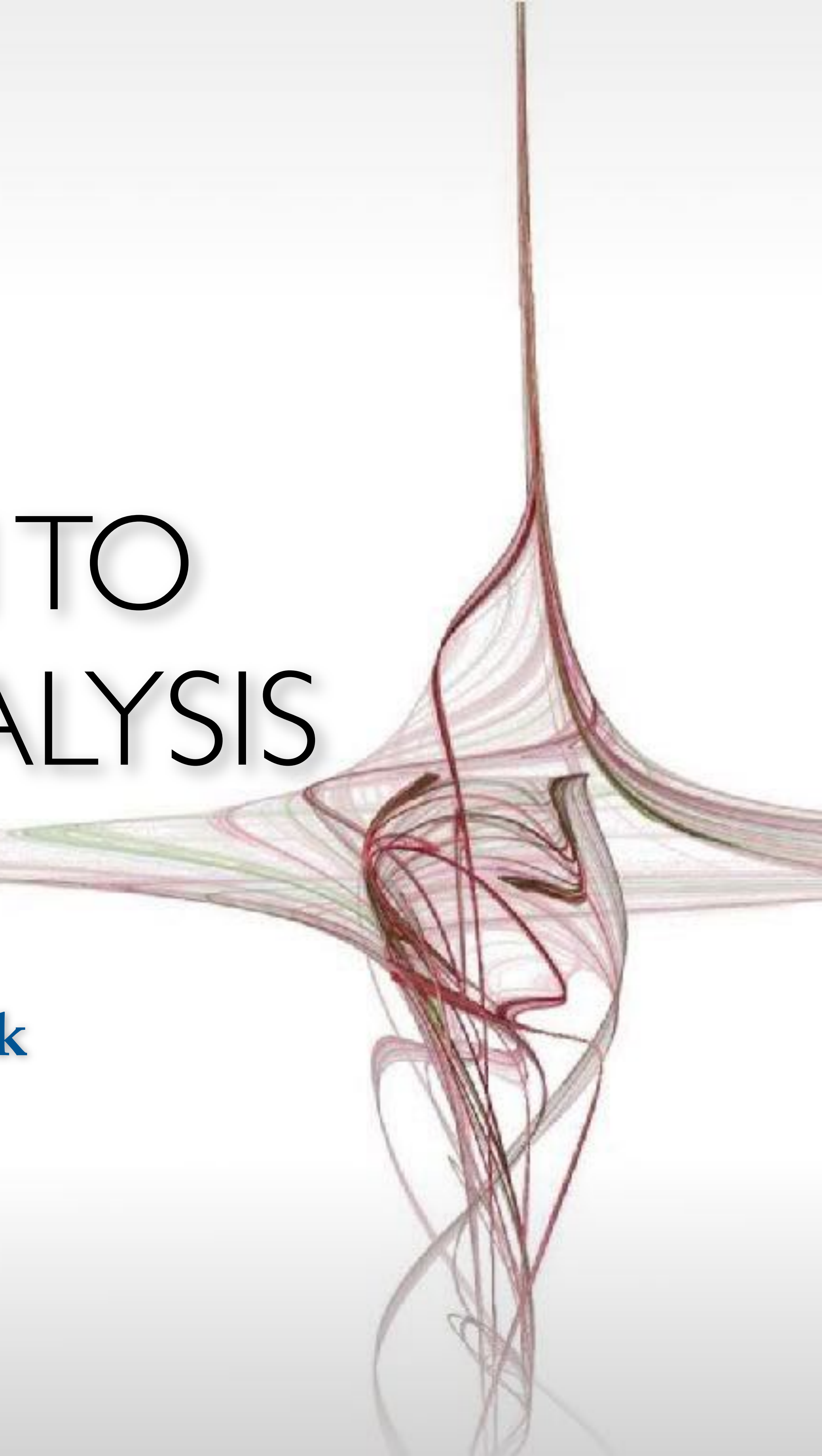
2020

INTRODUCTION TO NUMERICAL ANALYSIS



Lecture 3-3: Tricks for Improving Neural Network

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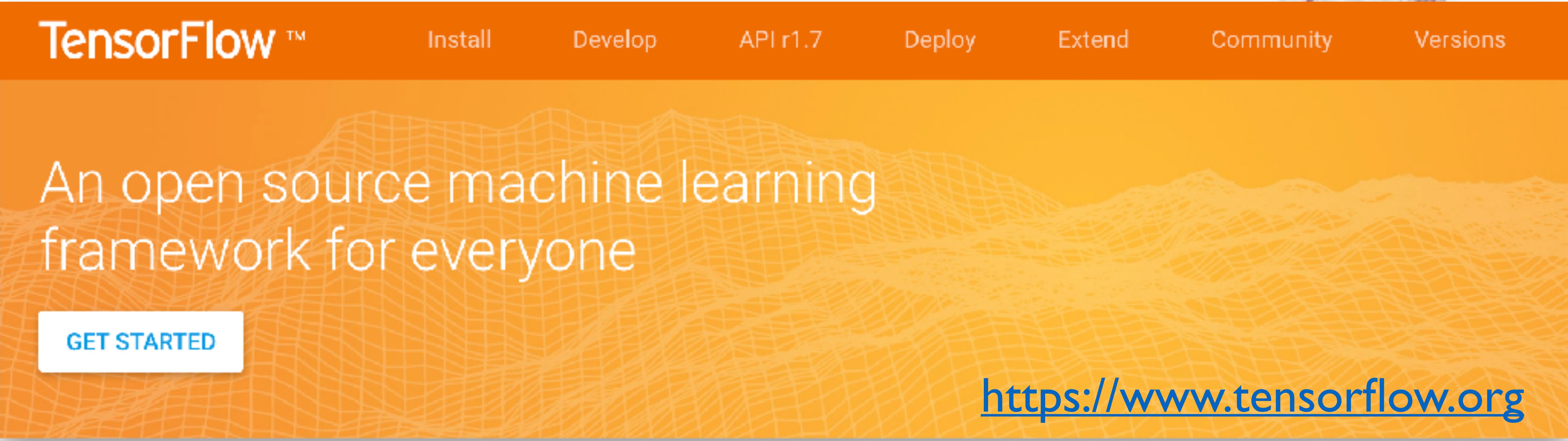
RECALL FROM THE LAST LECTURE…(AGAIN!)

- Last lecture we started to play with two nonlinear models, **SVM with non-linear kernel**, and the very classical **Neural Network**.
- Taking the MNIST data set as an benchmark, the SVM with Gaussian kernel can have a very good performance of ~98.4% accuracy!
- Our super simple neural network can already provide a good handwriting digits recognition with an accuracy of **~95%**. With a slightly better initial weights the performance can be pushed to **~96%**. Remember this was performed by a simple model of **784-30-10** network and only 20 epochs of training so far.
- Can we do better, by considering some of the state of arts techniques? Or can we further improve it by introducing a *deeper* network structure?

Time to tune
our network for
a better performance!

YOU MUST HAVE HEARD THE TENSORFLOW…

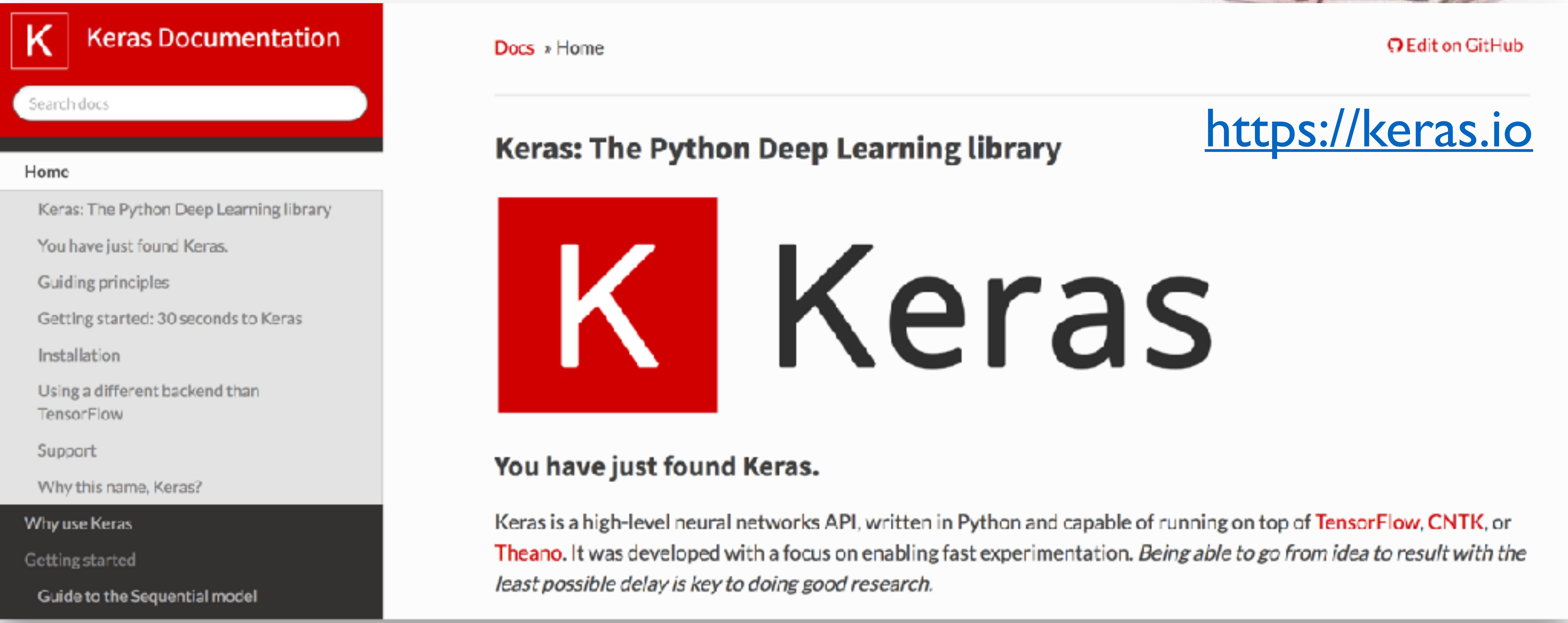


An open source machine learning framework for everyone

https://www.tensorflow.org

- **TensorFlow** is an open source software library for high performance numerical computation originally developed by Google. It comes with a strong support for machine learning and deep learning model and can run on CPU/GPU, or even the TPUs.
- But in order to have an even easier live, we will use something even simpler!

HERE COMES THE KERAS


Keras Documentation
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Keras: The Python Deep Learning library
You have just found Keras.
Guiding principles
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Why this name, Keras?
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Keras

Keras: The Python Deep Learning library

You have just found Keras.

Keras is a high-level neural networks API, written in Python and capable of running on top of TensorFlow, CNTK, or Theano. It was developed with a focus on enabling fast experimentation. *Being able to go from idea to result with the least possible delay is key to doing good research.*

https://keras.io

- **Keras** is a kind of "wrapper" or package which can help to build most of the conventional NN models, and the real calculation can be carried out by TensorFlow, as one of the supported backends.

INSTALLATION OF KERAS + TENORFLOW

- If you are using anaconda package, this can be done by typing this under your terminal:

```
conda install keras
```

- If it is working you will find both **keras** and **tensorflow** being installed. If you are not using anaconda, the package can be installed though pip:

```
pip install keras
```

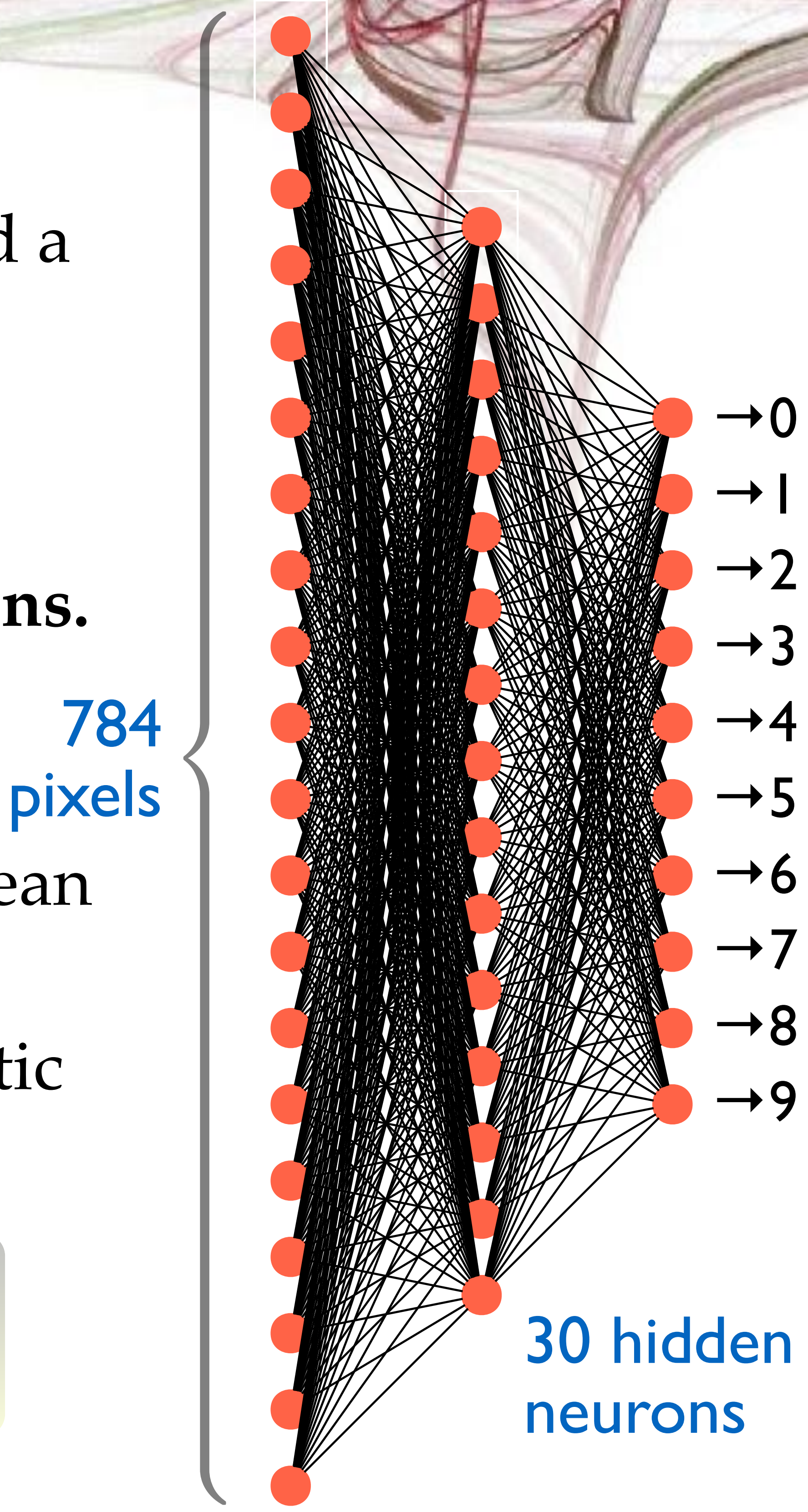
- A quick test can be made by just import the keras module directly:

```
% python
Python 3.6.4 |Anaconda custom (64-bit)| (default, Jan 16 2018,
12:04:33). . . .
>>> import keras
Using TensorFlow backend.
```

THE "BASELINE" NETWORK MODEL

- At the end of last lecture we have constructed a simple model with our own implementation. This serves as our starting point:
  - The network structure also consists with **3 layers, with one hidden layer of 30 neurons.**
  - The chosen activation function is also the **sigmoid function**.
  - The selected loss function is exactly the mean squared error, **MSE**.
  - The network will be trained using stochastic gradient descent **SGD** method.

What would be the performance if we construct exactly the same model with **Keras**?



