How to setup your Data Science project in 2021

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Foreword

- All conclusions are author's findings
  (personal opinion based on own experience, your may differ)
- Only bird's eye view - better dig yourself into links (plenty of them on slides)
- Additions, comments and discussions are welcome!

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Outline

1. Version control system
    a. Data version control
2. Data annotation
3. Jupyter notebooks
4. Code style
5. Dependencies and packaging
6. Models training
7. *Testing (not included, external video)*
8. *Inference (not included, external video)*

Version Control System (VCS)

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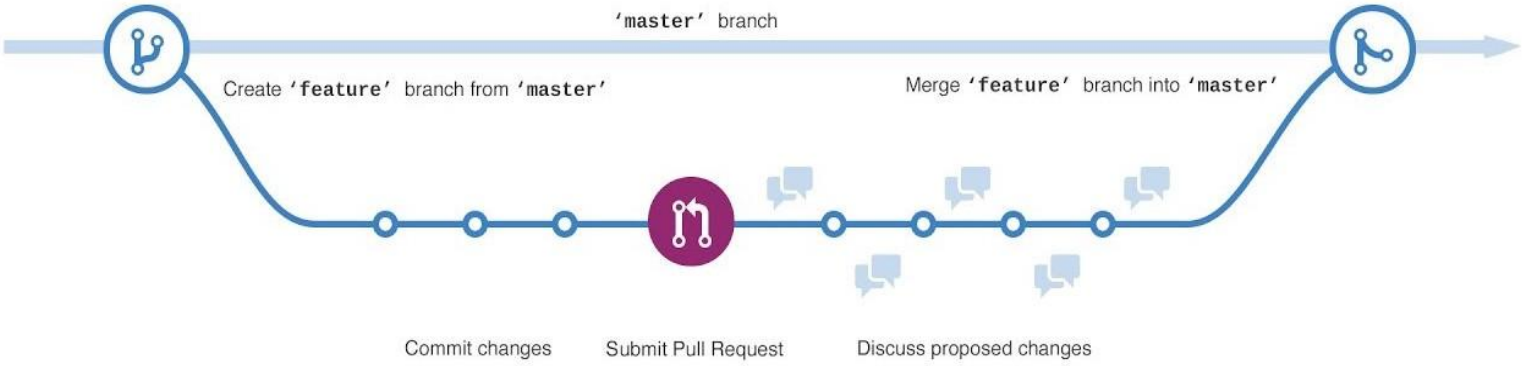
Version Control System

- Source code - git
- Cloud remote - gitlab or github
- Best practice - merge requests (pull requests)



