

Steps in deploying ML model using AWS EC2 instance

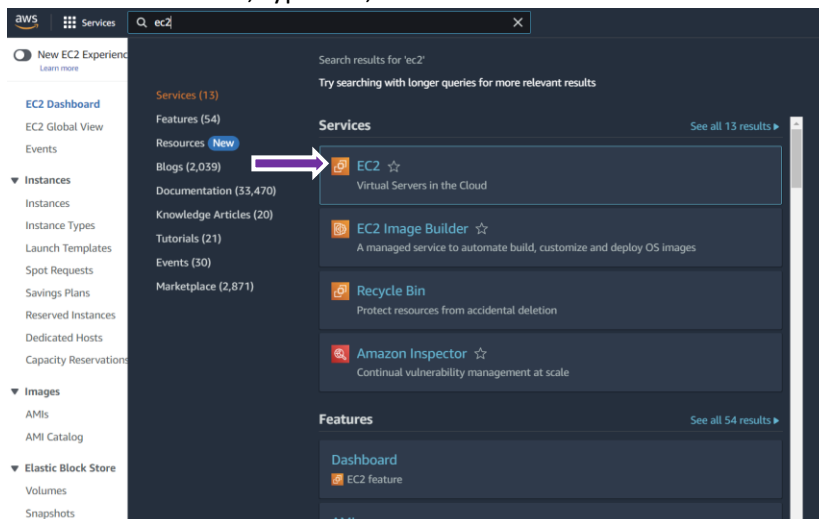
Part I

1. Create AWS Free Tier account

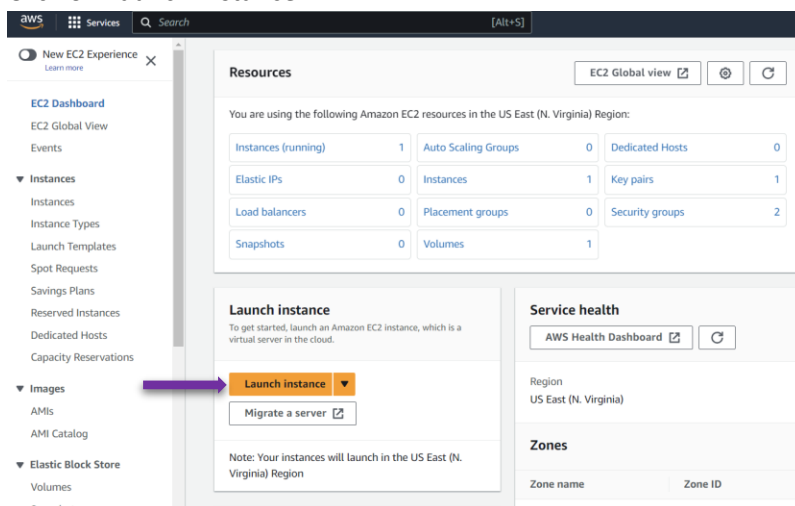


[AWS Free Tier](#)

2. Go to the search bar, type EC2, and click on EC2



3. Click on Launch instance



4. Give name for your app

Launch an instance Info

Amazon EC2 allows you to create virtual machines, or instances, that run on the AWS Cloud. Quickly get started by following the simple steps below.

Name and tags Info

Name

ML HOMO-LUMO-Gap

Add additional tags

5. Select the operating system

Application and OS Images (Amazon Machine Image) Info

An AMI is a template that contains the software configuration (operating system, application server, and applications) required to launch your instance. Search or Browse for AMIs if you don't see what you are looking for below

Q Ubuntu

×

Recents

Quick Start

Amazon Linux

aws

macOS

Mac

Ubuntu

ubuntu

Windows

Microsoft

Red Hat

Red Hat

SUSE Li

SUSE

Q

Browse more AMIs

Including AMIs from AWS, Marketplace and the Community

Q Ubuntu

×

▼

Quickstart AMIs (9)
Commonly used AMIs

My AMIs (0)
Created by me

AWS Marketplace AMIs (2178)
AWS & trusted third-party AMIs

Community AMIs (500)
Published by anyone

Refine results

Clear all filters

☐ Free tier only Info

OS category

☐ All Linux/Unix
 ☐ All Windows

Architecture

☐ 64-bit (Arm)
 ☐ 32-bit (x86)
 ☐ 64-bit (x86)