BUILDING NETWORK WITH KERAS

- It is more-or-less straightforward to build the network with Keras:

```
mnist = np.load('mnist.npz')
x_train = mnist['x_train']/255.
y_train = np.array([np.eye(10)[n] for n in mnist['y_train']])
x_test = mnist['x_test']/255.
y_test = np.array([np.eye(10)[n] for n in mnist['y_test']])

from keras.models import Sequential
from keras.layers import Dense, Reshape
from keras.optimizers import SGD

model = Sequential()                                      ⇐ build a 784-30-10
model.add(Reshape((784,), input_shape=(28,28)))             model
model.add(Dense(units=30, activation='sigmoid'))
model.add(Dense(units=10, activation='sigmoid'))

model.compile(loss='mean_squared_error', ⇐ Loss = MSE
              optimizer=SGD(lr=3.0), ⇐ training with SGD
              metrics=[‘accuracy']) ⇐ also output accuracy
```

1303-example-01.py (partial)

BUILDING NETWORK WITH KERAS (II)

```
model.fit(x_train, y_train, epochs=20, batch_size=10) ⇐ train for 20 epochs

print('Performance (training)')
print('Loss: %.5f, Acc: %.5f' % tuple(model.evaluate(x_train, y_train)))
print('Performance (testing)')
print('Loss: %.5f, Acc: %.5f' % tuple(model.evaluate(x_test, y_test)))
```

l303-example-01.py (partial)

```
Using TensorFlow backend.
Epoch 1/20
60000/60000 [==============] - 6s 100us/step - loss: 0.0205 - acc: 0.8841
. . . . . .
Epoch 20/20
60000/60000 [==============] - 6s 107us/step - loss: 0.0045 - acc: 0.9766
Performance (training)
60000/60000 [==============] - 1s 20us/step
Loss: 0.00437, Acc: 0.97785
Performance (testing)
10000/10000 [==============] - 0s 19us/step
Loss: 0.00622, Acc: 0.96620
```

Already get a similar/slightly better result? What are the **remaining wrongly tagged digits now**?

WRONGLY RECOGNIZED DIGITS?

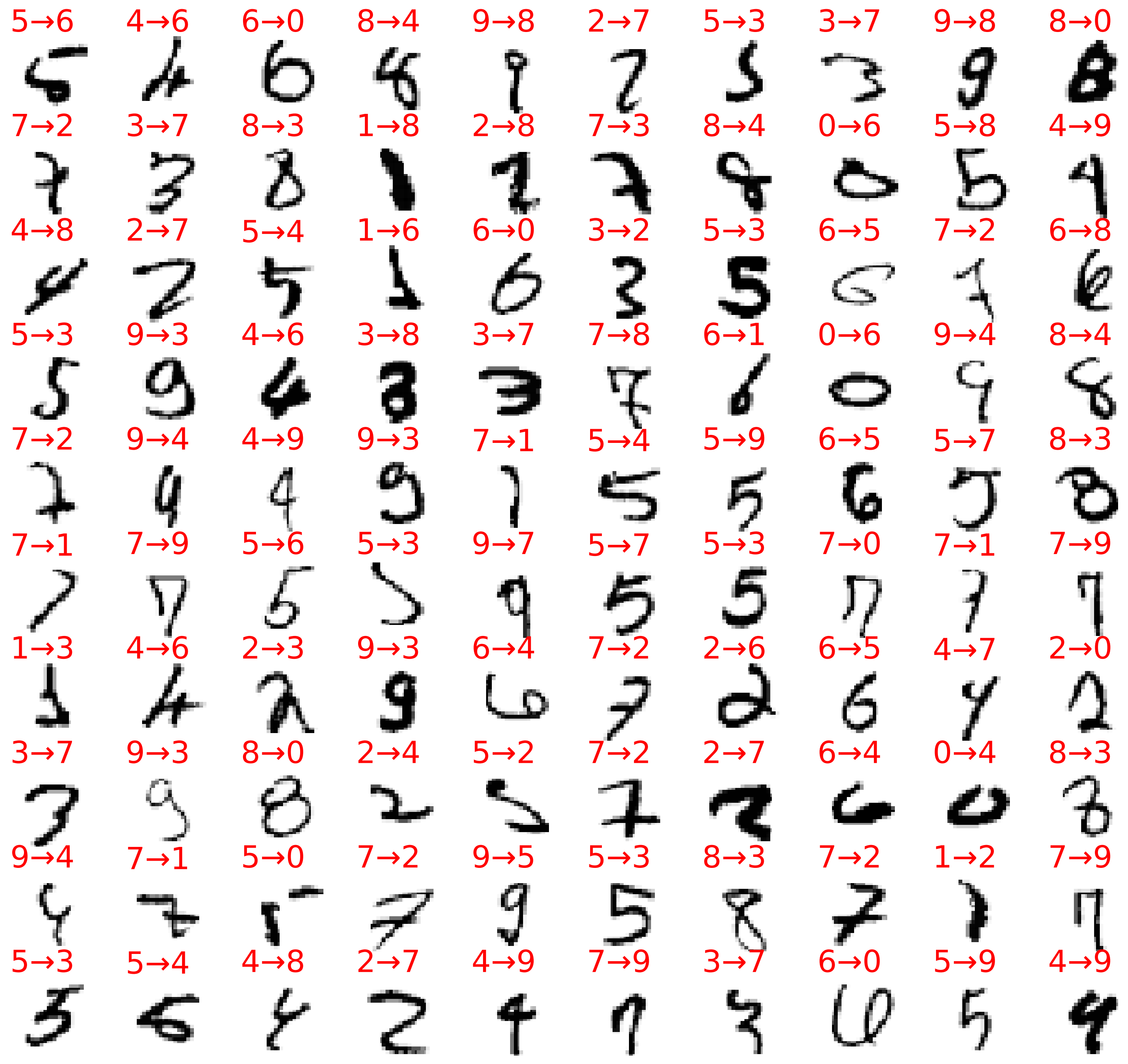
- At the end of the training we can feed the test data into the network and see the resulting "test" performance. An accuracy of **96.6%** means we have only around **~300 images** were wrongly tagged by our network.
- The following piece of code is prepared to show **first 100 of the wrongly tagged images**:

```
p_test = model.predict(x_test)
failedsample = [[img,y,p] for img,y,p in
zip(mnist['x_test'],y_test,p_test) if y.argmax()!=p.argmax()]

fig = plt.figure(figsize=(10,10), dpi=80)
for i in range(len(failedsample[:100])):
    plt.subplot(10,10,i+1)
    plt.axis('off')
    plt.imshow(failedsample[i][0], cmap='Greys')
    plt.text(0.,0.,'$%d\\to%d$' % (failedsample[i][1].argmax(),
             failedsample[i][2].argmax()),color='Red',fontsize=15)
plt.show()
```

⇑ pick up those wrongly tagged samples

1303-example-01a.py (partial)

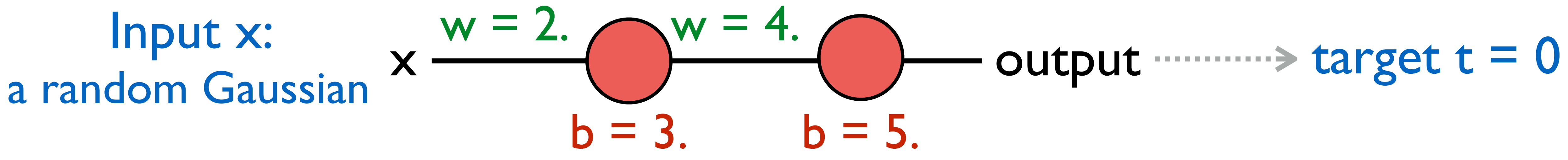
WRONGLY RECOGNIZED DIGITS? (II)



- You can see that there are still some handwriting digits are obviously wrongly tagged.
- But there are also some images can be easily mis-tagged!
- Nevertheless this is our starting point and we are going to discuss several techniques to improve the network!

SLOW LEARNING WITH BAD WEIGHTS

- Based on the NN model up to now, one of the typical issue we may face is this: when the initial weights are very far from the optimal, the learning is actually slower.
- This is very different from our intuition in fact — usually human beings **learn faster if they are very wrong**. But this is not the case for your NN.
- A demonstration simple network with only one input layer and one output layer, with 2 weights and 2 bias. Let's set the weights/bias by hand to some particular values:



SLOW LEARNING WITH BAD WEIGHTS (II)

- Such a model can be built with Keras easily as well:

```
x_train = np.random.randn(1000)
y_train = np.zeros(1000)

from keras.models import Sequential
from keras.layers import Dense
from keras.optimizers import SGD

model = Sequential()
model.add(Dense(units=1, activation='sigmoid', input_dim=1))
model.add(Dense(units=1, activation='sigmoid'))
model.compile(loss='mean_squared_error',
              optimizer=SGD(lr=1.0))

model.layers[0].set_weights([np.array([[2.]]),np.array([3.])])
model.layers[1].set_weights([np.array([[4.]]),np.array([5.])])

rec = model.fit(x_train, y_train, epochs=100, batch_size=100)

vep = np.linspace(1.,100.,100)
fig = plt.figure(figsize=(6,6), dpi=80)
plt.plot(vep,rec.history['loss'], lw=3)
plt.show()
```

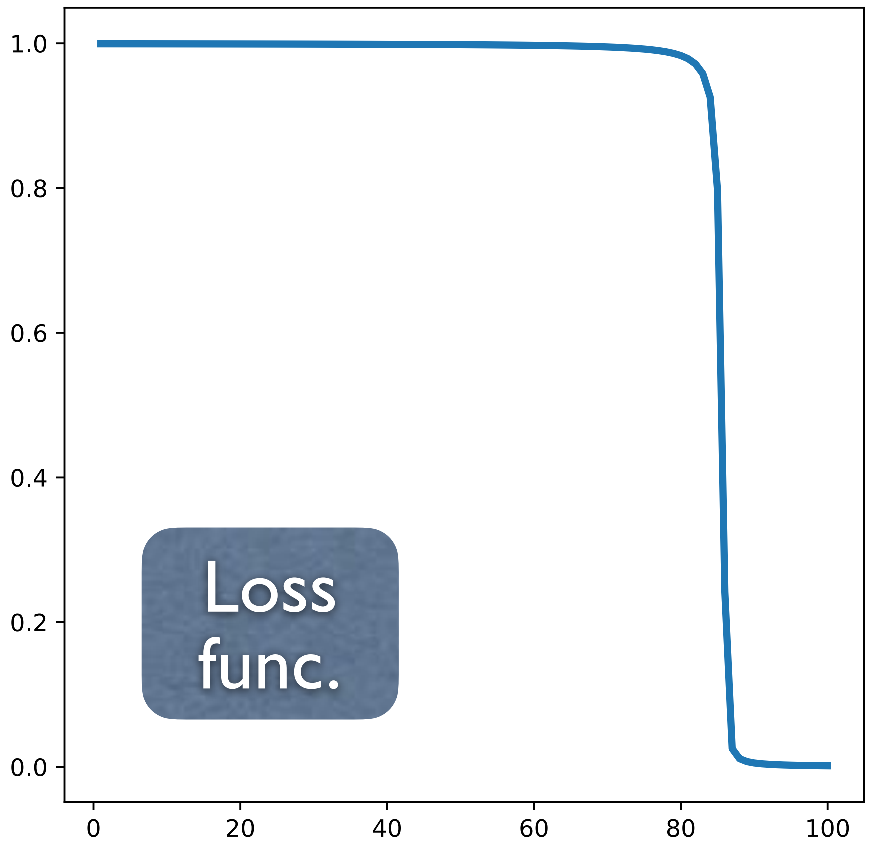
A simple sequential model
⇓with only 1 input / 1 output neuron

⇑ keep the history of training

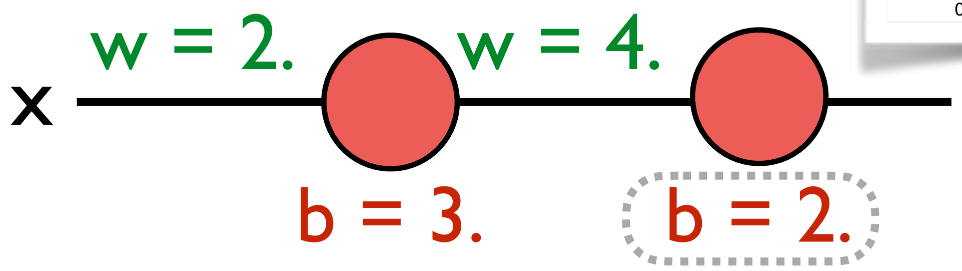
1303-example-02.py (partial)

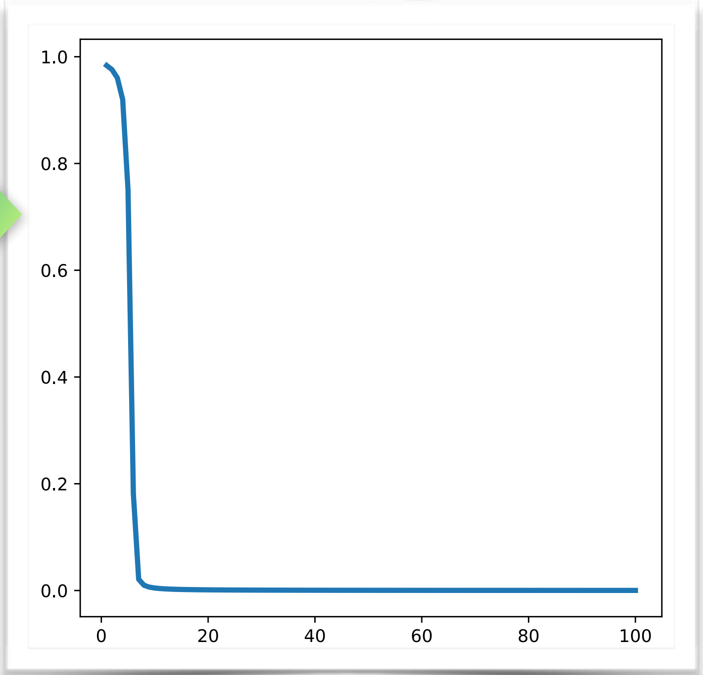
SLOW LEARNING WITH BAD WEIGHTS (III)

- This is what you may find: the loss function is large for initial epochs — and it takes for a while until the training really starts.
- Remember this network is already very simple with only 4 parameters to be tuned. But such a situation does happen.



Surely the situation is better if one uses a different initial values, e.g.





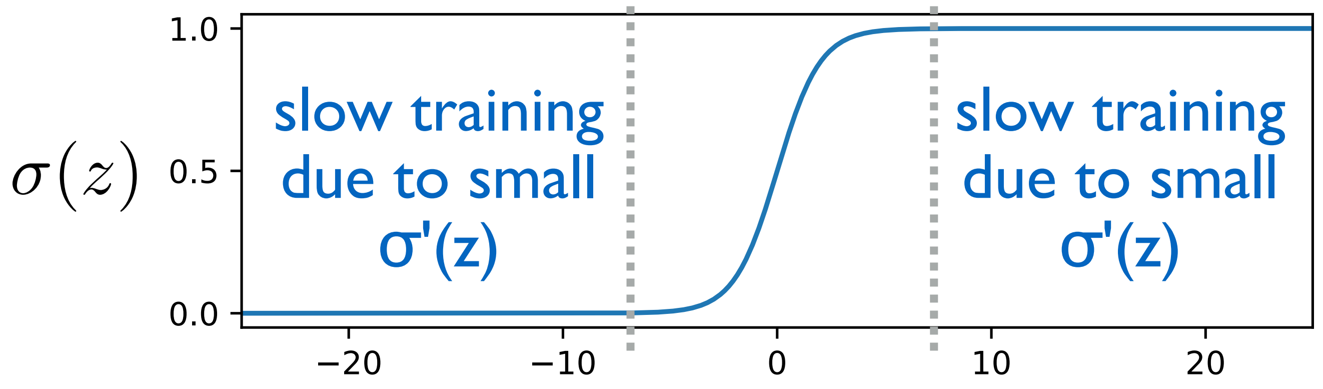
Both this also hints a problem of our network!

