Machine Learning with Python – SciKit-learn Part 3

Ramesh Shankar

UConn

Dimensionality reduction - PCA

- Principal Component Analysis – unsupervised data compression
  - Can help with computational efficiency – use lesser data for similar effect
  - Can also help reduce curse of dimensionality:
    - More dimentions – more volume of space – data becomes sparse
    - Therefore, it hinders efficient prediction or classification
  - PCA converts a set of possibly correlated variables (*d* variables) into fewer orthogonal (uncorrelated) variables *(k* variables)*:*

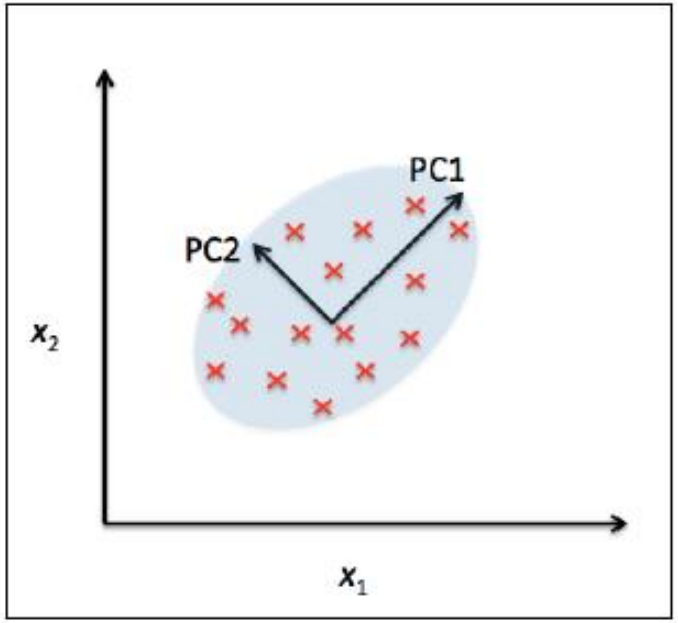
$$\boldsymbol{x} = [x_1, x_2, \ldots, x_d], \quad \boldsymbol{x} \in \mathbb{R}^d$$

$$\downarrow \boldsymbol{x}\boldsymbol{W}, \quad \boldsymbol{W} \in \mathbb{R}^{d \times k}$$

$$\mathbf{z} = [z_1, z_2, \ldots, z_k], \quad \mathbf{z} \in \mathbb{R}^k$$

PCA

- These principal components are the “directions of maximum variance” in the dataset:



Wine dataset

In [6]:
```
df_wine = pd.read_csv('https://raw.githubusercontent.com/rasbt/python-machine-learning-book/master/code/datasets/wine/wine.dat

df_wine.columns = ['Class label', 'Alcohol', 'Malic acid', 'Ash',
'Alcalinity of ash', 'Magnesium', 'Total phenols',
'Flavanoids', 'Nonflavanoid phenols', 'Proanthocyanins',
'Color intensity', 'Hue', 'OD280/OD315 of diluted wines', 'Proline']
df_wine.head()
```

Out[6]:

	Class label	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	Color intensity	Hue	OD280/OD315 of diluted wines	Proline
0	1	14.23	1.71	2.43	15.6	127	2.80	3.06	0.28	2.29	5.64	1.04	3.92	1065
1	1	13.20	1.78	2.14	11.2	100	2.65	2.76	0.26	1.28	4.38	1.05	3.40	1050
2	1	13.16	2.36	2.67	18.6	101	2.80	3.24	0.30	2.81	5.68	1.03	3.17	1185
3	1	14.37	1.95	2.50	16.8	113	3.85	3.49	0.24	2.18	7.80	0.86	3.45	1480
4	1	13.24	2.59	2.87	21.0	118	2.80	2.69	0.39	1.82	4.32	1.04	2.93	735

PCA - steps

- Standardize the d-dimensional dataset
- Construct covariance matrix:

$$\sigma_{jk} = \frac{1}{n}\sum_{i=1}^{n}\left(x_j^{(i)} - \mu_j\right)\left(x_k^{(i)} - \mu_k\right) \qquad \sum = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 \end{bmatrix}$$

- Obtain the eigenvectors (which are the principal components – the directions of maximum variance)
- And the eigenvalues (the scalar magnitudes of the eigenvectors)

Standardize the d-dimensional dataset

```
#·Download·data
df_wine·=·pd.read_csv('https://archive.ics.uci.edu/ml/'
····'machine-learning-databases/wine/wine.data',
····header=None)
df_wine.columns·=·['Class·label',·'Alcohol',·'Malic·acid',·'Ash',·
'Alcalinity·of·ash',·'Magnesium',·'Total·phenols',·
'Flavanoids',·'Nonflavanoid·phenols',·'Proanthocyanins',·
'Color·intensity',·'Hue',·'OD280/OD315·of·diluted·wines',·'Proline']
df_wine.head()

#·Split·data·into·train-test
from·sklearn.model_selection·import·train_test_split
X,·y·=·df_wine.iloc[:,·1:].values,·df_wine.iloc[:,·0].values
X_train,·X_test,·y_train,·y_test·=·\
····train_test_split(X,·y,·test_size=0.3,·random_state=0)

#·Standardize·the·data
from·sklearn.preprocessing·import·StandardScaler
sc·=·StandardScaler()
X_train_std·=·sc.fit_transform(X_train)
X_test_std·=·sc.transform(X_test)
```

Construct covariance matrix, obtain eigen values

```
#·Obtain·eigenvalues
import·numpy·as·np
cov_mat·=·np.cov(X_train_std.T)
eigen_vals,·eigen_vecs·=·np.linalg.eig(cov_mat)

print('\nEigenvalues·\n%s'·%·eigen_vals)
```

```
Eigenvalues
[ 4.8923083   2.46635032  1.42809973  1.01233462  0.84906459  0.60181514
  0.52251546  0.08414846  0.33051429  0.29595018  0.16831254  0.21432212
  0.2399553 ]
```

```
In [14]: eigen_vecs[0]
Out[14]:
array([  1.46698114e-01,   5.04170789e-01,  -1.17235150e-01,
         2.06254611e-01,  -1.87815947e-01,  -1.48851318e-01,
        -1.79263662e-01,  -5.54687162e-02,  -4.03054922e-01,
        -4.17197583e-01,   2.75660860e-01,   4.03567189e-01,
         4.13320786e-04])
```

```
In [16]: eigen_vals[0]
Out[16]: 4.8923083032737411
```

Computing a graph of variance explained

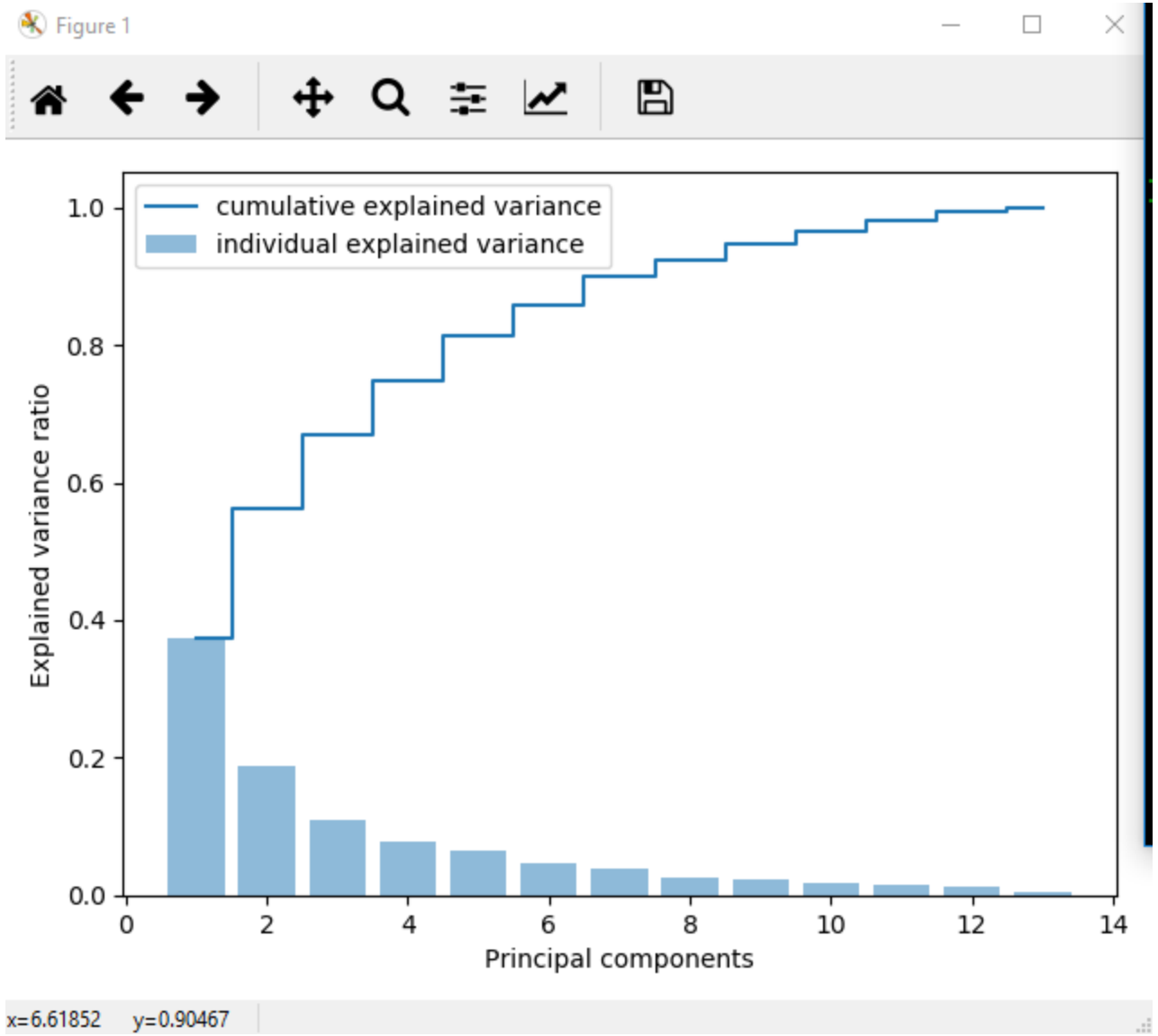
Variance explained ratio:

$$\frac{\lambda_j}{\sum_{j=1}^{d} \lambda_j}$$

```
#·Total·and·explained·variance
tot·=·sum(eigen_vals)
var_exp·=·[(i·/·tot)·for·i·in·sorted(eigen_vals,·reverse=True)]
cum_var_exp·=·np.cumsum(var_exp)
```

```
#·Plot·figure
import·matplotlib.pyplot·as·plt
plt.bar(range(1,·14),·var_exp,·alpha=0.5,·align='center',
·····label='individual·explained·variance')
plt.step(range(1,·14),·cum_var_exp,·where='mid',
·····label='cumulative·explained·variance')
plt.ylabel('Explained·variance·ratio')
plt.xlabel('Principal·components')
plt.legend(loc='best')
plt.tight_layout()
#·plt.savefig('./figures/pca1.png',·dpi=300)
plt.show()
```

