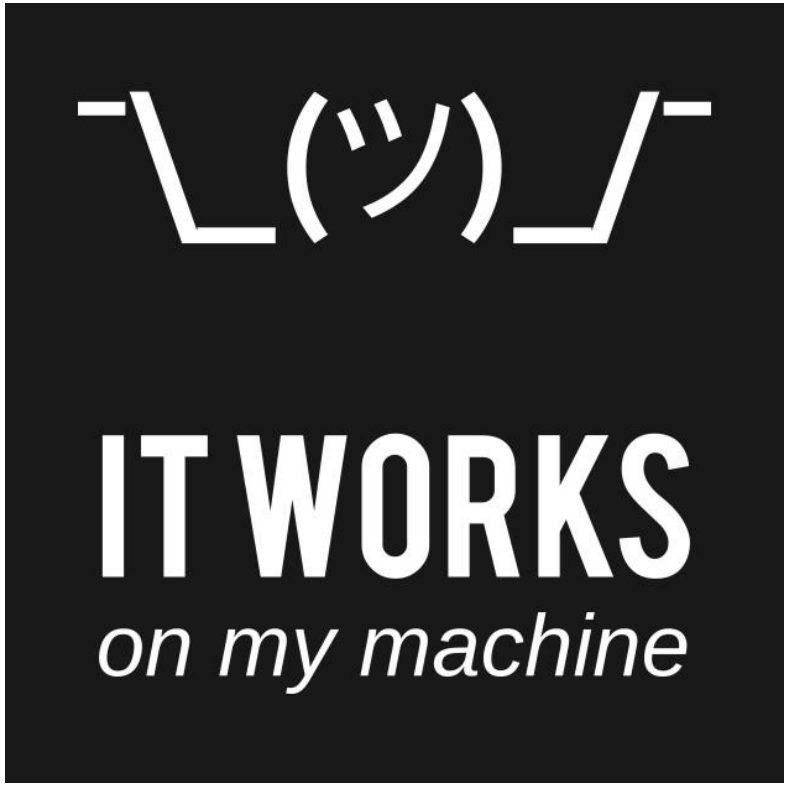
Docker for Reproducibility



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Agenda

- Why do we need containers?
- How can containers solve those problems?
- What is a Docker container?
  - How does Docker containerize?
- Demo: running r analysis in a container
- Reference

Why do we need containers?

- Scenario 1: rerun *my_analysis_12042018_KC.rmd* but get an error: *“Error in xx: could not find function ”xx"*

  - You then figure out the function xx is deprecated

Why do we need containers?

- Scenario 1: rerun *my_analysis_12042018_KC.rmd* but get an error: *"Error in xx: could not find function "xx"*

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- Scenario 2:

  - You send *analysis_12042019_KC.rmd* to your teammate, along with the *private library* stored in the project directory created by *packrat* to manage package dependencies

  - A few minutes later, your teammate pins you on Team and says he encountered an error: *"package 'X' is not available (for R version 3.3.0)"*

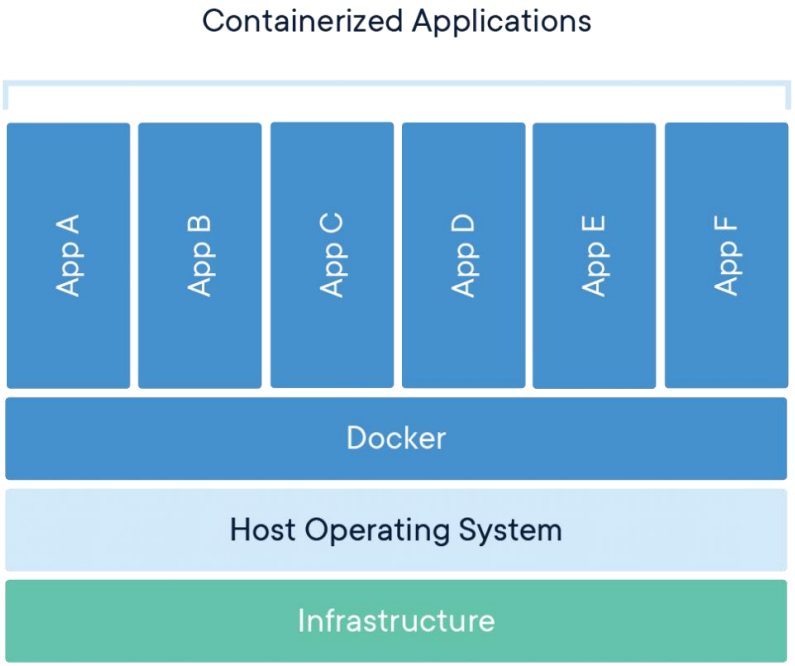
  - You two then figure out it's because the R version in your PC is 3.6.0, which is compatible for package X; however, your teammate has R version 3.3.0 installed in his PC