THE CHOICE OF LOSS

- In fact such a situation can be related to the definition of the loss function, and its gradient w.r.t. the weights and bias.
- Consider the current choice of loss, the **mean squared error**:

Consider only one output: $$L(w,b) = \frac{1}{2}|\sigma(z) - t|^2$$

Gradient is required in the training process:
$$\frac{\partial L}{\partial w} = [\sigma(z) - t]\sigma'(z)\frac{\partial z}{\partial w}$$
$$\frac{\partial L}{\partial b} = [\sigma(z) - t]\sigma'(z)\frac{\partial z}{\partial b}$$



The training speed is proportional to the **first derivative of the activation function**! If the z value is too large or too small, the training will be very

THE CHOICE OF LOSS (II)

- This can be improved by introducing a different loss function, for example, the **(binary) cross-entropy function**:

$$Loss(w_i, b_j) = \frac{-1}{n} \sum_{x}^{n} [t \ln y + (1-t)\ln(1-y)]$$

Consider only one output & replace y by σ(z):

$$L = -[t \ln \sigma(z) + (1-t)\ln(1-\sigma(z))]$$

Gradient w.r.t. weights/bias:

$$\frac{\partial L}{\partial w} = -t\frac{\sigma'(z)}{\sigma(z)}\frac{\partial z}{\partial w} + (1-t)\frac{\sigma'(z)}{1-\sigma(z)}\frac{\partial z}{\partial w}$$

$$= [\sigma(z) - t]\left\{\cancel{\frac{\sigma'(z)}{\sigma(z)[1-\sigma(z)]}}\right\}\frac{\partial z}{\partial w}$$

Cancelled

$$= [\sigma(z) - t]\frac{\partial z}{\partial w}$$

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

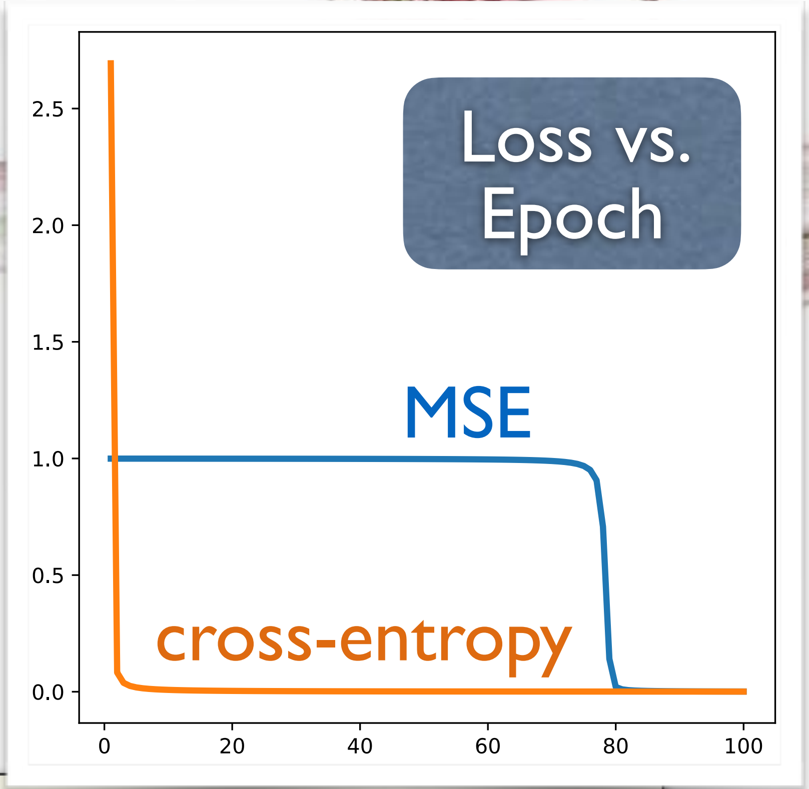
$$\Rightarrow \sigma'(z) = \sigma(z)[1-\sigma(z)]$$

A little bit of calculous…

Not depending on the first derivative **σ′(z)** anymore!

THE CHOICE OF LOSS (III)

- This effect can be tried easily!
- Indeed the cross-entropy function can speed up the learning even with bad initial weights!



```
model.compile(loss='mean_squared_error', optimizer=SGD(lr=1.0))
model.layers[0].set_weights([np.array([[2.]]),np.array([3.])])
model.layers[1].set_weights([np.array([[4.]]),np.array([5.])])

rec1 = model.fit(x_train, y_train, epochs=100, batch_size=100)

model.compile(loss='binary_crossentropy', optimizer=SGD(lr=1.0))
model.layers[0].set_weights([np.array([[2.]]),np.array([3.])])
model.layers[1].set_weights([np.array([[4.]]),np.array([5.])])

rec2 = model.fit(x_train, y_train, epochs=100, batch_size=100)

vep = np.linspace(1.,100.,100)
fig = plt.figure(figsize=(6,6), dpi=80)
plt.plot(vep,rec1.history['loss'], lw=3)
plt.plot(vep,rec2.history['loss'], lw=3)
plt.show()
```

l303-example-02a.py (partial)

THE CHOICE OF OUTPUT LAYER

- Another approach to the same problem is by introducing the **softmax layer**, instead of the classical sigmoid function.
- The softmax layer is a different type of output layer, it can be expressed as

$$y_j = \frac{\exp(z_j)}{\sum_k \exp(z_k)}$$

k: classes

- The output of the network ***y*** is replaced by the formula above. Given it is normalized (summing all of the outputs will be one by definition), another benefit of softmax layer is that the output values can be treated as a probability, which is not the case for the classical sigmoid function.
- By combining this with the **cross-entropy function**, it can be another remedy to the slow learning problem.

SOFTMAX + CROSS-ENTROPY LOSS

- The **(Categorical) cross-entropy loss function** for a given training sample is

$$L = -\sum_j t_j \ln(y_j) \quad \text{j: classes}$$

- You may find this is just an extended version of the previous cross-entropy function which was derived for 2 classes (binary case).
- Let's first calculate the partial derivate for y_j w.r.t. z_i (remember z_i is linear sum of weights times the outputs from previous layer + bias):

$$y_j = \frac{e^{z_j}}{\sum e^{z_k}} \rightarrow$$

If j≠i: $$\frac{\partial y_j}{\partial z_i} = \frac{-e^{z_j} e^{z_i}}{(\sum e^{z_k})^2} = -y_i y_j$$

If j=i: $$\frac{\partial y_i}{\partial z_i} = \frac{e^{z_i}(\sum e^{z_k}) - e^{z_i} e^{z_i}}{(\sum e^{z_k})^2} = y_i - y_i^2$$

SOFTMAX + CROSS-ENTROPY LOSS (II)

- Then the derivative for the loss function itself:

$$L = -\sum_j t_j \ln(y_j) \rightarrow \frac{\partial L}{\partial z_i} = -\sum_j t_j \frac{1}{y_j}\frac{\partial y_j}{\partial z_i}$$

$$\frac{\partial L}{\partial z_i} = -t_i \frac{1}{y_i}\frac{\partial y_i}{\partial z_i} - \sum_{j \neq i} t_j \frac{1}{y_j}\frac{\partial y_j}{\partial z_i}$$

$$= -t_i(1-y_i) + \sum_{j\neq i} t_j y_i = -t_i + t_i y_i + \sum_{j \neq i} t_j y_i$$

$$= -t_i + y_i \left(t_i + \sum_{j\neq i} t_j \right) = y_i - t_i$$

It ends up with the same results as before and no dependency on **σ′(z)**!

t_j = target value for class j
by definition $\Sigma t_j = 1$

It should solve the slow learning problem as well.

TRY IT OUT!

```
model = Sequential()
model.add(Reshape((784,), input_shape=(28,28)))
model.add(Dense(30, activation='sigmoid'))
model.add(Dense(10, activation='softmax'))

model.compile(loss='categorical_crossentropy',
              optimizer=SGD(lr=1.0),
              metrics=['accuracy'])

model.fit(x_train, y_train, epochs=20, batch_size=30)
```

l303-example-03.py (partial)

```
Using TensorFlow backend.
Epoch 1/20
60000/60000 [=============] - 3s 45us/step - loss: 0.2924 - acc: 0.9114
. . . . . .
Epoch 20/20
60000/60000 [=============] - 2s 41us/step - loss: 0.0465 - acc: 0.9850
Performance (training)
60000/60000 [=============] - 1s 22us/step
Loss: 0.04225, Acc: 0.98613
Performance (testing)
10000/10000 [=============] - 0s 23us/step
Loss: 0.13640, Acc: 0.96350
```

Although the performance for training sample is improved, but the performance for testing sample is still similar!

COMMENT

- We have two possible treatments that can be used in the classification problem:
  - **sigmoid activation + binary cross-entropy loss**
  - **softmax layer + categorical cross-entropy loss**
- You may find they have a very similar formulation and similar behavior. This is due to the fact that sigmoid is special case of softmax function (if you compare them carefully), and the binary cross-entropy loss can be considered as a "yes/no" problem for each output neuron.
- In our handwriting digits example one can solve "10 binary problems" with the binary cross-entropy loss, or "one out of 10 choices" with categorical cross-entropy loss.

Remark: Keras may give a different accuracy value if you do sigmoid activation + binary cross-entropy loss

INTERMISSION

- When introducing softmax layer + categorical cross-entropy loss, the output softmax function is :

$$y_j = \frac{\exp(z_j)}{\sum_k \exp(z_k)}$$

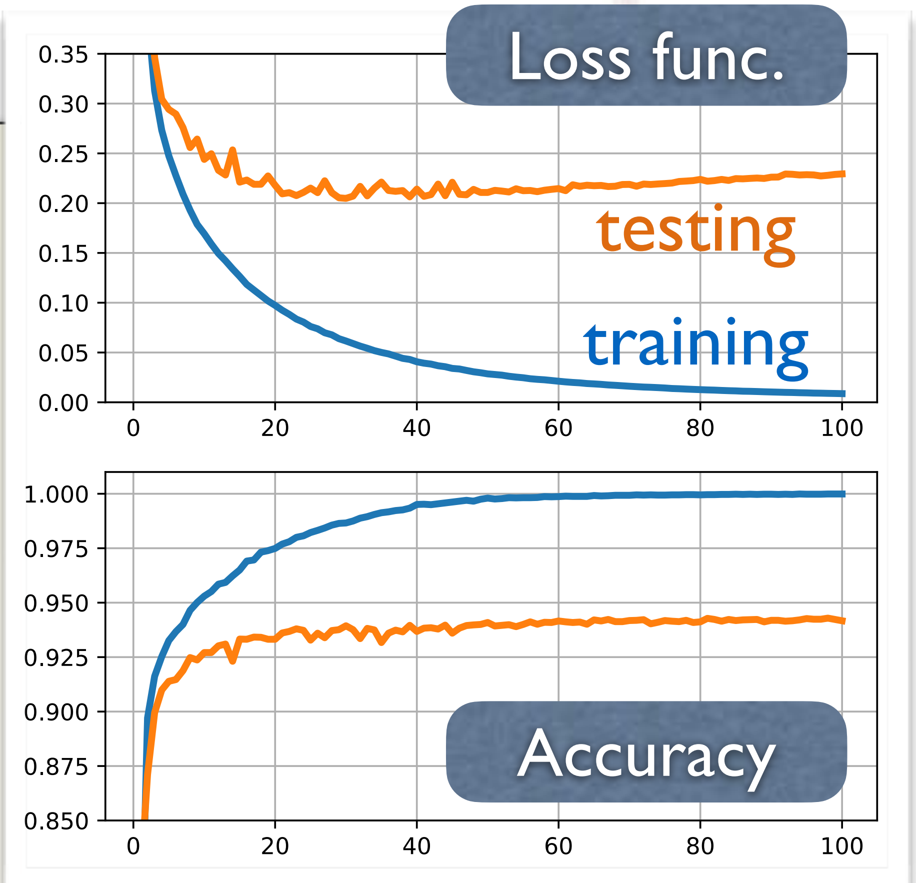
  which can be considered as **"probability"** out of the multiple choice, and this is one of the interesting aspect of the softmax layer.

- Try to extract output value of the best and second best options from the remaining wrongly tagged digits, see if their values are not too far from each other (ie. the second option has fairly good chance to be correct), given the probability interpretation of the softmax layer?

THE OVERTRAINING ISSUE

- We have touched slightly on this issue at the end of last lecture. Now we shall come back to it again.
- The training performance is indeed keeping improving with more epochs, but the testing performance saturated quickly.
- Demonstration with Keras tool again:

```
rec = model.fit(x_train, y_train,
        epochs=100, batch_size=120,
        validation_data=(x_test, y_test))

vep = np.linspace(1.,100.,100)
fig = plt.figure(figsize=(6,6), dpi=80)
plt.subplot(2,1,1)
plt.plot(vep,rec.history['loss'], lw=3)
plt.plot(vep,rec.history['val_loss'], lw=3)
plt.subplot(2,1,2)
plt.plot(vep,rec.history['acc'], lw=3)
plt.plot(vep,rec.history['val_acc'], lw=3)
plt.show()
```

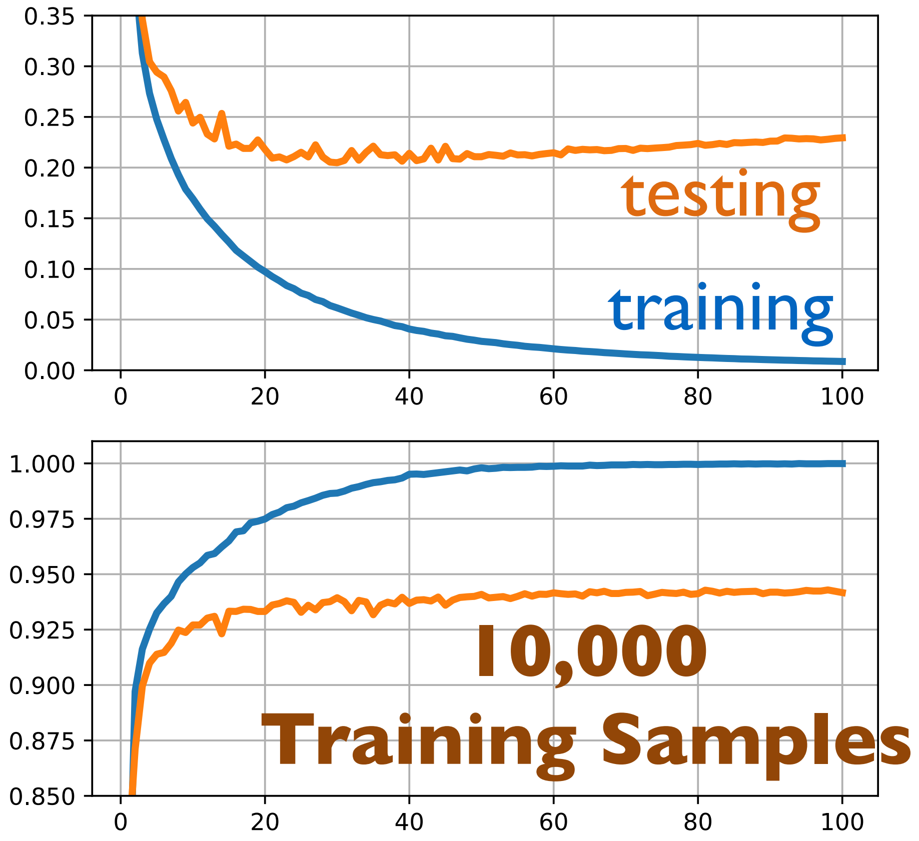


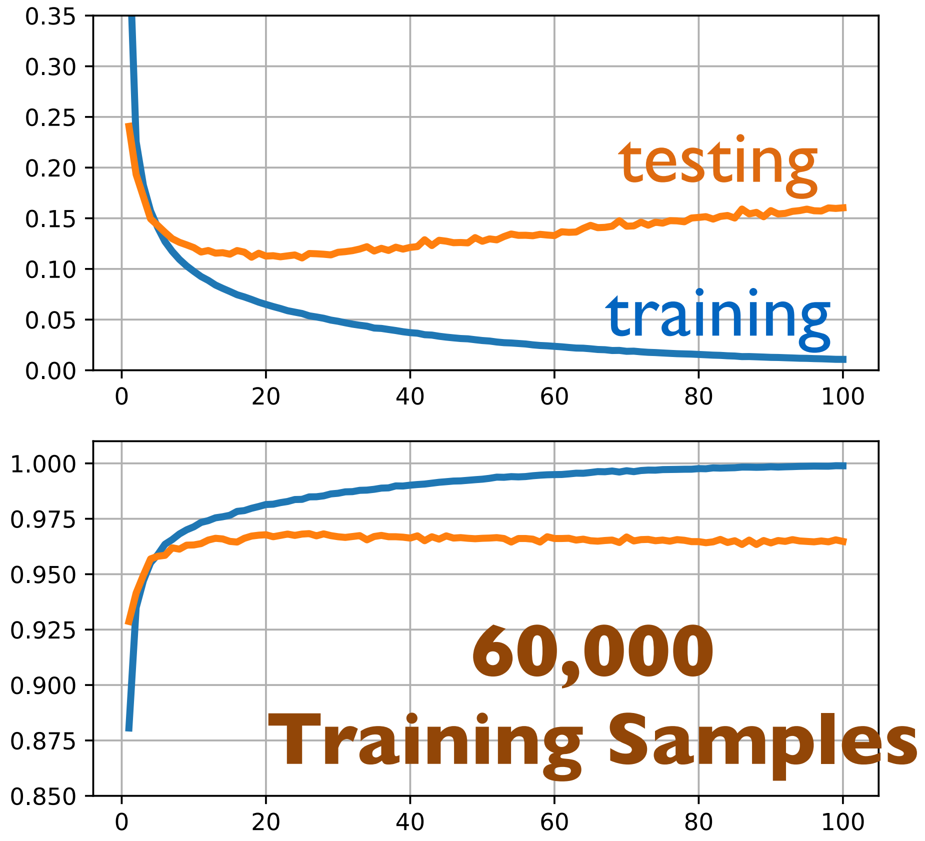
l303-example-04.py (partial)

TRAINING DATA DOES MATTER

- In the previous example we have only input 10K sets of training sample. By increasing the training data size the overtraining is indeed mitigated:

Loss func.





