Introduction to clustering

- *k*-means and agglomerative clustering
- Clustering with big data on the NCI

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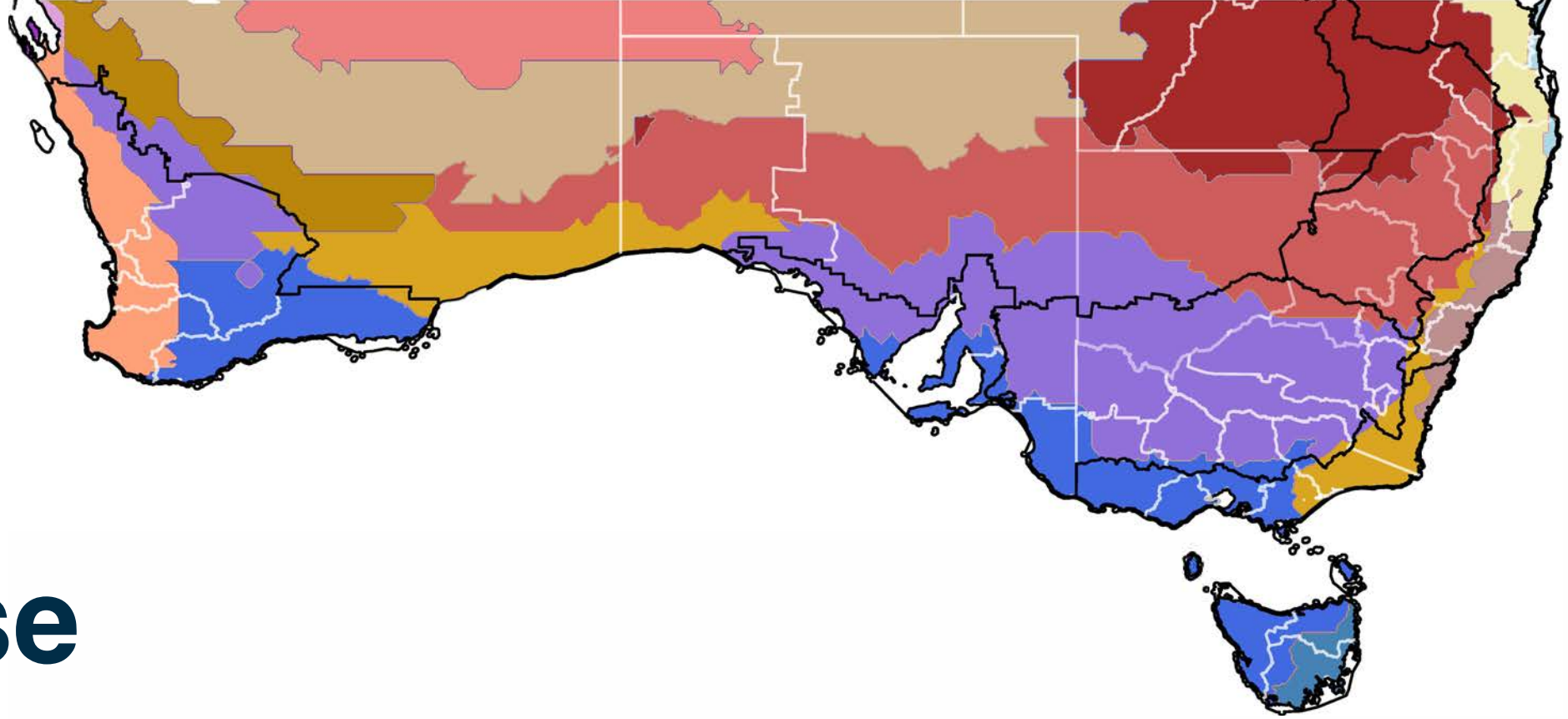
With help from Kate Saunders & acknowledgments to Acacia Pepler & Pandora Hope

AAPP
Australian Antarctic Program Partnership

The Australian Antarctic Program Partnership is led by the University of Tasmania, and includes the following partner agencies

The Australian Antarctic Program Partnership is funded by the Australian Government Department of Industry, Science, Energy and Resources through the Antarctic Science Collaboration Initiative.