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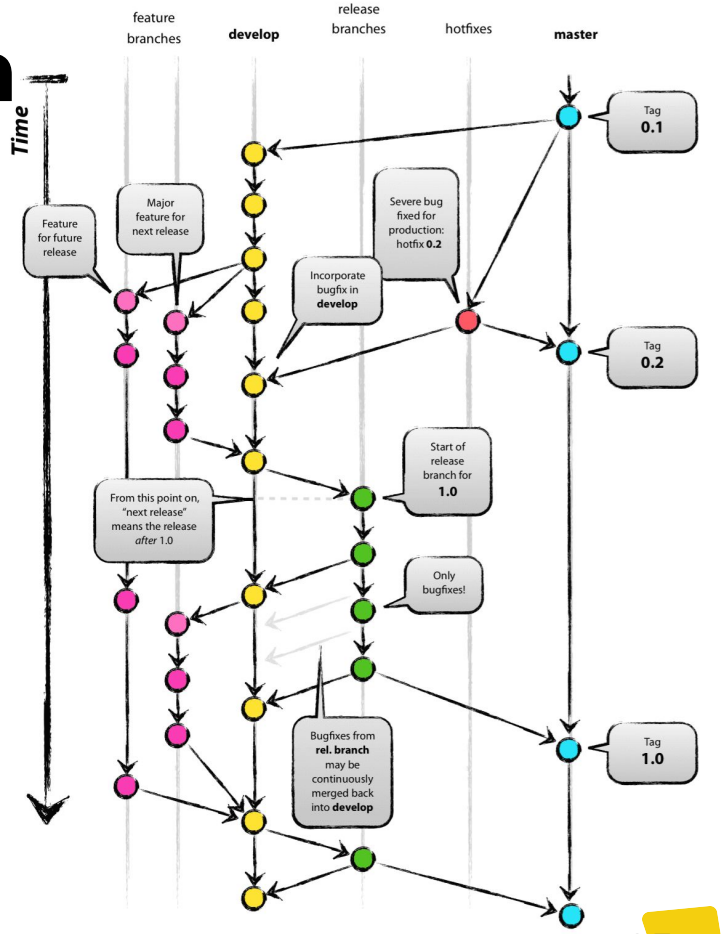
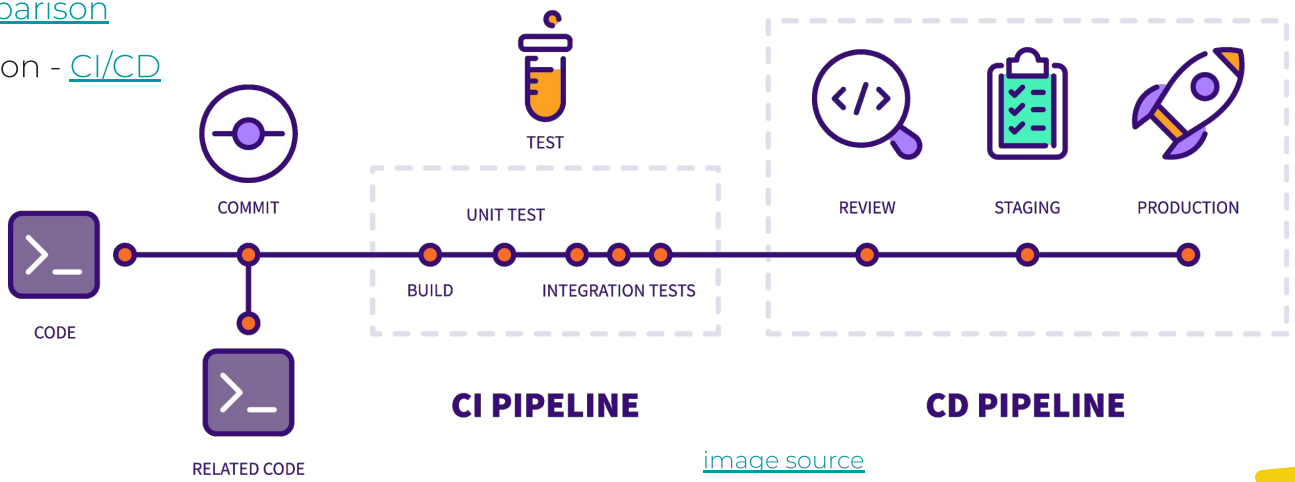
Version Control System

- Source code - [git]
- Cloud remote - gitlab or github
- Best practice - [merge requests (pull requests)]
    - Advanced - [Git Flow (original article)]
    - [Flows comparison]



Version Control System

- Source code - git
- Cloud remote - gitlab or github
- Best practice - merge requests (pull requests)
    - Advanced - Git Flow (original article)
    - Flows comparison
- Further automation - CI/CD



