NFM模型理论与实践

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一、理论部分

今天介绍一下NFM模型,NFM模型是FM模型的神经网络化尝试:即将FM的二阶交叉项作为 Deep模型的输入,以此加强模型的表达能力。

1. NFM数学表达式

经典的FM模型的数学表达式如公式 (1) 所示:

在数学形式上,NFM模型的主要思路是用一个表达能力更强的函数替代原FM中二阶隐向量内积部分。NFM的表达式如公式(2)所示:

$$\begin{split} \hat{y}_{NFM}(x) &= w_0 + \sum_{i=1}^n w_i x_i + deep\left(f(x)\right) \\ &= w_0 + \sum_{i=1}^n w_i x_i + deep\left(f_{BI}(V_x)\right) \\ &= w_0 + \sum_{i=1}^n w_i x_i + deep\left(\sum_{i=1}^n \sum_{j=i+1}^n (x_i v_i) \odot (x_j v_j)\right) \\ &= w_0 + \sum_{i=1}^n w_i x_i + deep\left(\frac{1}{2} \left[\left(\sum_{x=1}^n v_i x_i\right)^2 - \sum_{i=1}^n (x_i v_i)^2\right]\right) \end{split}$$

公式 (2)

2. NFM深度网络部分结构图

NFM模型的深度网络部分结构图如图(1)所示。

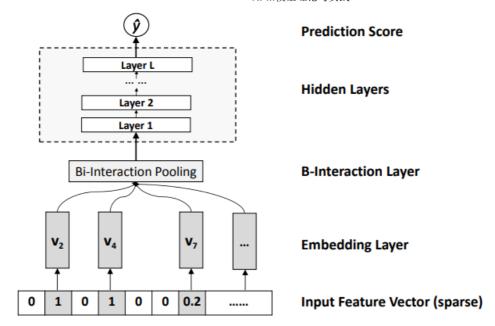


Figure 2: Neural Factorization Machines model (the first-order linear regression part is not shown for clarity).

图 (1) NFM模型的深度网络部分结构图

(2.1) 输入层、Embedding层、BI层

NFM网络架构的特点非常明显,就是在Embedding层和MLP隐层之间加入特征交叉池化层 (Bi-Interaction Pooling Layer)。假设是所有特征域的Embedding集合,特征交叉池化层的具体操作如公式(3)所示。

$$f_{BI}(V_x) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} (x_i v_i) \odot (x_j v_j)$$

(公式 3)

在进行两两 **K维** Embedding向量的元素积操作后,对交叉特征向量求和,得到池化层的 **K** 维输出向量。再把该向量输入到上层的MLP全连接神经网络中,进行下一步的交叉。

(2.2) MLP全连接层

MLP隐层部分就是常规的nn全连接,结构如下所示:

$$\mathbf{z}_1 = \sigma_1(\mathbf{W}_1 f_{BI}(\mathcal{V}_X) + \mathbf{b}_1),$$

$$\mathbf{z}_2 = \sigma_2(\mathbf{W}_2 \mathbf{z}_1 + \mathbf{b}_2),$$
.....
$$\mathbf{z}_L = \sigma_L(\mathbf{W}_L \mathbf{z}_{L-1} + \mathbf{b}_L),$$

其中: W_l , b_l 分别表示参数矩阵与偏置向量; σ_l 表示激活函数,可以取 sigmoid, tanh, relu等。

(2.3) 预测层

最后一层隐藏层加上一个线性变换,作为结果输出,即: $f^{(x)}=h^Tz_L$ 。向量 h 是输出层的权重值。

3. NFM模型的学习过程

由以上分析可知,公式(2)可以写为公式(4)

$$\hat{y}_{NFM}(x) = w_0 + \sum_{i=1}^n w_i x_i + h^T \sigma_L \left(W_L(...\sigma_1(W_1 f_{BI}(V_X) + b_1)...) + b_L \right)$$

采用SGD方式链式法则求解,此处只给出Bi-interaction层的求导,其他的都是常规的nn的求导。

$$rac{df_{BI}(V_x)}{d_{v_i}} = (\sum_{j=1}^n x_j ec{v}_j) x_i - x_i^2 ec{v}_i = \sum_{j=1, j
eq i}^n x_i x_j ec{v}_j$$