But in many of the cases training samples are difficult to collect and expensive. Can we do something without just adding more the data?

REGULARIZATION

- A method is called “Regularization” or “weight decay” may help to reduce the overtraining situation.
- The idea is to introduce an additional term to the loss function:

$$L = L_0 + \frac{\lambda}{n}\sum |w| \quad \text{or} \quad L = L_0 + \frac{\lambda}{2n}\sum w^2$$

- The form given above is usually called the **L1/L2 regularization**, where the ***λ*** is the *regularization parameter* (***λ*>0**) and ***n*** is the size of training sample.
- One can see the gradient of the loss function will be modified and change the learning step (taking L2 regularization as an example):

$$\frac{\partial L}{\partial w} = \frac{\partial L_0}{\partial w} + \frac{\lambda}{n}w \quad \Longrightarrow \quad w \Rightarrow w - \eta\frac{\partial L_0}{\partial w} - \eta\frac{\lambda}{n}w$$

The weights will “decay” by a factor during the training process.

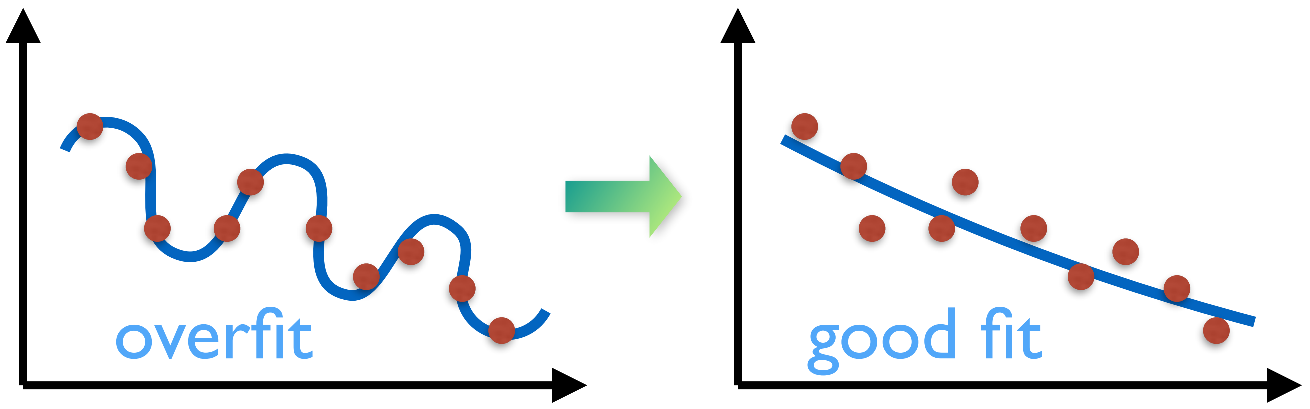
$$= \boxed{\left(1 - \eta\frac{\lambda}{n}\right)} w - \eta\frac{\partial L_0}{\partial w}$$

REGULARIZATION (II)

- By introducing such a "weight decay" to the training, the weights will be pushed toward smaller values. But why a network with smaller weights can have a smaller overtraining problem?
- Consider a fit to the data points along the x-axis, the "weights" are just the coefficients of the polynomial terms:

$$f(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^2 + w_4 x^4 + w_5 x^5 + \cdots$$

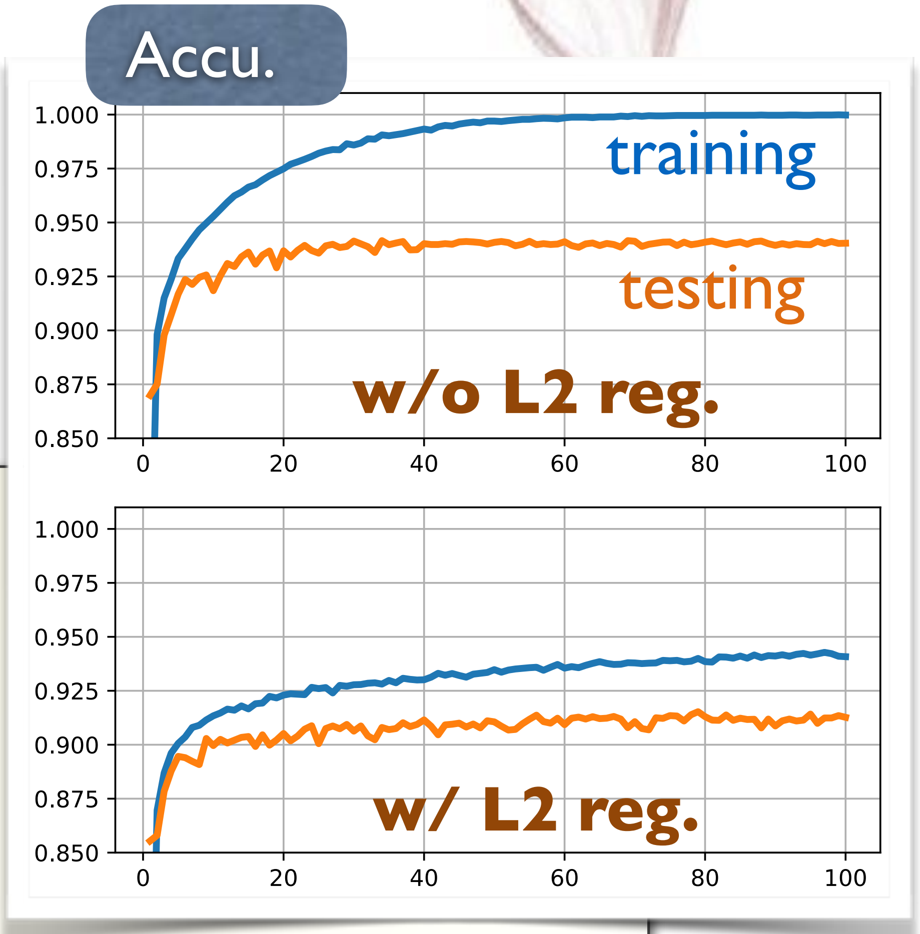
$$\Rightarrow f(x) = w_0 + w_1 x + w_2 x^2 + {\color{red}0x^2} + {\color{red}0x^4} + {\color{red}0x^5} + \cdots$$



By reducing the weights for all terms, it actually removes the higher order term and make the fit to be less sensitive to the noise (local fluctuation), and resulting a more robust model.

REGULARIZATION (III)

- Let's try this method quickly with Keras. If we simply add this weight decay feature to *the weights of the output layer*, one can see the overtraining effect is reduced:

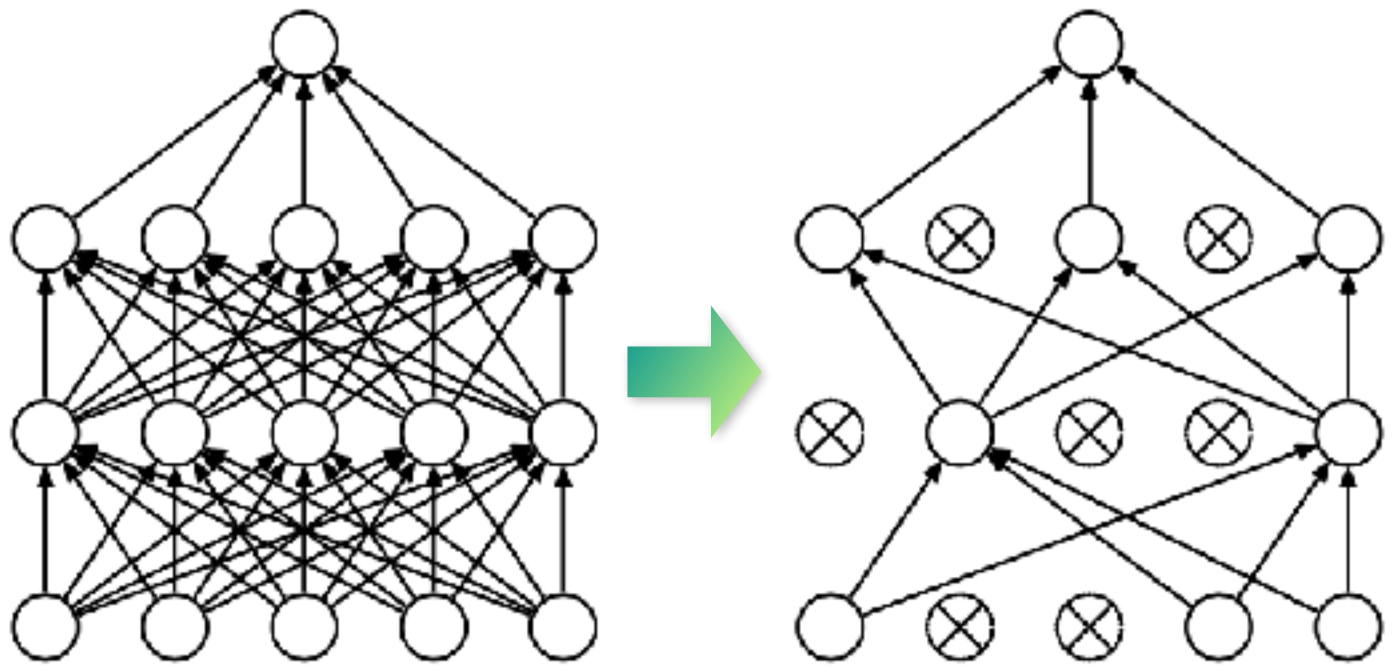


```
. . . . . .
from keras.regularizers import l2

m2 = Sequential()
m2.add(Reshape((784,), input_shape=(28,28)))
m2.add(Dense(30, activation='sigmoid'))
m2.add(Dense(10, activation='softmax',
kernel_regularizer=l2(0.01)))
m2.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=1.0), metrics=['accuracy'])
. . . . . .
```

l303-example-04a.py (partial)

DROPOUT

- Another useful method to reduce the overtraining is the **dropout** technique. Dropout does not change the loss function, but change the network structure itself.
- That is, one can randomly disconnect some of the inputs of a specific layer/neurons at each training cycle:



The dropout method would reduce the dependence of the network to some specific neurons or weights, and hence it will be less sensitive to the noise and become more robust against the overtraining.

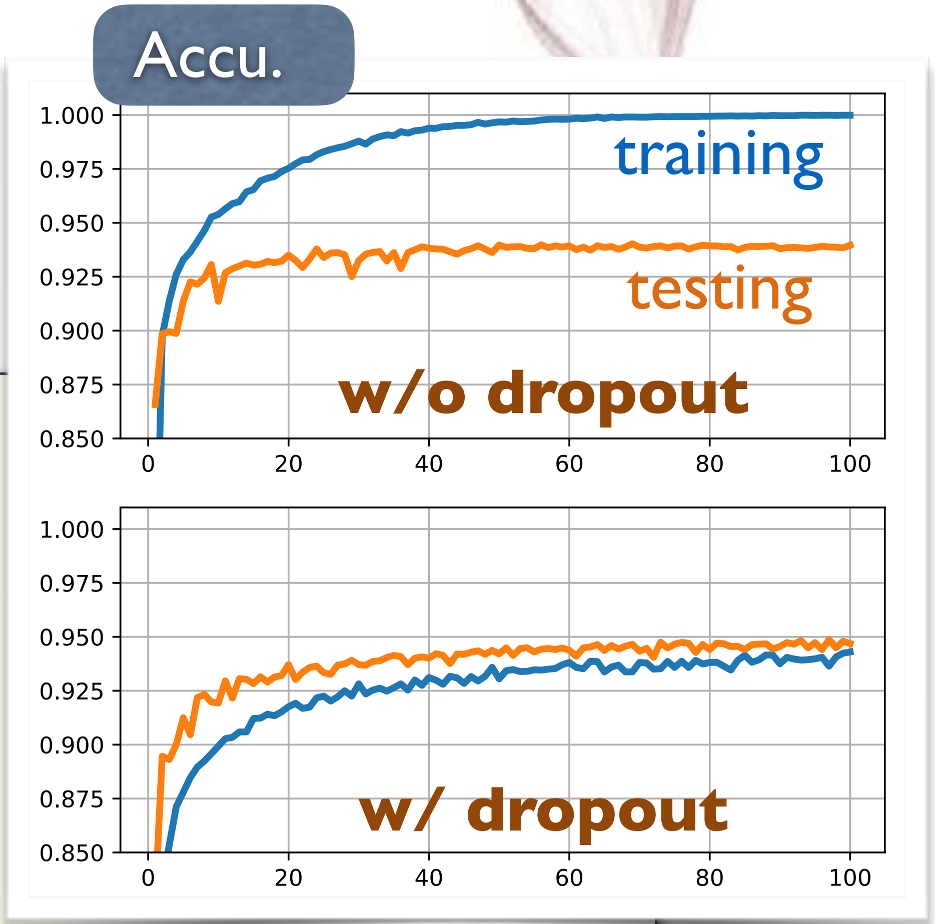
DROPOUT (II)

- And you can find that the dropout method is actually very helpful in terms of against overtraining:

Drop 20% of the inputs randomly

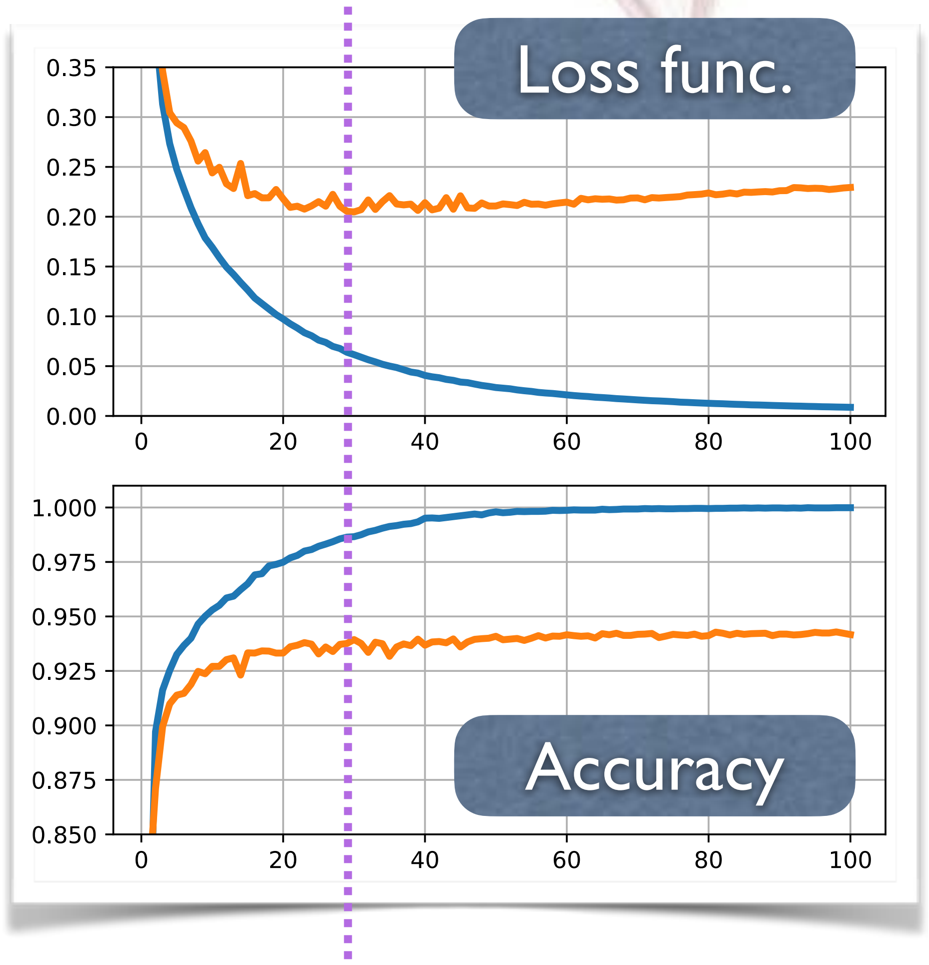
```
. . . . . .
from keras.layers import Dropout

m2 = Sequential()
m2.add(Reshape((784,), input_shape=(28,28)))
m2.add(Dropout(0.2))
m2.add(Dense(30, activation='sigmoid'))
m2.add(Dropout(0.2))
m2.add(Dense(10, activation='softmax'))
m2.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=1.0), metrics=['accuracy'])
. . . . . .
```

l303-example-04b.py (partial)



EARLY STOPPING

- In fact one can even think of something super simple: why cannot we just stop training immediately when we find the model just becomes overtrained?
- Such a scenario is usually called **"Early Stopping"**. This can be achieved by monitoring the performance of the model during the training process, and terminate the job when the model stop improving.
- It is usually recommended to adopt this criteria on **an independent validation sample** (not the training, nor the testing samples!)



