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Introduction to Scientific Computation
Lecture 8
Fall 2020

Packaging, Unsupervised learning: t-SNE

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Package types:

A package can be essentially in two forms:

- source
- binary

Focusing now on the Python world:
As Python is a dynamic language, this distinction can get a bit blurred:
There is little difference between a source and binary package *for a pure python package*
But if there is any compiled code in there, building from source can be a challenge:

- Binary packages are very helpful

Source Packages

A source package is all the source code required to build the package.
Package managers (like pip) can automatically build your package from source.
But:

- Your system needs the correct tools installed, compilers, build tools, etc
- You need to have the dependencies available
- Sometimes it takes time, sometimes a LONG time

Binary Packages

A collection of code all ready to run.

- Everything is already compiled and ready to go – makes it easy.

But:

- It's likely to be platform dependent
- May require dependencies to be installed

Python Packaging

There are two package managers widely used for Python.

pip: The "official" solution.

- Pulls packages from PyPI
- Handles both source and binary packages (wheels)
- Python only

conda: Widely used in the scipy community.

- Pulls packages from anaconda.org
- Binary only (does not compile code when installing)
- Supports other languages / libraries: C, Fortran, R, Perl, Java (anything, really)
- Manages Python itself!

WHY ARE WE DOING THIS?

One of the most powerful things about coding for the sciences is that it costs nothing to re-use code we've written in the past, allowing us to build on past work rather than starting over every project or paper.

However, one practice we see again and again is copying and pasting code from one project into another. Sometimes it will just be a function, other times (coughMATLABcough) it's files.

Assembling code in packages makes it really easy to re-use old code: all the scripts and functions end up in a central location and can be called and imported from anywhere on the computer - just like the famous packages `numpy` or `matplotlib`.

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SETTING UP

1. THE BASICS

The most basic directory structure for a Python package looks like this:

```
project
|
|__ setup.py
|
|__ myPackage
     |
     |_  somePython.py
     |_  __init__.py
```

But at the moment, we've just got some flat files.

```
project
|
|__ norms.py
|__ metrics.py
```

So, the first step is to move files around. First comes the hardest part: choosing a package name. I'll call mine `measure`. Create a directory with that name, and move the python files in there.

```
project
|
|__ measure
     |__ norms.py
     |__ metrics.py
```

There is one more crucial file: `__init__.py` lets the Python interpreter know that there are importable modules in this directory. This is the script that gets run when you execute `import measure`. For more about what you can do with modules, you can see the (Python docs)[https://docs.python.org/3/tutorial/modules.html]. After adding `__init__.py`, the project directory should be

```
project
|
|__ measure
     |__ __init__.py
     |__ norms.py
     |__ metrics.py
```

2. SETUP.PY

At this point, the library can be imported if we're in the same directory, but it isn't a package. To let setuptools and `pip` know how to handle it, we need to add the `setup.py` file.

A very basic version of `setup.py` is

```
from setuptools import setup

setup(
    # Whatever arguments you need/want
)
```

If you were to run that file, you'd get a whole bunch of warnings, and nothing would actually get packaged. As a bare minimum, here is our `setup.py` for it to work.

```
from setuptools import setup

setup(
    # Needed to silence warnings (and to be a worthwhile package)
    name='Measurements',
    url='https://github.com/jladan/package_demo',
    author='John Ladan',
    author_email='jladan@uwaterloo.ca',
    # Needed to actually package something
    packages=['measure'],
    # Needed for dependencies
    install_requires=['numpy'],
    # *strongly* suggested for sharing
    version='0.1',
    # The license can be anything you like
    license='MIT',
    description='An example of a python package from pre-existing code',
    # We will also need a readme eventually (there will be a warning)
    # long_description=open('README.txt').read(),
)
```

```
project
|
|__ setup.py
|__ MANIFEST.in
|
|__ measure
|    |__ __init__.py
|    |__ norms.py
|    |__ metrics.py
|
|__ tests
|    |__ test_suite.py
|
|__ doc
|    |__ docs.rst
|
|__ scripts
|    |__ hello.py
|
|__ README.txt
|__ CHANGES.txt
|__ LICENSE.txt
```