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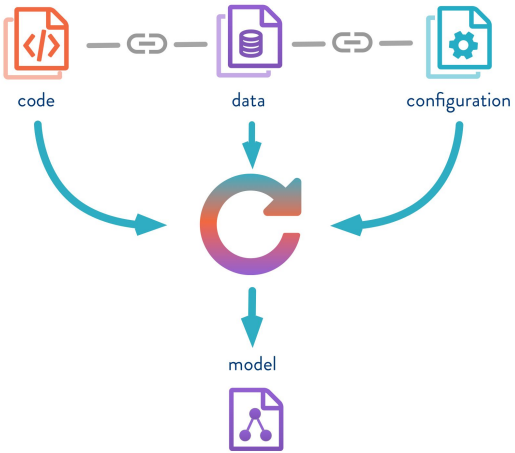
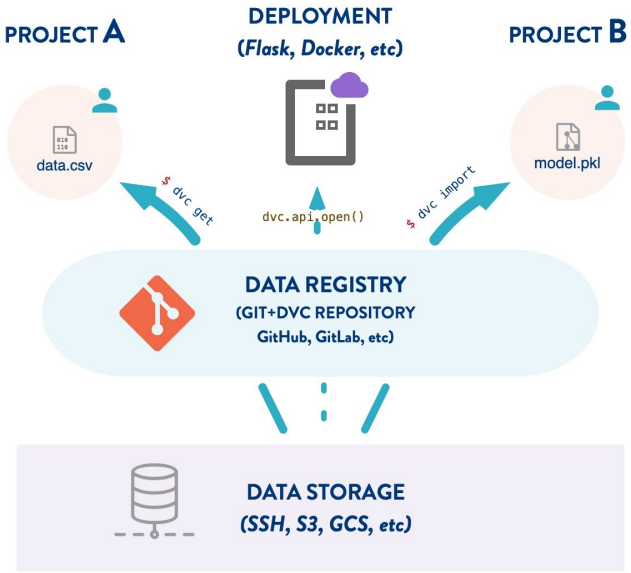
Data Version Control (DVC)

- git for data is DVC (tutorials: one, two)
- use only Versioning and Access

  (Pipelines and Experiments are still raw)





Data Annotation

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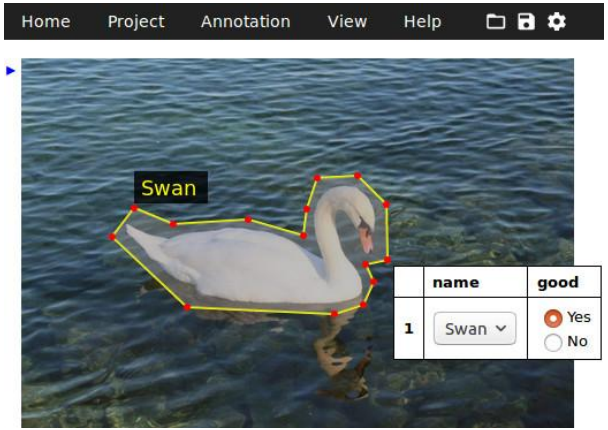
Data Annotation

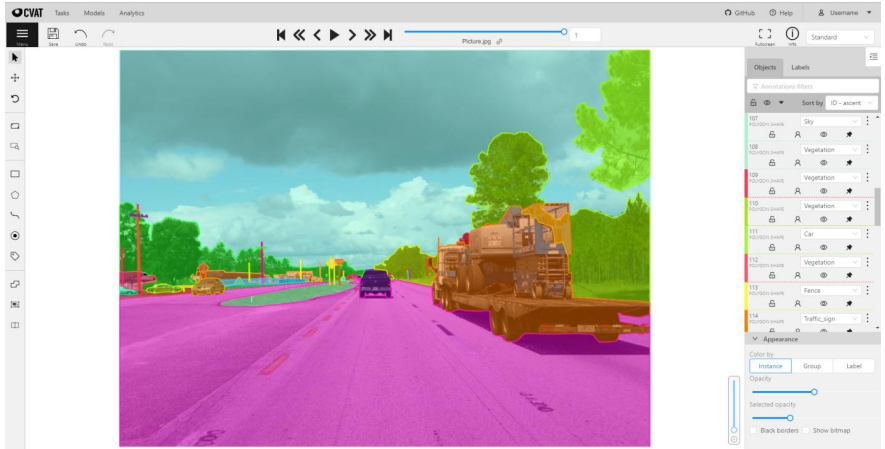


Solutions specific to Computer Vision

- simple cases - VIA (free software, standalone)
- scalable solution - CVAT (free software, server based)
- special cases - hasty.ai (proprietary, server based)

All of them are web based

Suggest your favorite tools in comments! (especially for other tasks)