Why use clustering?

Fiddes et al. (2021) Redefining Southern Australia's climate regions and seasons

Want to organise data into ‘clusters’ that are internally (within cluster) similar and externally (between cluster) different

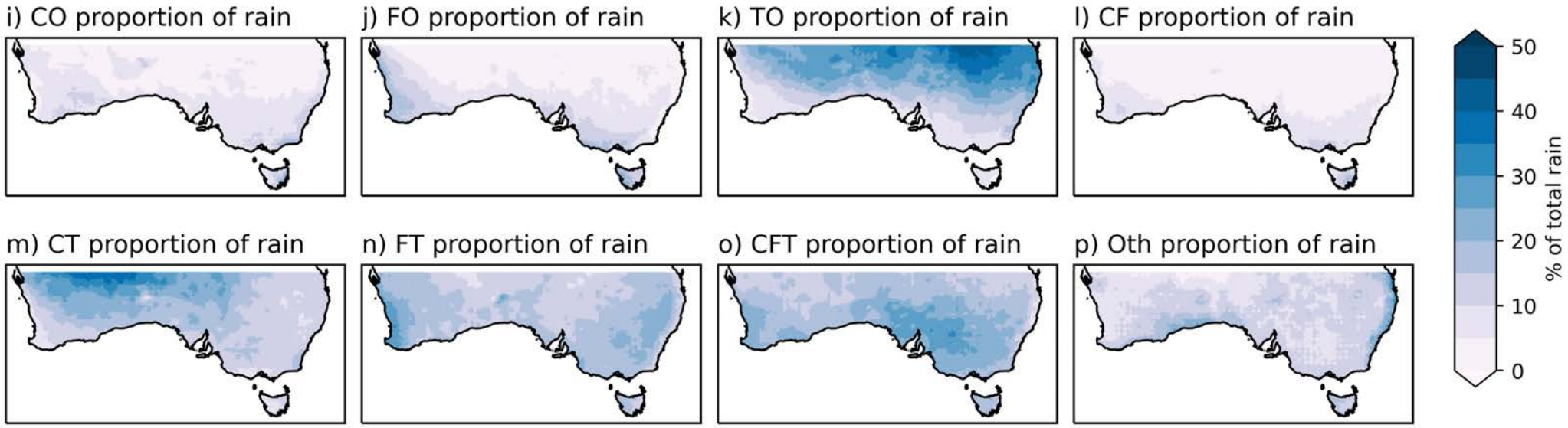
Do not know what these clusters look like

Unsupervised machine learning

Fiddes et al. (2021) Redefining Southern Australia’s climate regions and seasons

Example: Fiddes et al. (2021) wanted to know where different climate regions existed across Southern Australia, based on the proportion of rain produced by weather systems.

We did not know where these boundaries would fall, or how many clusters there should be.



Fiddes et al. (2021) Redefining Southern Australia's climate regions and seasons

Some terminology:

