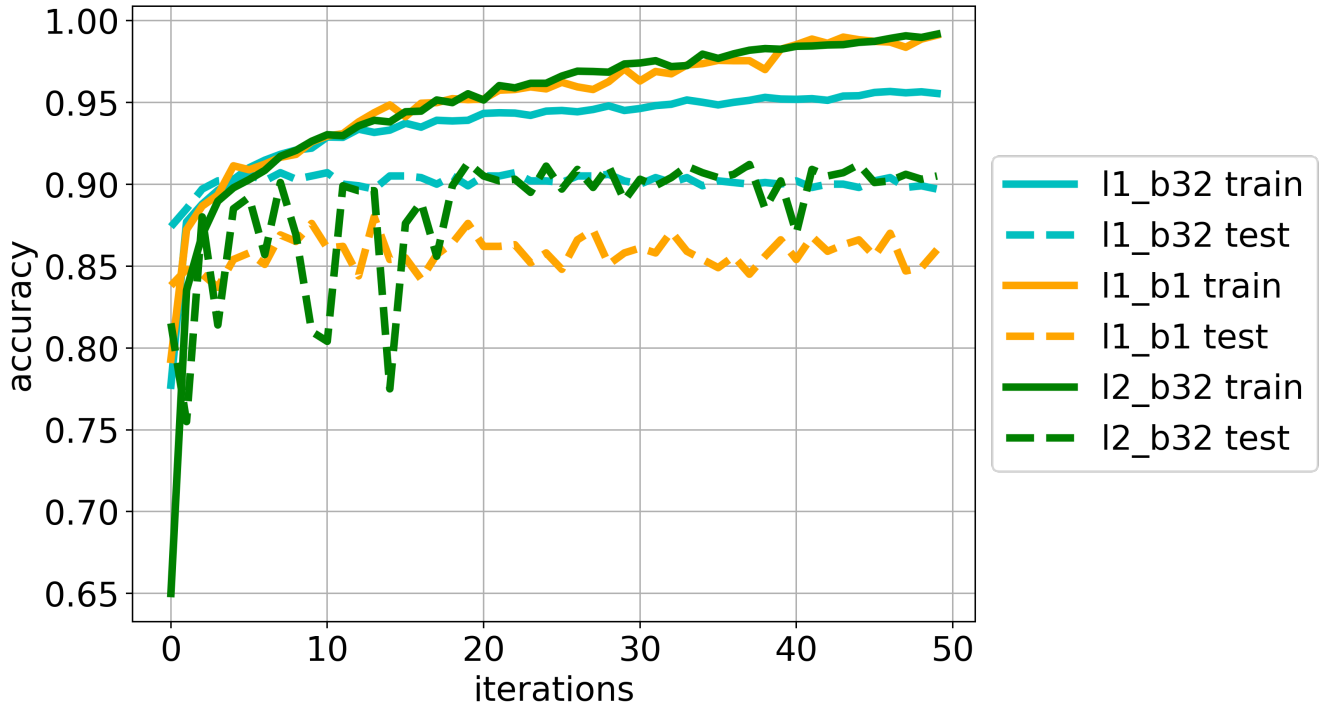
Learning behaviors
[layers,batchsize]



Param size 7850

- l1_b32: one layer, batch size 32 <=> Softmax regression
- l1_b1: one layer, batch size 1 <=> Softmax regression **SGD**
- L2_b32: two layers, batch size 32 **Param size 7960**
- L2_b1: two layers, batch size 1 **SGD**