Plot cumulative explained variance



Feature transformation

Sort eigen vectors in descending order of eigen values:

```
In [17]: eigen_pairs = [(np.abs(eigen_vals[i]), eigen_vecs[:, i])
    ...:                for i in range(len(eigen_vals))]
    ...:
    ...: # Sort the (eigenvalue, eigenvector) tuples from high to low
    ...: eigen_pairs.sort(key=lambda k: k[0], reverse=True)
    ...:
```

```
In [20]: eigen_pairs
Out[20]:
[(4.8923083032737411,
  array([ 0.14669811, -0.24224554, -0.02993
          0.38934455,  0.42326486, -0.30634
          0.30032535,  0.36821154,  0.29259
 (2.4663503157592306,
  array([ 0.50417079,  0.24216889,  0.28698
          0.09363991,  0.01088622,  0.01870
         -0.27924322, -0.174365  ,  0.36315
 (1.4280997275048442,
  array([-0.11723515,  0.14994658,  0.65639
          0.18080442,  0.14295933,  0.17223
```

Construct pairs of eigen vectors (eigen_pairs):

```
In [18]: w = np.hstack((eigen_pairs[0][1][:, np.newaxis],
    ...:                eigen_pairs[1][1][:, np.newaxis]))
    ...: print('Matrix W:\n', w)
    ...:
```

```
Matrix W:
 [[ 0.14669811  0.50417079]
 [-0.24224554  0.24216889]
 [-0.02993442  0.28698484]
 [-0.25519002 -0.06468718]
 [ 0.12079772  0.22995385]
 [ 0.38934455  0.09363991]
 [ 0.42326486  0.01088622]
 [-0.30634956  0.01870216]
 [ 0.30572219  0.03040352]
 [-0.09869191  0.54527081]
 [ 0.30032535 -0.27924322]
 [ 0.36821154 -0.174365  ]
 [ 0.29259713  0.36315461]]
```

Create the new features:

$$x' = xW$$

```
#·Create·the·new·features·with·our·eigen·vectors
X_train_pca·=·X_train_std.dot(w)
colors·=·['r',·'b',·'g']
markers·=·['s',·'x',·'o']

import·matplotlib.pyplot·as·plt

for·l,·c,·m·in·zip(np.unique(y_train),·colors,·markers):
····plt.scatter(X_train_pca[y_train·==·l,·0],·
····················X_train_pca[y_train·==·l,·1],·
····················c=c,·label=l,·marker=m)

plt.xlabel('PC·1')
plt.ylabel('PC·2')
plt.legend(loc='lower·left')
plt.tight_layout()
#·plt.savefig('./figures/pca2.png',·dpi=300)
plt.show()
```

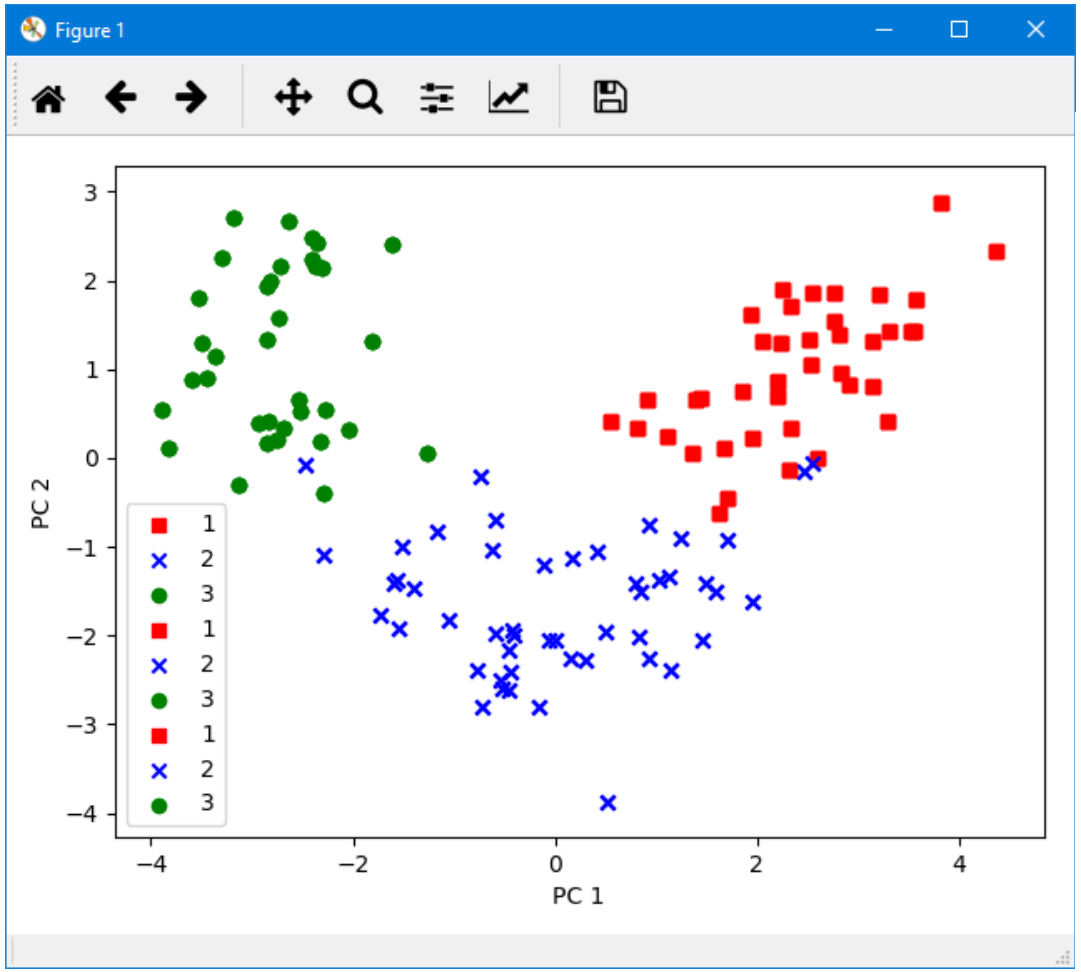
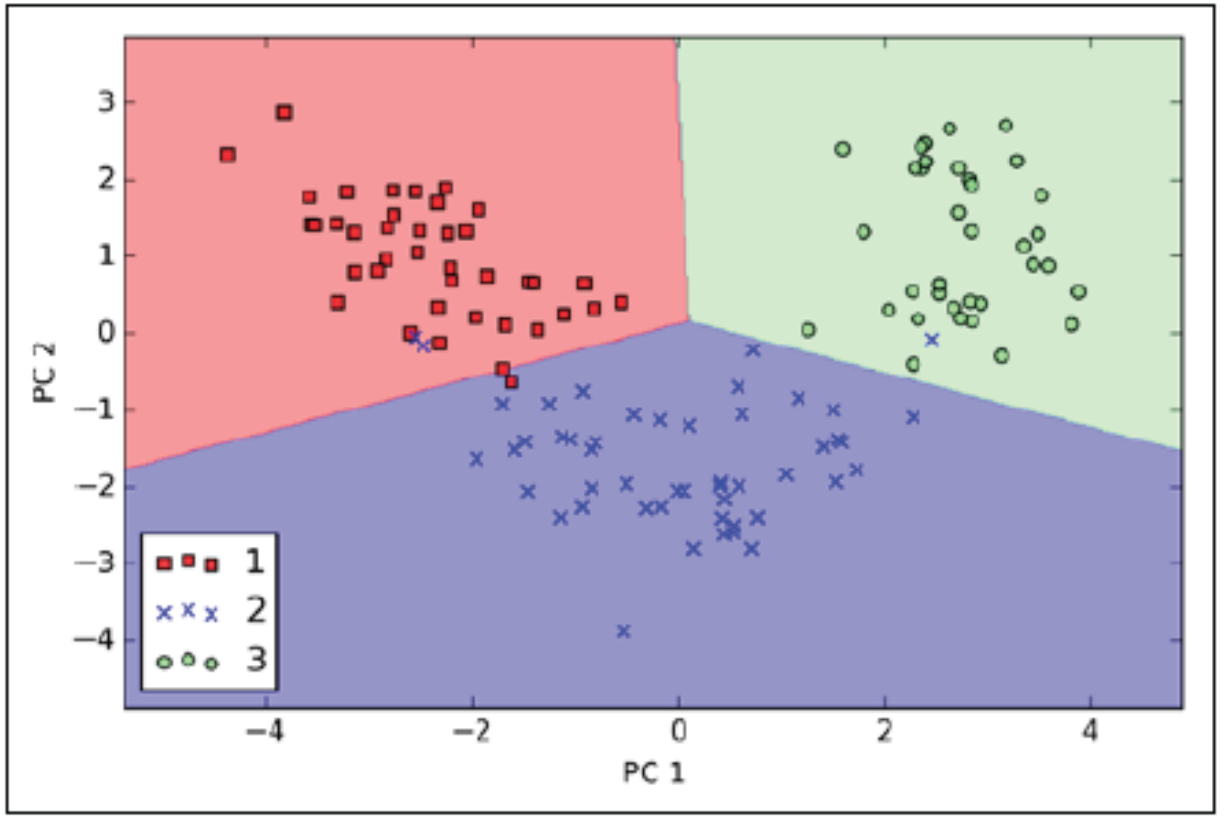