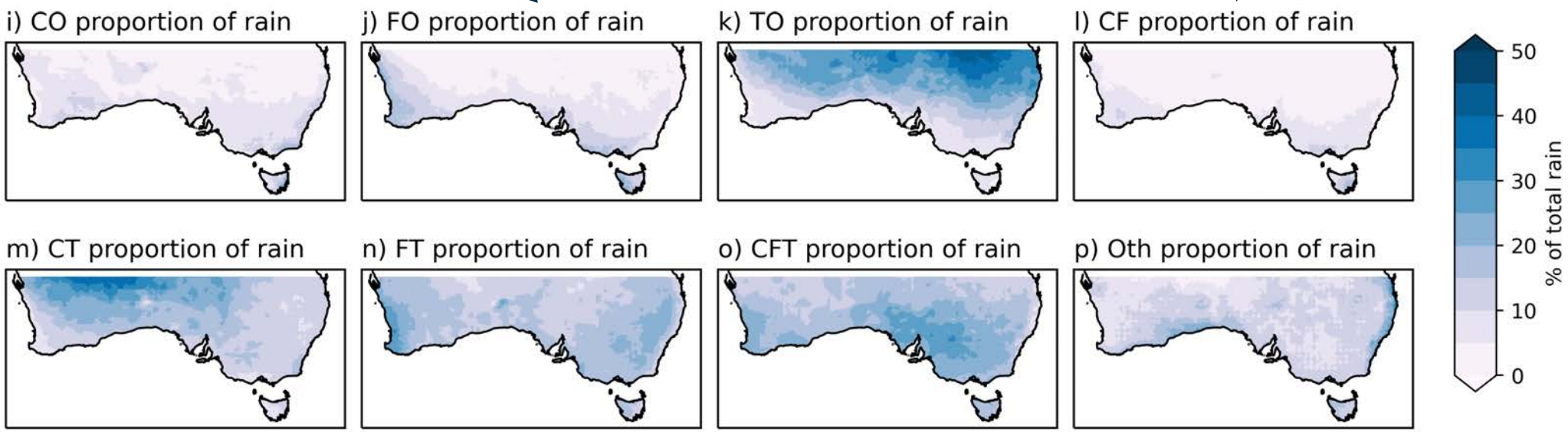
***n* : Number of clusters**

***i* : Number of observations**

***j*: Number of attributes**

In this case:
i = number of grid points
j = 8

Attributes



Fiddes et al. (2021) Redefining Southern Australia's climate regions and seasons

How do we define similar?

The majority of clustering algorithms use a 'dissimilarity matrix' *D:* the sum of attribute dissimilarity d_j between observations *i* and *i'*

$$D(x_i, x_{i'}) = \sum_{j=1}^{p} d_j(x_{ij}, x_{i'j})$$

Hastie et al. (2009) Elements of statistical learning

The most common measure of dissimilarity is the squared distance (but there are a number of other options)

$$d_j(x_{ij}, x_{i'j}) = (x_{ij} - x_{i'j})^2$$

Hastie et al. (2009) Elements of statistical learning

Are all attributes equal?

No. Most commonly, clustering uses the Euclidean distance (there are other options).

If one attribute (and its dissimilarities) is larger in magnitude than another, this attribute will contribute more to the clustering decisions.

Fiddes et al. (2021) was interested in how the relationship of rainfall and weather types influence climate. Rainfall and days exist on different scales (note plot is showing %)