实践中一般采用mini-batch的方式,采用Adagrad做优化。

4. 防止过拟合措施

防止模型的过拟合风险,采用以下两种手段提高模型的泛化能力。

(4.1) dropout

将dropout技术用在Bi-interaction层,即:获取 $f_{BI}(V_x)$ (**K维**向量)之后,随机drop掉o百分 比的latent factors,这相当于是对于FM的一种新的正则约束形式。同时在隐层也可以应用 dropout技术。

(4.2) Batch Normalization

$$BN(ec{x}_i) = \gamma \odot (rac{ec{x}_i - \mu_B}{\sigma_B}) + eta$$
中的堂规操作:

NN中的常规操作:

其中: μ B 是该mini-batch的均值, σ B 是mini-batch的方差, γ 和 β 是可以训练的参数, 用来控制normalization的缩放和平移。对于NFM,对Bi-interaction层的输出也进行BN操 作。

二、实践环节

1. 首先来看看特征交叉池化层 (Bi-Interaction Pooling Layer) 的实现

```
# Bi-Interaction Pooling Layer
from tensorflow.python.keras import backend as K
import tensorflow as tf
a = \lceil
               [[3., 0., 1., 0.],
                 [1., 2., 3., 4.],
                 [4., 5., 6., 1.]
       7
concated embeds value = tf.convert to tensor(a)
square of sum = tf.square(tf.reduce sum(concated embeds value, axis=1, keepdims=True))
sum of square = tf.reduce sum(concated embeds value * concated embeds value, axis=1, keep
cross term = 0.5 * (square of sum - sum of square)
sess = tf. InteractiveSession()
square of sum = sess.run(square of sum)
print(square of sum)
# [[ 64. 49. 100. 25. ]]]
```

```
sess = tf.InteractiveSession()
sum_of_square = sess.run(sum_of_square)
print(sum_of_square)

# [[[26. 29. 46. 17.]]]

sess = tf.InteractiveSession()
cross_term = sess.run(cross_term)
print(cross_term)

# [[[19. 10. 27. 4.]]]
```

2. 从实际例子应用一下NFM模型

(2.1) 准备数据

titanic数据集 的目标是根据乘客信息预测他们在Titanic号撞击冰山沉没后能否生存。结构化数据一般会使用Pandas中的DataFrame进行预处理。

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split

df_data = pd.read_csv('data/train.csv')
```

titanic数据集下载地址: https://www.kaggle.com/c/titanic/data

字段说明:

```
• Survived: 0代表死亡, 1代表存活
                                 【y标签】
• Pclass: 乘客所持票类,有三种值(1,2,3)
                                 【类别变量】
• Name: 乘客姓名
                                 【舍去】

    Sex: 乘客性别

                                 【类别变量】
• Age: 乘客年龄(有缺失)
                                 【数值特征】
• SibSp: 乘客兄弟姐妹/配偶的个数(整数值)
                                 【数值特征】
• Parch: 乘客父母/孩子的个数(整数值)
                                 【数值特征】
• Ticket: 票号(字符串)
                                 <del>【舍去】</del>

    Fare: 乘客所持票的价格(浮点数, 0-500不等) 【数值特征】

• Cabin: 乘客所在船舱(有缺失)
                                 【类别变量】
• Embarked: 乘客登船港口:S、C、Q(有缺失) 【类别变量】
```

```
# 类别变量重新编码
#数值变量,用0填充缺失值
sparse_feature_list = ["Pclass", "Sex", "Cabin", "Embarked"]
dense_feature_list = ["Age", "SibSp", "Parch", "Fare"]
sparse_feature_reindex_dict = {}
for i in sparse feature list:
       cur_sparse_feature_list = df_data[i].unique()
       sparse_feature_reindex_dict[i] = dict(zip(cur_sparse_feature_list, \)
               range(1, len(cur_sparse_feature_list)+1)
                                                                      )
                                                              )
       df data[i] = df data[i].map(sparse feature reindex dict[i])
for j in dense_feature_list:
       df data[j] = df data[j].fillna(0)
# 分割数据集
data = df_data[sparse_feature_list + dense_feature_list]
label = df data["Survived"].values
xtrain, xtest, ytrain, ytest = train_test_split(data, label, test_size=0.2, random_state=
```