Ubuntu (9 filtered, 9 unfiltered)

ubuntu

Free tier eligible

Verified provider

Ubuntu Server 22.04 LTS (HVM), SSD Volume Type

ami-053b0d53c279acc90 (64-bit (x86)) / ami-0a0c8eebcd6dcbd0 (64-bit (Arm))

Select

64-bit (x86)

64-bit (Arm)

Platform: ubuntu

Root device type: ebs

Virtualization: hvm

ENA enabled: Yes

ubuntu

Free tier eligible

Verified provider

Ubuntu Server 20.04 LTS (HVM), SSD Volume Type

ami-0261755bbcb8c4a84 (64-bit (x86)) / ami-097d5b19d4f1a7d1b (64-bit (Arm))

Select

64-bit (x86)

64-bit (Arm)

Platform: ubuntu

Root device type: ebs

Virtualization: hvm

ENA enabled: Yes

Q Ubuntu

×

AMI from catalog

Recents

Quick Start

Amazon Machine Image (AMI)

ubuntu/images/hvm-ssd/ubuntu-jammy-22.04-amd64-server-20230516

ami-053b0d53c279acc90

Verified provider

Free tier eligible

Q

Browse more AMIs

Including AMIs from AWS, Marketplace and the Community

Catalog	Published	Architecture	Virtualization	Root device type	ENA Enabled
Quickstart AMIs	2023-05-16T03:38:03.000Z	x86_64	hvm	ebs	Yes

2

6. Create key-pair and save .pem file in your computer.

▼ Key pair (login) Info

You can use a key pair to securely connect to your instance. Ensure that you have access to the selected key pair before you launch the instance.

Key pair name - required

Select

Create new key pair

Create key pair

7. Use the remaining default values and launch the instance.

▼ Network settings Info

Network info

vpc-099ac967ccf8300a6

Subnet info

No preference (Default subnet in any availability zone)

Auto-assign public IP info

Enable

Firewall (security groups) info

A security group is a set of firewall rules that control the traffic for your instance. Add rules to allow specific traffic to reach your instance.

Create security group Select existing security group

We'll create a new security group called 'launch-wizard-1' with the following rules:

Allow SSH traffic from Anywhere 0.0.0.0/0

Allow HTTPS traffic from the internet

Allow HTTP traffic from the internet

Rules with source of 0.0.0.0/0 allow all IP addresses to access your instance. We recommend setting security group rules to allow access from known IP addresses only.

▼ Summary

Number of instances Info

1

Software Image (AMI)

Ubuntu Server 22.04 LTS (HVM)...read more

ami-053b0653c279ac9d0

Virtual server type (instance type)

t2.micro

Firewall (security group)

New security group

Storage (volumes)

1 volume(s) - 8 GiB

Free tier: In your first year includes 750 hours of t2.micro (or t3.micro in the Regions in which t2.micro is unavailable) instance usage on free tier AMIs per month.

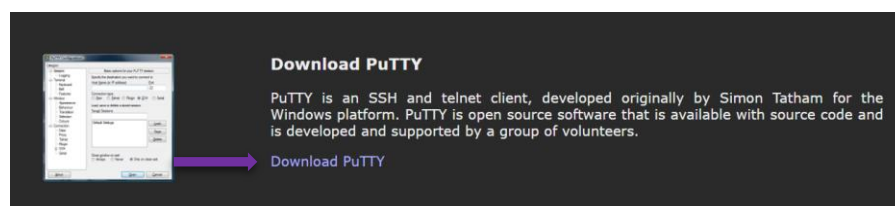
Launch instance

Review commands

Part II

1. Install three software packages (Putty, PuttyGen and WinSCP)

<https://www.putty.org/>



<https://www.puttygen.com/download-putty>


Choose the appropriate windows installer version (32-bit or 64-bit) and click on it.