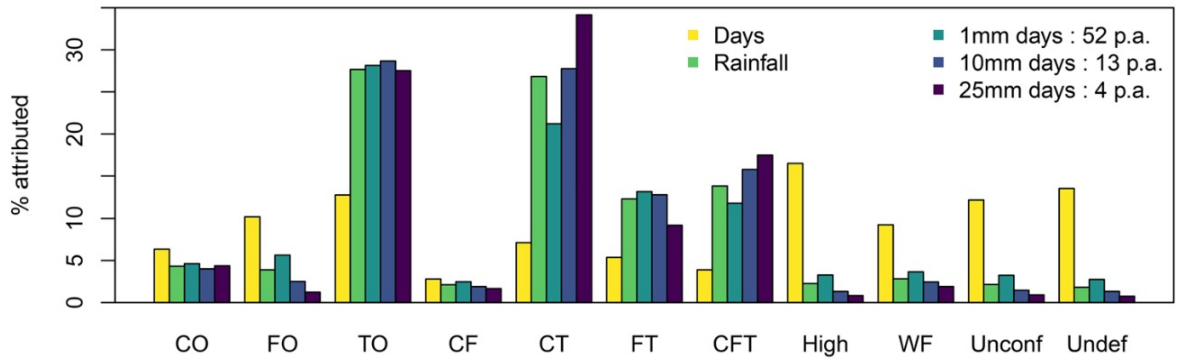


Fig. 6 Annual percentage contribution of each weather system type to rainfall in the 0.05° AWAP gridded analyses between 1979 and 2015, averaged across all land areas of Australia south of 25° S. Bars show the percentage of all days influenced by each weather type (days), the total annual precipitation from each type (rainfall), and the proportion of all days with rainfall exceeding a given threshold (1 mm, 10 mm and 25 mm) that are associated with a given weather type. Legend shows the average number of days p.a. for each rainfall threshold

Pepler et al. (2020) The contributions of fronts, lows and thunderstorms to southern Australian rainfall

Data processing

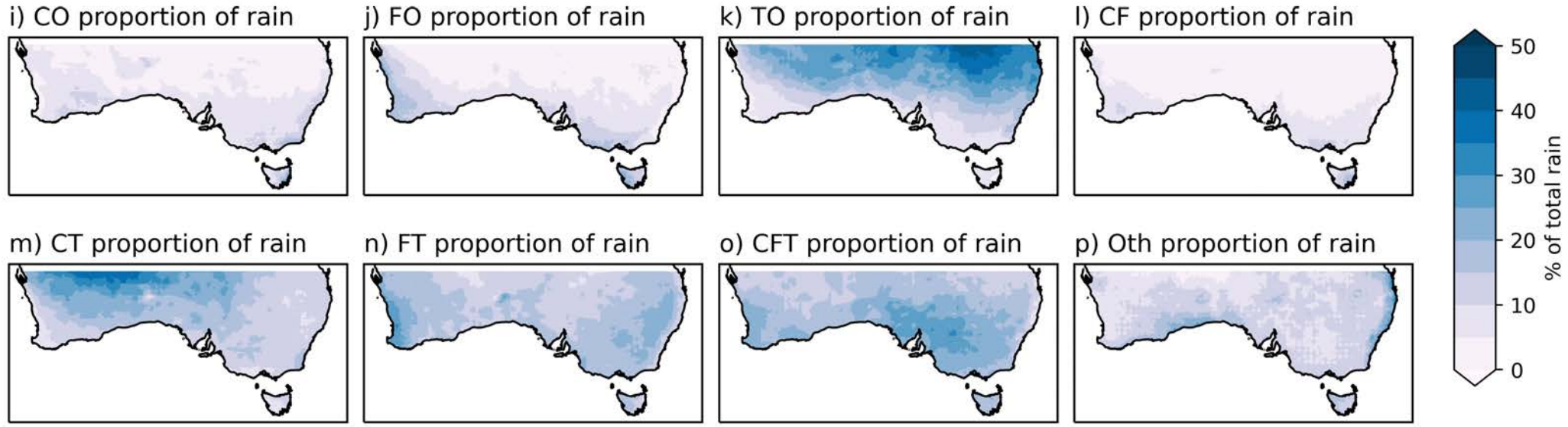
In order to ensure your attributes contribute equally to the clustering algorithm, you can:

- **Weight them (*w*)**
- **Normalise them**
- **Choose different attributes**
- **Use another method to reduce data 'dimensionality' eg. Principal Component Analysis**

$$D(x_i, x_{i'}) = \sum_{j=1}^{p} w_j \cdot d_j(x_{ij}, x_{i'j}); \quad \sum_{j=1}^{p} w_j = 1.$$

Hastie et al. (2009) Elements of statistical learning

In Fiddes et al. (2021), we chose to cluster on the proportion of rain brought by each weather type, instead of using total rainfall amount or number of days for each weather type