Why do we need containers?

- challenge:
  - the computation environment where the analyses build is **different** from where the analyses execute
  - replicating prior analysis or allowing other users to reproduce your analysis in their machines become troublesome
    - computation environment, in the context of analysis in R programming, is included functions in the packages, packages, and R version, etc.

How can containers solve those problems?

- *containerize* the computation environment as code
  - containerize analyses with their computation environment in separated containers
  - Run each analysis in its container to replicate same results
    - isolate from computation environment in main PC



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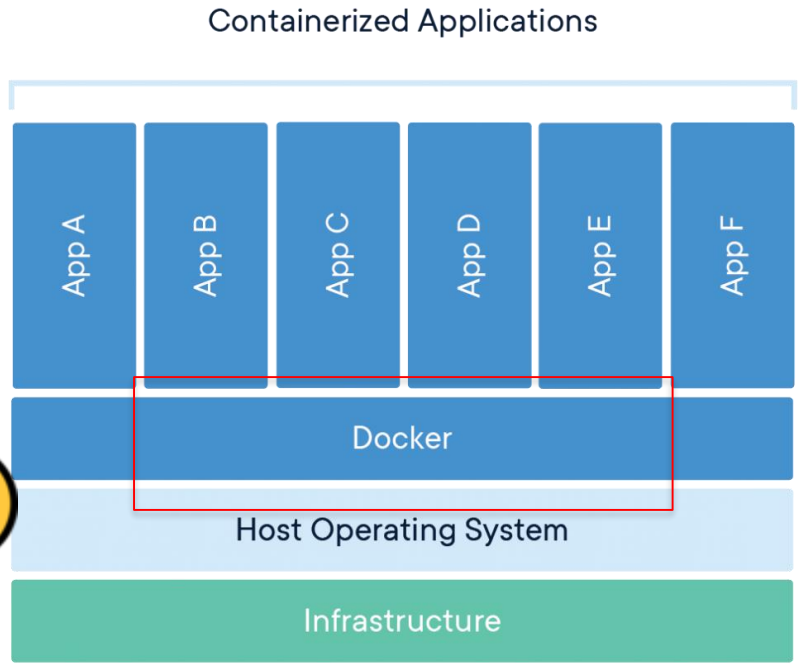
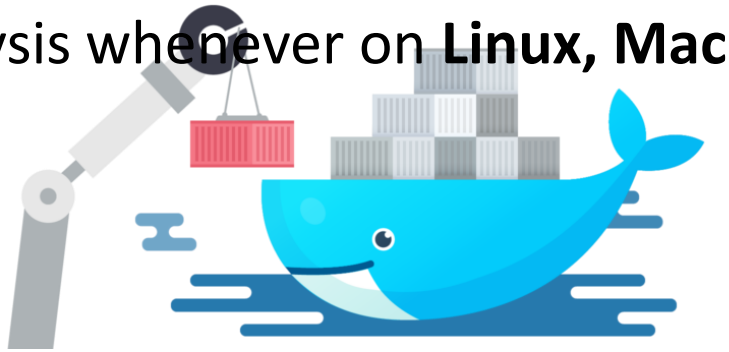


What is a Docker container?