Stop training here?

EARLY STOPPING (II)

- This can be carried out by a "callback" function within Keras:

```
mnist = np.load('mnist.npz')
x_train = mnist['x_train'][:10000]/255.
y_train = np.array([np.eye(10)[n] for n in mnist['y_train'][:10000]])
x_valid = mnist['x_train'][50000:]/255.
y_valid = np.array([np.eye(10)[n] for n in mnist['y_train'][50000:]])
x_test = mnist['x_test']/255.
y_test = np.array([np.eye(10)[n] for n in mnist['y_test']])
. . . . . .
from keras.callbacks import EarlyStopping

rec = model.fit(x_train, y_train, epochs=100, batch_size=120,
        validation_data=(x_valid, y_valid),
        callbacks=[EarlyStopping(monitor='val_loss', patience=3)])

print('Performance (training)')
print('Loss: %.5f, Acc: %.5f' % tuple(model.evaluate(x_train, y_train)))
print('Performance (validation)')
print('Loss: %.5f, Acc: %.5f' % tuple(model.evaluate(x_valid, y_valid)))
print('Performance (testing)')
print('Loss: %.5f, Acc: %.5f' % tuple(model.evaluate(x_test, y_test)))
```

l303-example-04c.py (partial)

EARLY STOPPING (III)

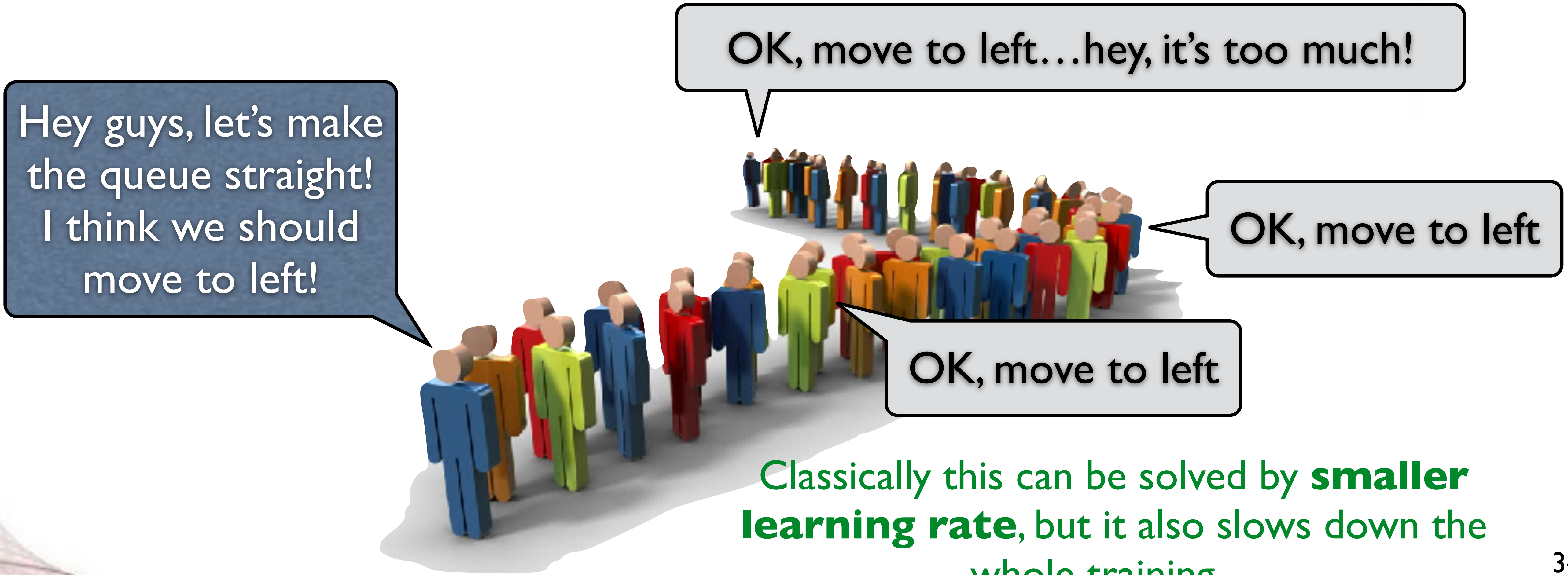
- The learning process is stopped automatically after 21 epochs:

```
Train on 10000 samples, validate on 10000 samples
Epoch 1/100
10000/10000 [==============] - 0s 27us/step - loss: 0.9330 - acc: 0.7552 -
val_loss: 0.5119 - val_acc: 0.8510
Epoch 21/100
10000/10000 [==============] - 0s 21us/step - loss: 0.0876 - acc: 0.9783 -
val_loss: 0.2068 - val_acc: 0.9373
Performance (training)
Loss: 0.09317, Acc: 0.97770
Performance (validation)
Loss: 0.20682, Acc: 0.93730
Performance (testing)
Loss: 0.21634, Acc: 0.93480
```

The reason to setup another **validation sample** here is to keep that the **testing sample always provides a unbiased performance estimate**. The validation sample here is "used" to decide the ending of the training process already. This validation setup is also recommended for hyper parameter and model tuning.

INTERNAL COVARIATE SHIFT

- **Internal covariate shift** is a kind of problem which may shows up when the network goes deeper. This is due to the distributions of the activations are always changing during training, and the training of the intermediate layers may not be able to catch up the situation and then slows down the learning process.


Hey guys, let's make the queue straight! I think we should move to left!
OK, move to left…hey, it's too much!
OK, move to left
OK, move to left

Classically this can be solved by **smaller learning rate**, but it also slows down the whole training…

BATCH NORMALIZATION

- The **Batch Normalization** is a method to mitigate this kind of issue.
- The key idea is to normalize the inputs of each layer, try to make it closer to a standard Gaussian (normal) distribution.
- First calculate the mean and variance of the input:

$$\mu_B = \frac{1}{m}\sum_{i=1}^{m} x_i$$

$$\sigma_B^2 = \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_B)^2$$

- Normalize the inputs using the previously calculated batch statistics:

$$\overline{x_i} = \frac{x_i - \mu_B}{\sigma_B}$$

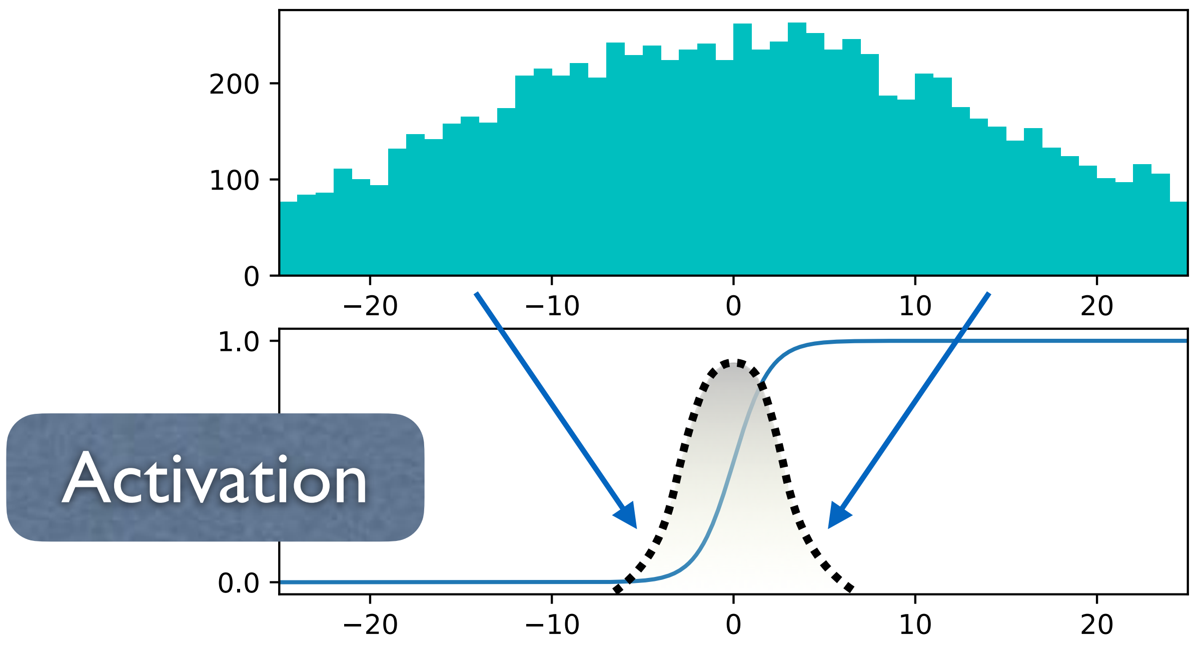
- Then shift/scale the input:

$$y_i = \gamma\overline{x_i} + \beta$$

The **γ**,**β** are trained together with other parameters of the network.

BATCH NORMALIZATION (II)

- You may already observed this should also reduce the problem of bad initial weights that we have already discussed in the previous lecture, ie.



The batch normalization can reduce the gradient vanishing problem, and internal covariate shift problem; mild improvement on the overtraining.

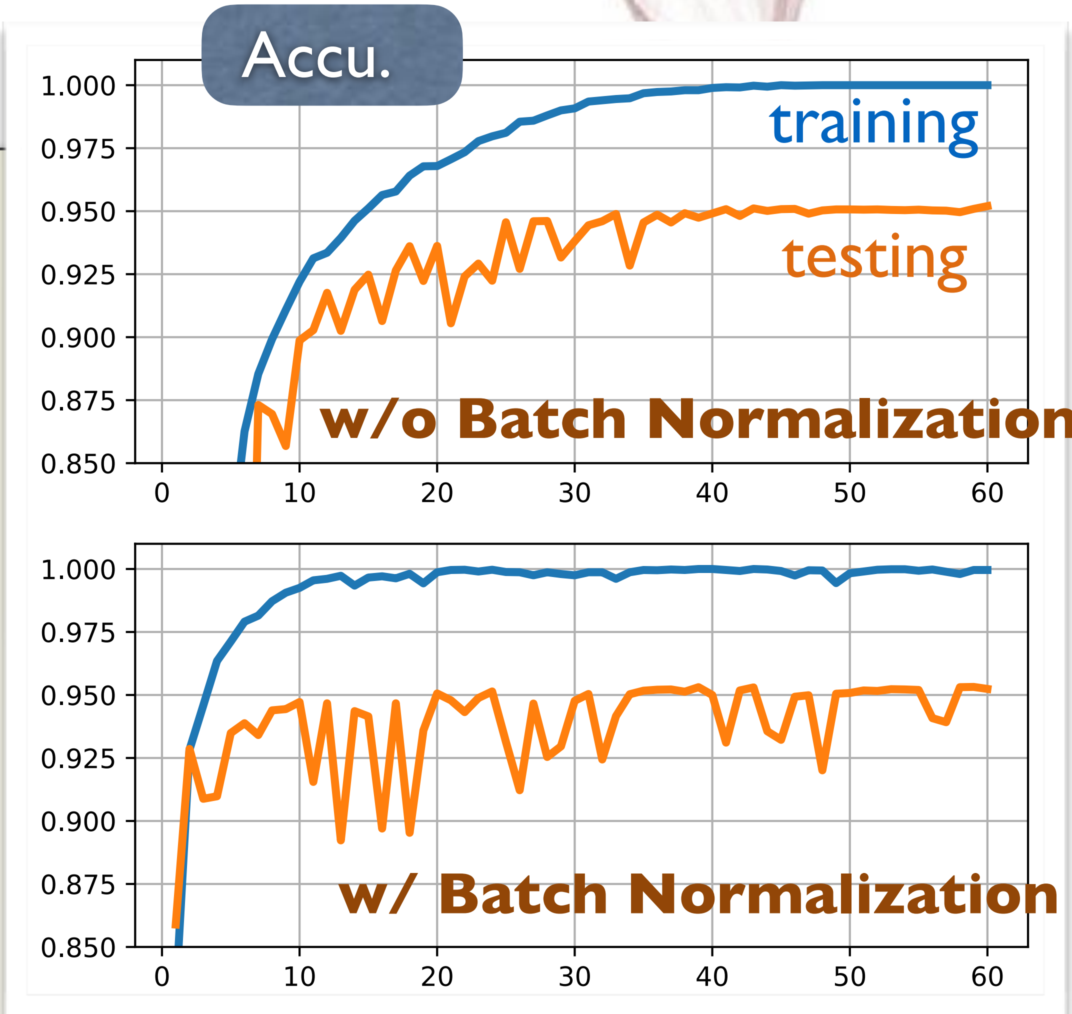
- Generally this method works for larger/deeper network with **sigmoid** or **tanh** activation. But usually it is a bad idea to mix it with dropout since dropout may interfere with the normalization calculation.

BATCH NORMALIZATION (III)

- Let's test with a larger/deeper network like 784–128–128–128–10 and with 60 epochs of training.

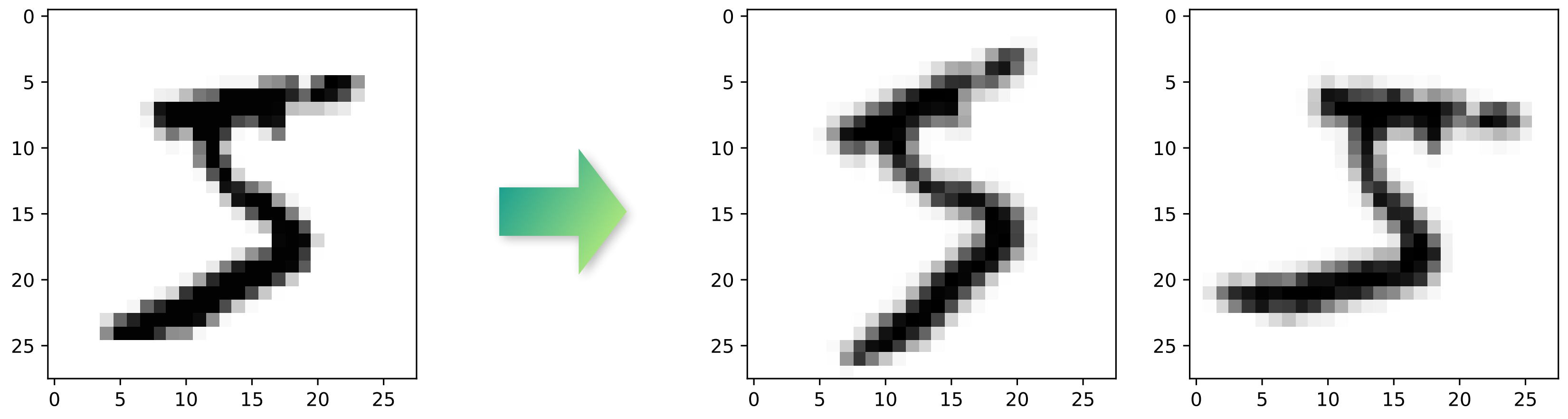
```
from keras.models import Sequential
from keras.layers import Dense, Reshape
from keras.layers import BatchNormalization
from keras.optimizers import SGD

m2 = Sequential()
m2.add(Reshape((784,), input_shape=(28,28)))
m2.add(BatchNormalization())
m2.add(Dense(128, activation='sigmoid'))
m2.add(BatchNormalization())
m2.add(Dense(128, activation='sigmoid'))
m2.add(BatchNormalization())
m2.add(Dense(128, activation='sigmoid'))
m2.add(BatchNormalization())
m2.add(Dense(10, activation='softmax'))
m2.compile(loss='categorical_crossentropy',
```

l303-example-04d.py (partial)



