機器學習於材料資訊的應用
Machine Learning on Material Informatics

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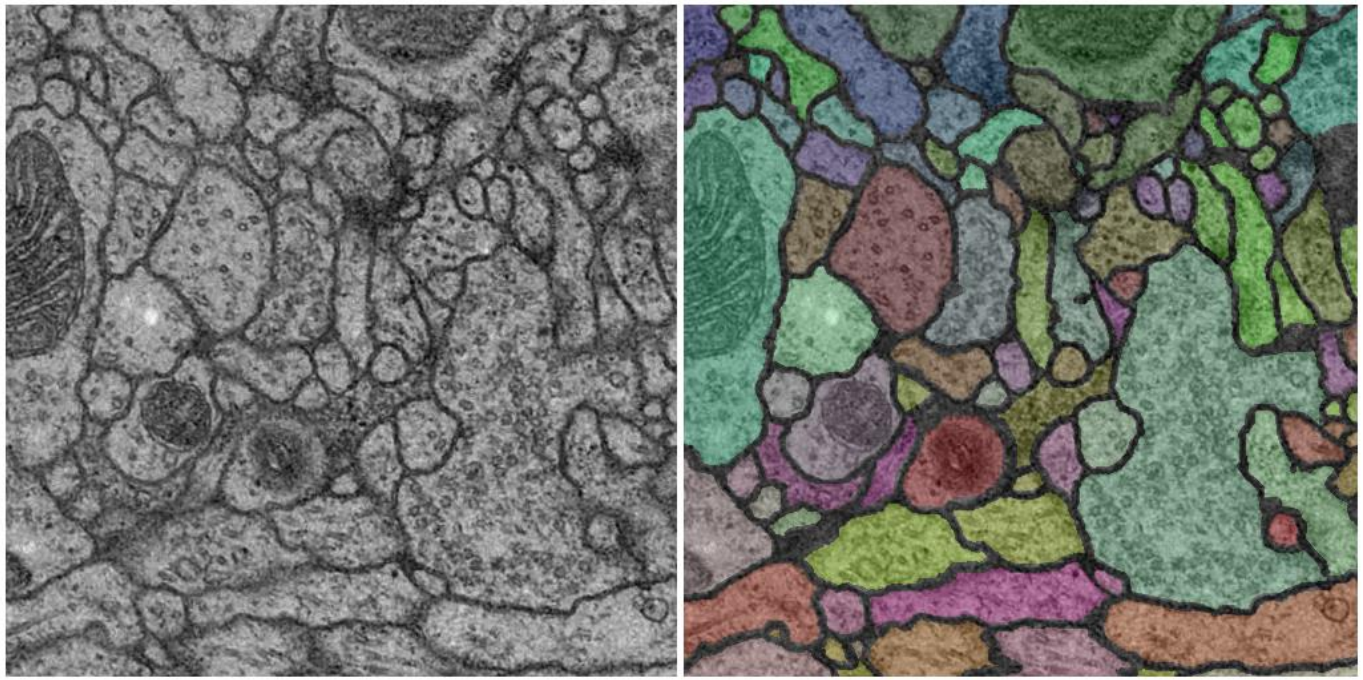
2D EM segmentation challenge

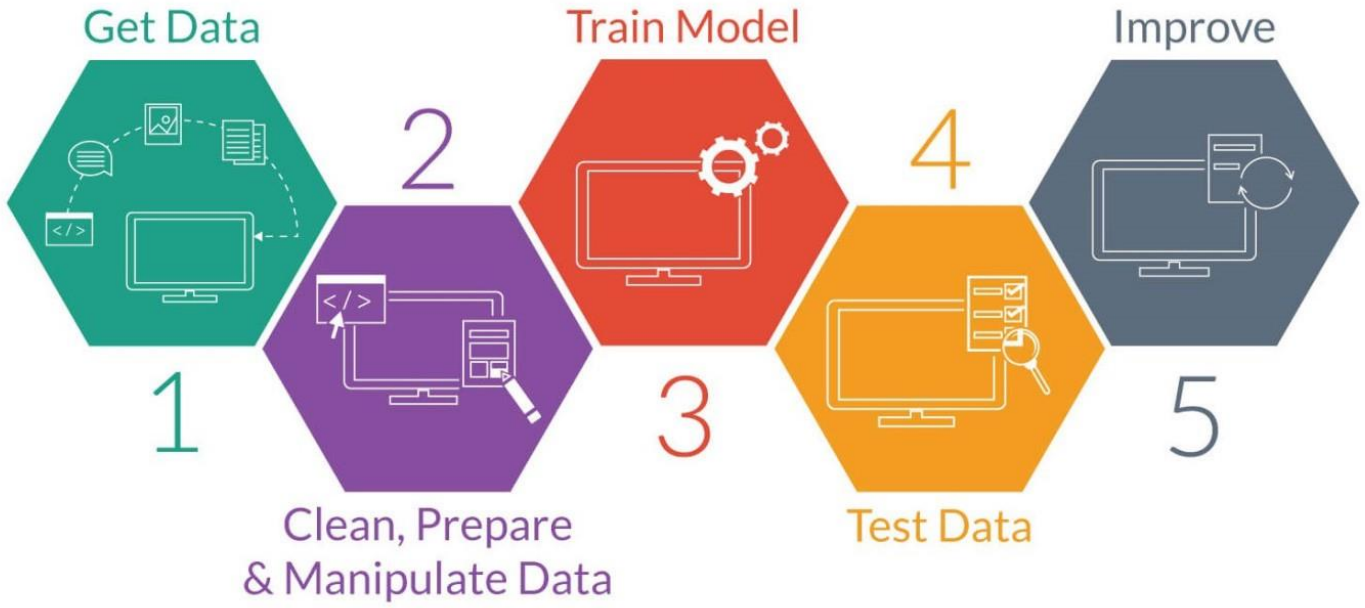
ISBI Challenge
Segmentation of neuronal structures in EM stacks



http://brainiac2.mit.edu/isbi_challenge/

ISBI Challenge

- This challenge was part of a workshop previous to the IEEE International Symposium on Biomedical Imaging (ISBI) 2012.
- First challenge on 2D segmentation of neuronal processes in EM images
- The training data is a set of 30 sections from a serial section Transmission Electron Microscopy (ssTEM) data set of the Drosophila first instar larva ventral nerve cord (VNC)神經索. The microcube measures 2 x 2 x 1.5 microns approx., with a resolution of 4x4x50 nm/pixel.
- The results are expected to be submitted as a 32-bit TIFF 3D image, which values between 0 (100% membrane certainty) and 1 (100% non-membrane certainty).