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Jupyter Notebooks

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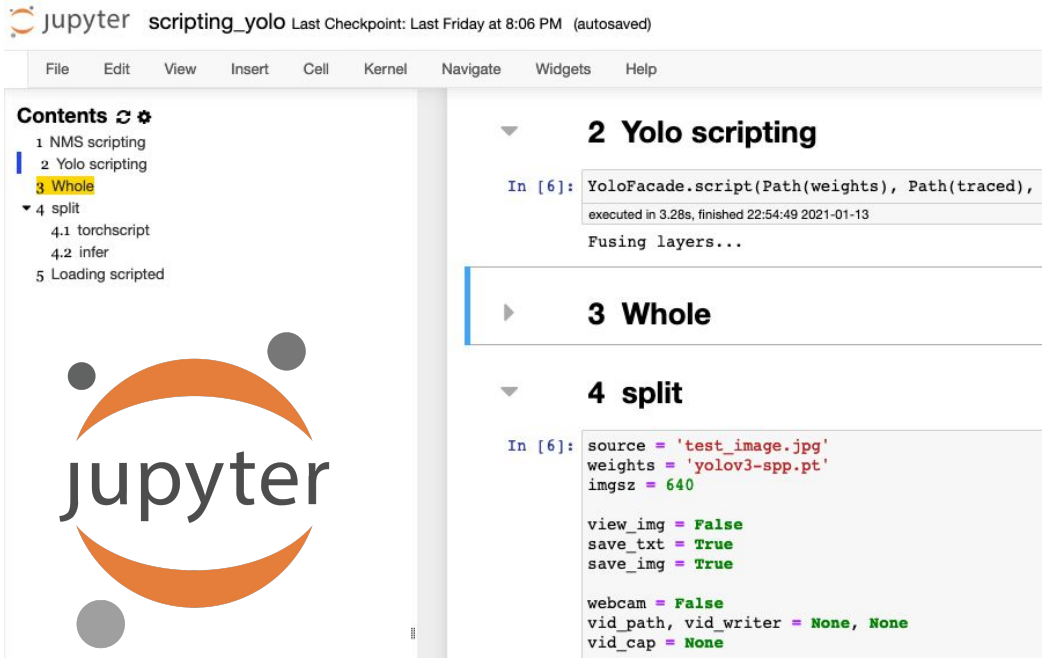
Jupyter Notebooks

- One server for all kernels with [nb_conda_kernels]
- Advanced features functionality with [extensions] and [configurator]
- Notebooks are not added to git
- Used only for prototyping, transfer to .py files (repo) as soon as possible!!! (if you hit one cell at least twice)



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Code Style

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Code Style

- pre-commit

  uses git hooks to run common utilities before git commands processing

```
$ pre-commit install
pre-commit installed at /home/asottile/workspace/pytest/.git/hooks/pre-commit
$ git commit -m "Add super awesome feature"
black.....................................................................Passed
blacken-docs.........................................(no files to check)Skipped
Trim Trailing Whitespace.................................................Passed
Fix End of Files.........................................................Passed
Check Yaml...........................................(no files to check)Skipped
Debug Statements (Python)................................................Passed
Flake8...................................................................Passed
Reorder python imports...................................................Passed
pyupgrade................................................................Passed
rst ``code`` is two backticks........................(no files to check)Skipped
rst..................................................(no files to check)Skipped
changelog filenames..................................(no files to check)Skipped
[master 146c6c2c] Add super awesome feature
 1 file changed, 1 insertion(+)
```

Code Style

- pre-commit
- black (PyCon talk)

  The uncompromising code formatter

  Other solutions:

  - yapf
  - autopep8

```
class Foo  (     object  ):
  def f    (self
  ):
    return       37*-2
  def g(self, x,y=42):
      return y
def f  (   a: List[ int ]) :
  return      37-a[42-u :  y**3]
```

```
class Foo(object):
    def f(self):
        return 37 * -2

    def g(self, x, y=42):
        return y


def f(a: List[int]):
    return 37 - a[42 - u : y ** 3]
```

Code Style

- pre-commit
- black
- isort

  Configurable

  Sorts import to 3 categories:

  - standard library
  - external (third party)
  - internal (this project and associatives)

isort your imports, so you don't have to.

```
import os
from math import ceil
import myproject.test

import .utils
from math import sqrt
import django.settings
```

```
from math import ceil, sqrt
import os

import django.settings

import myproject.test
```

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Code Style

- pre-commit
- black
- isort
- flake8

  List of rules explained

Example of rules:

- F401: Module imported but unused
- E402: Module level import not at top of file
- F811: Redefinition of unused name from line n