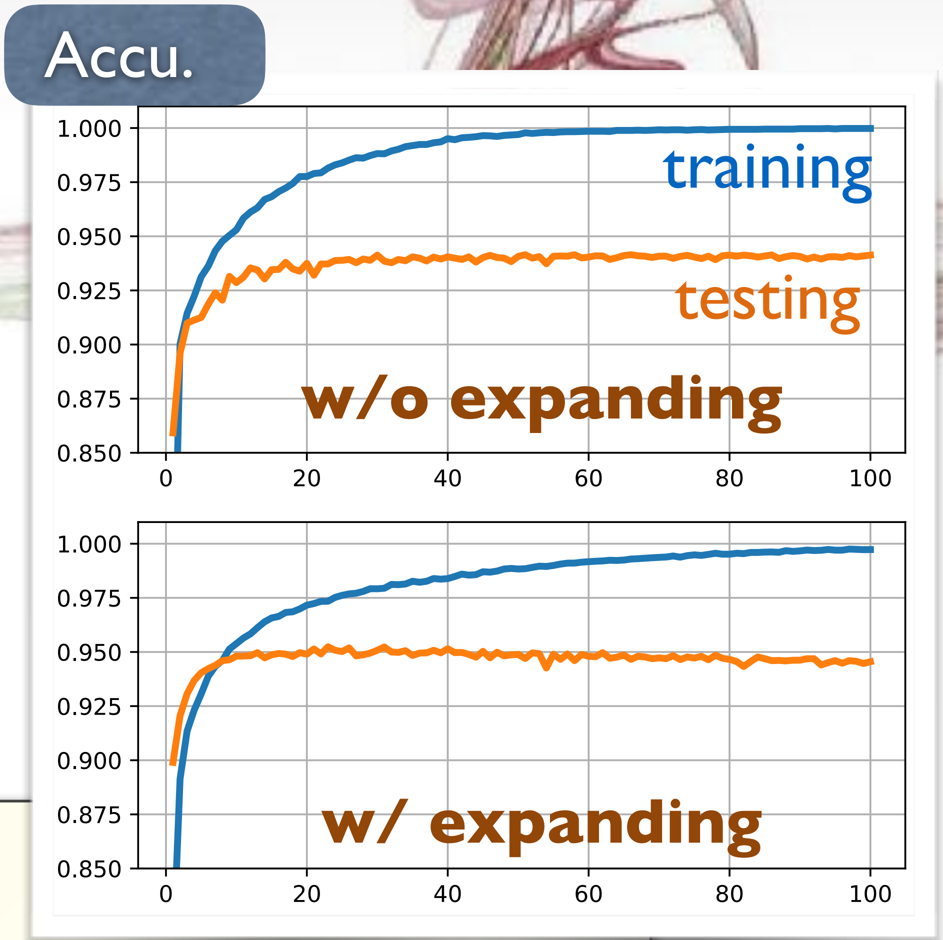
WHAT ELSE WE CAN DO?

- As we mentioned earlier, the size of training sample does matter. With a larger training sample size, the issue of overtraining can be mitigated. But if we cannot collect more data?
- A method can still be tried is **artificially increasing the training data**. This is in fact a very reasonable technique — remember in our example the training data are just images of handwriting digits. One can, slightly, twist or rotate the input images and it can be used as another training sample. This will help the network to catch the correct feature of the input images but not the small distortion nor the local noise.



ARTIFICIAL DATA EXPANDING

- Let's **triple the training data** by randomly rotate the images either +5º~+25º, or –5º~–25º. Some positive effect found!



```
. . . . . .
from skimage.transform import rotate
ext1 = np.array([rotate(img,np.random.uniform(+5.,+25.)) for
img in x_train])
ext2 = np.array([rotate(img,np.random.uniform(-25.,-5.)) for
img in x_train])
x_train_ext = np.vstack([x_train,ext1,ext2])
y_train_ext = np.vstack([y_train,y_train,y_train])
. . . . . .
rec1 = m1.fit(x_train, y_train, epochs=100,
    batch_size=120,validation_data=(x_test, y_test))
rec2 = m2.fit(x_train_ext, y_train_ext, epochs=100,
    batch_size=120,validation_data=(x_test, y_test))
. . . . . .
```

l303-example-05.py (partial)

INTERMISSION

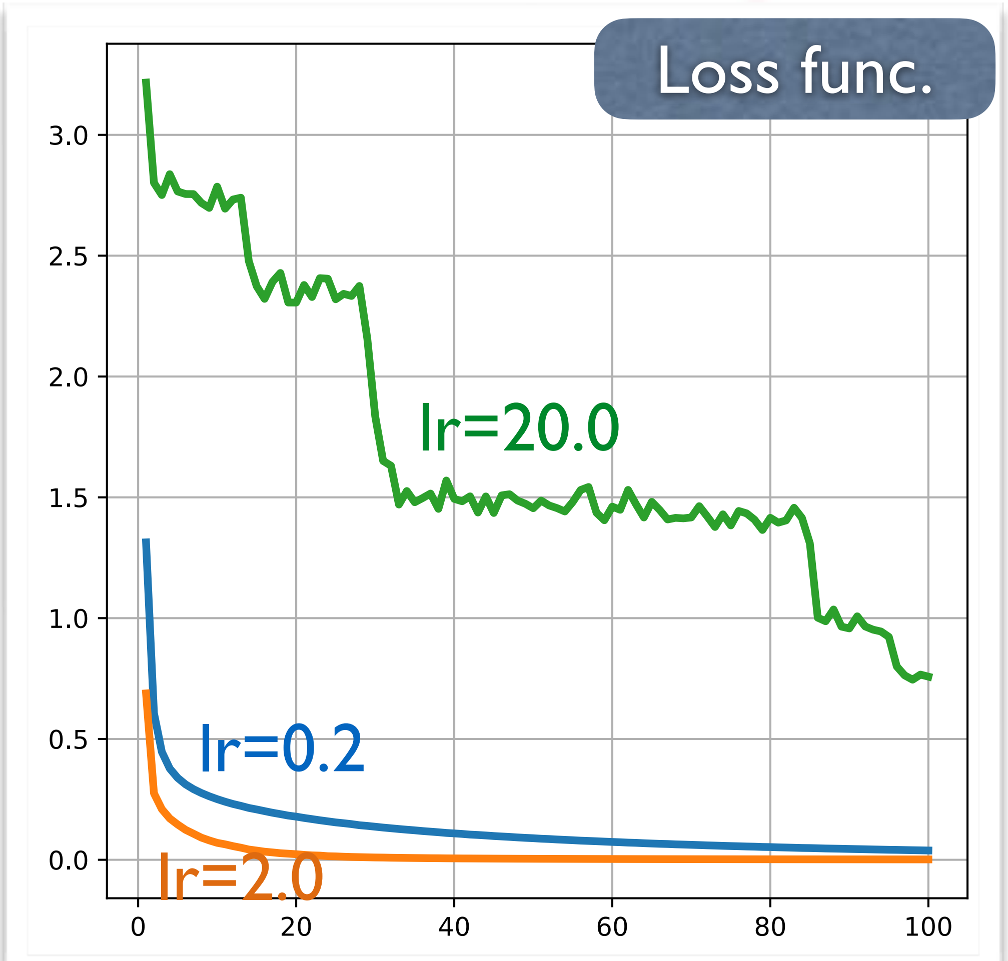
- We have introduced several methods to improve the learning speed, and touched the issue of overtraining. If port (some of) them back to the original example `l303-example-01a.py`, what's the performance you can reach by now already?
- Surely this will take a long time to run, in particular if you expand the training data size! Be aware!

CAN WE DO SOMETHING WITH THE LEARNING METHOD?

- So far we are always using standard stochastic gradient descent method with a given learning rate. Will a large/smaller learning rate helps, or can one do something else to improve the learning?
- Let's examine this by comparing the results with different learning rates:

```
. . . . . .
m1.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=0.2))

m2 = clone_model(m1)
m2.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=2.0))

m3 = clone_model(m1)
m3.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=20.))
. . . . . .
```

l303-example-06.py (partial)

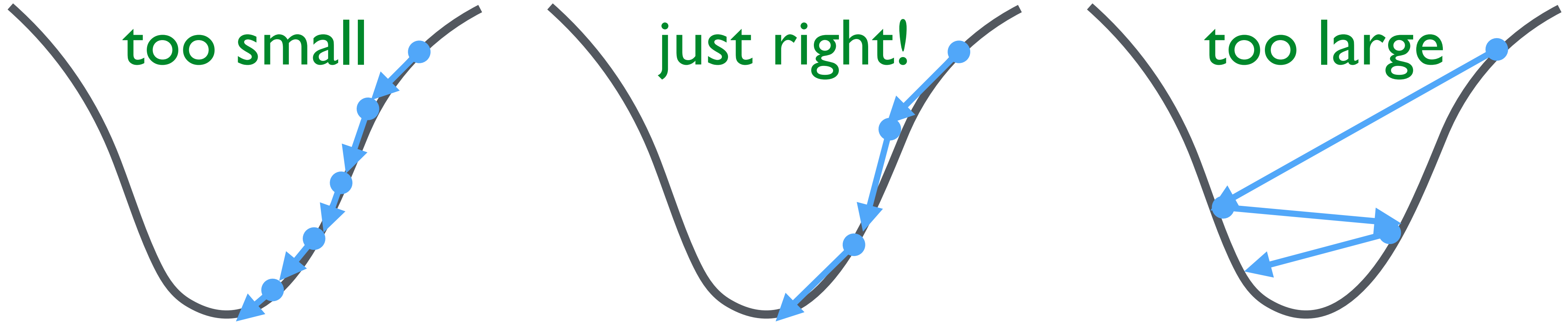


LEARNING RATE

- Come back to the definition of the learning method itself:

$$\theta \to \theta' = \theta - \eta \nabla L$$

- The learning rate basically decide how much we should move at each step. Too small learning rate will take a long time to train the network (*but you can already image for a super long run this might be better!*); too large rate will make the learning more likely a random walk.
- Sometimes it might be a good idea to **decrease the learning rate over epoch** and it might end up with a slightly better network, if the network training already saturated quickly.

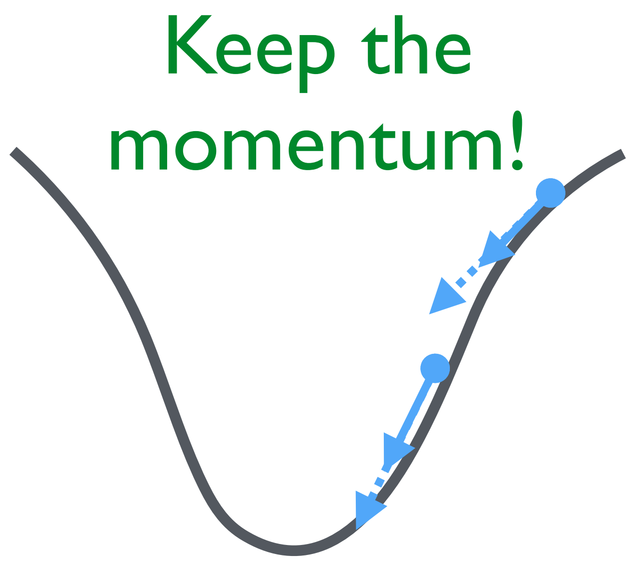


KEEP THE MOMENTUM?

- One can imagine the training with SGD is more likely to go downhill in a valley. If the current direction is good (obviously going toward lower altitude), why not to keep the **MOMENTUM** of your moving?
- This can be also an option within SGD algorithm to enable a momentum based update. It might speed up the training with a proper setup.
- Both of the options (decay of learning rate, momentum) are supported within the framework of Keras:

```
keras.optimizers.SGD(lr=0.01,
momentum=0.0, decay=0.0, nesterov=False)
```

Note: the "nesterov" option is a kind of improved momentum method!

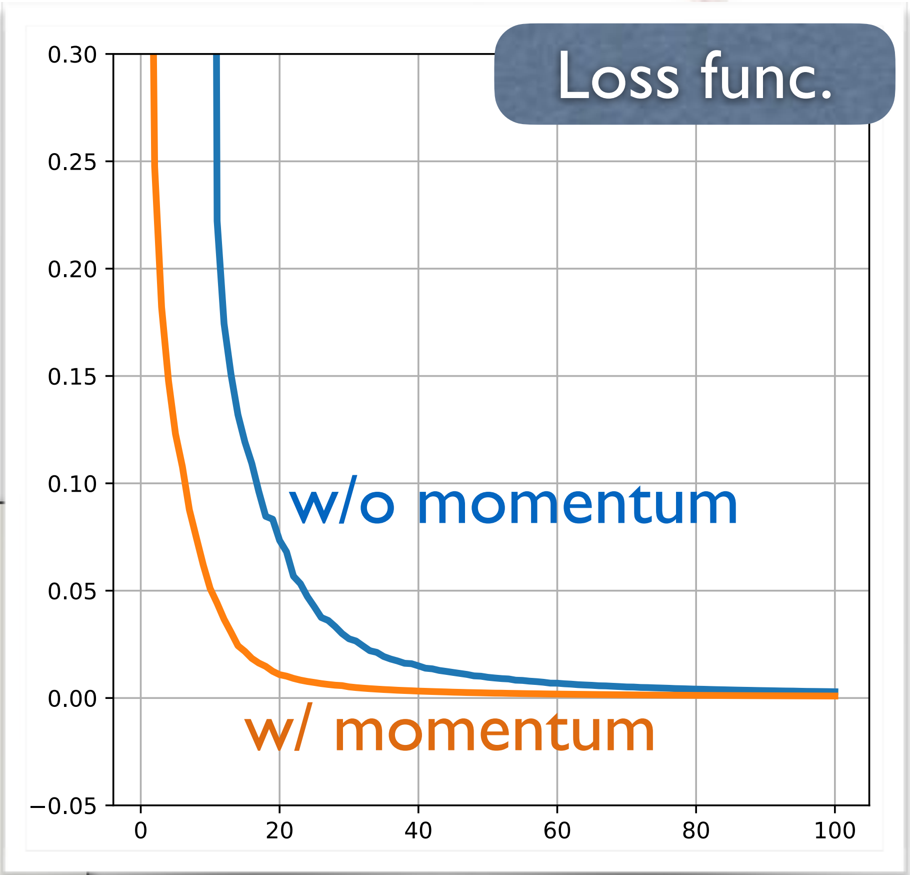


KEEP THE MOMENTUM? (II)

- Again, let's try these option(s)!
- We only tested "momentum" since it can speed up of the training, while the decay of learning rate is generally for the network fine-tune and it is hard to see the effect quickly.
- The loss function converges quicker with momentum method!

```
. . . . . .
m1.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=2.0))

m2 = clone_model(m1)
m2.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=2.0, momentum=0.4))
. . . . . .
```

l303-example-06a.py (partial)

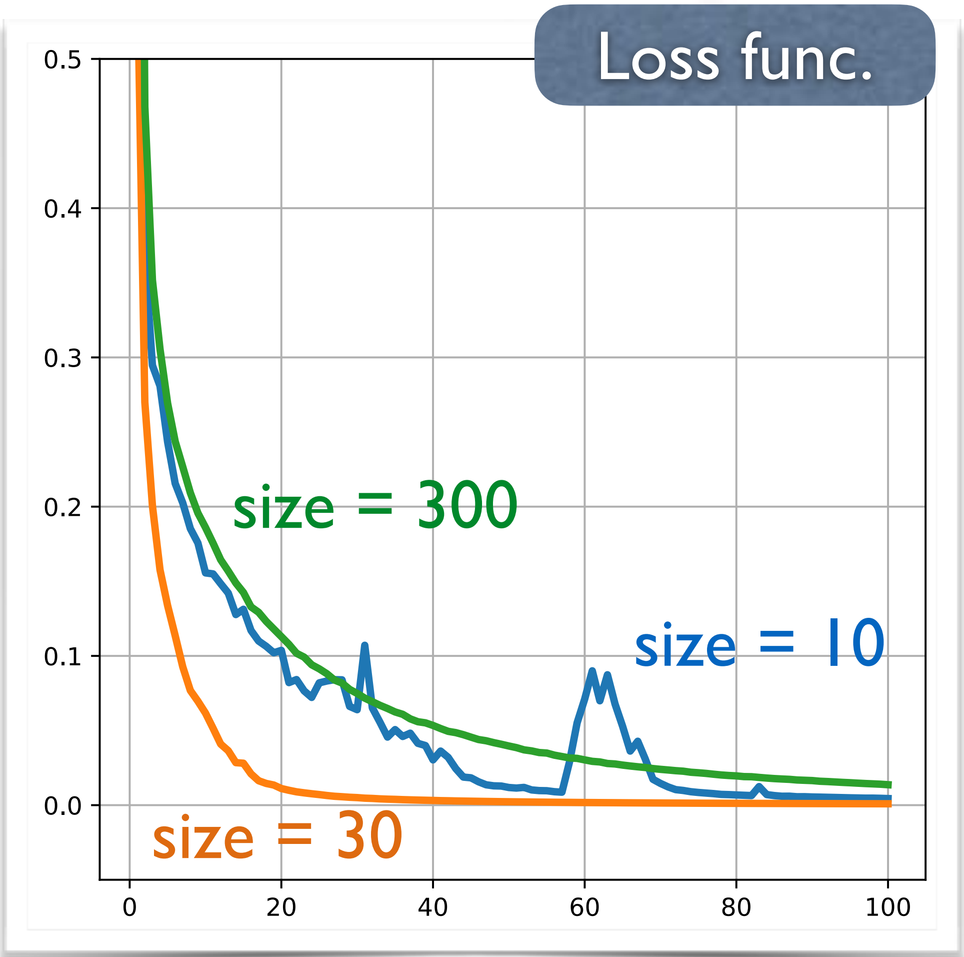


SIZE OF MINI-BATCH?