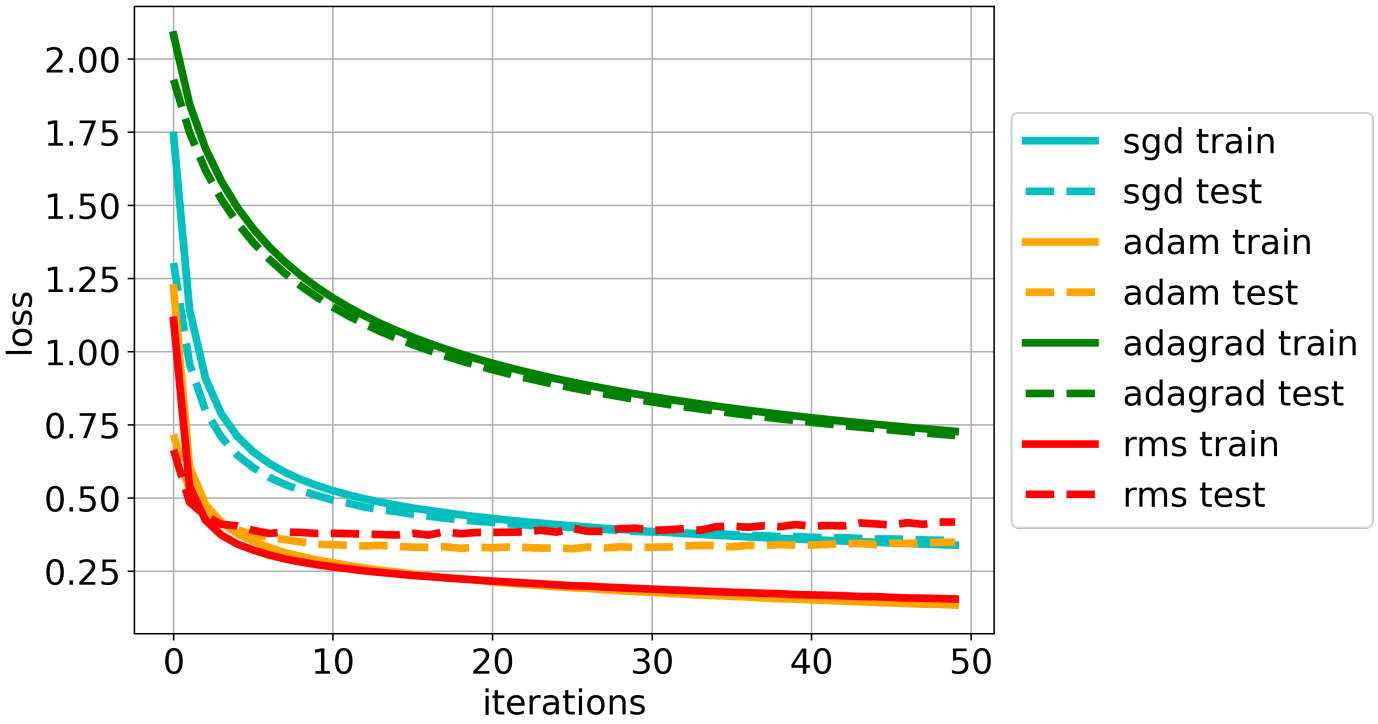
Learning behaviors
[layers,batchsize]



- l1_b1 and l2_b32 fit the training set better than l1_b32
- However, l1_b32 achieves stable generalization for the test set
- l1_b1 has the worst accuracy in test set

Behaviors of different optimizers

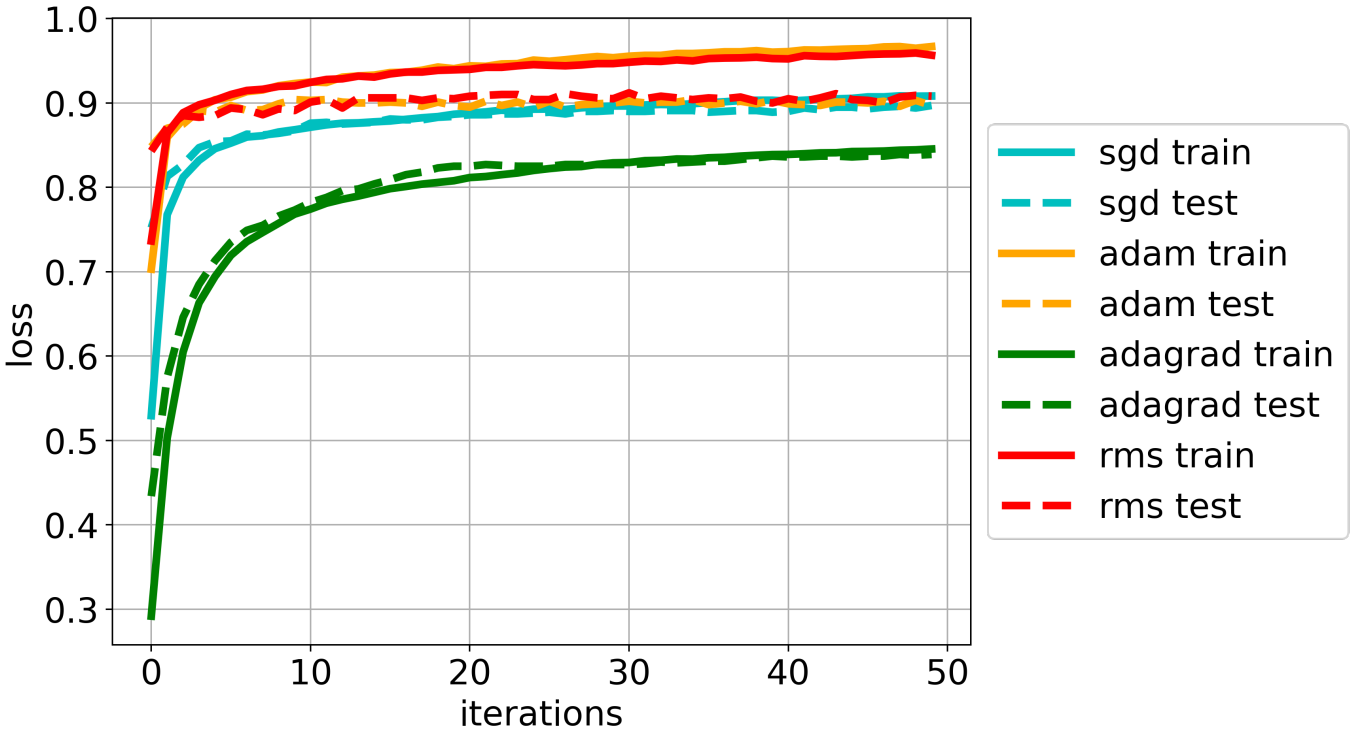
[layer : 1, batch: 32]