```
xtrain data = {"Pclass": np.array(xtrain["Pclass"]), \
                            "Sex": np.array(xtrain["Sex"]), \
                           "Cabin": np. array(xtrain["Cabin"]), \
                           "Embarked": np.array(xtrain["Embarked"]), \
                           "Age": np.array(xtrain["Age"]), \
                           "SibSp": np.array(xtrain["SibSp"]), \
                           "Parch": np. array(xtrain["Parch"]), \
                            "Fare": np. array(xtrain["Fare"])}
xtest data = {"Pclass": np.array(xtest["Pclass"]), \
                            "Sex": np. array(xtest["Sex"]), \
                            "Cabin": np.array(xtest["Cabin"]), \
                           "Embarked": np.array(xtest["Embarked"]), \
                           "Age": np. array(xtest["Age"]), \
                           "SibSp": np. array(xtest["SibSp"]), \
                           "Parch": np. array(xtest["Parch"]), \
                           "Fare": np. array(xtest["Fare"])}
```

(2.2) 构建模型

(2.2.1) 加载python模块

(2.2.2) 定义类别变量的输入层、Embedding层

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```
input_layer = Input(shape=[shape, ], name=name)
embedding_layer = Embedding(vocabulary_size, embedding_dim)(input_layer)
return input_layer, embedding_layer
```

(2.2.3) 定义 线性层、Bi-Interaction层、DNN层、预测层

```
class Linear (Layer):
       def init (self, 12 reg=0.0, mode=2, use bias=True, **kwargs):
               self.12\_reg = 12\_reg
               if mode not in [0, 1, 2]:
                       raise ValueError("mode must be 0, 1 or 2")
               self.mode = mode
               self.use bias = use bias
               super(Linear, self). __init__(**kwargs)
       def build(self, input_shape):
               if self.use bias:
                       self.bias = self.add weight (name='linear bias',
                                                                              shape=(1,),
                                                                              initializer=
                                                                              trainable=Ti
               if self.mode == 1:
                       self.kernel = self.add weight(
                               'linear kernel',
                               shape=[int(input shape[-1]), 1],
                               initializer=tf.keras.initializers.glorot normal(),
                               regularizer=tf.keras.regularizers.12(self.12_reg),
                               trainable=True)
               elif self. mode == 2:
                       self.kernel = self.add weight(
                               'linear kernel',
                               shape=[int(input shape[1][-1]), 1],
                               initializer=tf.keras.initializers.glorot_normal(),
                               regularizer=tf.keras.regularizers.12(self.12 reg),
                               trainable=True)
               super(Linear, self).build(input shape)
       def call(self, inputs, **kwargs):
```

```
if self.mode == 0:
                       sparse input = inputs
                       linear_logit = reduce_sum(sparse_input, axis=-1, keep_dims=True)
               elif self. mode == 1:
                       dense input = inputs
                       fc = tf. tensordot(dense_input, self.kernel, axes=(-1, 0))
                       linear logit = fc
               else:
                       sparse_input, dense_input = inputs
                       fc = tf. tensordot(dense input, self. kernel, axes=(-1, 0))
                       linear_logit = tf.reduce_sum(sparse_input, axis=-1, keep_dims=Fals
               if self.use bias:
                       linear_logit += self.bias
               return linear_logit
       def compute output shape (self, input shape):
               return (None, 1)
       def compute_mask(self, inputs, mask):
               return None
       def get config(self, ):
               config = {'mode': self.mode, '12 reg': self.12 reg, 'use bias':self.use bi
               base_config = super(Linear, self).get_config()
               return dict(list(base_config.items()) + list(config.items()))
class BiInteractionPooling(Layer):
        """Bi-Interaction Layer used in Neural FM, compress the
         pairwise element-wise product of features into one single vector.
           Input shape
               - A 3D tensor with shape: `(batch size, field size, embedding size)`.
           Output shape
               - 3D tensor with shape: ``(batch size, 1, embedding size)``.
           References
               - [He X, Chua T S. Neural factorization machines for sparse predictive an
       def init (self, **kwargs):
               super(BiInteractionPooling, self). init (**kwargs)
       def build(self, input_shape):
               if len(input shape) != 3:
                       raise ValueError(
```

def call(self, inputs, **kwargs):

if K.ndim(inputs) != 3:

super(BiInteractionPooling, self).build(input shape)