- We have not discussed the mini-batch size, but you may / can already tried to train your network with different mini-batch size!
- In principle larger mini-batch will reduce the “randomness” of the SGD algorithm and results a smoother training, but it also suffers from less frequent updates. But too small mini-batch will also make your training like a random walk.

```
. . . . . .
rec1 = m1.fit(x_train, y_train, epochs=100,
batch_size=10)
rec2 = m2.fit(x_train, y_train, epochs=100,
batch_size=30)
rec3 = m3.fit(x_train, y_train, epochs=100,
batch_size=300)
. . . . . .
```

l303-example-06b.py (partial)



DIFFERENT TRAINING ALGORITHM?

- SGD algorithm is powerful and easy to understand / implement, but there are some issues indeed:
  - Only depends on the gradient calculated by the batched data.
  - Difficult to choose a proper learning rate, and all parameters are learning with the same speed (*only a global learning rate*).
  - May run into a local minimum instead of the global one.
- This is the reason why there are many other algorithms developed to improve these points.
- Many of these SGD variations introduce an **adaptive learning rate** according to the situation of the network training.

DIFFERENT TRAINING ALGORITHM? (II)

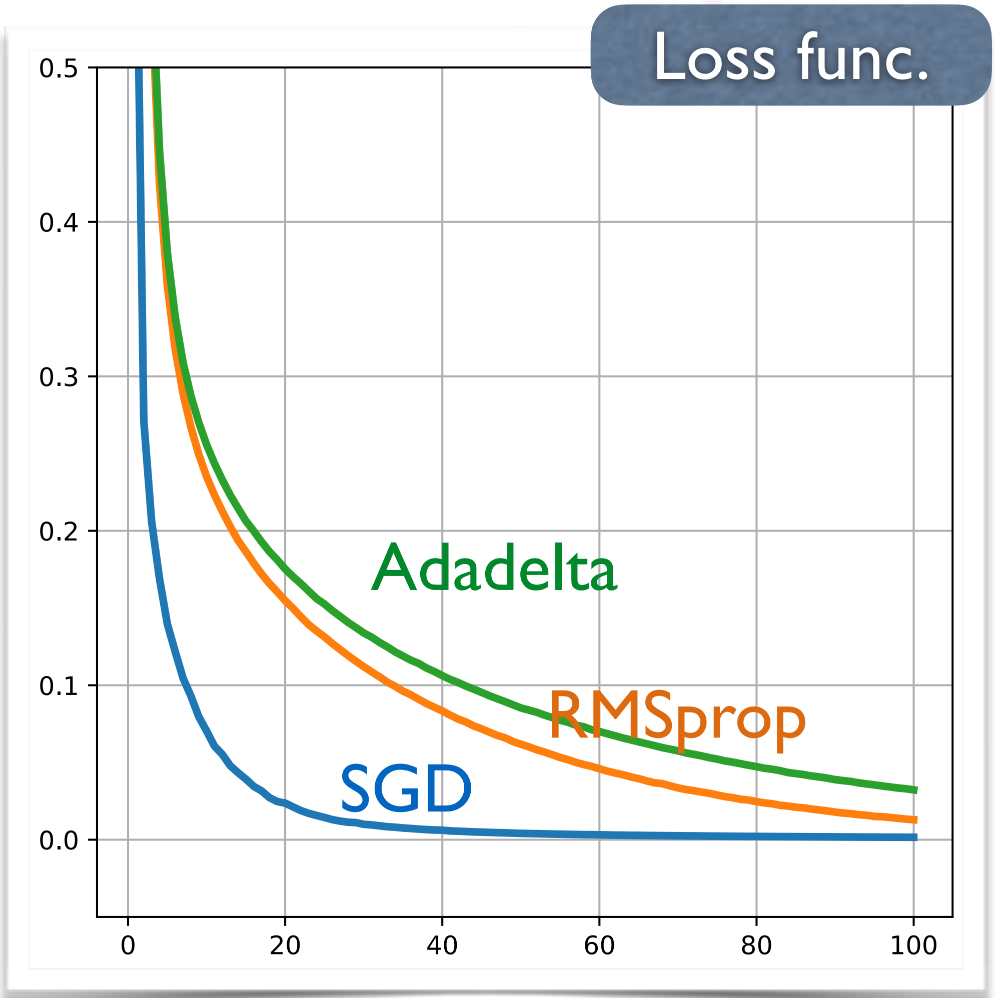
- **Adagrad**: applying regularization to the learning rate. Larger/smaller gradient would give smaller/larger learning rate.
- **Adadelta** : extended Adagrad with simplification and reduced the dependence to the global learning rate.
- **RMSprop**: a kind of variation of Adagrad and regularization with RMS of gradient. Good for large variant case.
- **Adam**: a kind of variation of RMSprop + momentum. Combining the good features of Adagrad and RMSprop.
- **Adamax**: variation of Adam, with simplified learning rate regularization formula.
- **Nadam**: Adam + Nesterov momentum.

DIFFERENT TRAINING ALGORITHM? (III)

- In general SGD is slower but very robust with good parameters.
- If you want a quicker converge with a complex network, those algorithms with adaptive learning can be better.
- *With our simple network SGD actually performs very well!*

```
. . . . . .
m1.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=2.0))

m2 = clone_model(m1)
m2.compile(loss='categorical_crossentropy',
           optimizer=RMSprop())

m3 = clone_model(m1)
m3.compile(loss='categorical_crossentropy',
           optimizer=Adadelta())
. . . . . .
```

l303-example-06c.py (partial)

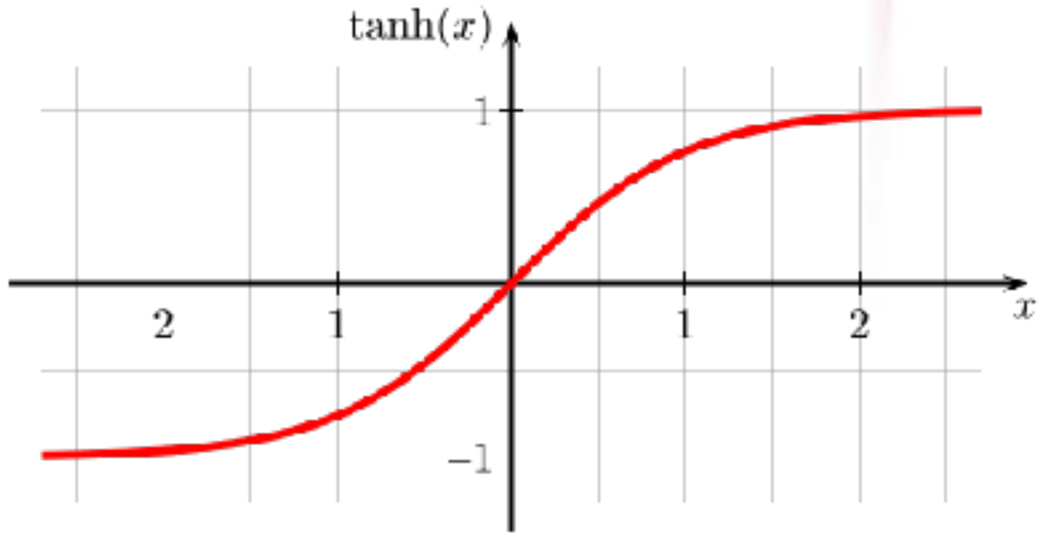


DIFFERENT ACTIVATION FUNCTION?

- Up to now we are mostly using the sigmoid function as our activation. The only exception is the output layer, where a softmax function has been introduced.
- A different choice is the **hyperbolic tangent**. It is very close to the sigmoid function but with –1 as the non-active value instead of zero:

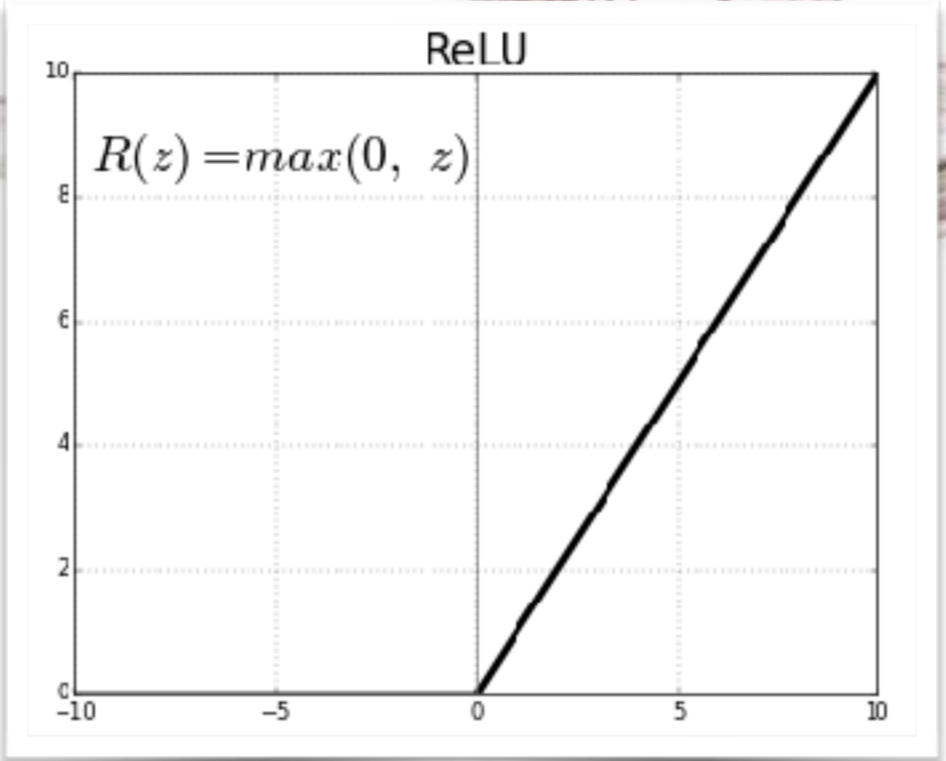
$$\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$\sigma(z) = \frac{1 + \tanh(z/2)}{2}$$



- Using hyperbolic tangent requires a slightly different scale since the out range becomes [–1, +1]. Some studies suggest tanh can have a better performance in some of the cases since it has a symmetric response.

DIFFERENT ACTIVATION FUNCTION? (II)



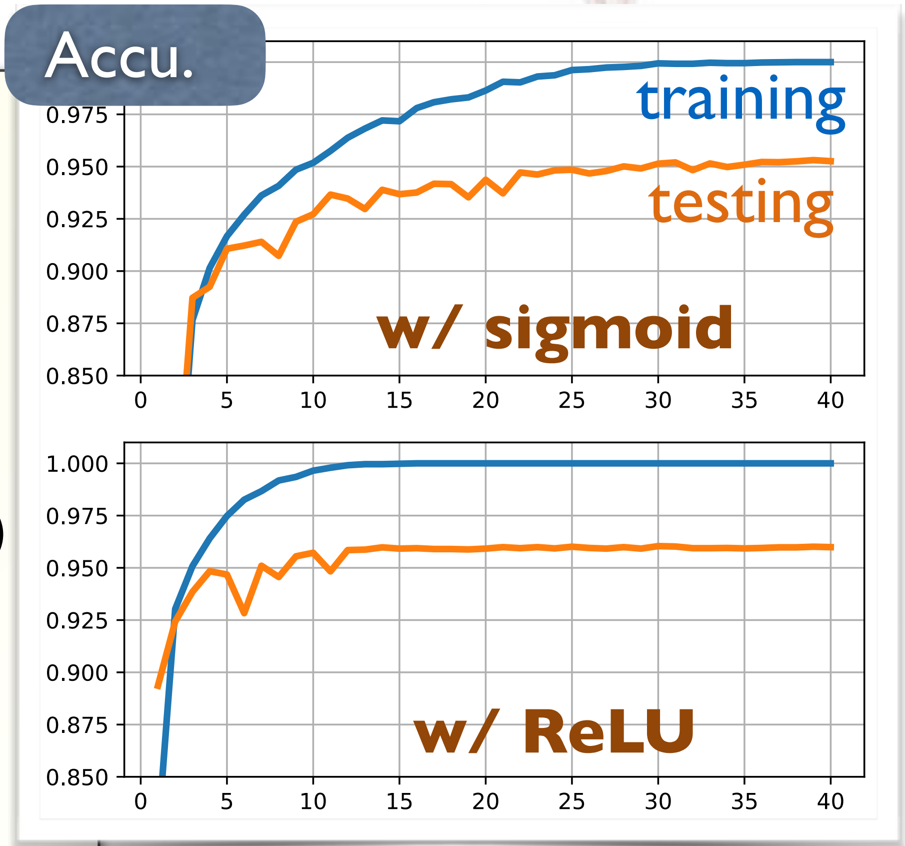
- In fact, the most common selection of activation function in modern network is the **rectified linear unit "ReLU"** (*not the sigmoid function!*), and it looks like this:
- Obviously this is very different from the sigmoid or tanh! Why this works better than the classical choices?
- One obvious feature is that the **gradient will not vanish with large input z**! This will not slow down the training speed as usually happening for the sigmoid-like functions.
- Another good feature is the ReLU function can **"switch-off" subset of the neurons** with an output zero. This can reduce the overtraining issue. *But it might be hard to "switch-on" those neurons again*.