從ssTEM取得資料

檔案處理

人工標記

建立網路

分類演算法

用測試資料檢驗演算法

改善人工標記

data.py

dataPrepare.ipynb

model.py

trainUnet.ipynb

main.py

資料夾結構

aug
擴增影像的存放位置

image
原始影像資料

label
標記資料(mask)

test
測試資料

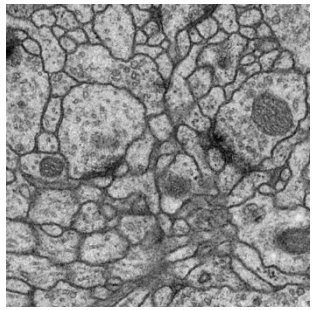
Fixed
標記影像斷點位置用的dataset

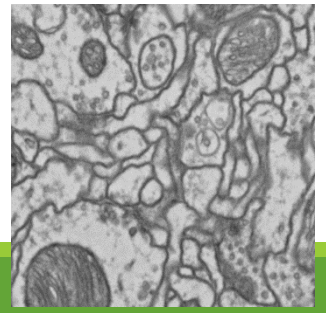
Membrane
分離細胞膜用的dataset

Mitochondrion
分離粒線體用的dataset

image

label

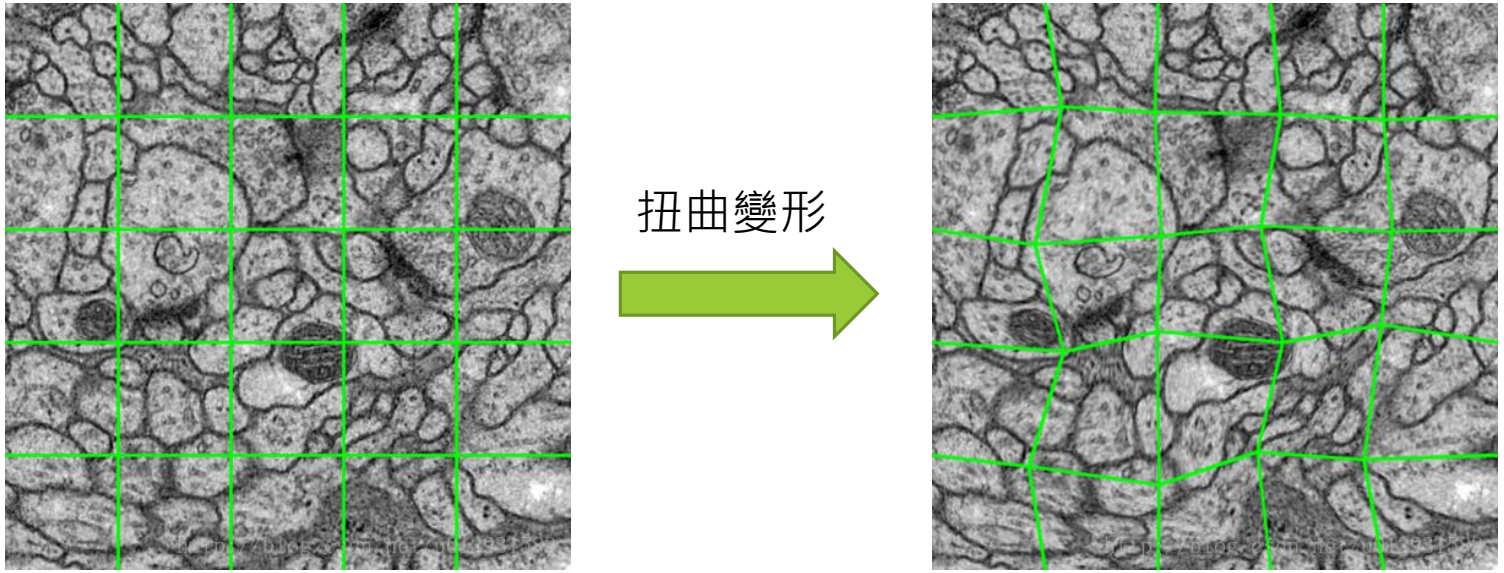




檔案處理

- 檔案處理主要仰賴keras.preprocessing.image 的 ImageDataGenerator功能。(https://keras.io/api/preprocessing/image/)
- 之所以可以進行資料擴增完全是基於一個假設:

扭曲圖像對於分類結果影響不大!!



檔案處理-dataPrepare.ipynb

- 資料擴增的引數透過dict形式存放，因為我們是依照ImageDataGenerator實作，所以我們的自訂函數也必須遵照ImageDataGenerator的設計。

```
data_gen_args = dict(rotation_range=20,
                     width_shift_range=0.05,
                     height_shift_range=0.05,
                     shear_range=0.05,
                     zoom_range=0.05,
                     horizontal_flip=True,
                     fill_mode='nearest')
```

rotation_range: 隨機旋轉的範圍
width_shift_range: 進行影像處理的範圍
height_shift_range:進行影像處理的範圍
shear_range: 扭曲的程度(逆時針扭)
zoom_range: 隨機縮放的範圍
horizontal_flip: 隨機水平翻轉
fill_mode: 填空模式

檔案處理-data.py

```
def trainGenerator(batch_size,train_path,image_folder,mask_folder,aug_dict,image_color_mode = "grayscale",
                   mask_color_mode = "grayscale",image_save_prefix  = "image",mask_save_prefix  = "mask",
                   flag_multi_class = False,num_class = 2,save_to_dir = None,target_size = (512,512),seed = 1):
```

```
train_path: ” Fixed”, “Membrane”, “Mitochondrion”三項任務擇一
image_folder: 影像存放位置 image
mask_folder: 標記資料存放位置label
```

檔案處理-data.py

- 同步處理影像集標記資料。

```
def trainGenerator(batch_size,train_path,image_folder,mask_folder,aug_dict,image_color_mode = "grayscale",
                   mask_color_mode = "grayscale",image_save_prefix  = "image",mask_save_prefix  = "mask",
                   flag_multi_class = False,num_class = 2,save_to_dir = None,target_size = (512,512),seed = 1):
```

```
image_generator =
image_datagen.flow_from_directory(
        train_path,
        classes = [image_folder],
        class_mode = None,
        color_mode = image_color_mode,
        target_size = target_size,
        batch_size = batch_size,
        save_to_dir = save_to_dir,
        save_prefix  = image_save_prefix,
        seed = seed)
```

```
mask_generator =
mask_datagen.flow_from_directory(
        train_path,
        classes = [mask_folder],
        class_mode = None,
        color_mode = mask_color_mode,
        target_size = target_size,
        batch_size = batch_size,
        save_to_dir = save_to_dir,
        save_prefix  = mask_save_prefix,
        seed = seed)
```