"Unexpected inputs dimensions %d, expect to be 3 dimension

```
raise ValueError(
                               "Unexpected inputs dimensions %d, expect to be 3 dimension
               concated embeds value = inputs
               square_of_sum = tf.square(tf.reduce_sum(concated_embeds_value, axis=1, ke
               sum of square = tf.reduce sum(concated embeds value * concated embeds val
               cross_term = 0.5 * (square_of_sum - sum_of_square)
               return cross_term
       def compute output shape (self, input shape):
               return (None, 1, input_shape[-1])
class DNN(Laver):
        """The Multi Layer Percetron
           Input shape
               - nD tensor with shape: ``(batch_size, ..., input_dim)``. The most common
           Output shape
               - nD tensor with shape: ``(batch size, ..., hidden size[-1])``. For insta
           Arguments
               - **hidden units**:list of positive integer, the layer number and units i
               - **activation**: Activation function to use.
               - **12 reg**: float between 0 and 1. L2 regularizer strength applied to t
               - **dropout rate**: float in [0,1). Fraction of the units to dropout.
               - **use bn**: bool. Whether use BatchNormalization before activation or n
               - **seed**: A Python integer to use as random seed.
        11 11 11
       def __init__(self, hidden_units, activation='relu', 12_reg=0, dropout_rate=0, us
               self.hidden units = hidden units
               self.activation = activation
               self.dropout rate = dropout rate
               self.seed = seed
               self. 12 reg = 12 reg
               self.use bn = use bn
               super(DNN, self). __init__(**kwargs)
       def build(self, input shape):
```

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```
# if len(self.hidden units) == 0:
        # raise ValueError("hidden units is empty")
        input size = input shape[-1]
       hidden units = [int(input size)] + list(self.hidden units)
       self.kernels = [self.add weight(name='kernel' + str(i),
                                                                      shape=(hidde
                                                                      initializer:
                                                                      regularizer
                                                                      trainable=T1
       self.bias = [self.add weight(name='bias' + str(i),
                                                                shape=(self.hidde
                                                                initializer=Zeros
                                                                trainable=True) f
       if self.use bn:
               self.bn_layers = [tf.keras.layers.BatchNormalization() for _ in
       self.dropout layers = [tf.keras.layers.Dropout(self.dropout rate, seed=se
                                                    range (len (self. hidden units))
       self.activation layers = [tf.keras.layers.Activation(self.activation) \
                                                          for _ in range(len(se
       super(DNN, self).build(input_shape)
def call(self, inputs, training=None, **kwargs):
       deep_input = inputs
       for i in range (len (self. hidden units)):
               fc = tf. nn. bias add(tf. tensordot(
                       deep input, self.kernels[i], axes=(-1, 0)), self.bias[i])
               # fc = Dense(self.hidden_size[i], activation=None,
               # kernel_initializer=glorot_normal(seed=self.seed),
               # kernel regularizer=12(self.12 reg)) (deep input)
               if self.use bn:
                       fc = self.bn layers[i](fc, training=training)
               fc = self.activation layers[i](fc)
               fc = self.dropout layers[i](fc, training=training)
               deep input = fc
       return deep input
def compute output shape (self, input shape):
```

```
if len(self.hidden units) > 0:
                       shape = input_shape[:-1] + (self.hidden_units[-1],)
               else:
                       shape = input shape
               return tuple (shape)
       def get_config(self, ):
               config = {'activation': self.activation, 'hidden_units': self.hidden_unit
                                  '12 reg': self.12 reg, 'use bn': self.use bn, 'dropout
               base_config = super(DNN, self).get_config()
               return dict(list(base_config.items()) + list(config.items()))
class PredictionLayer(Layer):
           Arguments
                 - **task**: str, ``"binary"`` for binary logloss or ``"regression"`` fo
                 - **use bias**: bool. Whether add bias term or not.
        11 11 11
       def init (self, task='binary', use bias=True, **kwargs):
               if task not in ["binary", "multiclass", "regression"]:
                       raise ValueError("task must be binary, multiclass or regression")
               self.task = task
               self.use bias = use bias
               super(PredictionLayer, self). init (**kwargs)
       def build(self, input shape):
               if self.use bias:
                       self.global bias = self.add weight(
                               shape=(1,), initializer=Zeros(), name="global bias")
               super(PredictionLayer, self).build(input shape)
       def call(self, inputs, **kwargs):
               x = inputs
               if self.use bias:
                       x = tf.nn.bias add(x, self.global bias, data format='NHWC')
               if self.task == "binary":
                       x = tf. sigmoid(x)
               output = tf. reshape(x, (-1, 1))
```

```
def compute_output_shape(self, input_shape):
    return (None, 1)

def get_config(self, ):
    config = {'task': self.task, 'use_bias': self.use_bias}
    base_config = super(PredictionLayer, self).get_config()
    return dict(list(base_config.items()) + list(config.items()))
```

(2.2.4) 定义NFM模型结构

return output