DIFFERENT ACTIVATION FUNCTION? (III)

- Let's try to compare ReLU and sigmoid activations, but with a much larger/complicated network of **768-256-256-10** structure.
- See how good we can reach within 40 epochs of training:

```
m1 = Sequential()
m1.add(Reshape((784,), input_shape=(28,28)))
m1.add(Dense(256, activation='sigmoid'))
m1.add(Dense(256, activation='sigmoid'))
m1.add(Dense(10, activation='softmax'))
m1.compile(loss='categorical_crossentropy',
    optimizer=SGD(lr=1.0), metrics=['accuracy'])

m2 = Sequential()
m2.add(Reshape((784,), input_shape=(28,28)))
m2.add(Dense(256, activation='relu'))
m2.add(Dense(256, activation='relu'))
m2.add(Dense(10, activation='softmax'))
m2.compile(loss='categorical_crossentropy',
    optimizer=SGD(lr=0.2), metrics=['accuracy'])
```

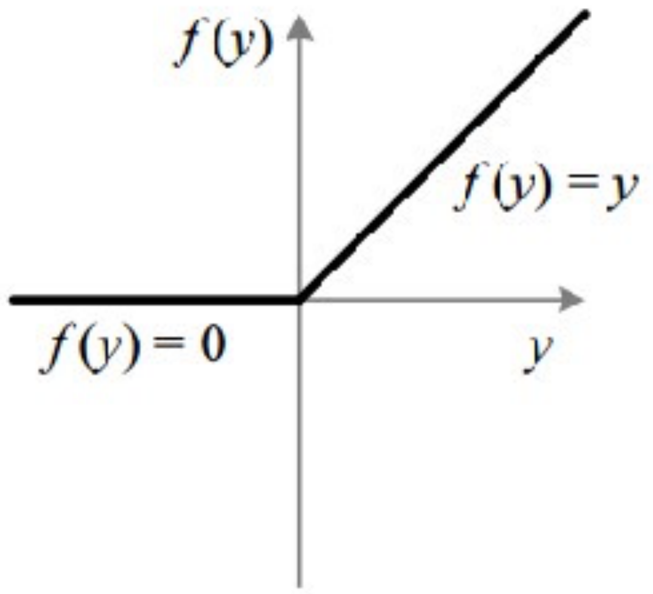
l303-example-06d.py (partial)



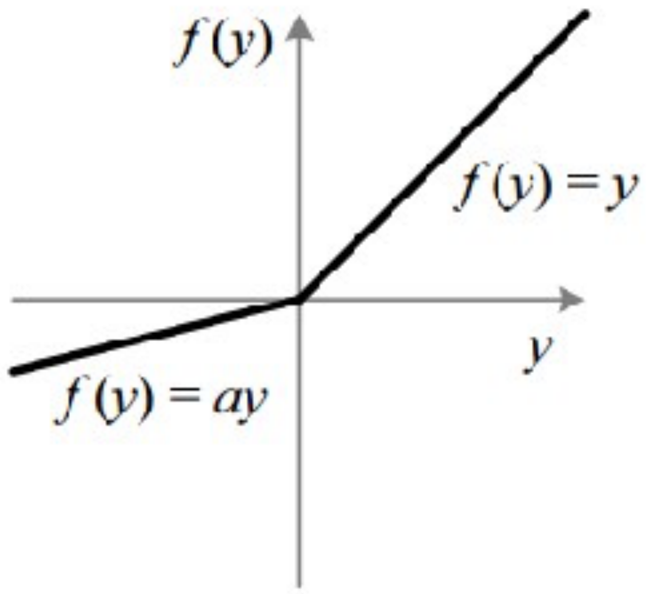
It improves!

DIFFERENT ACTIVATION FUNCTION? (IV)

- The **Leaky ReLU** or **Parametric ReLU** are variations of the ReLU function to reduce the issue of "switch-off" problem (*ie. when the input stay at the "off" region, no chance to get it back…*).



ReLU



Leaky ReLU / PReLU

Leaky ReLU treat the slope (α) as a fixed hyper parameter, while **PReLU** include it as a parameter in the training.

- There are few more variations of the ReLU functions, left for your own study!

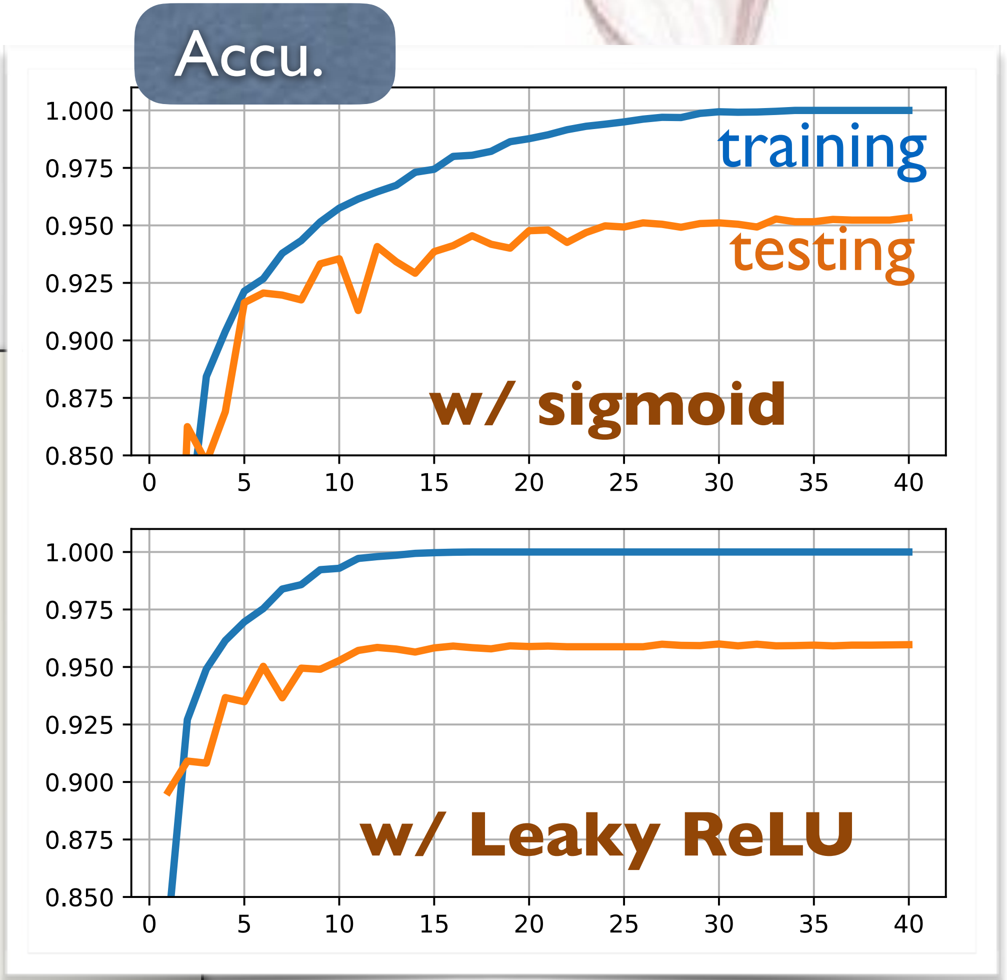
DIFFERENT ACTIVATION FUNCTION? (V)

- Let's replace the previous example of using ReLU with Leaky ReLU function, and see the resulting performance:

In Keras those advanced activation function has to be imported from layers.

```
from keras.layers import LeakyReLU
from keras.optimizers import SGD
. . . . . .
m2 = Sequential()
m2.add(Reshape((784,), input_shape=(28,28)))
m2.add(Dense(256))
m2.add(LeakyReLU(alpha=0.1))
m2.add(Dense(256))
m2.add(LeakyReLU(alpha=0.1))
m2.add(Dense(10, activation='softmax'))
m2.compile(loss='categorical_crossentropy',
           optimizer=SGD(lr=0.2),...
```

l303-example-06e.py (partial)



The results are similar to standard ReLU in this example.

LARGER/DEEPER NETWORK?

- Now finally — can we improve our network with more hidden neurons and/or more hidden layers?
- Let's integrated several improvements discussed up to now: Full training sample + ReLu activation + Adadelta optimizer + Dropout + a much larger network of **2 hidden layers of 512 neurons**:

```
. . . . . . .
model = Sequential()
model.add(Reshape((28*28,), input_shape=(28,28)))
model.add(Dense(512, activation='relu'))
model.add(Dropout(0.2))
model.add(Dense(512, activation='relu'))
model.add(Dropout(0.2))
model.add(Dense(10, activation='softmax'))

model.compile(loss='categorical_crossentropy',
              optimizer=Adadelta(), metrics=['accuracy'])

model.fit(x_train, y_train, epochs=20, batch_size=128)
. . . . . . .
```

l303-example-07.py (partial)

This network has **669,706** parameters to be tuned.

LARGER/DEEPER NETWORK? (II)

- We can have a great performance of 98.5% accuracy which matches to our performance from SVM with Gaussian kernel!

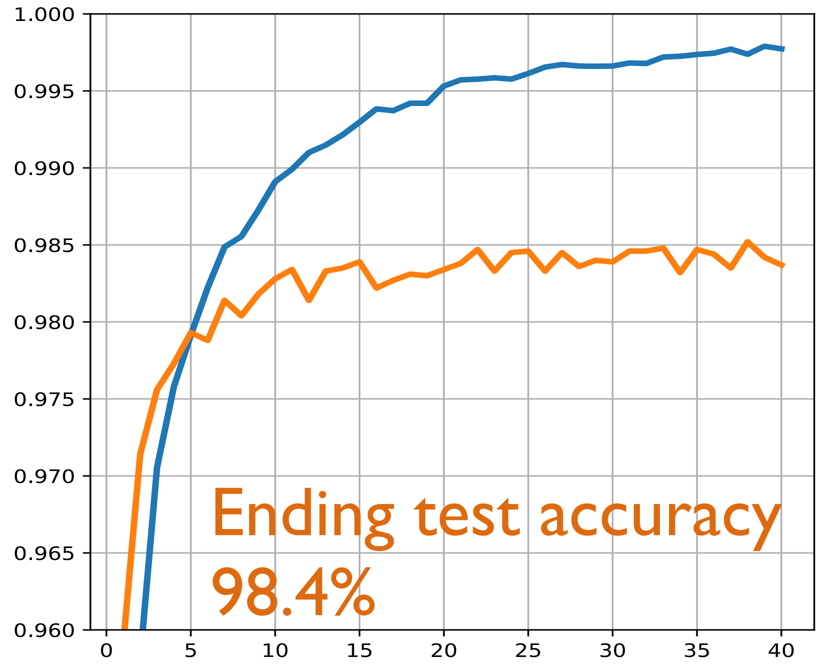
```
. . . . . .
Epoch 20/20
60000/60000 [===========] - 5s 91us/step - loss: 0.0065 - acc: 0.9979
Performance (training)
Loss: 0.00114, Acc: 0.99987
Performance (testing)
Loss: 0.06721, Acc: 0.98490
```

- **Can we do *even better* with a deeper network?** e.g. adding a couple of big layers or many smaller layers?
- In fact it is not so obvious. A larger network will definitely have much more parameters to be optimized and have a stronger capability to describe the data, but it is definitely much more difficult to train. In particular, **a deeper network will be even harder**.

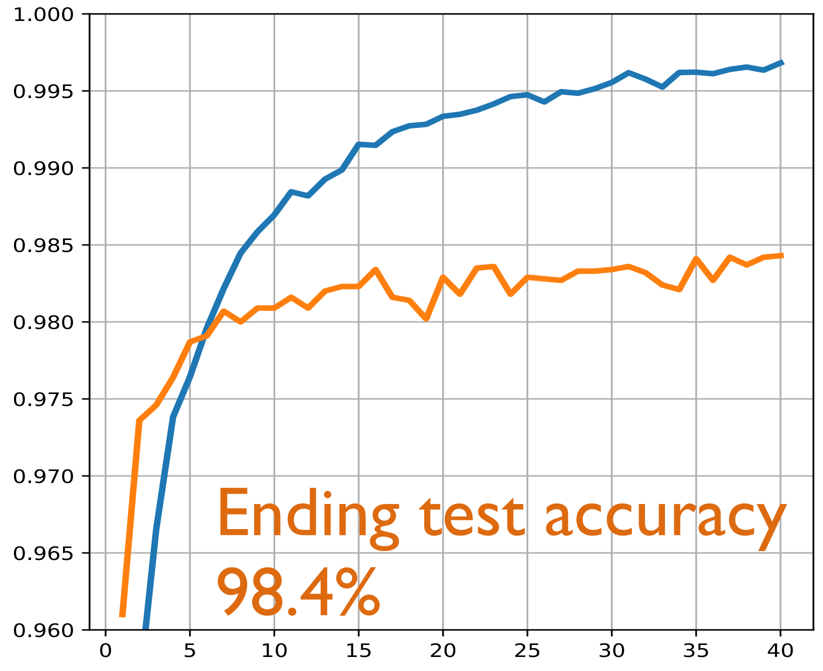
LARGER/DEEPER NETWORK? (III)

- Let's try several different network models and see if we can have interesting findings?

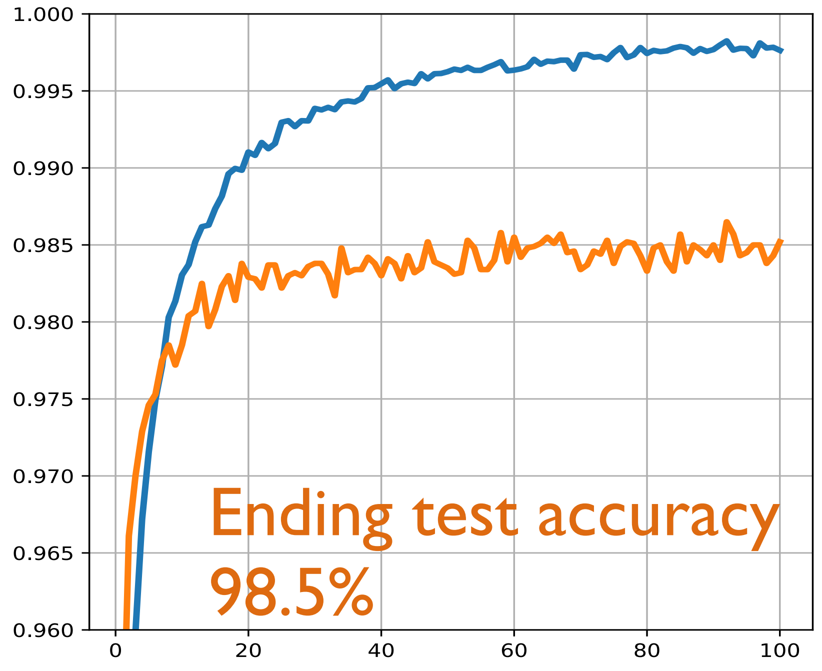
784-(256x2)-10
train for 40 epochs



784-(256x4)-10
train for 40 epochs



784-(256x8)-10
train for 100 epochs

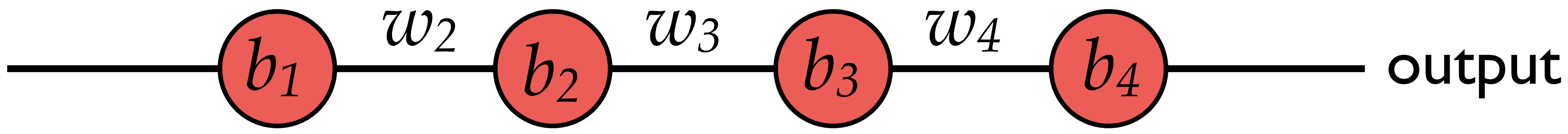


A more complex network does require a longer training time.
Why it is difficult to train a deeper network?

WHY IT IS DIFFICULT TO TRAIN A DEEP NETWORK?

- Surely a deeper network does contain much more weights/bias to be tuned. But this is not the only reason — **vanishing gradients with a deeper network**. Small gradients = slow learning.
- Let's consider a chain of neurons and calculate the gradient according to back propagation:

$$\frac{\partial L}{\partial b_4} = \sigma'(z_4) \cdot \frac{\partial L}{\partial y}$$



$$\frac{\partial L}{\partial b_1} = \sigma'(z_1) \cdot w_2 \cdot \sigma'(z_2) \cdot w_3 \cdot \sigma'(z_3) \cdot w_4 \cdot \sigma'(z_4) \cdot \frac{\partial L}{\partial y}$$

Generally the weights are small (<1) after training, and σ'(z) is less then 0.25 by definition, if the sigmoid function is used. This will enforce $\frac{\partial L}{\partial b_1} < 0.0156 \frac{\partial L}{\partial b_4}$

The updating on b1 will be much slower than b4.

WHY IT IS DIFFICULT TO TRAIN A DEEP NETWORK? (II)

- And this is not the full story. The small $\sigma'(z)$ is not a problem for ReLU activation. However, if we have large weights, say >> 1, the gradient will become very large when network goes deeper. Then we are going to have an **exploding gradient problem** instead.
- The intrinsic problem is that the **gradients are unstable with deeper network**, given they are evaluated with a production of many layers of weights and derivatives.
- In fact such unstable gradient problem is a complex issue and depending one many other factor (and hyperparameters) as well. Although it sounds difficult to get a decent deep network trained, but one can, still get a better performing deep network, **with a different network structure**.

HANDS-ON SESSION

- **Practice 01:**
  - Trial #1:
    In the `l303-example-04a.py` we have tried a L2 regularization method to reduce the overtraining issue. What will be the situation if we switched to L1 regularization?

HANDS-ON SESSION

- **Practice 02:**
  Up to now we are always using the same testing sample to measure the performance. But what will happen if we rotate our testing data and see how good we can still separate the handwriting digits?
- You can take one of the ending example, e.g. `l303-example-08.py` or `l303-example-08a.py`, train your network, but in the end use the rotated test sample to see the performance. The method/code to rotate your images can be found in `l303-example-05.py`.

```
Performance (training):
Loss: 0.xxxx, Acc: 0.yyyy
Performance (testing):
Loss: 0.xxxx, Acc: 0.yyyy
```