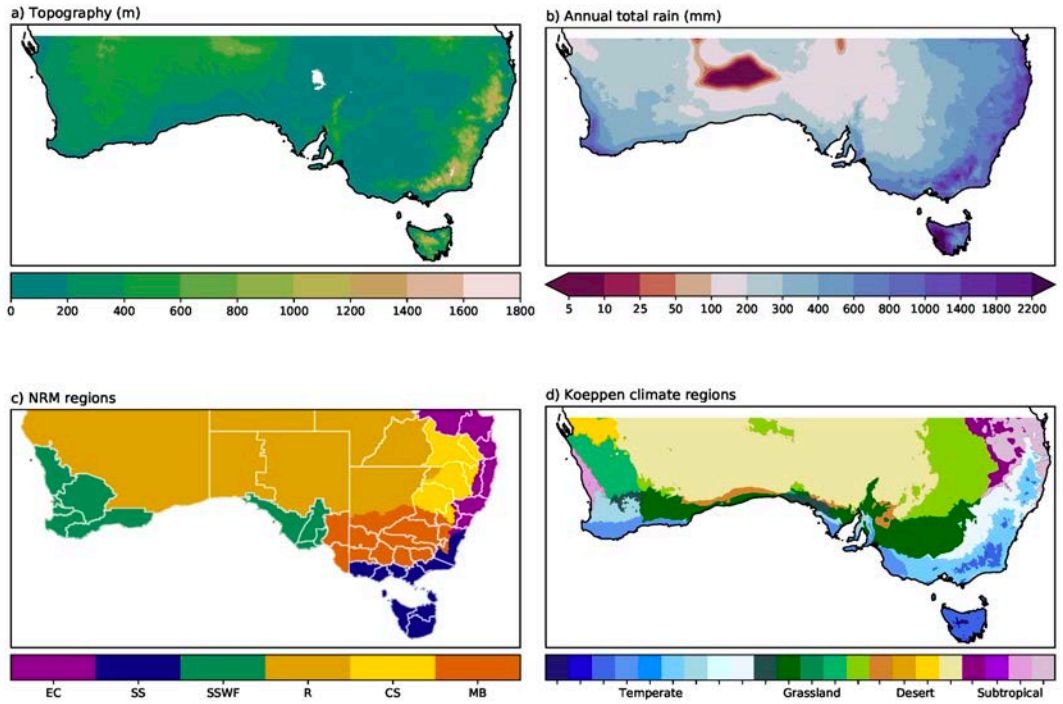


Fiddes et al. (2021) Redefining Southern Australia's climate regions and seasons

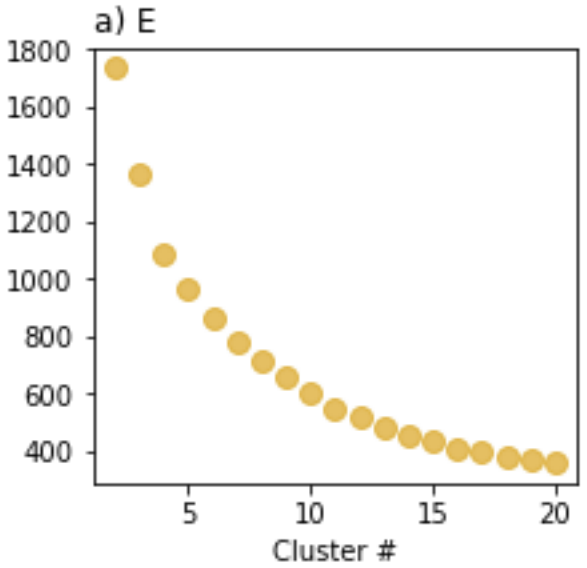
How many clusters?