- Adam and RMSprop are relatively better than SGD and Adagrad

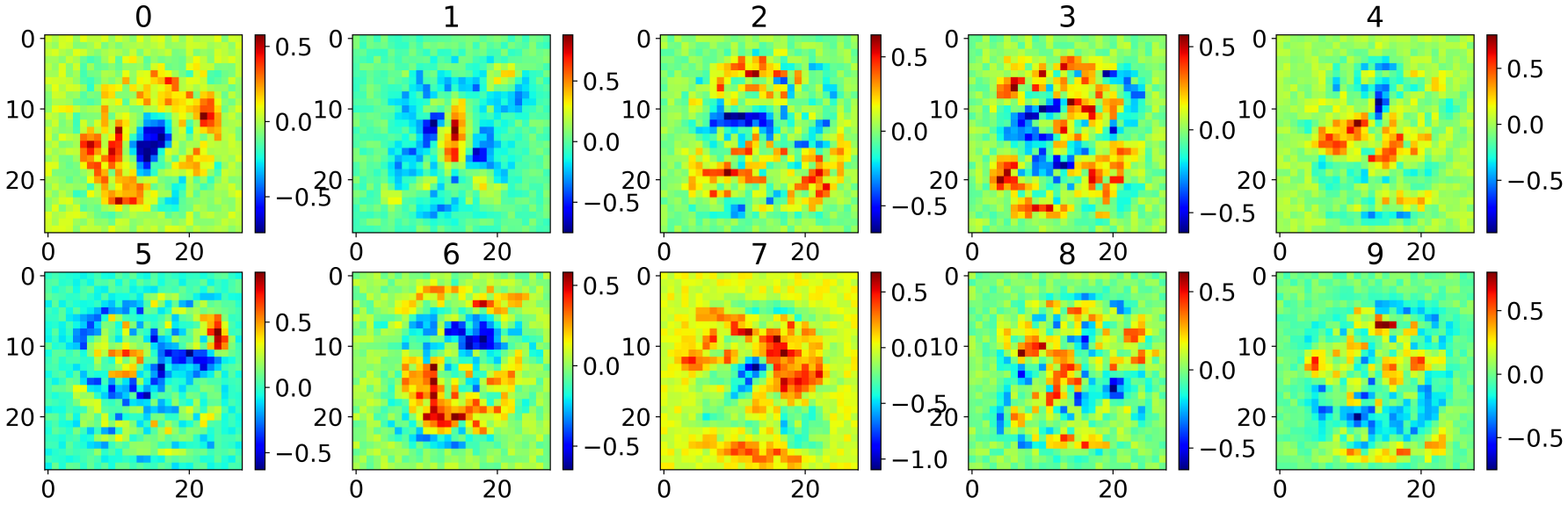
Behaviors of different optimizers

[layer : 1, batch: 32]



- Final accuracies on test sets are similar among SGD, Adam and RMSprop, however, Adam and RMSprop converge faster

Weights visualization for softmax regression (one-layer MLP)



Weights visualization for two-layer MLP