檔案處理-data.py

```
## zip() 函数用于將可疊代的物件作為參數，將物件中對應的元素打包成元組，然後返回由這些元組組成的物件。
## zip 方法在 Python 2 和 Python 3 中的不同：
## 在 Python 2.x zip() 返回的是一个列表。
## 在 Python 3.x 中為了減少記憶體，zip() 返回的是一個物件。如需展示列表，需手動使用 list() 轉換。
    train_generator = zip(image_generator, mask_generator)
    for (img,mask) in train_generator:
        …..
```

檔案處理-data.py

```
#調整成one-hot label
def adjustData(img,mask,flag_multi_class,num_class):
#產生測試資料
def testGenerator(test_path,num_image = 30,target_size = (512,512),flag_multi_class =
False,as_gray = True):
#以numpy格式存放資料
def geneTrainNpy(image_path,mask_path,flag_multi_class = False,num_class = 2,image_prefix
= "image",mask_prefix = "mask",image_as_gray = True,mask_as_gray = True):
#將結果套用顏色
def labelVisualize(num_class,color_dict,img):

def saveResult(save_path,npyfile,flag_multi_class = False,num_class = 2):
```

檔案處理-dataPrepare.ipynb

- 呼叫方式為:

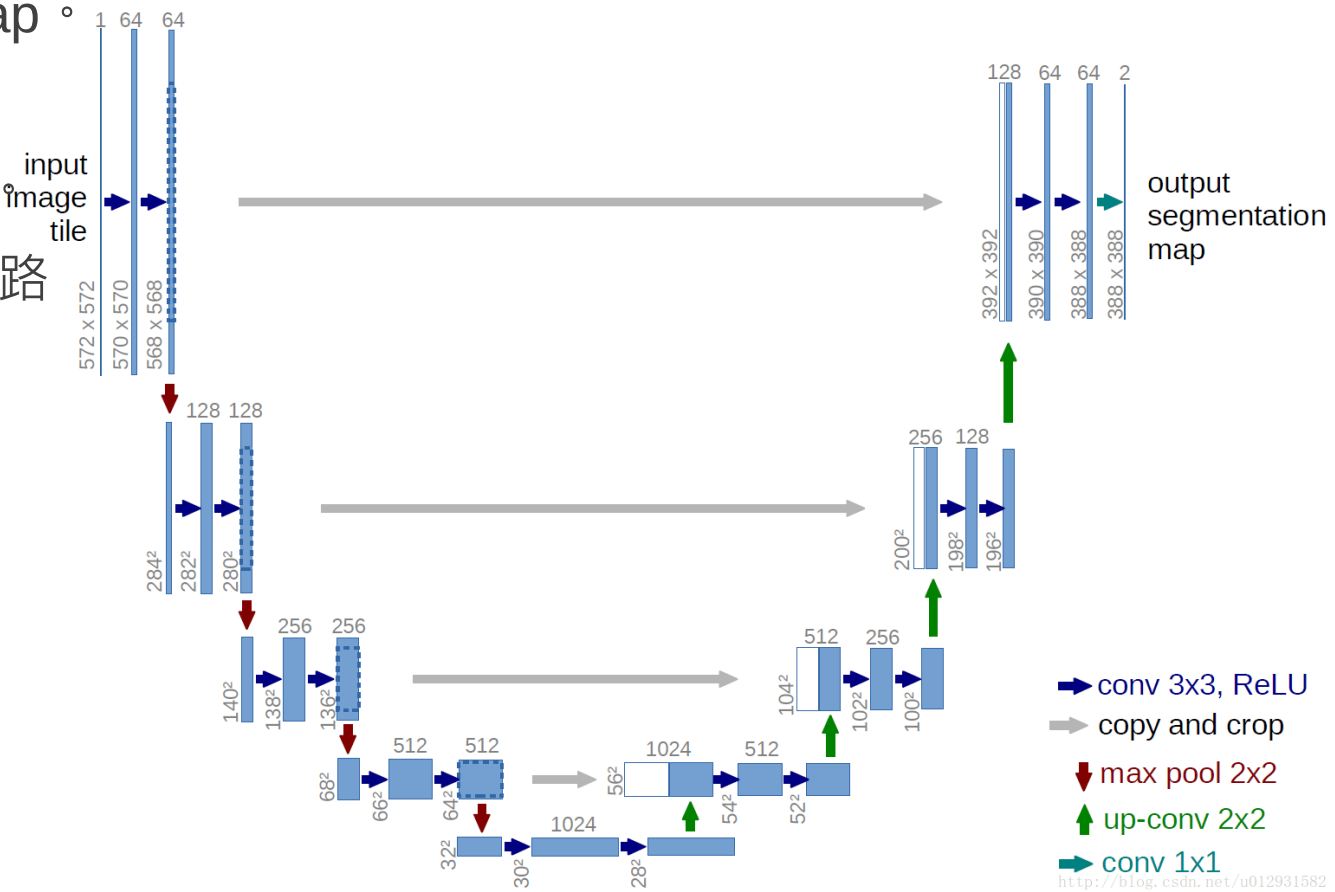
```
myGenerator = trainGenerator(BatchSize,'Membrane','image','label',data_gen_args,save_to_dir = "Membrane/aug")
```

人工標記

- 需要影像專家花時間投入。
- 感謝時任中研院物理所博士後研究員王定遠博士的高品質標記資料。

建立網路

- 每個藍色方塊代表的是multi-channel feature map。
- 藍色方塊上的數字代表的是channel數量。
- x-y-size代表影像本身的尺寸，標記在方塊左側
- 白色方塊代表透過直通路徑 concatenate左側網路的feature map。
- 不同顏色箭頭代表不同的操作
  - 藍色:conv 3X3 ReLu
  - 白色: copy
  - 紅色: max pool 2X2
  - 綠色: up-conv 2X2
  - 藍綠: conv 1X1