MSI ('Windows Installer for putty')			
32-bit:	putty-0.79-installer.msi	(via FTP)	(signature)
64-bit:	putty-64bit-0.79-installer.msi	(via FTP)	(signature)
64-bit x86:	putty-arm64-0.79-installer.msi	(via FTP)	(signature)
Unix source archive for putty			
.tar.gz:	putty-0.79.tar.gz	(via FTP)	(Signature)

<https://winscp.net/eng/download.php>

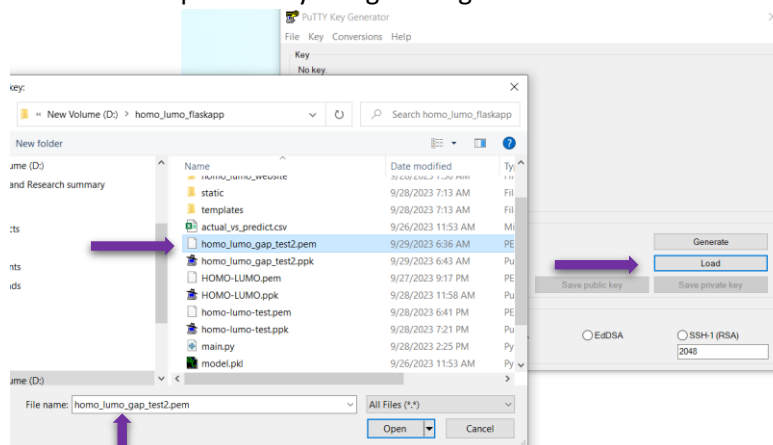
WinSCP 6.1 is a major application update. New features and enhancements include:

- Local file manager mode (two local panels).
- Windows 11 flat style graphics.
- SSH core upgraded to PuTTY 0.78. That includes support for OpenSSH certificates.
- Ongoing delete operation can be moved to background queue.
- Showing directory size in file panel.
- [List of all changes.](#)

[DOWNLOAD WINSCP 6.1.2 \(11 MB\)](#)  Get it from Microsoft [OTHER DOWNLOADS](#)

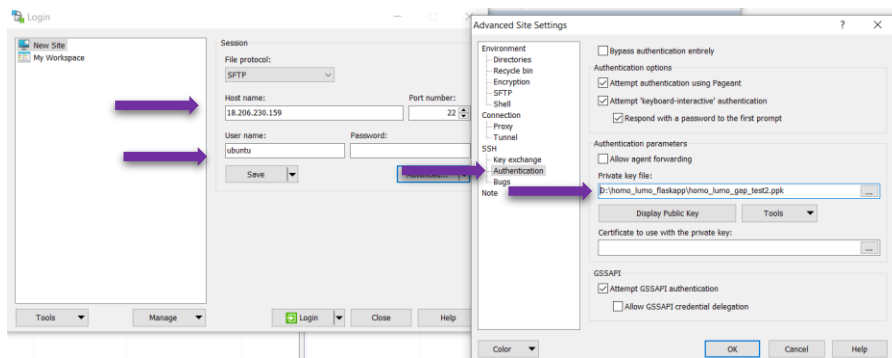
264,868 downloads since 2023-09-19 [What is this?](#)

2. Generate the private key using PuTTYgen

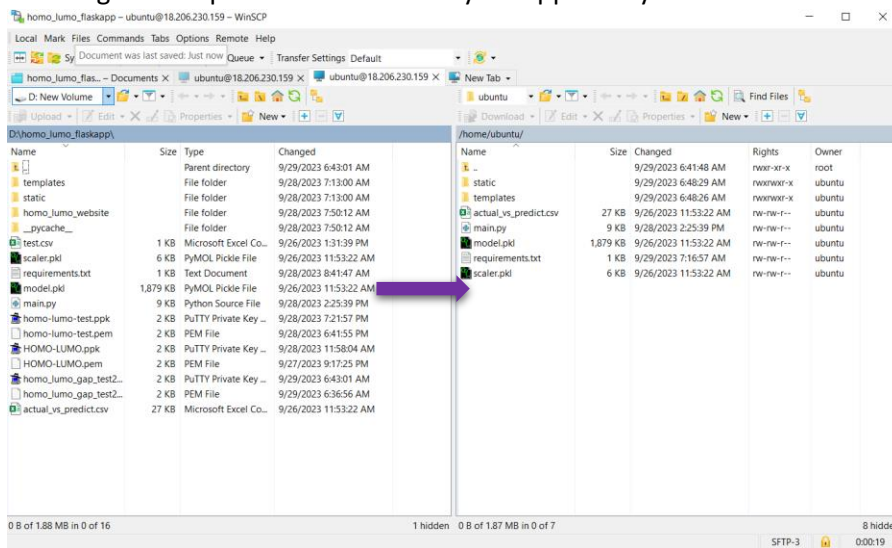


3. Use WinSCP to move your files by drag and drop to your EC2 instance storage

- First connect to EC2 instance using its public IP address or Public IPv4 DNS and using the private key generated using PuTTYgen.