```
def nfm(sparse_feature_list, \
                sparse_feature_reindex_dict, \
                dense_feature_list, \
                dnn_hidden_units=(128, 128), \
                12 reg embedding=1e-5, \
                12_reg_linear=1e-5, \
                12 reg dnn=0, \
                init_std=0.0001, \
                seed=1024, \
                bi dropout=0.2,
                dnn_dropout=0.2, \
                dnn activation='relu', \
                task='binary'):
        sparse_input_layer_list = []
        sparse embedding layer list = []
        dense input layer list = []
        # 1. Input & Embedding sparse features
        for i in sparse feature list:
                shape = 1
                name = i
                vocabulary_size = len(sparse_feature_reindex_dict[i]) + 1
                embedding \dim = 64
                cur_sparse_feaure_input_layer, cur_sparse_feaure_embedding_layer = \
                        input embedding layer(
                                shape = shape, \
                               name = name, \setminus
                               vocabulary size = vocabulary size, \
```

```
embedding_dim = embedding_dim)
```

```
sparse input layer list.append(cur sparse feaure input layer)
       sparse_embedding_layer_list.append(cur_sparse_feaure_embedding_layer)
# 2. Input dense features
for j in dense_feature_list:
       dense_input_layer_list.append(Input(shape=(1, ), name=j))
# === linear ===
sparse_linear_input = Concatenate(axis=-1)(sparse_embedding_layer_list)
dense_linear_input = Concatenate(axis=-1) (dense_input_layer_list)
linear_logit = Linear()([sparse_linear_input, dense_linear_input])
# === nfm cross ===
nfm input = Concatenate(axis=1) (sparse embedding layer list)
bi_out = BiInteractionPooling() (nfm_input)
if bi dropout:
       bi_out = tf.keras.layers.Dropout(bi_dropout)(bi_out, training=None)
bi_out = Flatten()(bi_out)
dnn_input = Concatenate(axis=-1)([bi_out, dense_linear_input])
dnn_output = DNN(dnn_hidden_units, dnn_activation, 12_reg_dnn, dnn_dropout, False
dnn_logit = tf.keras.layers.Dense(1, use_bias=False, activation=None)(dnn_output)
# === finally dense ===
out = PredictionLayer(task) (tf.keras.layers.add([linear logit, dnn logit]))
nfm_model = Model(inputs = sparse_input_layer_list + dense_input_layer_list, outp
return nfm model
```

(2.2.5) 应用NFM模型

(2.2.6) 打印NFM模型 summary

print(nfm_model.summary())

Layer (type)	Output	Sha	ipe	Param #	Connected to
Pclass (InputLayer)	(None,	1)	========	0	
Sex (InputLayer)	(None,	1)		0	
Cabin (InputLayer)	(None,	1)		0	
Embarked (InputLayer)	(None,	1)		0	
embedding_76 (Embedding)	(None,	1,	64)	256	Pclass[0][0]
embedding_77 (Embedding)	(None,	1,	64)	192	Sex[0][0]
embedding_78 (Embedding)	(None,	1,	64)	9536	Cabin[0][0]
embedding_79 (Embedding)	(None,	1,	64)	320	Embarked[0][0]
concatenate_72 (Concatenate)	(None,	4,	64)	0	embedding_76[0][0] embedding_77[0][0] embedding_78[0][0] embedding_79[0][0]
bi_interaction_pooling_19 (BiIn	(None,	1,	64)	0	concatenate_72[0][0]
Age (InputLayer)	(None,	1)		0	
SibSp (InputLayer)	(None,	1)		0	
Parch (InputLayer)	(None,	1)		0	
Fare (InputLayer)	(None,	1)		0	
dropout_26 (Dropout)	(None,	1,	64)	0	bi_interaction_pooling_19[0][0]

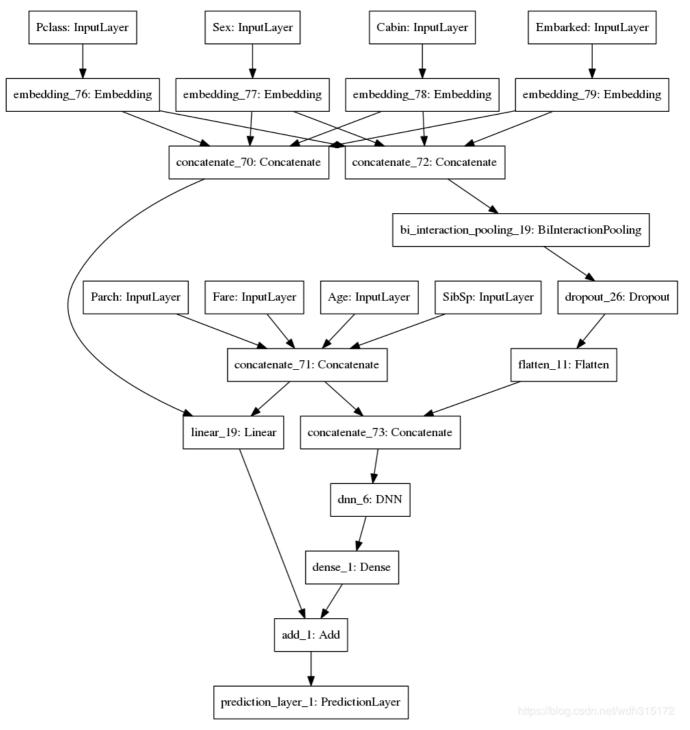
0/10/2		NFIMI快至理化与头	《
concatenate_71 (Concatenate)	(None, 4)	0	Age[0][0] SibSp[0][0] Parch[0][0] Fare[0][0]
flatten_11 (Flatten)	(None, 64)	0	dropout_26[0][0]
concatenate_73 (Concatenate)	(None, 68)	0	flatten_11[0][0] concatenate_71[0][0]
concatenate_70 (Concatenate)	(None, 1, 256)	0	embedding_76[0][0] embedding_77[0][0] embedding_78[0][0] embedding_79[0][0]
dnn_6 (DNN)	(None, 128)	25344	concatenate_73[0][0]
linear_19 (Linear)	(None, 1)	5	concatenate_70[0][0] concatenate_71[0][0]
dense_1 (Dense)	(None, 1)	128	dnn_6[0][0]
add_1 (Add)	(None, 1)	0	linear_19[0][0] dense_1[0][0]
prediction_layer_1 (PredictionL	(None, 1)	1	add_1[0][0]

Total params: 35,782 Trainable params: 35,782 Non-trainable params: 0

https://blog.csdn.net/wdh315172

(2.2.7) 输出NFM模型结构图

plot_model(nfm_model, to_file='nfm_model.png')



(2.2.8) 编译 NFM 模型, 训练模型

history = nfm_model.fit(xtrain_data, ytrain, epochs=5, batch_size=32, validation_data=(x1