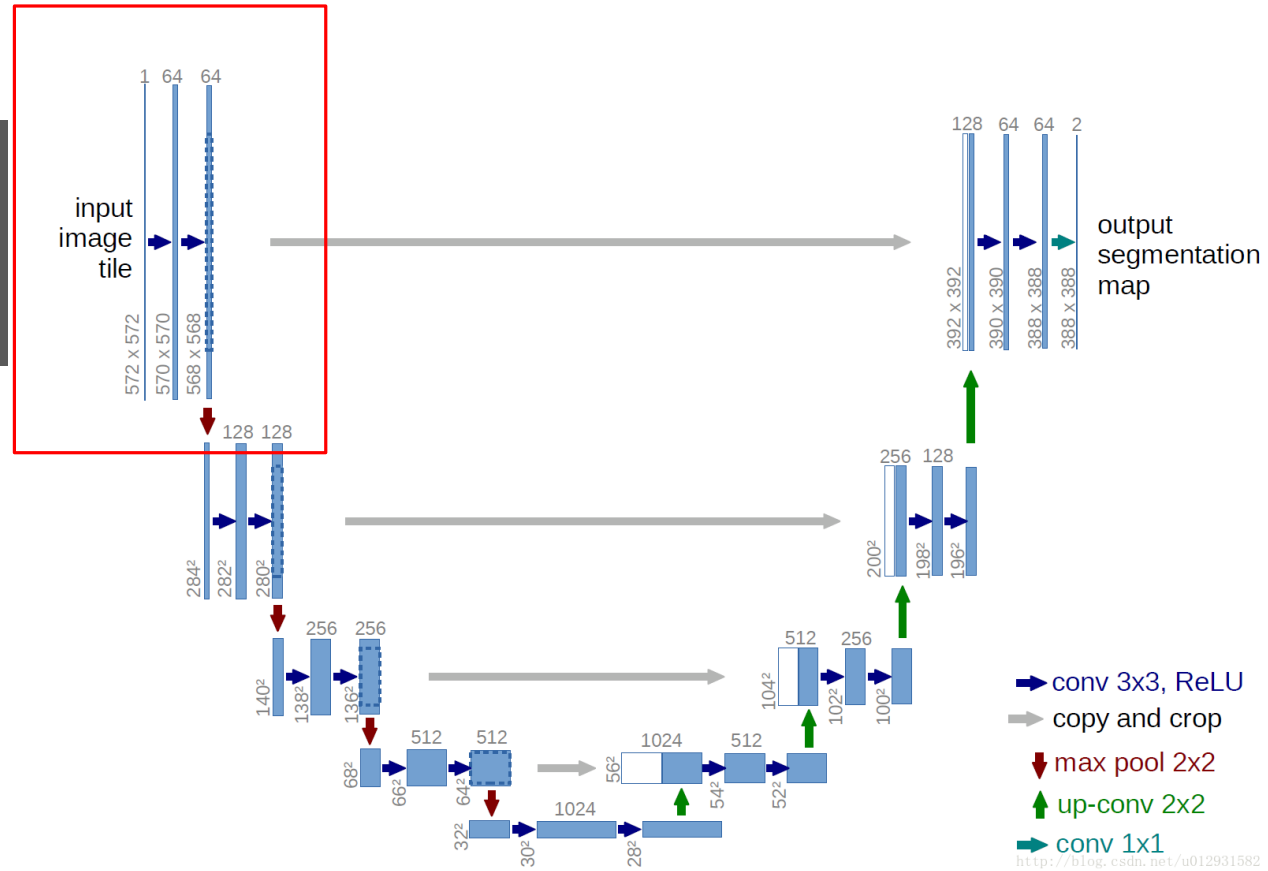
https://lmb.informatik.uni-freiburg.de/people/ronneber/u-net/

建立網路

```
import numpy as np
import os
import skimage.io as io
import skimage.transform as trans
import numpy as np
from keras.models import *
from keras.layers import *
from keras.optimizers import *
from keras.callbacks import ModelCheckpoint, LearningRateScheduler
from keras import backend as keras
```

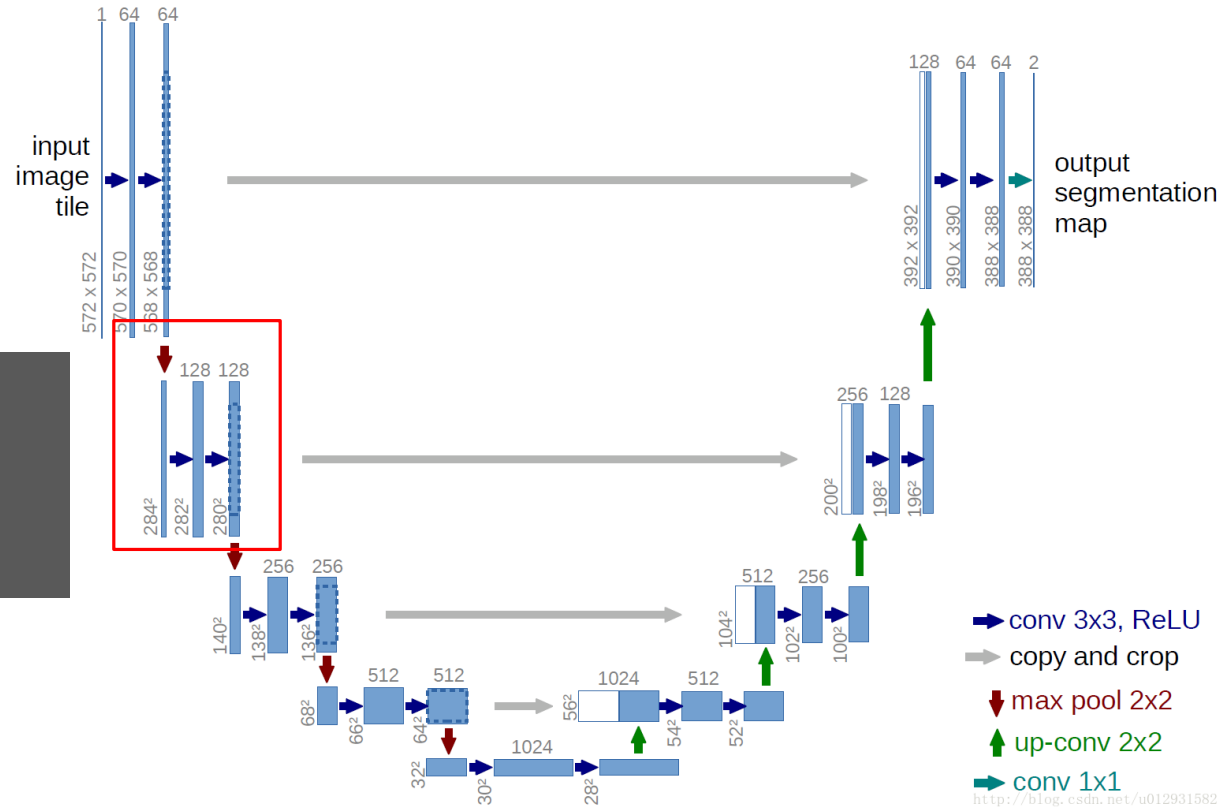
建立網路

```
inputs = Input(input_size)
conv1 = Conv2D(64, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(inputs)
conv1 = Conv2D(64, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(conv1)
```