Ultimately, if you do not know the underlying structure of your data, *there is no 'right' or 'wrong' answer.*

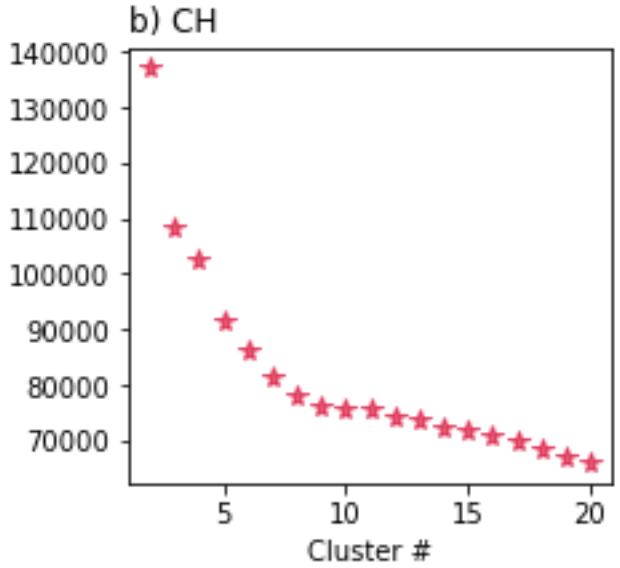
You need to understand the physical meaning of your data to help make this decision.



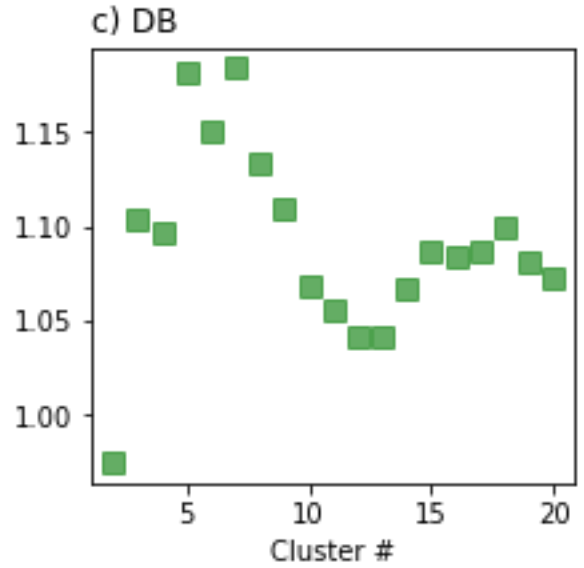
There are some metrics to help, but be warned: often they don't.



Elbow plots – find the elbow.