Basic definitions

We have a set of objects: X

And the set of possible answers: Y

We define the target function: $y^* : X \rightarrow Y$

Supervised

Unsupervised $Y \in \emptyset$

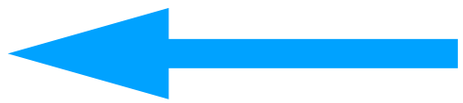
Unsupervised

We have a set of objects: X

And the set of possible answers: Y

Unsupervised

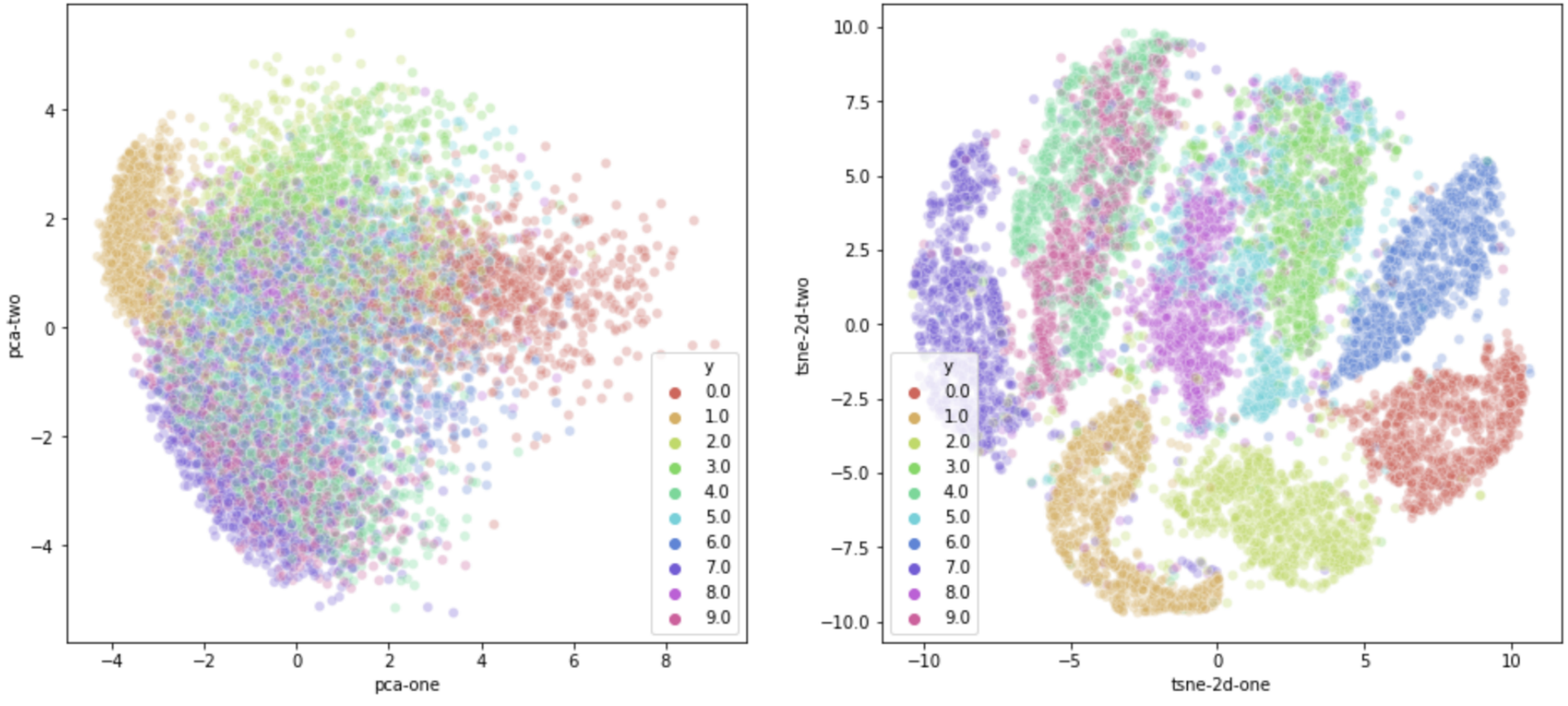
We have a set of objects: X

And the set of possible answers: Y  This one we don't have

Unsupervised

We have a set of objects: X

And the set of possible answers: Y ← This one we don't have



(c) https://towardsdatascience.com/visualising-high-dimensional-datasets-using-pca-and-t-sne-in-python-8ef87e7915b

SNE

- “Encode” high-dimensional information into distribution
- Random walk between data points
  - Higher probability to jump to a closer point
- Find low dimensional points with similar neighbourhood distribution
- Not easy to embed new points

Neighbourhood distributions

- Consider the neighbourhood around an input data point $x_i \in \mathbb{R}^d$
- Imagine Gaussian distribution centred around x_i
- The probability that x_i chooses some other datapoint x_j as neighbour is proportional to the area under gaussian curve.
- The point closer to x_i is more likely than a further one

- The $i \rightarrow j$ probability to choose point j from i
- $$P_{j|i} = \frac{\exp(-||x_i - x_j||^2/\sigma_i^2)}{\sum_{k \neq i} \exp(-||x_i - x_k||^2/\sigma_i^2)}$$
- $P_{i|i} = 0$
- σ_i sets the size of neighbourhood:
  - Low - always choose nearest point
  - High - uniform weights

- σ_i is chosen differently for each data point
- The distribution is symmetric: $P_{ij} = \frac{1}{2N}(P_{i|j} + P_{j|i})$
  - Pick i or j uniformly and jump according to distribution

Perplexity

- For each $P_{j|i}$ (depends on σ_i) perplexity:
  - $\text{perp}(P_{j|i}) = 2^{H(P_{j|i})}, H(P_i) = -\sum_i P_i \log(P_i)$
- If P is uniform over k elements, perplexity is k
  - Smooth version of k in kNN
  - Low perplexity - small σ_i
  - Large perplexity - large σ_i
- σ_i sets the size of neighbourhood:
  - Low - always choose nearest point
  - High - uniform weights

SNE objective

- Given $x^{(1)}, \ldots, x^{(N)} \in \mathbb{R}^d$ we define distribution P_{ij}
- Goal: find good embedding $y^{(1)}, \ldots, y^{(N)} \in \mathbb{R}^{\hat{d}}$, where $\hat{d} < d$ (normally 2 or 3)
- For points $y^{(1)}, \ldots, y^{(N)} \in \mathbb{R}^{\hat{d}}$ we can define distribution Q (no σ_i and not symmetric):
- $$Q = \frac{\exp(-||y_i - y_j||^2)}{\sum_k \sum_{k \neq i} \exp(-||y_i - y_k||^2)}$$
- Optimize Q to be close to P
  - Use KL-divergence

KL

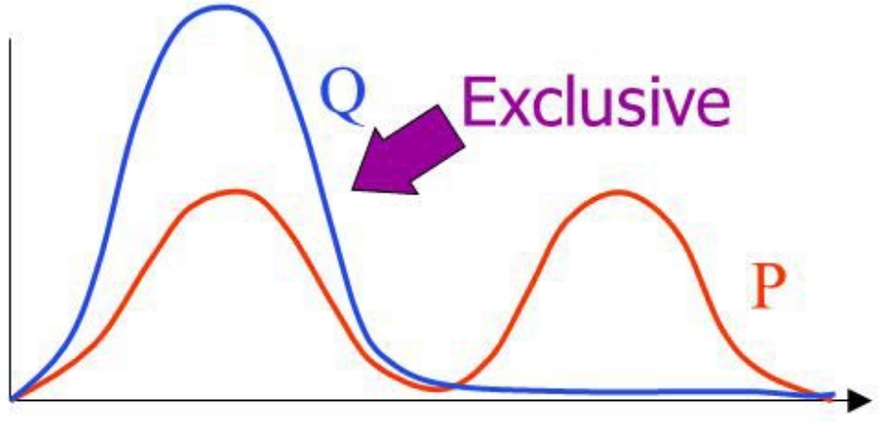
- $KL(P||Q) = \sum_{ij} Q_{ij} \log \frac{Q_{ij}}{P_{ij}}$
- Not a metric function - not symmetric
- $KL(Q||P) = -\sum_{ij} P_{ij} \log Q_{ij} + \text{const}$
- In lower dimensions it is harder to pack neighbours than in high dimension: crowding problem
- t-SNE: change gaussian in Q to a heavy tailed distribution