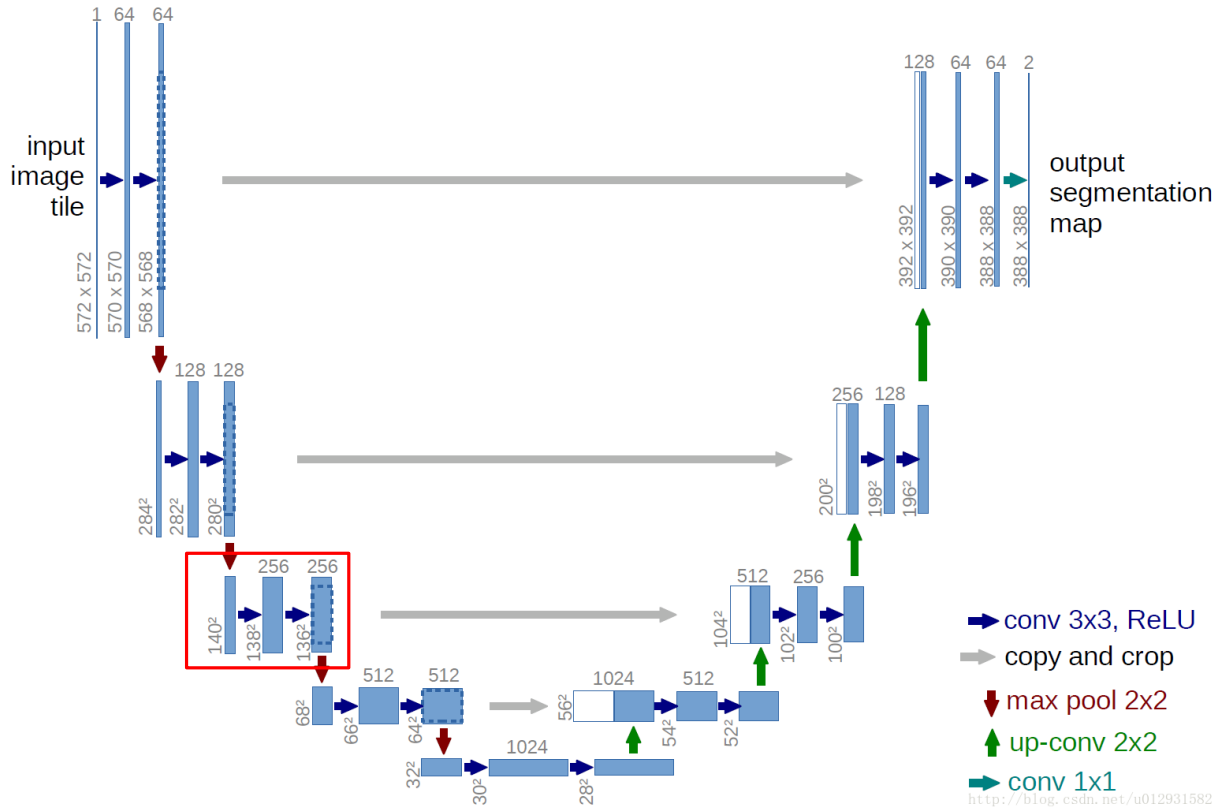
建立網路

```
pool1 = MaxPooling2D(pool_size=(2, 2))(conv1)
conv2 = Conv2D(128, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(pool1)
conv2 = Conv2D(128, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(conv2)
```



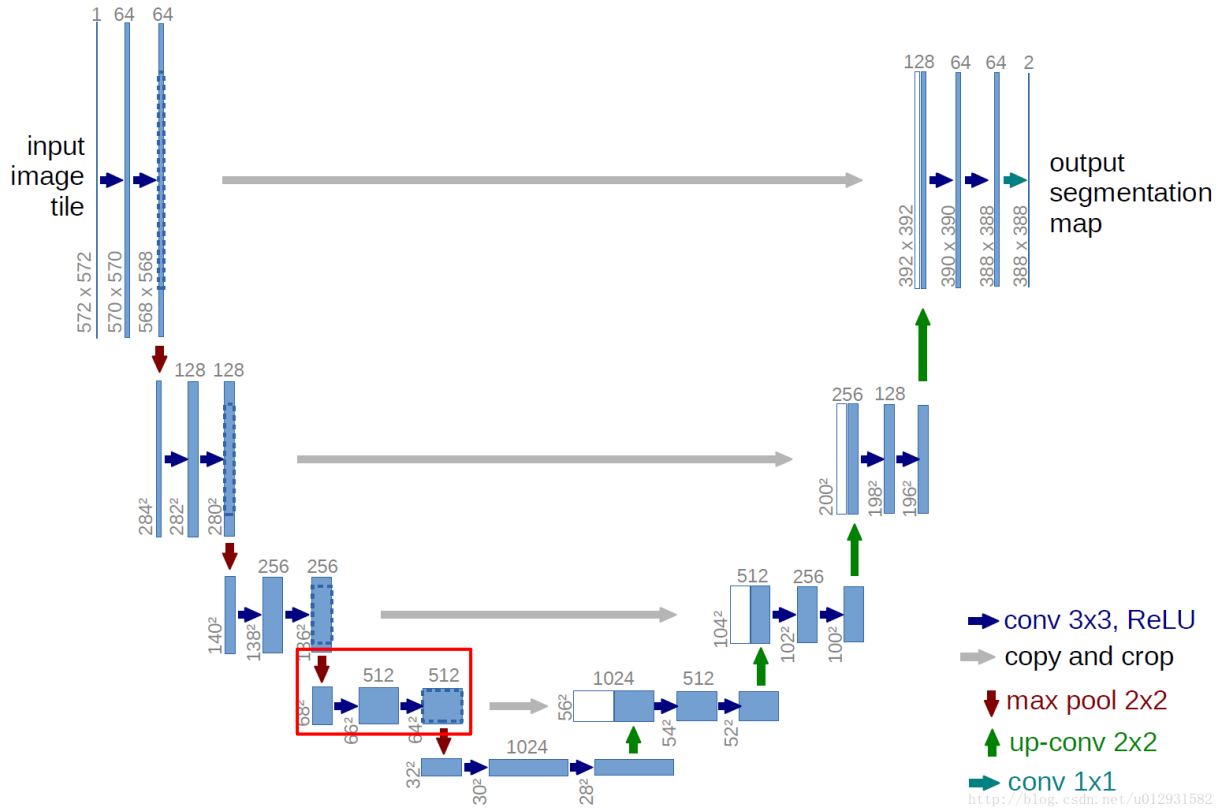
建立網路

```
pool2 = MaxPooling2D(pool_size=(2, 2))(conv2)
    conv3 = Conv2D(256, 3, activation = 'relu', padding =
'same', kernel_initializer = 'he_normal')(pool2)
    conv3 = Conv2D(256, 3, activation = 'relu', padding =
'same', kernel_initializer = 'he_normal')(conv3)
```