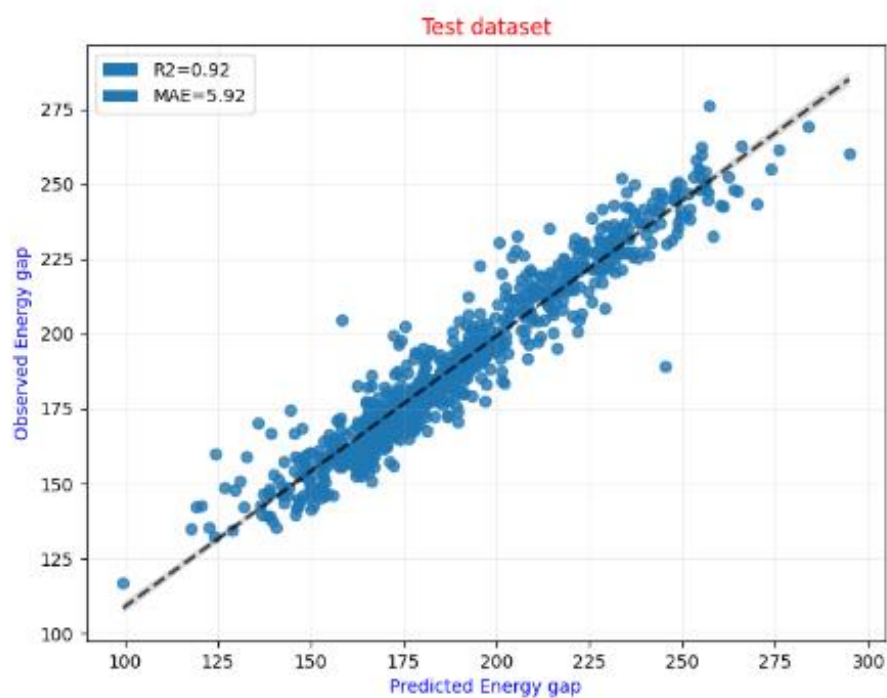
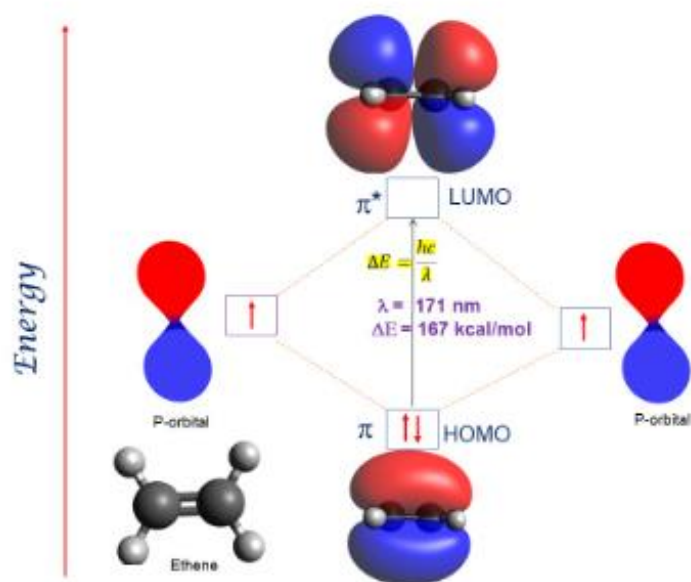


- Drag and drop files needed to run your app from your local folder to EC2 instance storage.



I deployed a ML web app for HOMO-LUMO gap prediction using AWS CE2 instance

HOMO-LUMO Energy Gap Prediction



Enter SMILES or few SMILES in single or double quotations separated by comma such as ["CCC","CCO"] :

Upload CSV file:

Choose File

No file chosen

Predict

See the Results Below:

	SMILES	Predicted
0	CCCCCCC	262.72
1	C=CCCCC	226.81
2	C=CC=CCC	187.56
3	C=CC=CC=C	179.67
4	C=CC=CC=CC=C	173.84

[Download predicted_HOMO-LUMO energygap.csv](#)

Structures from CSV file:

Search

Text

SMARTS



Sort



☐ 0



262.72

☐ 1



226.81

☐ 2



187.56

☐ 3



179.67

☐ 4



173.84