Figure 1
PC 2
PC 1
1
2
3
1
2
3
1
2
3


PC 2
PC 1
1
2
3

PCA in Scikit-learn

```
# PCA in Scikit-learn:

from sklearn.decomposition import PCA
pca = PCA()
X_train_pca = pca.fit_transform(X_train_std)
pca.explained_variance_ratio_

import matplotlib.pyplot as plt
plt.bar(range(1, 14), pca.explained_variance_ratio_, alpha=0.5, align='center')
plt.step(range(1, 14), np.cumsum(pca.explained_variance_ratio_), where='mid')
plt.ylabel('Explained variance ratio')
plt.xlabel('Principal components')
plt.show()

pca = PCA(n_components=2)
X_train_pca = pca.fit_transform(X_train_std)
X_test_pca = pca.transform(X_test_std)

plt.scatter(X_train_pca[:, 0], X_train_pca[:, 1])
plt.xlabel('PC 1')
plt.ylabel('PC 2')
plt.show()
```

Streamlining workflows with pipelines

- Can add different preprocessing techniques into a pipeline – e.g.
  - Standardization for feature scaling
  - Data compression – e.g. principal component analysis – for dimensionality reduction
- Example: Wisconsin Breast Cancer dataset
  - 569 samples of malignant and benign tumor cells
  - Column 1: Unique ID of sample
  - Column 2: diagnosis (M = malignant, B = benign)
  - Columns 3 – 32: 30 real-value features computed from digitized images of cell nuclei – can be used to build model to predict whether tumor B or M

Loading dataset

```
# Import Wisconsin Breast Cancer dataset
import pandas as pd

# Read dataset from website
df = pd.read_csv('https://archive.ics.uci.\
edu/ml/machine-learning-databases/breast-cancer-\
wisconsin/wdbc.data', header=None)
```

```
# Assign columns 2 through 30 to the variable X
X = df.loc[:, 2:].values
# Assign column 1 to the variable y
y = df.loc[:, 1].values
# Using LabelEncoder, transform class labels to integers
from sklearn.preprocessing import LabelEncoder
le = LabelEncoder()
y = le.fit_transform(y)
# The above transforms M as 1, B as 0
# Check that using this command:
le.transform(['M', 'B'])
```

```
# Divide dataset into separate training (80%)
# and test dataset
from sklearn.cross_validation import train_test_split
X_train, X_test, y_train, y_test = \
train_test_split(X, y, test_size=0.20, random_state=1)
```

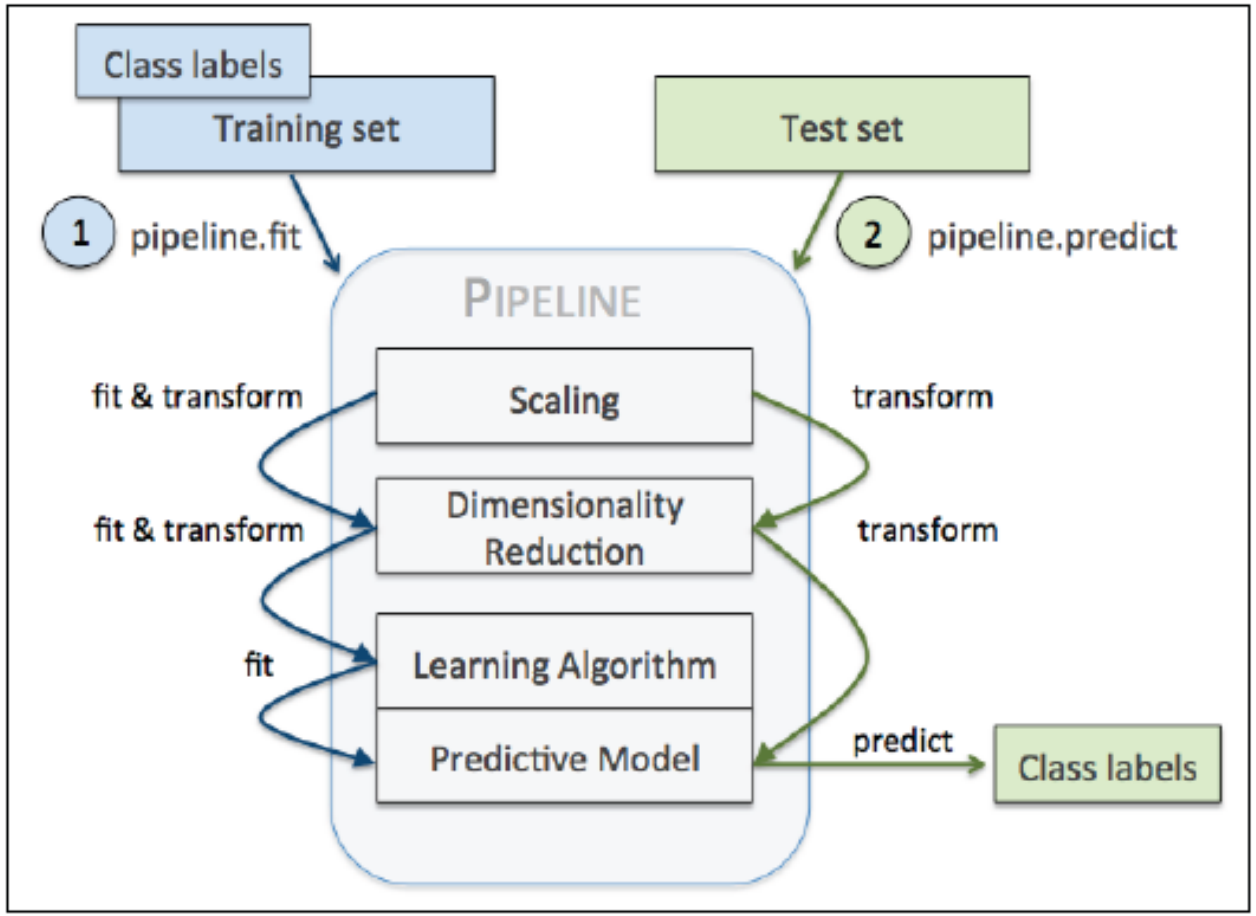
Combining steps into pipeline

- Standardize columns to ensure they are on same scale
- Reduce dimensionality of 30 attributes using Principal Component Analysis (PCA)
- Pineline:

(1) Identifier

(2) Transformer or estimator

```
# Combine standardization and PCA
# into one pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
pipe_lr = Pipeline([('scl', StandardScaler()),
('pca', PCA(n_components=2)),
('clf', LogisticRegression(random_state=1))])
pipe_lr.fit(X_train, y_train)
print('Test Accuracy: %.3f' % pipe_lr.score(X_test, y_test))
```


Class labels
Training set
Test set
1
pipeline.fit
2
pipeline.predict
PIPELINE
fit & transform
Scaling
transform
fit & transform
Dimensionality Reduction
transform
fit
Learning Algorithm
Predictive Model
predict
Class labels

Cross-validation to assess model performance

- Key goal: estimate performance on data the model has not seen
- Model can suffer from underfitting (high bias) or overfitting (high variance)
- To find acceptable bias-variance tradeoff, evaluate model
- Hold-out cross-validation, K-fold cross-validation

Holdout method

- Split initial dataset into training, validation and test datasets
- Use training dataset for model training
- Use validation set for model selection
  - Select optimal values of tuning parameters (hyperparameters)
- Use test dataset to estimate performance – test ability of model to generalize to new data
- Disadvantage: performance estimate is sensitive to how we partition training set into training and validation subsets.

K-fold cross validation

- Randomly split training dataset into k folds without replacement
  - Typically k = 10
- Use k-1 folds for model training
- Use 1 fold for validation
- Calculate average performance of models based on different folds – performance estimate less sensitive to data partitioning
- Perform model tuning – find hyperparameters with satisfactory general performance
- Then, retrain model on complete training set, obtain performance estimate using independent test set


Training set
Training folds
Test fold
1st iteration
2nd iteration
3rd iteration
10th iteration
E_1
E_2
E_3
E_{10}
$E = \frac{1}{10}\sum_{i=1}^{10} E_i$

K-fold cross validation

- Stratified k-fold cross-validation: yields better bias and variance estimates. (Kohavi et al., 1995).
- Each fold is representative of the class-proportions of the training dataset.

```
# Stratified K-fold cross-validation
import numpy as np
from sklearn.model_selection import StratifiedKFold
# Initialize the StratifiedKFold iterator
# with class-labels y_train in training set
skf = StratifiedKFold(n_splits=10)
skf.get_n_splits(X_train, y_train)


# Define array "scores"
scores = []
# Loop through each of the k folds
k = 0
for train, test in skf.split(X_train, y_train):
    k += 1
    pipe_lr.fit(X_train[train], y_train[train])
    score = pipe_lr.score(X_train[test], y_train[test])
    scores.append(score)
    print('Fold: %s, Class dist.: %s, Acc: %.3f' % (k,
          np.bincount(y_train[train]), score))
```

Alternate method:

```
from sklearn.model_selection import cross_val_score
scores = cross_val_score(estimator=pipe_lr,
                         X=X_train,
                         y=y_train,
                         cv=10,
                         n_jobs=1)
print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))
```

Fine-tuning models via grid search

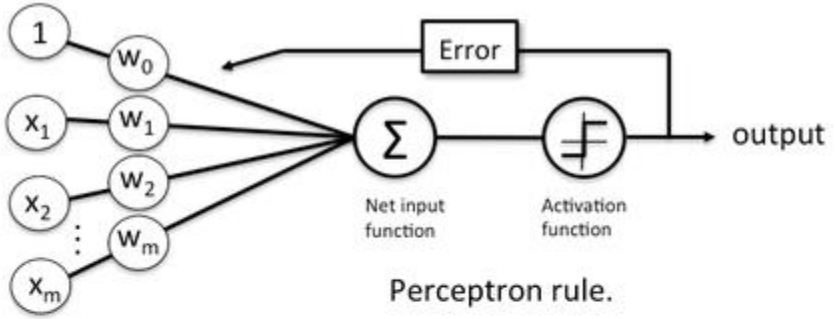
- Two types of parameters
  - Those learned from data
  - Those we specify – hyperparameters (e.g. regularization parameter in Logistic Regression)
- How to choose optimum hyperparameters?
  - Grid Search

```
# Initiallize GridSearchCV object from
# sklearn.grid_search module
from sklearn.grid_search import GridSearchCV
from sklearn.svm import SVC

# Create pipeline for SVM
pipe_svc = Pipeline([('scl', StandardScaler()),
                     ('clf', SVC(random_state=1))])
# Set parameter range
param_range = [0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0, 1000.0]
# Set param_grid to a list of
# dictionaries - specify parameters to tune
param_grid = [{'clf__C': param_range,
               'clf__kernel': ['linear']},
              {'clf__C': param_range,
               'clf__gamma': param_range,
               'clf__kernel': ['rbf']}]
```

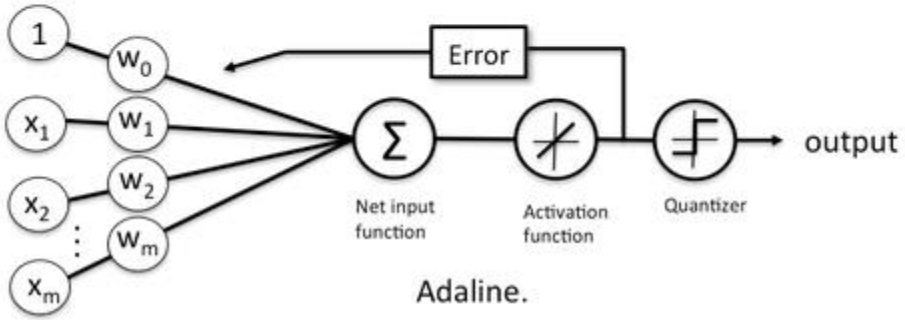
```
# set up k-fold cross-validation
gs = GridSearchCV(estimator=pipe_svc,
                  param_grid=param_grid,
                  scoring='accuracy',
                  cv=10,
                  n_jobs=-1)

# Use training data to perform grid search
gs = gs.fit(X_train, y_train)

# Obtain the score of the best-performing model
print(gs.best_score_)

# print the parameters of the best-performing model
print(gs.best_params_)

# Use independent test dataset
# to estimate performance of best-selected model
clf = gs.best_estimator_
clf.fit(X_train, y_train)
print('Test accuracy: %.3f' % clf.score(X_test, y_test))
```

Introduction to Deep Learning

- Perceptron vs Adaline (single layer neural network)

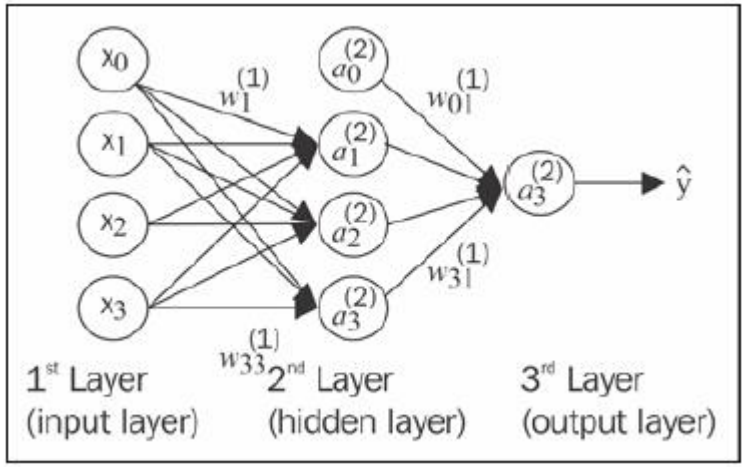


Perceptron rule.

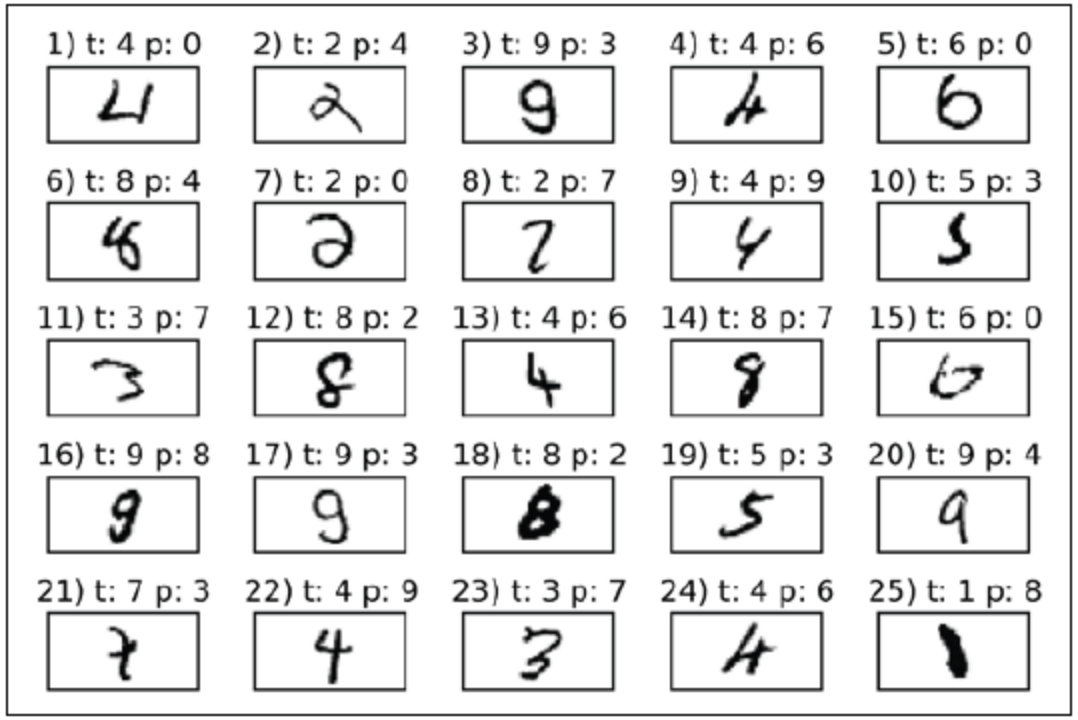


Adaline.

Multi-layer neural network



MNIST dataset

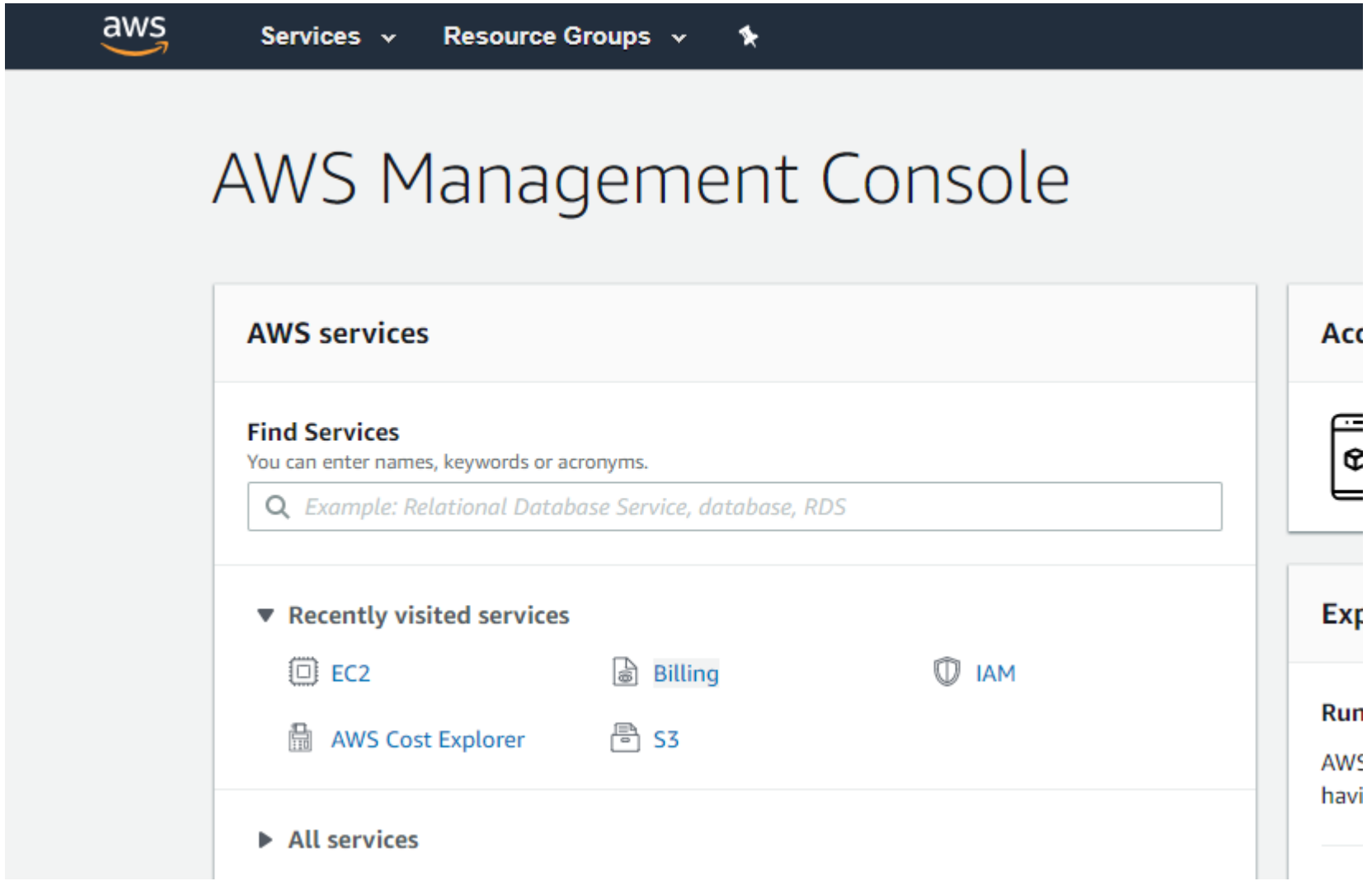


TensorFlow or Keras?

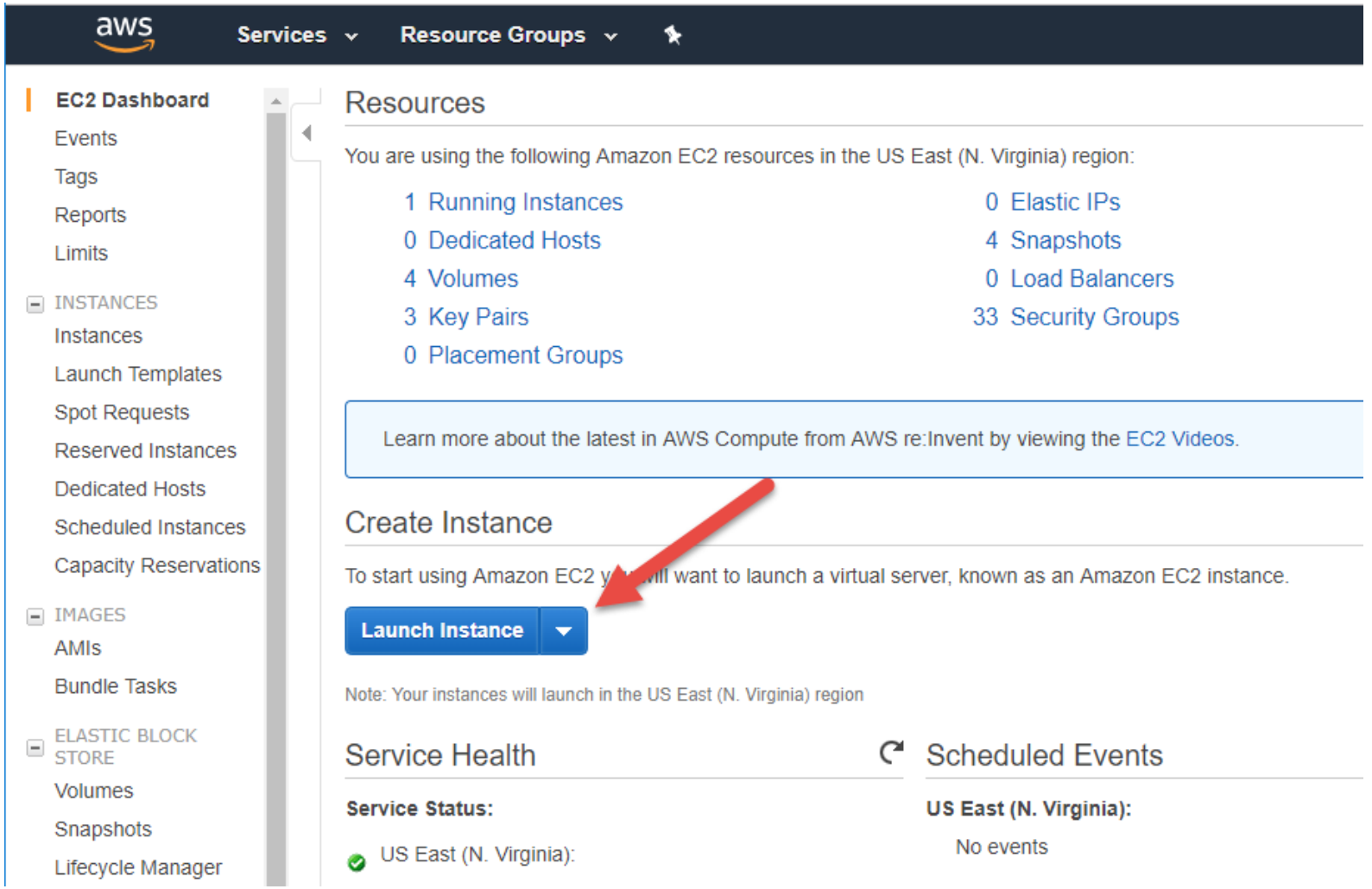
- https://medium.com/implodinggradients/tensorflow-or-keras-which-one-should-i-learn-5dd7fa3f9ca0

Deep learning with Python on AWS EC2

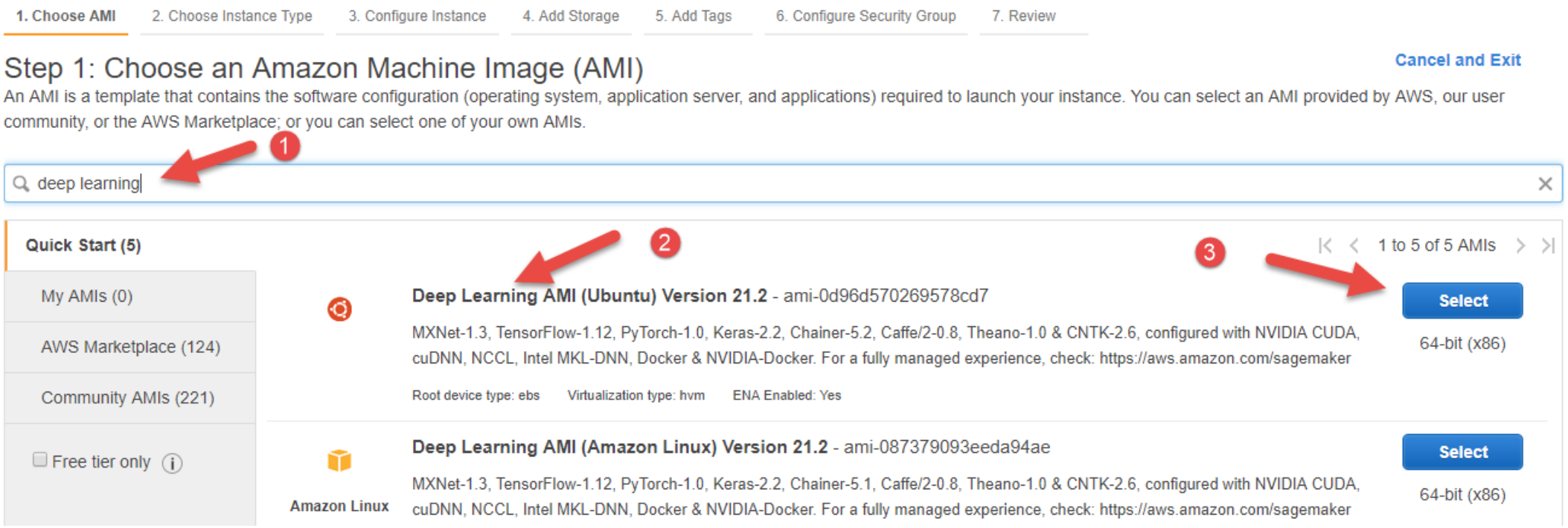
- Login:



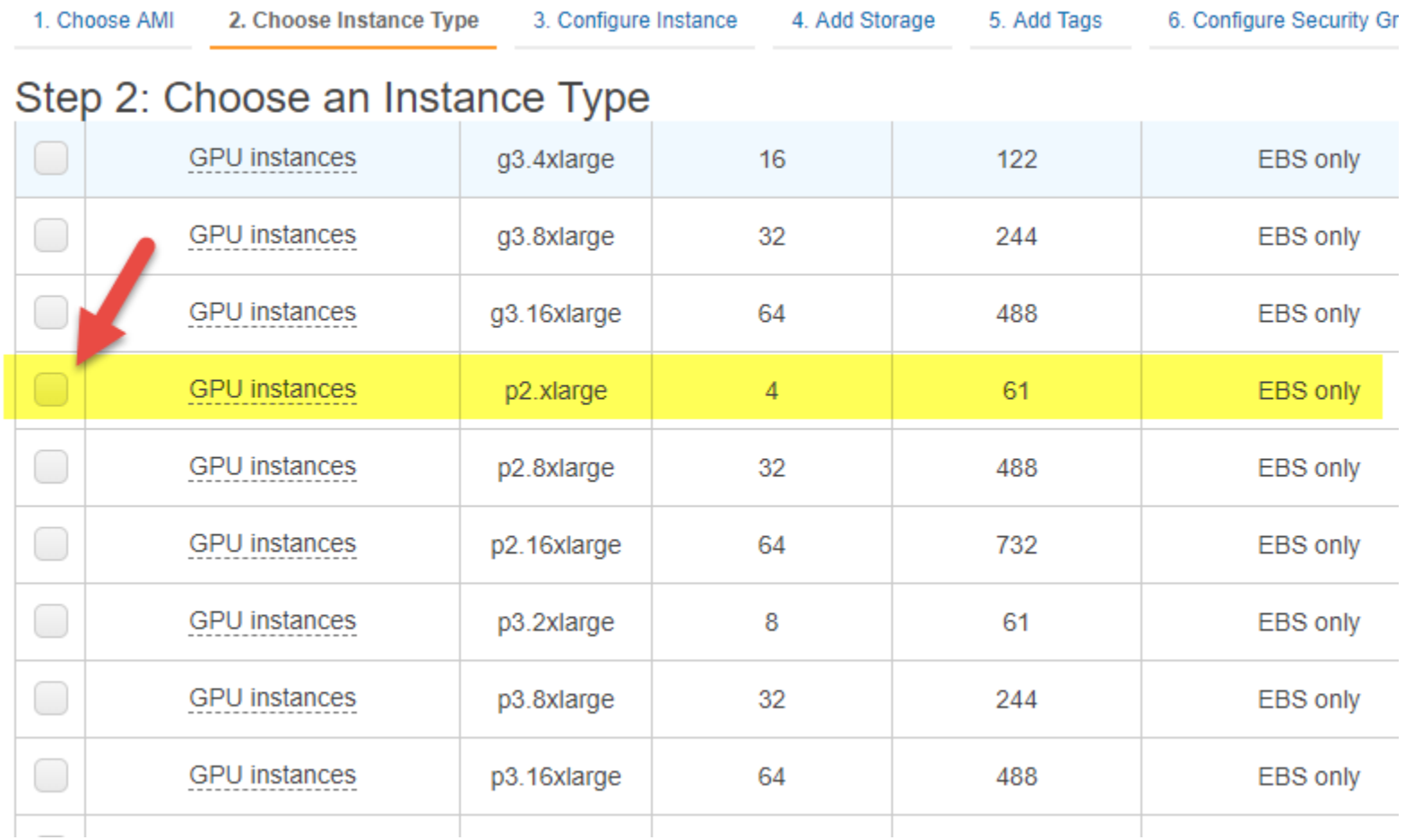
Navigate to EC2



Choose the appropriate AMI



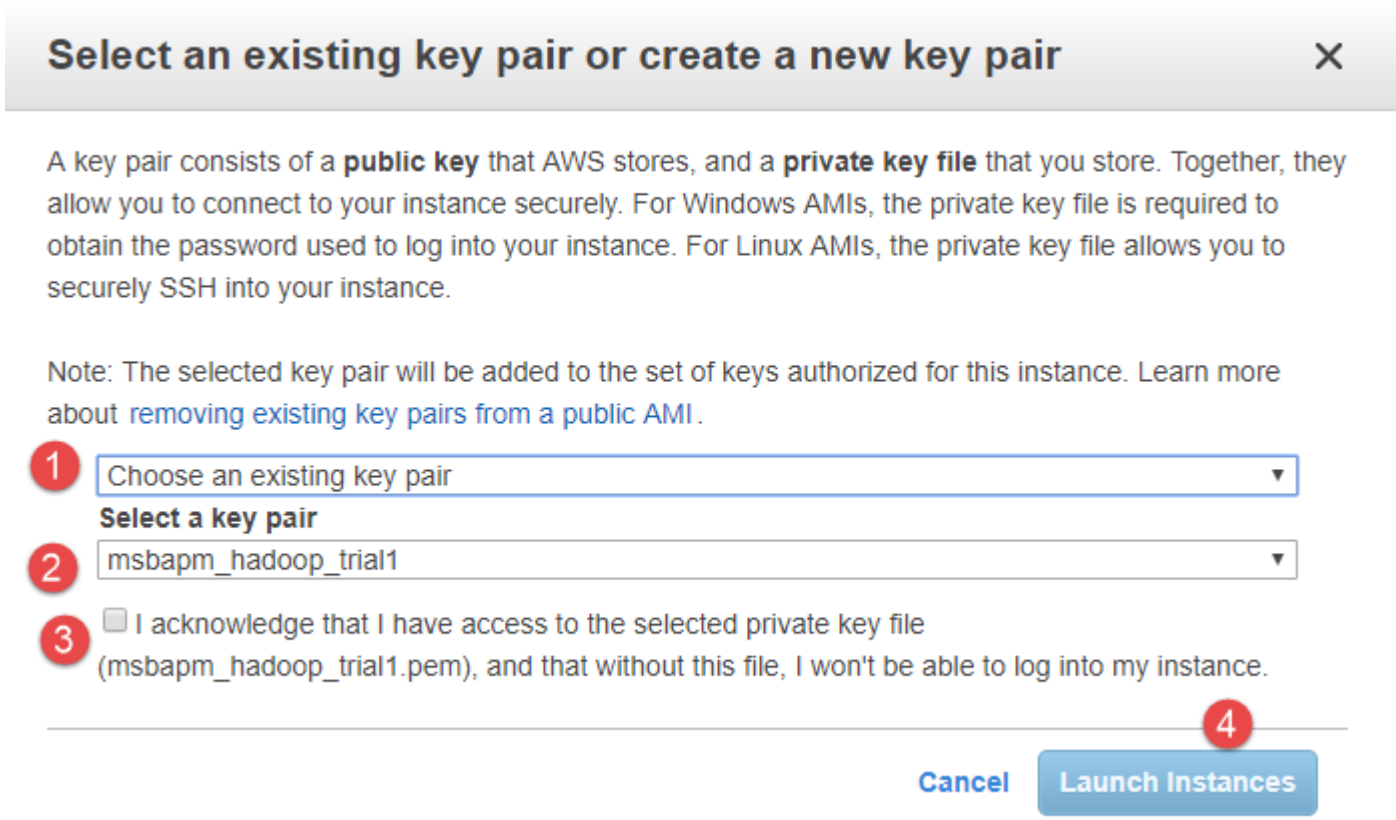
Choose the appropriate instance type (GPU)



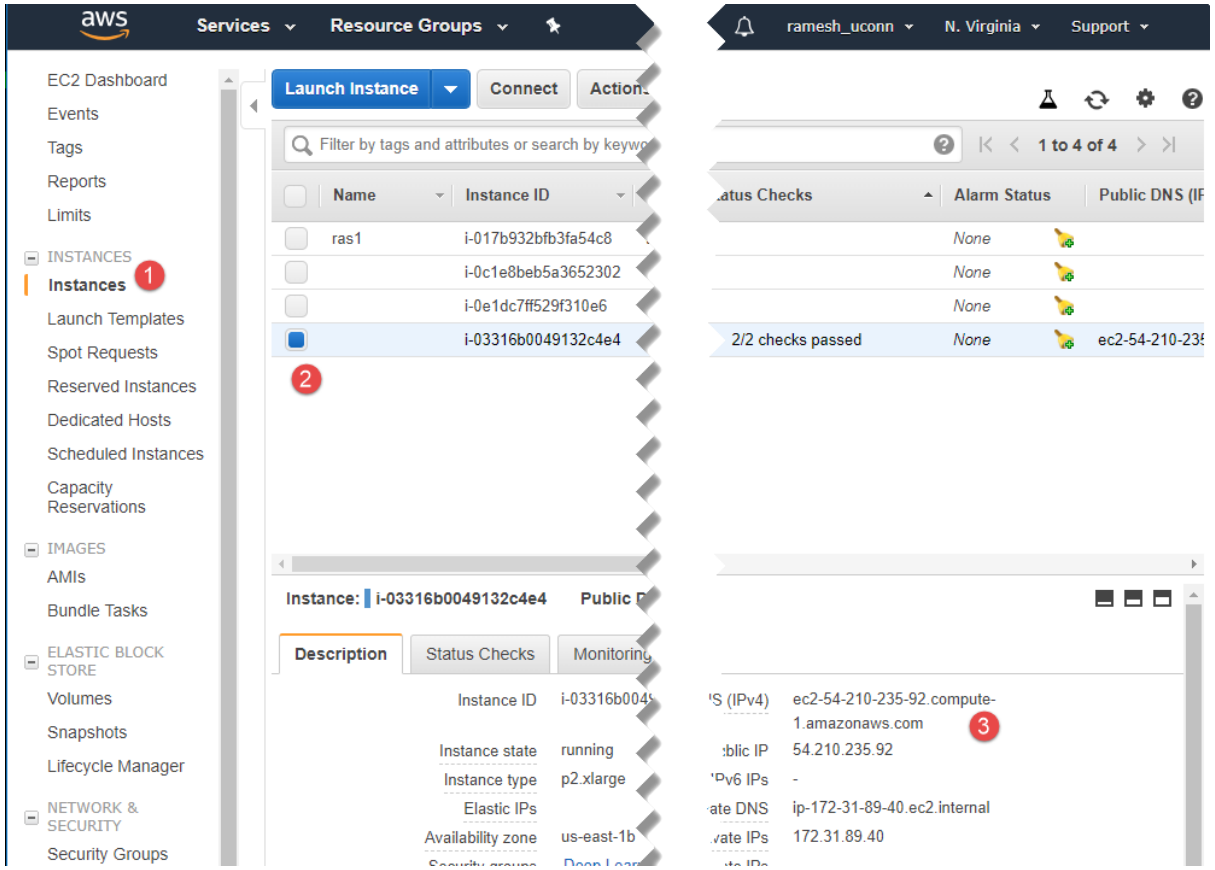
Click “review and launch”

Launching:

1. Choose a SSH key – existing pair or create a new pair
2. Choose the name
3. Acknowledge (check box)
4. Launch instance