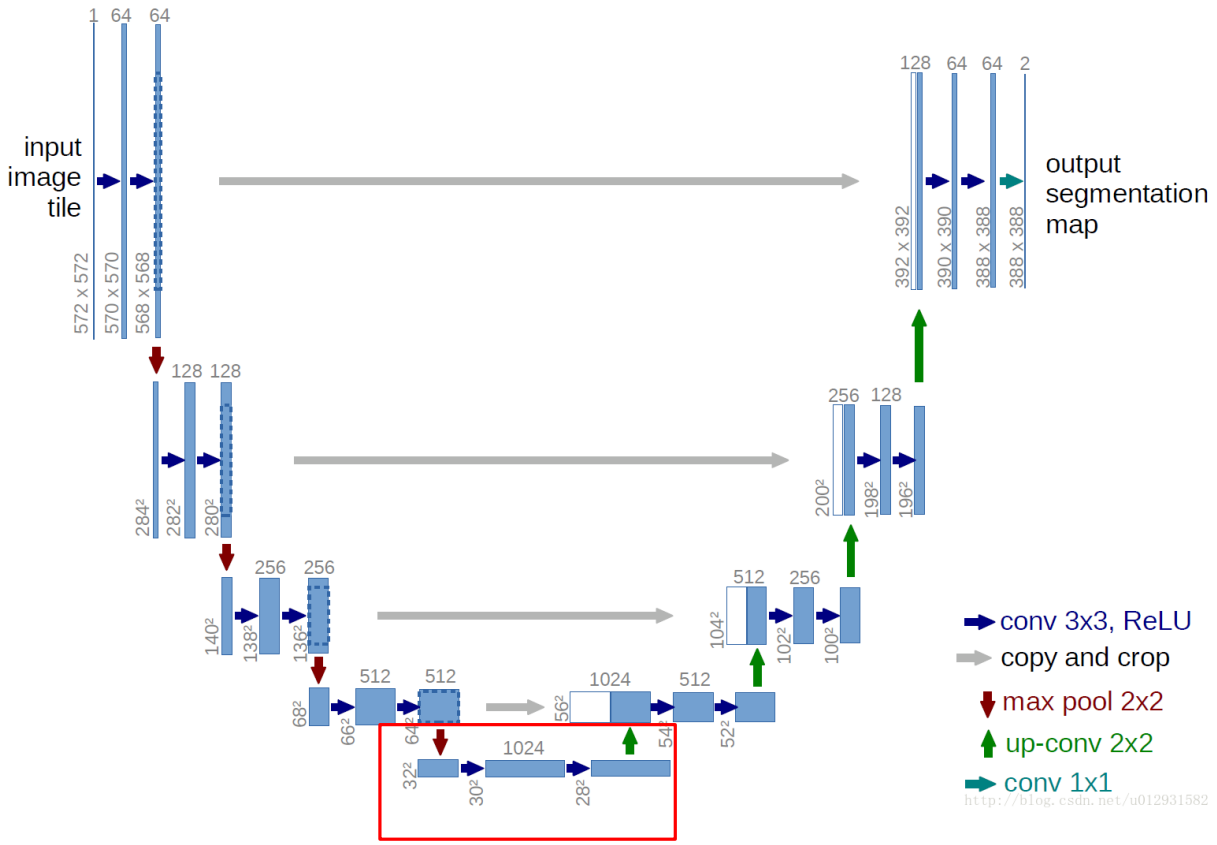


建立網路

```
pool3 = MaxPooling2D(pool_size=(2, 2))(conv3)
    conv4 = Conv2D(512, 3, activation = 'relu', padding =
'same', kernel_initializer = 'he_normal')(pool3)
    conv4 = Conv2D(512, 3, activation = 'relu', padding =
'same', kernel_initializer = 'he_normal')(conv4)
    drop4 = Dropout(0.5)(conv4)
    pool4 = MaxPooling2D(pool_size=(2, 2))(drop4)
```