```
Train on 712 samples, validate on 179 samples
WARNING: tensorflow: From \ /opt/conda/lib/python3.6/site-packages/tensorflow/python/ops/math\_ops.py: 3066: to\_int32 \ (from \ tensorflow.) and the sum of the sum 
python.ops.math_ops) is deprecated and will be removed in a future version.
Instructions for updating:
Use tf.cast instead.
Epoch 1/5
712/712 [=
                                                 Epoch 2/5
712/712 [===========] - 0s 143us/sample - loss: 5.1172 - acc: 0.5126 - val_loss: 2.5739 - val_acc: 0.6145
Epoch 3/5
                                 =============================== - 0.6320 - val_loss: 2.2888 - val_acc: 0.6201
712/712 [=
Epoch 4/5
                                            712/712 [=:
Epoch 5/5
```

(2.2.9) 绘制损失函数图

```
import matplotlib.pyplot as plt

loss = history.history['loss']

val_loss = history.history['val_loss']

epochs = range(1, len(loss) + 1)

plt.figure()

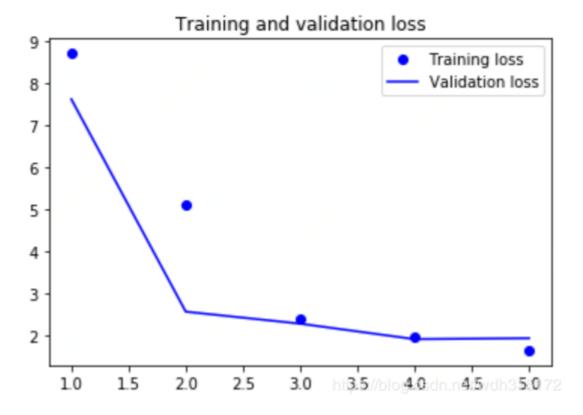
plt.plot(epochs, loss, 'bo', label='Training loss')

plt.plot(epochs, val_loss, 'b', label='Validation loss')

plt.title('Training and validation loss')

plt.legend()

print(plt.show())
```



参考: