

1092_BioInfomatics_FP

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Outline

- Project Goal
- Problems & Solutions
- Deployment
- Conclusion



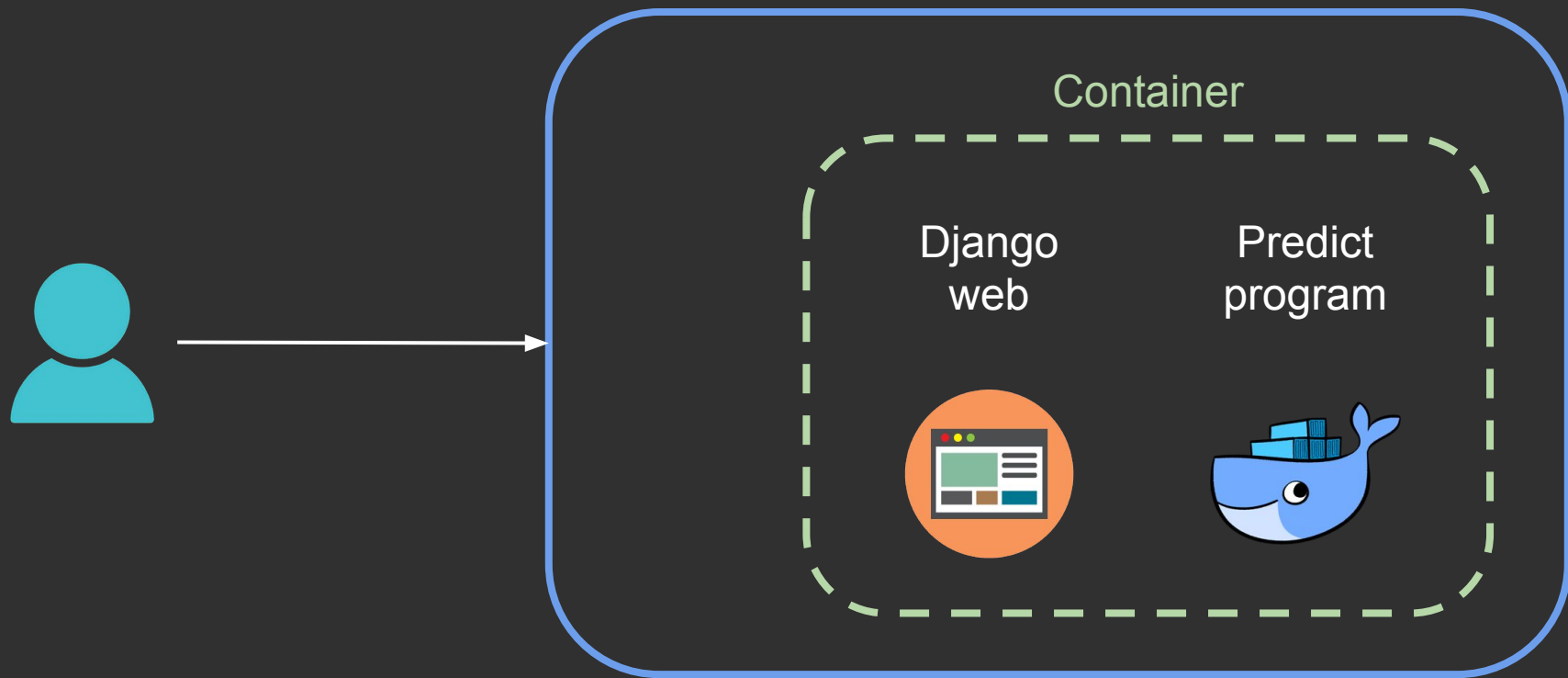
Project Goal



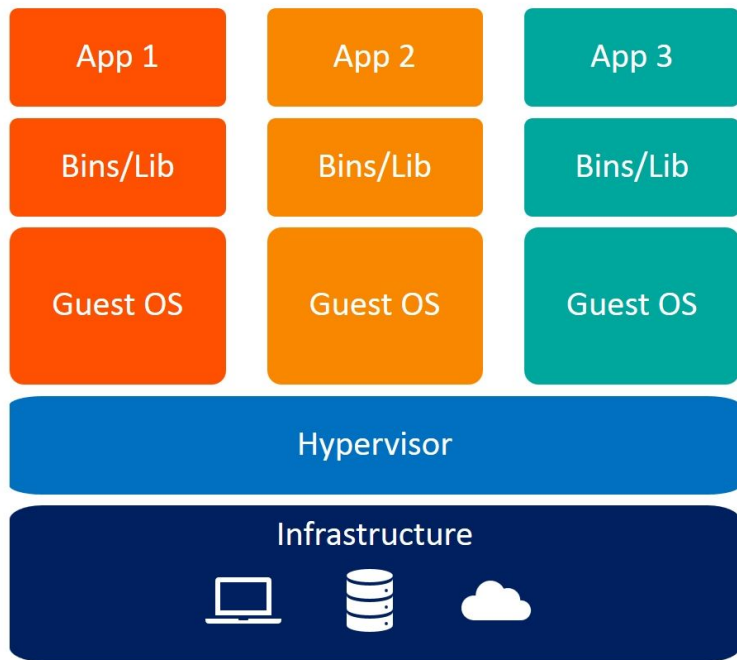
Goal

- Source
 - [Predict app docker image \(36G\)](#)
 - [GODoc web code](#)
- Make it runnable
- Re-pack docker image
- Deploy to remote server

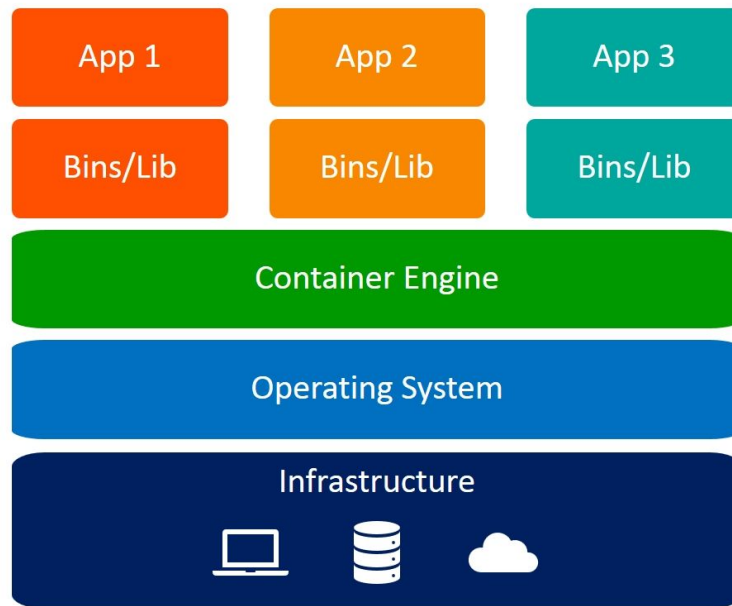
Architecture



VM v.s. Container

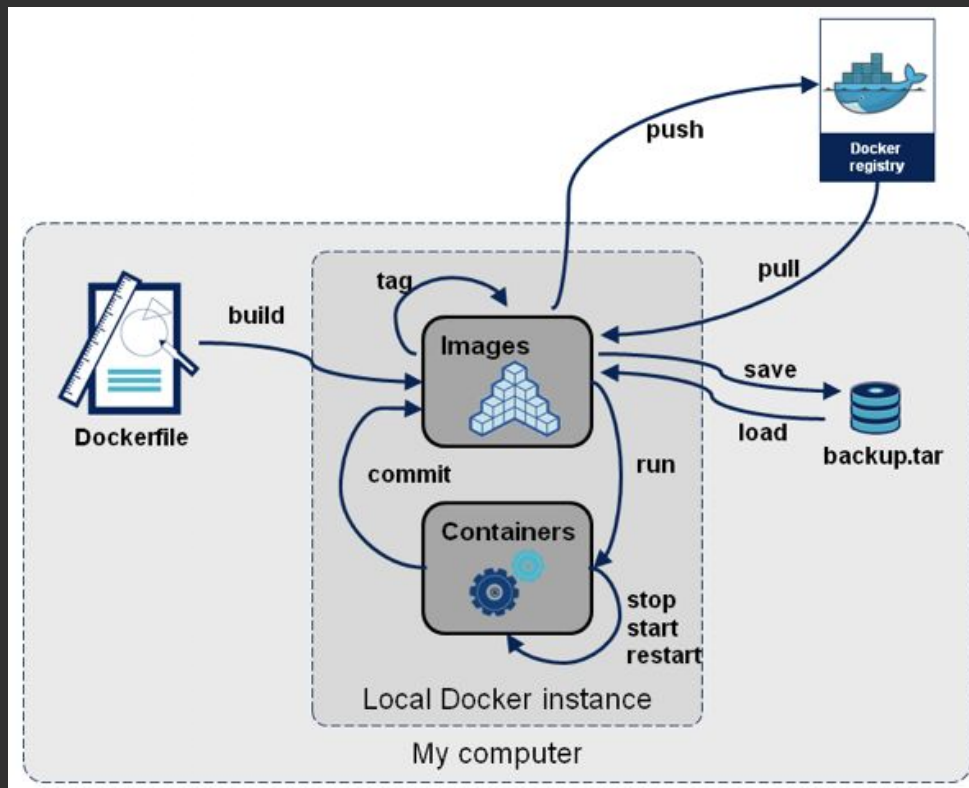


Virtual Machines



Containers

Docker Basic Flow



Problems & Solutions



Container run but failed

```
# roberson @ LAPTOP-BICQ1LBS in /mnt/c/Users/rober [2:57:49]
```

```
$ docker run --name pps-v2-app pps:v2
```

```
# roberson @ LAPTOP-BICQ1LBS in /mnt/c/Users/rober [2:57:53]
```

```
$ docker ps -a | grep pps-v2-app
```

```
700e440efab7    pps:v2          "bash"
```

```
8 seconds ago
```

```
Exited (0) 7 seconds ago
```

```
pps-v2-app
```

```
$ docker image history pps:v2
```

IMAGE	CREATED	CREATED BY	SIZE	COMMENT
382482bdb9ef	3 years ago	bash	36GB	Add prediction
<missing>	3 years ago	/bin/sh -c #(nop) CMD ["/bin/bash"]	0B	
<missing>	3 years ago	/bin/sh -c mkdir -p /run/systemd && echo 'do...	7B	
<missing>	3 years ago	/bin/sh -c sed -i 's/^#\s*(deb.*universe\)\$...	2.76kB	
<missing>	3 years ago	/bin/sh -c rm -rf /var/lib/apt/lists/*	0B	
<missing>	3 years ago	/bin/sh -c set -xe && echo '#!/bin/sh' > /...	195kB	
<missing>	3 years ago	/bin/sh -c #(nop) ADD file:f5013009a258adf00...	221MB	

Indicate cmd with interactive mode

```
# roberston @ LAPTOP-BICQ1LBS in /mnt/c/Users/rober [3:30:00]
$ docker run -it --name pps-v2-app pps:v2 /bin/bash
root@0bd5688b6e07:/# ls
bin boot dev etc home lib lib64 media mnt opt proc root run sbin srv sys tmp usr var ~
root@0bd5688b6e07:/# ls root/
anaconda2 blast cafa3 data nextflow pps predict
root@0bd5688b6e07:/#
```

Mount web from desktop into container

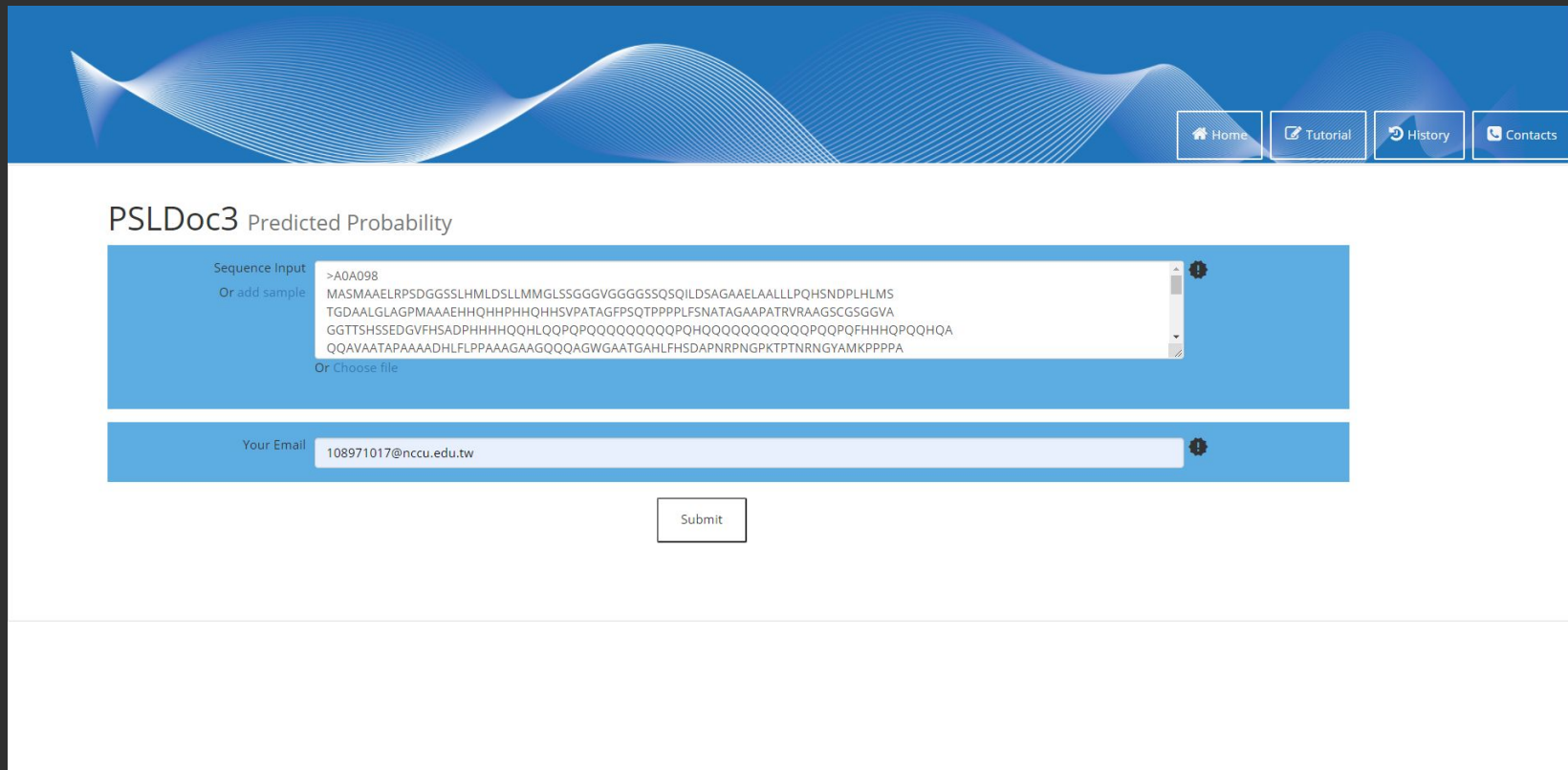
```
$ docker run -it --name pps-v2-app --mount "type=bind,source=/mnt/c/Users/rober/Desktop/G0Doc/web,target=/web" pps:v2 /bin/bash
root@6aa485da8b1f:/# ls web/
Data Project Protein README.md Upload data.csv db.sqlite3 images manage.py venv
root@6aa485da8b1f:/# cp -R web/ root/web/
root@6aa485da8b1f:/# ls root/web/
Data Project Protein README.md Upload data.csv db.sqlite3 images manage.py venv web
root@6aa485da8b1f:/# ls root/
anaconda2 blast cafa3 data nextflow pps predict web
root@6aa485da8b1f:/# |
```

Fixed some bugs of web app

- Upload sequence folder not exist.
- File encoding error.
- Change & apply Smtip token.



Make it worked locally!



The image shows a web application interface for PSLDoc3. The header is blue with a white wavy line pattern and contains four navigation buttons: Home, Tutorial, History, and Contacts. The main content area is white and features the title 'PSLDoc3 Predicted Probability'. Below the title is a large blue input box. Inside this box, on the left, are labels 'Sequence Input' and 'Or add sample'. To the right of these labels is a text area containing a long sequence of amino acid codes. Below the text area is a link 'Or Choose file'. Below the blue input box is a light blue box containing a label 'Your Email' and a text input field with the email address '108971017@nccu.edu.tw'. At the bottom center of the form is a 'Submit' button.

PSLDoc3 Predicted Probability

Sequence Input >A0A098

Or add sample MASMAAELRP5DGGSSLHMLDSLMMGLSSGGVGGGGSSQ5ILDSAGAAELAALLPQHSNDPLHMS
TGDAALGLAGPMAAAEHQHHPHQHHSVPATAGFPSQTPPPLFSNATAGAAPTRVRAAGSCSGGVA
GGTTSSESDEGVFHSADPHHHHQHLQQPQQQQQQQQQHQQQQQQQQQQQPQFHHHPQQHQA
QQAVAATAPAAAADHLFPAAAGAAGQQAGWGAATGAHLFHSADPNRPNPKPTNRRNGYAMKPPPPA

Or Choose file

Your Email 108971017@nccu.edu.tw

Submit

docker commit & built new image

```
FROM pps:v4.1
EXPOSE 80
WORKDIR /root/web/

RUN cd /root/web
ENTRYPOINT ["/root/anaconda2/bin/python", "manage.py", "runserver", "0.0.0.0:80"]
```

```
# rober @ LAPTOP-BICQ1LBS in ~\Desktop\GODOC on git:master ≡ 18 ~2 [22:03:55]
$ docker build -t psldoc3:v5.0.0 .
    0.0s
    0.0s
=> [internal] load metadata for docker.io/library/pps:v4.1
=> [1/3] FROM docker.io/library/pps:v4.1
=> CACHED [2/3] WORKDIR /root/web/
=> CACHED [3/3] RUN cd /root/web
=> exporting to image
=> => exporting layers
=> => writing image sha256:eba789acef8901b36cff35fe92b1ae3779fb976b7e15ba2f24f9c5e81c57ca09
=> => naming to docker.io/library/psldoc3:v5.0.0
```

```
0.0s
0.0s
0.0s
0.0s
0.0s
0.0s
0.0s
0.0s
```

But got error after pack new image...

Command output:

```
N E X T F L O W ~ version 0.26.3
Launching `/root/predict/tfpssm_db.nf` [suspicious_wing] - revision: 81feca8167
[warm up] executor > local
[08/6841d6] Submitted process > blast (1)
Save PSI-BLAST result to /root/predict/Output/47805/88524/psiBlastResult/A0A098.txt
[59/04a865] Submitted process > tfpssm (1)
Save tfpssm result to /root/predict/Output/47805/88524/tfpssm/A0A098.txt
```

Command error:

```
Traceback (most recent call last):
  File "/root/predict/pca_folder.py", line 3, in <module>
    import pandas
  ImportError: No module named pandas
```

Use symbolic link to redirect the cmd

Before

```
lrwxrwxrwx 1 root root          9 Dec 21  2013 python -> python2.7
lrwxrwxrwx 1 root root          9 Dec 21  2013 python2 -> python2.7
-rwxr-xr-x 1 root root 3341288 Nov 23  2017 python2.7
lrwxrwxrwx 1 root root          9 Mar 23  2014 python3 -> python3.4
-rwxr-xr-x 2 root root 3693624 Nov 17  2016 python3.4
```

After

```
lrwxrwxrwx 1 root root          26 Jun 14 13:20 python -> /root/anaconda2/bin/python
lrwxrwxrwx 1 root root          9 Dec 21  2013 python-bk -> python2.7
lrwxrwxrwx 1 root root          9 Dec 21  2013 python2 -> python2.7
-rwxr-xr-x 1 root root 3341288 Nov 23  2017 python2.7
lrwxrwxrwx 1 root root          9 Mar 23  2014 python3 -> python3.4
-rwxr-xr-x 2 root root 3693624 Nov 17  2016 python3.4
```


Output new docker image

```
# roberson @ LAPTOP-BICQ1LBS in /mnt/c/Users/rober/Desktop [8:54:25] C:1
$ docker save -o psldoc-image/psldoc3-v0.0.5.tar.gz psldoc3:v0.0.4
|
```

名稱	修改日期	類型	大小	
 psldoc3-v0.0.4.tar.gz	2021/6/14 下午 11:22	WinRAR 壓縮檔	11,982,732 KB	11G

Deployment



TWCC - centos VM

- Install docker in centos.
- Upload docker image & run.
- Enable 80 port from security group rule.

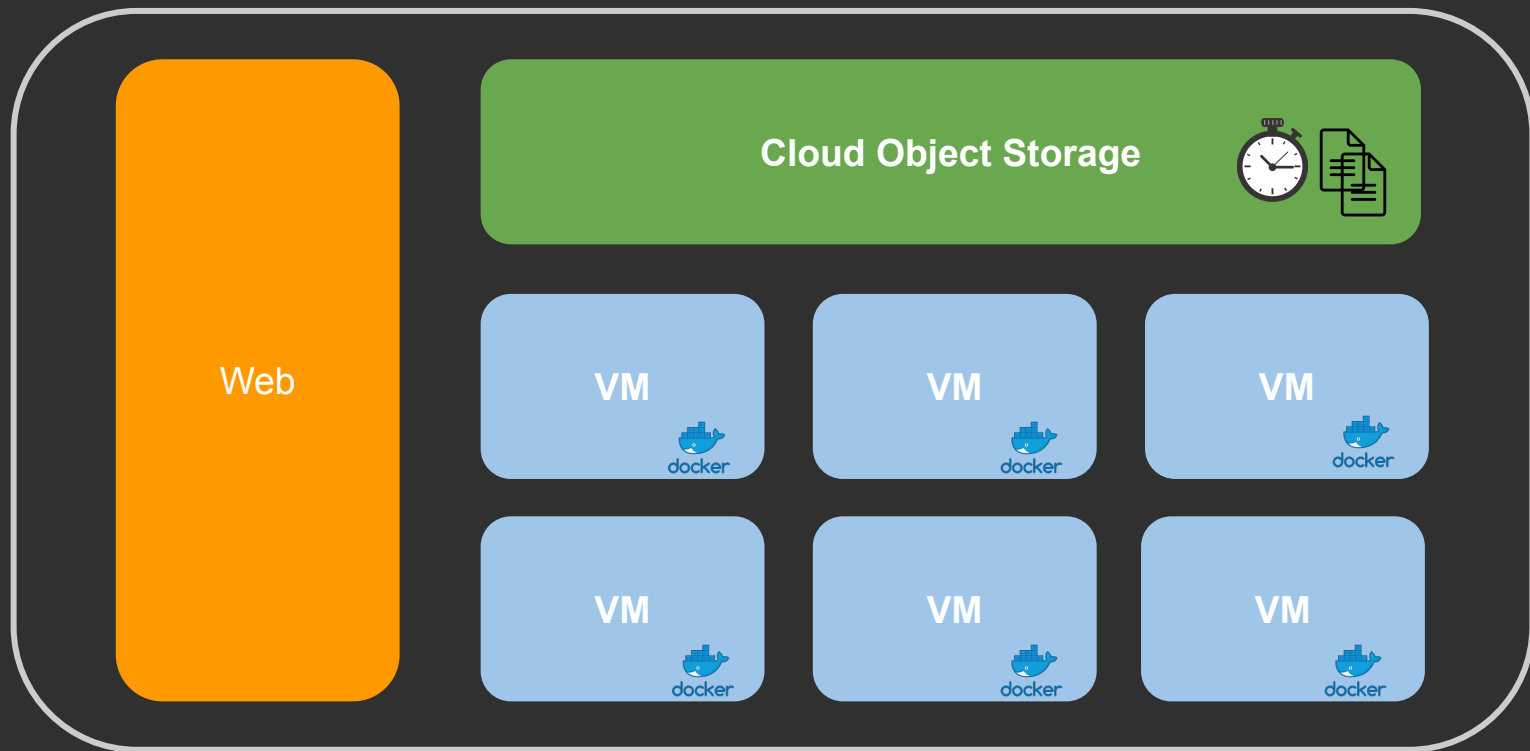
<input type="checkbox"/>	ID ↓	Direction	Network Type	Port Range (Min)	Port Range (Max)	Protocol	CIDR	
<input type="checkbox"/>	fbd79c87-ddab-423f-94b8-364b3d05a441	ingress	IPv4	22	22	tcp	0.0.0.0/0	⋮
<input type="checkbox"/>	cfacc3d6-6c6c-406a-a989-1b26667b1342	ingress	IPv4	80	80	tcp	0.0.0.0/0	⋮
<input type="checkbox"/>	c7e065d5-9888-4e75-af8c-e2cf4bab1851	egress	IPv4			ANY	0.0.0.0/0	⋮
<input type="checkbox"/>	b5e4bf02-6409-45ab-a7fb-7e669858cfd0	ingress	IPv4			icmp	0.0.0.0/0	⋮
<input type="checkbox"/>	9fef602-f674-450d-b264-022df9614076	egress	IPv6			ANY	::/0	⋮
<input type="checkbox"/>	9ebaa6c5-1434-4163-9672-e8b935097bff	ingress	IPv4	443	443	tcp	0.0.0.0/0	⋮

Conclusion

- <https://changlabserver.com//psldoc3>
- The docker image cannot be reduced.
- The web has large coupling with predict app.



Extensible Architecture



The End