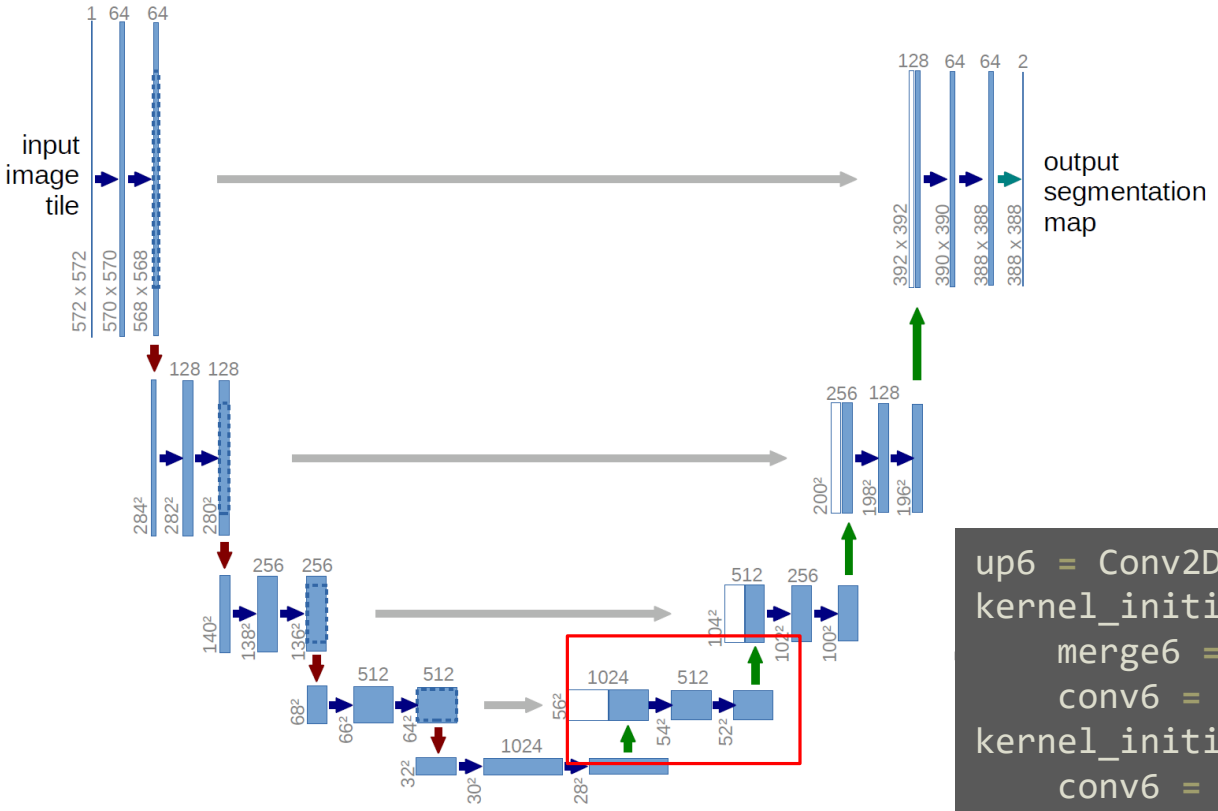


建立網路



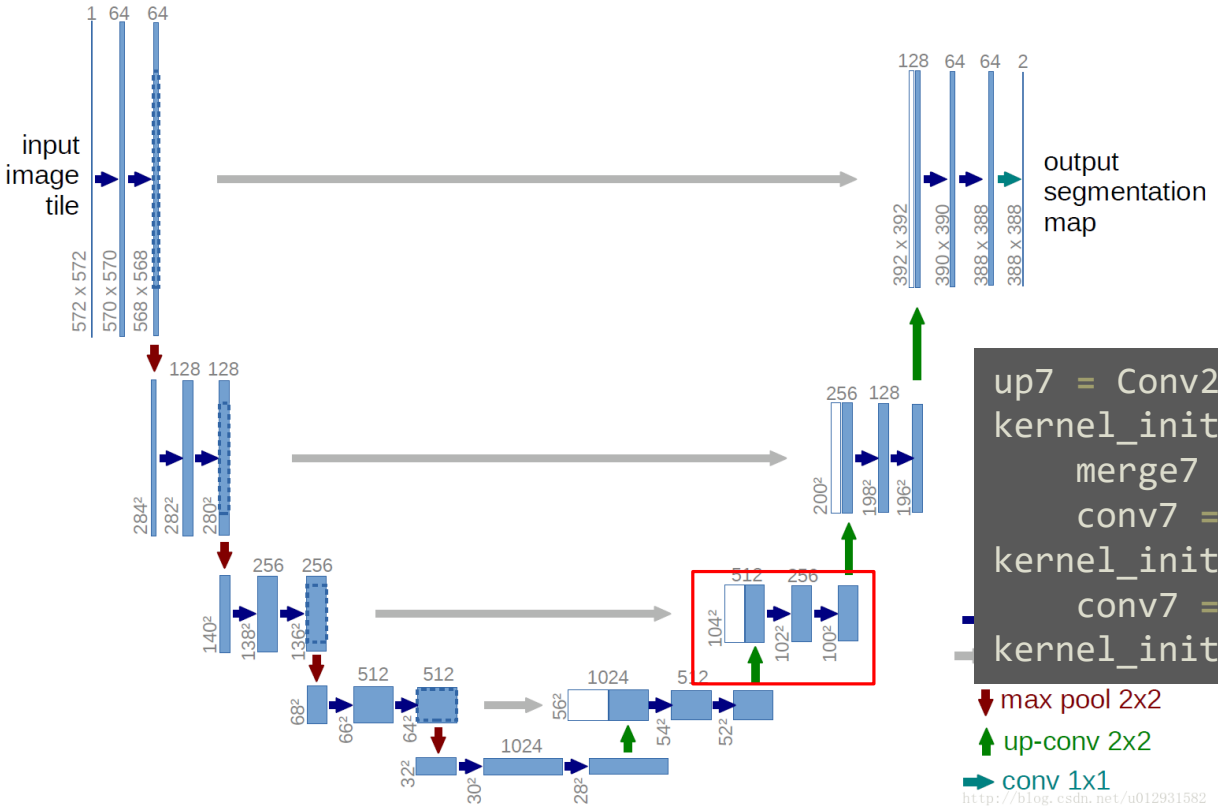

```
conv5 = Conv2D(1024, 3, activation = 'relu', padding =
'same', kernel_initializer = 'he_normal')(pool4)
    conv5 = Conv2D(1024, 3, activation = 'relu', padding =
'same', kernel_initializer = 'he_normal')(conv5)
    drop5 = Dropout(0.5)(conv5)
```