KL

- $KL(Q||P) \geq 0$ and 0 if $Q = P$
- $KL(Q||P)$ is convex
- If $P_{ii} = 0$ but $Q_{ii} > 0$ then $KL(Q||P) = \infty$

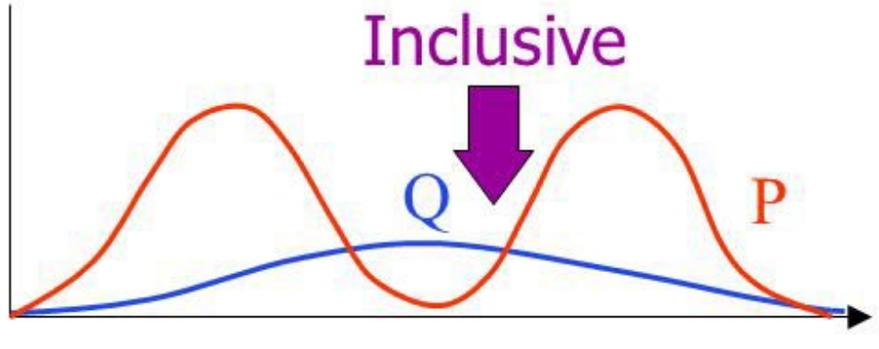
Minimising
$KL(Q||P)$

$$= \sum_H Q(H) \ln \frac{Q(H)}{P(H|V)}$$



Minimising
$KL(P||Q)$

$$= \sum_H P(H|V) \ln \frac{P(H|V)}{Q(H)}$$



(c) https://timvieira.github.io/blog/post/2014/10/06/ kl- divergence- as- an- objective- function/

Algorithm

- We optimise $KL(P||Q)$ by choosing $y^{(1)}, \ldots, y^{(N)} \in \mathbb{R}^{\hat{d}}$
- $$\frac{\partial KL(P||Q)}{\partial y^{(i)}} = \sum_j (P_{ij} - Q_i j)(y^{(i)} - y^{(j)})$$

- Not a convex problem! No garanties, we can use multiple restarts
- Main issue: crowding problem
- In lower dimensions it is harder to pack neighbours than in high dimension: crowding problem
- t-SNE: change gaussian in Q to a heavy tailed distribution

t-SNE

- Student t-probability density $p(x) \propto (1 + \frac{x^2}{v})^{-(v+1)/2}$
- Probability goes to zero much slower than for Gaussian (that's heavy tailed)
- $Q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_k \sum i \neq k (1 + ||y_i - y_k||^2)^{-1}}$
- $\frac{\partial KL(P||Q)}{\partial y^{(i)}} = \sum_j (P_{ij} - Q_i j)(y^{(i)} - y^{(j)})(1 + ||y_i - y_j||^2)^{-1}$

t-SNE algorithm

- We learn $y^{(1)}, \ldots, y^{(N)} \in \mathbb{R}^{\hat{d}}$
- Compute P_{ij} with perplexity
- Make P_{ij} symmetric
- Sample initial solution $y^{(1)}, \ldots, y^{(N)} \in \mathbb{R}^{d}$
- For T iterations:
  - Compute Q_{ii}
  - Compute gradient of the loss
  - Update $y^{(1)}, \ldots, y^{(N)} \in \mathbb{R}^{\hat{d}}$