More solutions from Python Code Quality Authority:

- bandit

Code Style

- pre-commit
- black
- isort
- flake8
- mypy

  Best for code editors,

  not pre-commit

: my[py]

Seamless dynamic and static typing

From Python...

```
def fib(n):
    a, b = 0, 1
    while a < n:
        yield a
        a, b = b, a+b
```

...to statically typed Python

```
def fib(n: int) -> Iterator[int]:
    a, b = 0, 1
    while a < n:
        yield a
        a, b = b, a+b
```

Code Style

- pre-commit
- black
- isort
- flake8
- mypy
- nbQA

  То же самое для Jupyter Notebooks!

  Поддерживает pre-commit

nbQA

Quality Assurance For Jupyter Notebooks

Code Style

- pre-commit
- black
- isort
- flake8
- mypy
- nbQA
- Documentation Driven Development (docstrings)
- Sphinx
- annotations, typing module
- pathlib

Dependencies and Packaging

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Dependencies and Packaging

First - follow python package structure

- common extensible format
- able to be packaged

Second - dependencies management and packaging

- requirements.txt
- pip-tools
- pipx
- Pipfile and pipenv
- **poetry**

```
sound/                          Top-level package
      __init__.py               Initialize the sound package
      formats/                  Subpackage for file format conversions
              __init__.py
              wavread.py
              wavwrite.py
              aiffread.py
              aiffwrite.py
              auread.py
              auwrite.py
              ...
      effects/                  Subpackage for sound effects
              __init__.py
              echo.py
              surround.py
              reverse.py
              ...
      filters/                  Subpackage for filters
              __init__.py
              equalizer.py
              vocoder.py
              karaoke.py
              ...
```

Dependencies and Packaging

One tool for all - poetry

- dares to install ONE tool per OS
- better conflicts resolving

Creates two files:

- `pyproject.toml` - initial dependencies, config for all tools
- `poetry.lock` - all concrete dependencies (platform agnostic)

If using conda environments:

```
poetry config virtualenvs.create false
```

For installing dependencies:

```
poetry install --no-root --remove-untracked
```

Also it is able to build and publish to PyPI or your own package registry

```
poetry build && poetry publish
```

Models Training

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Models Training Framework

- Deep Learning
  - Pytorch
  - Tensorflow
- Gradient boosting
  - LightGBM
  - XGboost
  - CatBoost
- Others
  - Sklearn
  - Vowpal Wabbit
  - MLlib
  - .....

Experiments Runner

- Pytorch
  - Ignite
  - **Catalyst**
  - Lightning
- DVC Experiments
- MLFlow Experiments
- pachyderm
- .....

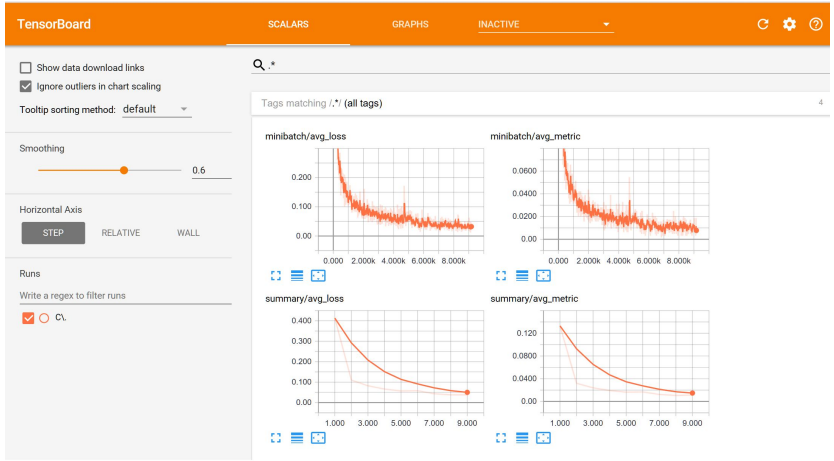
Catalyst

PyTorch Ignite

PyTorch Lightning

Experiments Tracker

- Tensorboard
- **MLFlow**
- sacred
- Kubeflow
- neptune.ai
- weights and biases
- .....



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Thanks for attention!

Questions? Additions? Welcome!

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