建立網路



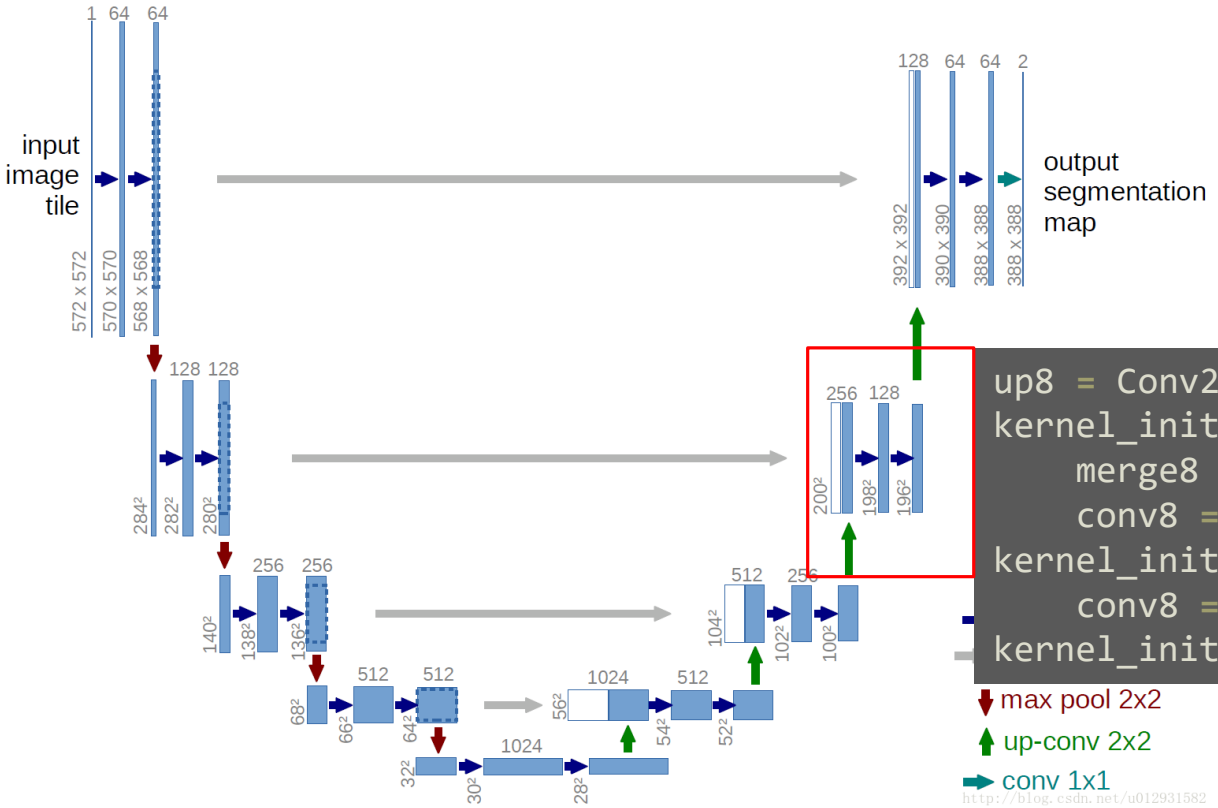

```
up6 = Conv2D(512, 2, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(UpSampling2D(size = (2,2))(drop5))
    merge6 = concatenate([drop4,up6], axis = 3)
    conv6 = Conv2D(512, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(merge6)
    conv6 = Conv2D(512, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(conv6)
```

建立網路



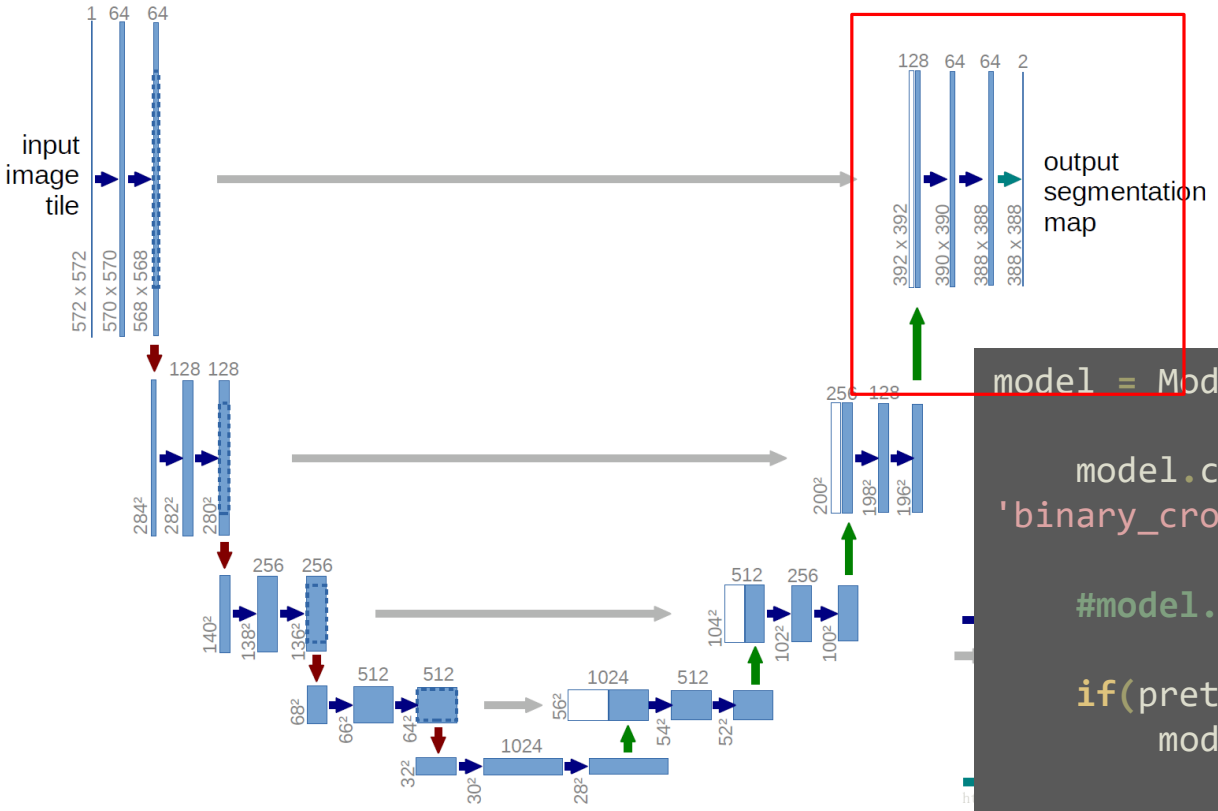

```
up7 = Conv2D(256, 2, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(UpSampling2D(size = (2,2))(conv6))
    merge7 = concatenate([conv3,up7], axis = 3)
    conv7 = Conv2D(256, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(merge7)
    conv7 = Conv2D(256, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(conv7)
```

建立網路




```
up8 = Conv2D(128, 2, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(UpSampling2D(size = (2,2))(conv7))
    merge8 = concatenate([conv2,up8], axis = 3)
    conv8 = Conv2D(128, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(merge8)
    conv8 = Conv2D(128, 3, activation = 'relu', padding = 'same',
kernel_initializer = 'he_normal')(conv8)
```

建立網路




```
model = Model(input = inputs, output = conv10)

    model.compile(optimizer = Adam(lr = 1e-4), loss =
'binary_crossentropy', metrics = ['accuracy'])

    #model.summary()

    if(pretrained_weights):
        model.load_weights(pretrained_weights)

    return model
```

訓練網路

```
myGene =
trainGenerator(BatchSize,'membrane/train','image','label',data_gen_
args,save_to_dir = None)

model = unet()
model_checkpoint = ModelCheckpoint('unet_membrane.hdf5',
monitor='loss',verbose=1, save_best_only=True)
model.fit_generator(myGene,steps_per_epoch=300,epochs=1,callbacks=[
model_checkpoint])
```