- Docker: shipping companies, which carry containers from one part of the world to another
  - no containers:
    - everything needs to be transported are individually loaded into the ship but that makes loading and unloading of goods difficult
  - with containers:
    - everything can be loaded or unloaded quickly using cranes and that helps shipping companies to transport goods more easily

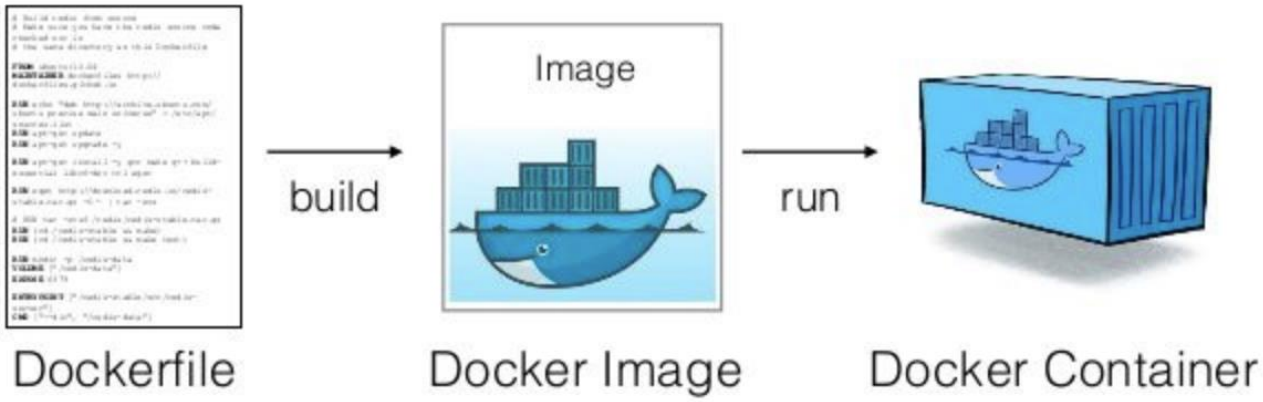
What is a Docker container?

- Docker ships containers in which containerize **analyses**
  - analysis: a collection of computation pieces included packages, system dependencies, codes, reports, etc.
  - Docker creates a **“containerized”** version of the analysis, and everything needed to run the analysis is included
    - allow reproducing the analysis whenever on **Linux, Mac or Windows**



What is a Docker container? - how does Docker containerize?

- *build* an image from Dockerfile, and *spin up* a running container from that image
  - Dockerfile: a list of commands in a special text file to create an image
  - Docker image: a template of your analyses computation environment
  - Docker container: a running instance of a Docker image



Demo: running r analysis in container

- repo: https://github.com/jiatingchen/docker-for-reproducibility
- step:
  - `docker build` *Dockerfile*
  - `docker run` image-nme
  - `render` *my_analysis.rmd* to *my_analysis.html* in container
  - copy *my_analysis.html* to local machine
- walk through Dockerfile:
  - rocker: https://www.rocker-project.org/
  - FROM RUN COPY CMD
  - differences between computation env in container vs that in my PC

```
library(e1071)
library(caret)
sessionInfo()
## R version 3.6.0 (2019-04-26)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
## other attached packages:
## [1] caret_6.0-81    ggplot2_3.2.1   lattice_0.20-38 e1071_1.7-0.1
```

  - build repo in binder

Reference

https://reproducible-analysis-workshop.readthedocs.io/en/latest/8.Intro-Docker.html

https://arxiv.org/pdf/1410.0846.pdf

https://hackernoon.com/5-free-online-courses-to-learn-docker-for-beginners-492cfc488ecb

https://cloudblogs.microsoft.com/opensource/2019/07/15/how-to-get-started-containers-docker-kubernetes/

https://nickjanetakis.com/blog/understanding-how-the-docker-daemon-and-docker-cli-work-together

https://ropenscilabs.github.io/r-docker-tutorial/

https://machinelearningmastery.com/machine-learning-in-r-step-by-step/

https://colinfay.me/docker-r-reproducibility/

Thank you!