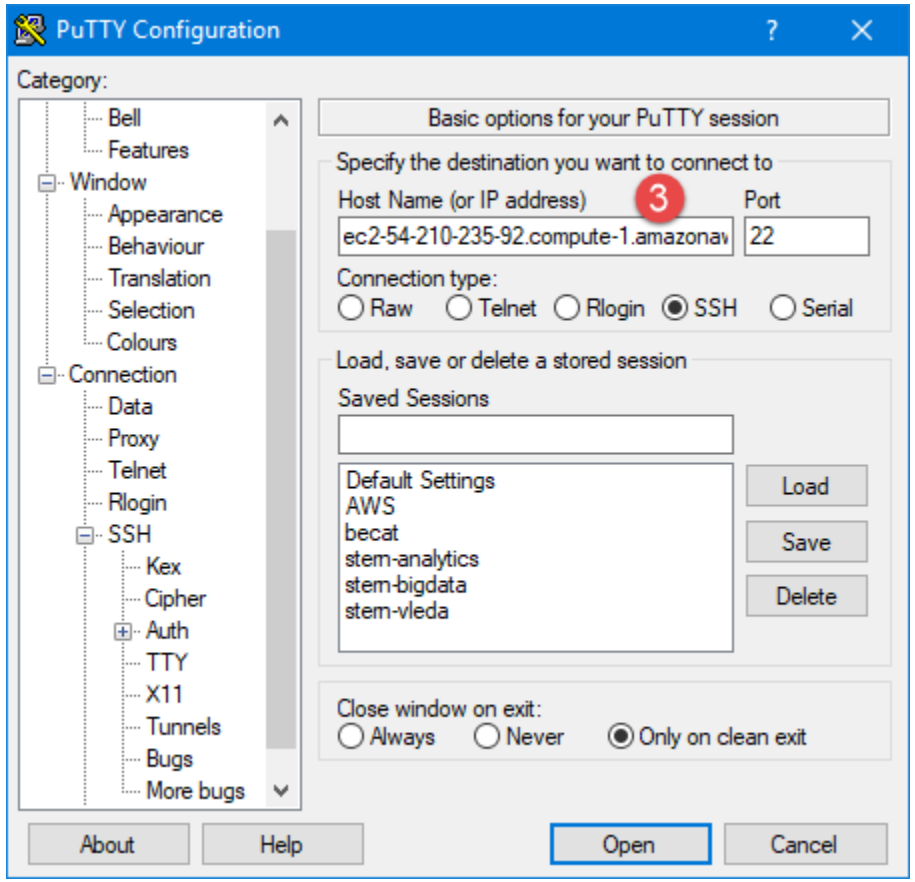


Login via Putty



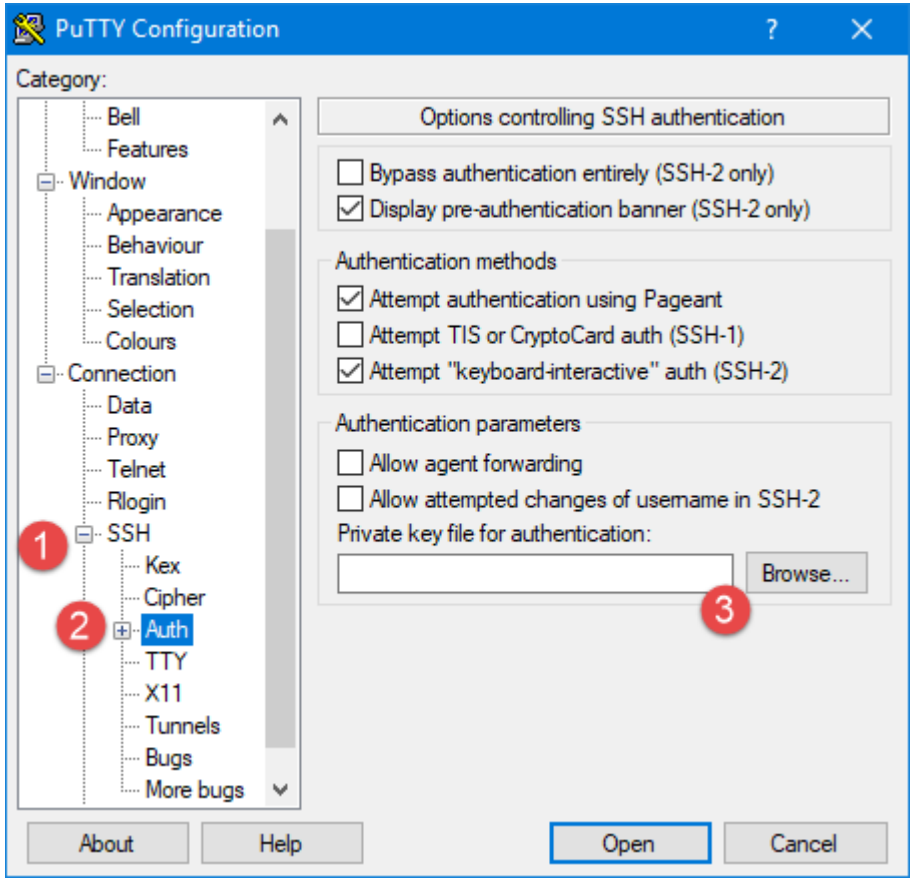
Login via putty

- Paste #3 from previous image: the EC2 instance URL

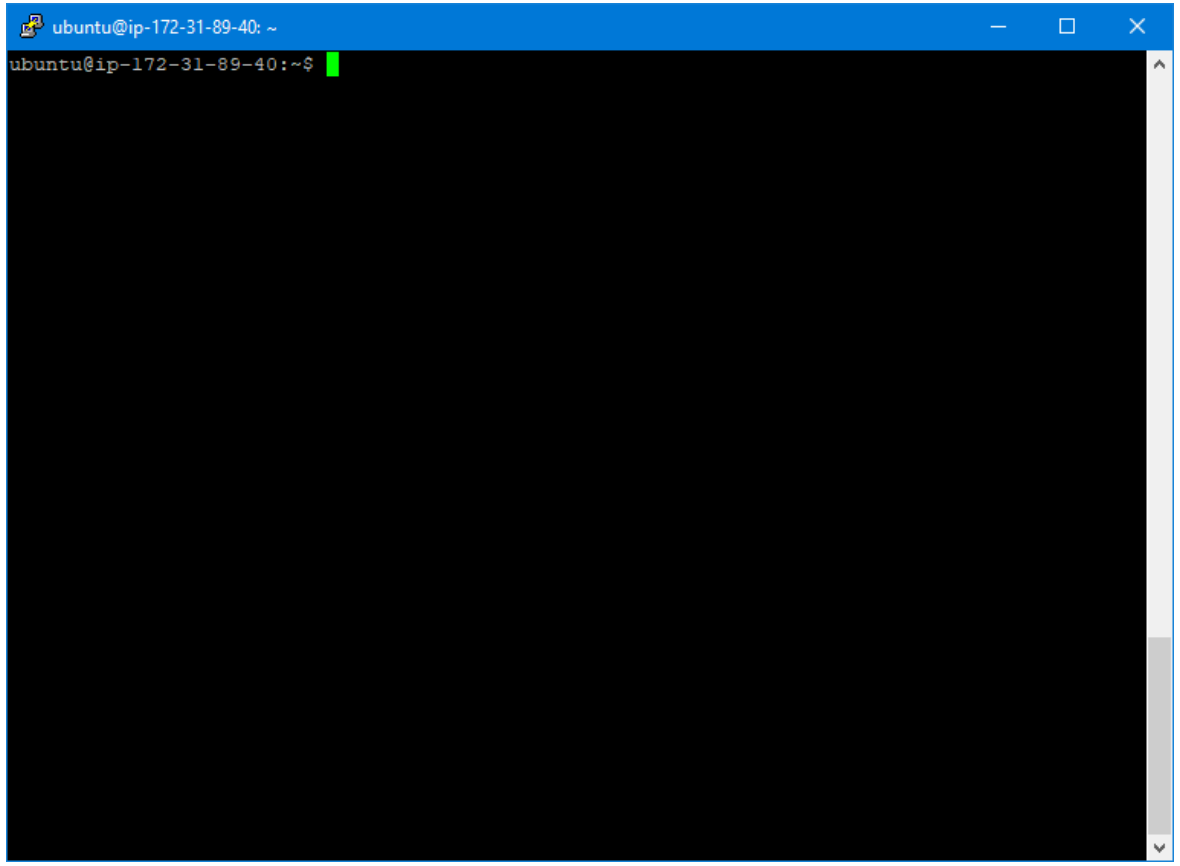


Login via putty

1. Click on SSH
2. Click on Auth
3. Choose (browse to) the .ppk file that you already created
4. (If necessary, use puttygen to convert .pem to .ppk)



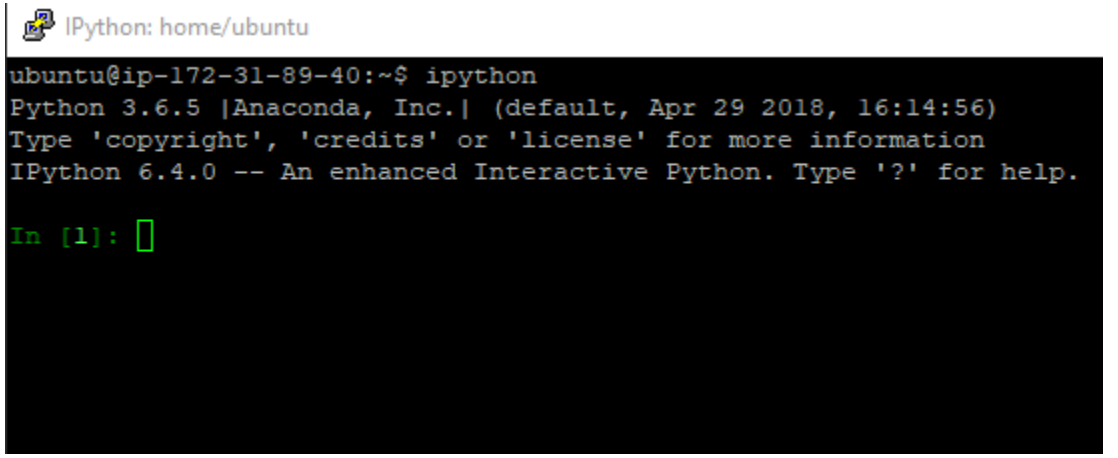
Your AWS EC2 Ubuntu screen



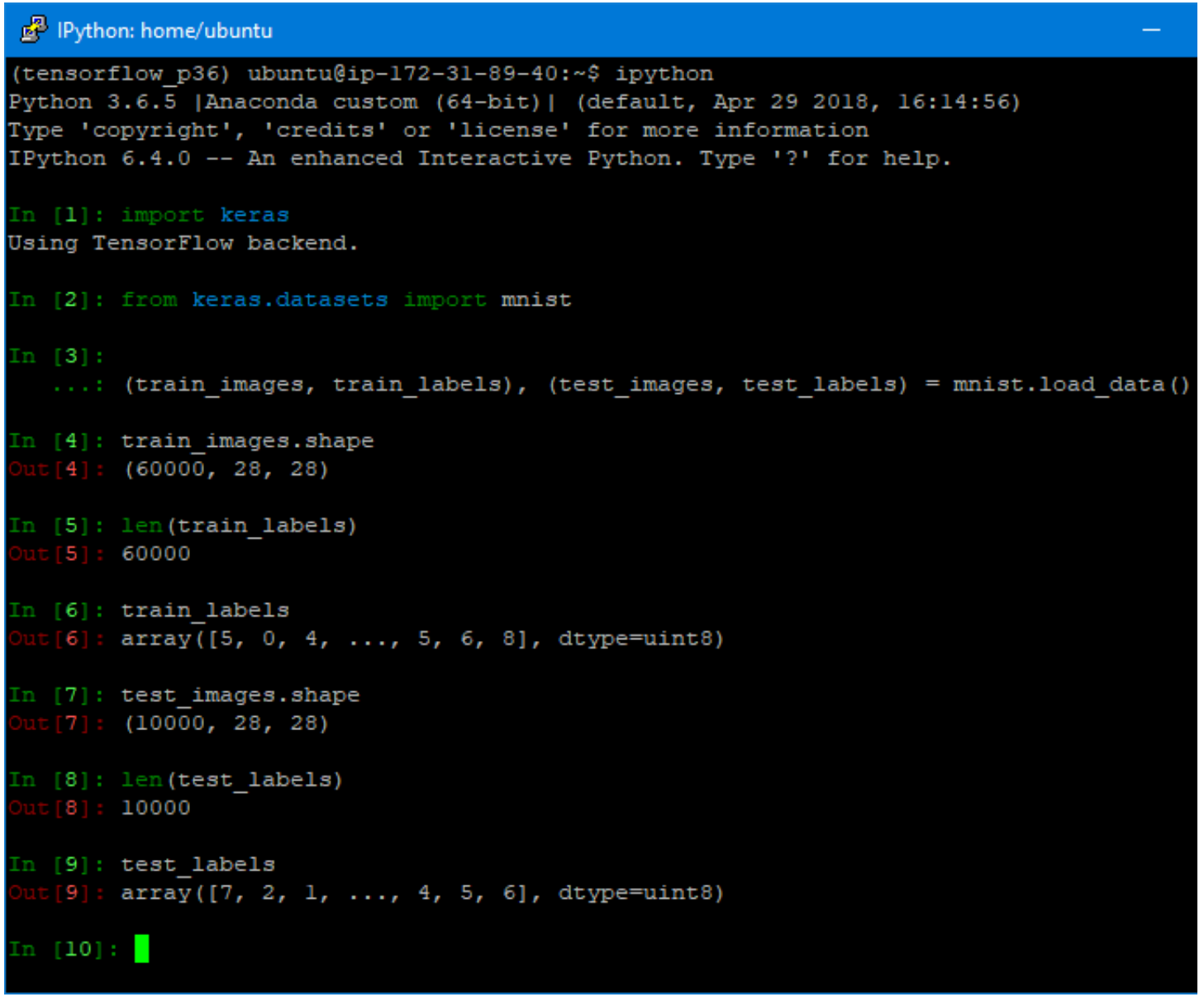
- Run these three commands:

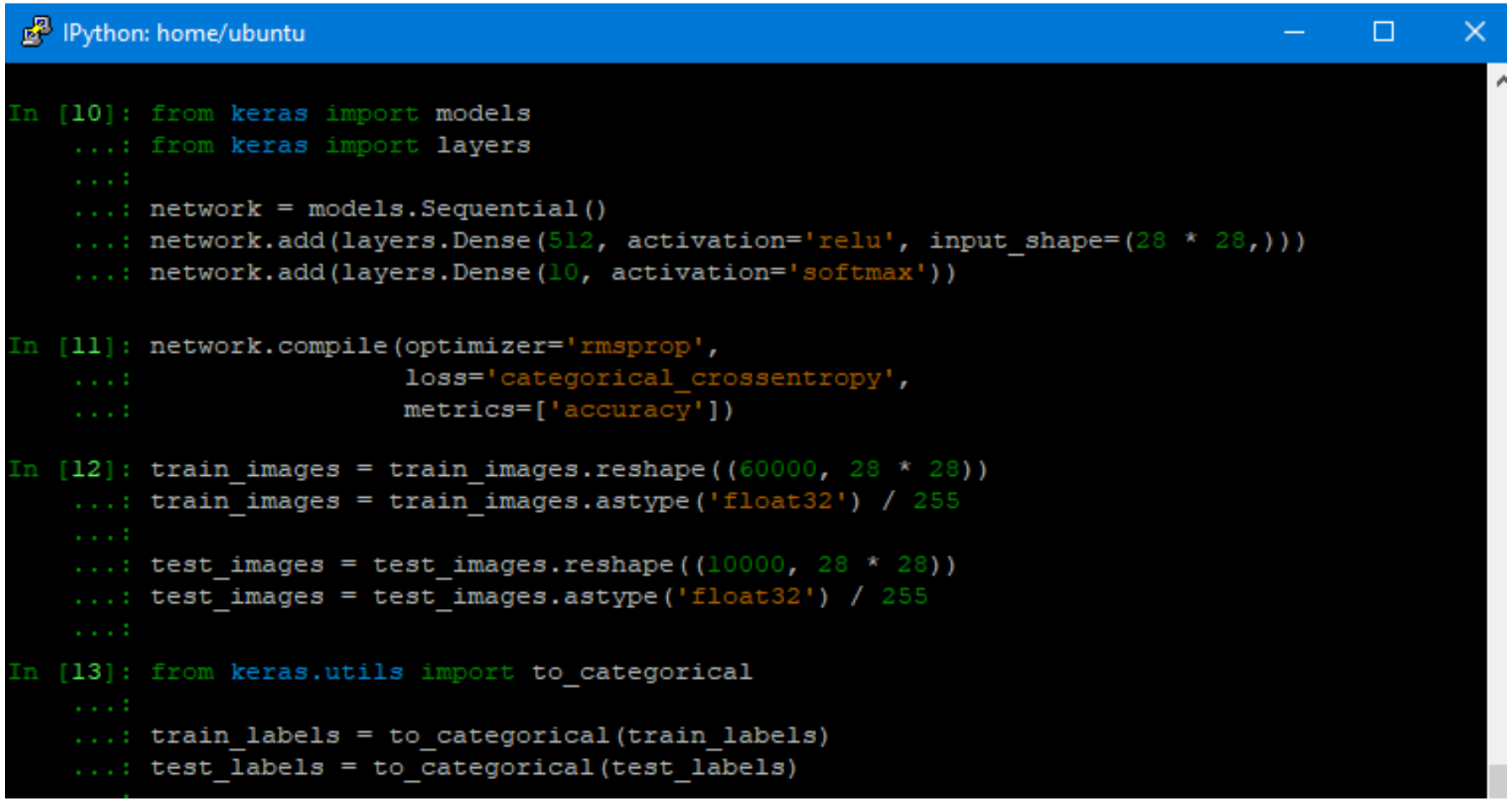
```
sudo pip3 install keras
sudo pip3 install --upgrade tensorflow-gpu
source activate tensorflow_p36
```

- Then, run iPython:



Code here: https://nbviewer.jupyter.org/github/fchollet/deep-learning-with-python-notebooks/blob/master/2.1-a-first-look-at-a-neural-network.ipynb




IPython: home/ubuntu
In [10]: from keras import models
...: from keras import layers
...:
...: network = models.Sequential()
...: network.add(layers.Dense(512, activation='relu', input_shape=(28 * 28,)))
...: network.add(layers.Dense(10, activation='softmax'))
In [11]: network.compile(optimizer='rmsprop',
...: loss='categorical_crossentropy',
...: metrics=['accuracy'])
In [12]: train_images = train_images.reshape((60000, 28 * 28))
...: train_images = train_images.astype('float32') / 255
...:
...: test_images = test_images.reshape((10000, 28 * 28))
...: test_images = test_images.astype('float32') / 255
...:
In [13]: from keras.utils import to_categorical
...:
...: train_labels = to_categorical(train_labels)
...: test_labels = to_categorical(test_labels)

```
In [14]:

In [14]: network.fit(train_images, train_labels, epochs=5, batch_size=128)
Epoch 1/5

60000/60000 [==============================] - 5s 80us/step - loss: 0.2586 - acc: 0.9248
Epoch 2/5
60000/60000 [==============================] - 2s 26us/step - loss: 0.1051 - acc: 0.9691
Epoch 3/5
60000/60000 [==============================] - 2s 26us/step - loss: 0.0687 - acc: 0.9794
Epoch 4/5
60000/60000 [==============================] - 2s 25us/step - loss: 0.0501 - acc: 0.9850
Epoch 5/5
60000/60000 [==============================] - 2s 25us/step - loss: 0.0376 - acc: 0.9889
Out[14]: <keras.callbacks.History at 0x7f441071b3c8>

In [15]:

In [15]: test_loss, test_acc = network.evaluate(test_images, test_labels)
10000/10000 [==============================] - 0s 37us/step

In [16]:

In [16]: print('test_acc:', test_acc)
test_acc: 0.9714
```