Calinski-Harabasz score – higher score: better defined clusters



Davies-Bouldin index – lower score: clusters with least similarity

Types of clustering

There are many types of clustering available

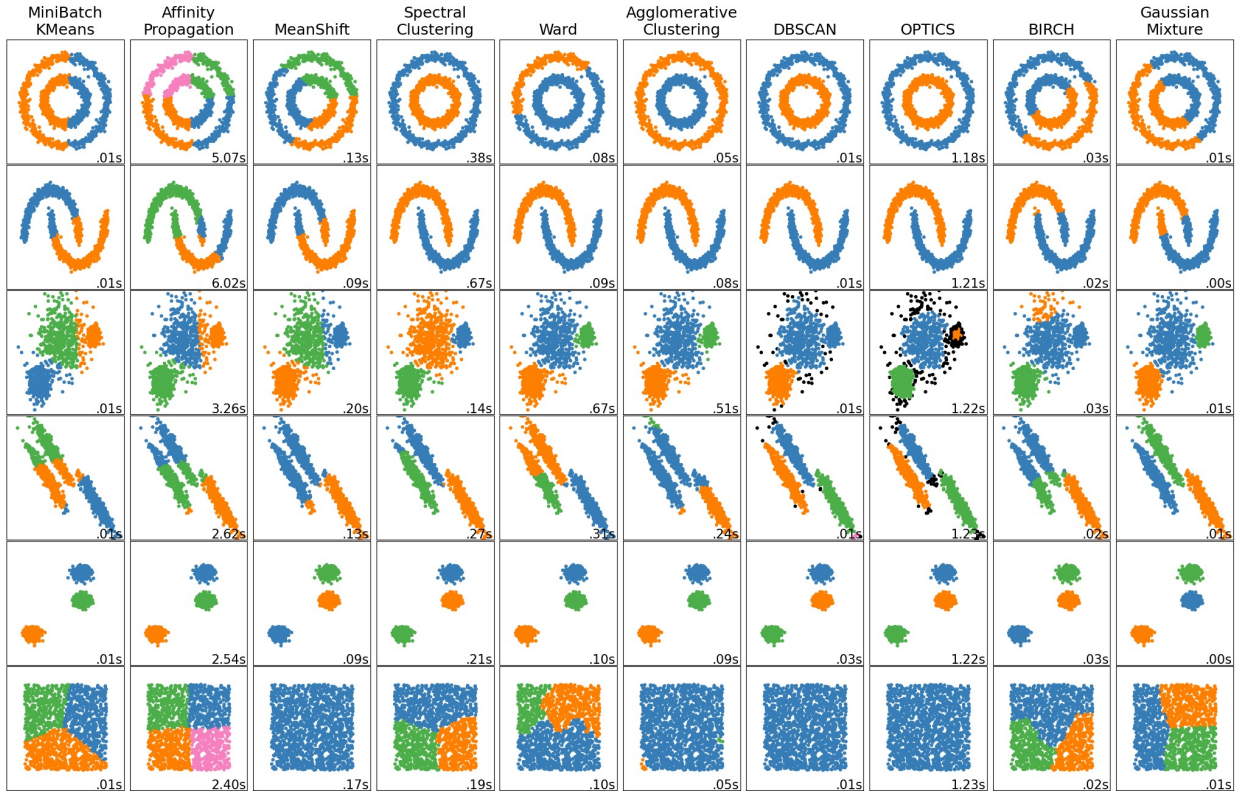


Image: https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html

K-means

Uses the squared Euclidean distance as it's dissimilarity metric

Minimizes with-in cluster variance

1. Randomly assign observations to clusters

2. Work out the cluster means (cluster centres)

3. Update assignment of observations to the nearest cluster centre*

*** Repeat 2-3 until the change in cluster means is very small (a given threshold) i.e the assignments do not change**

Hastie et al. (2009) Elements of statistical learning

Assumptions

Clusters are spatially grouped (spherically)

Assumes that each cluster has a roughly equal number of observations (ie. equal probability)

Does not like ‘high-dimensional’ spaces (because it uses the Euclidean distance). I.e. attributes have the same variance

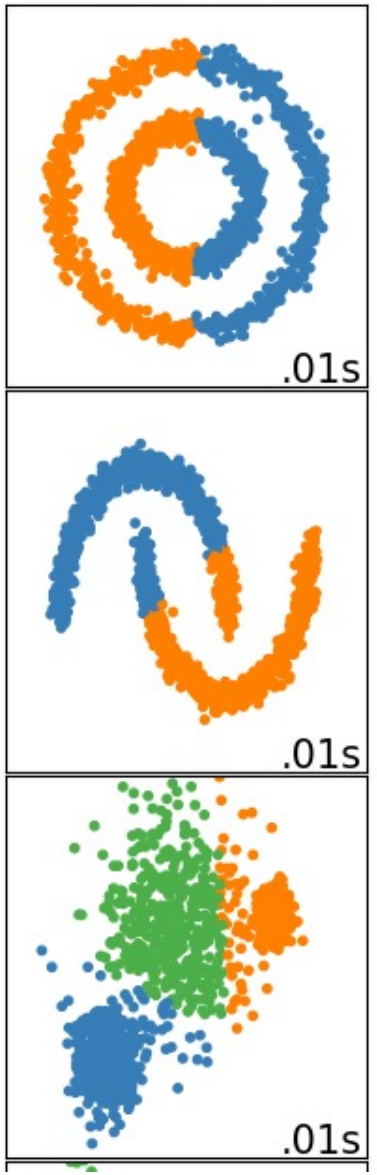


Image: https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html

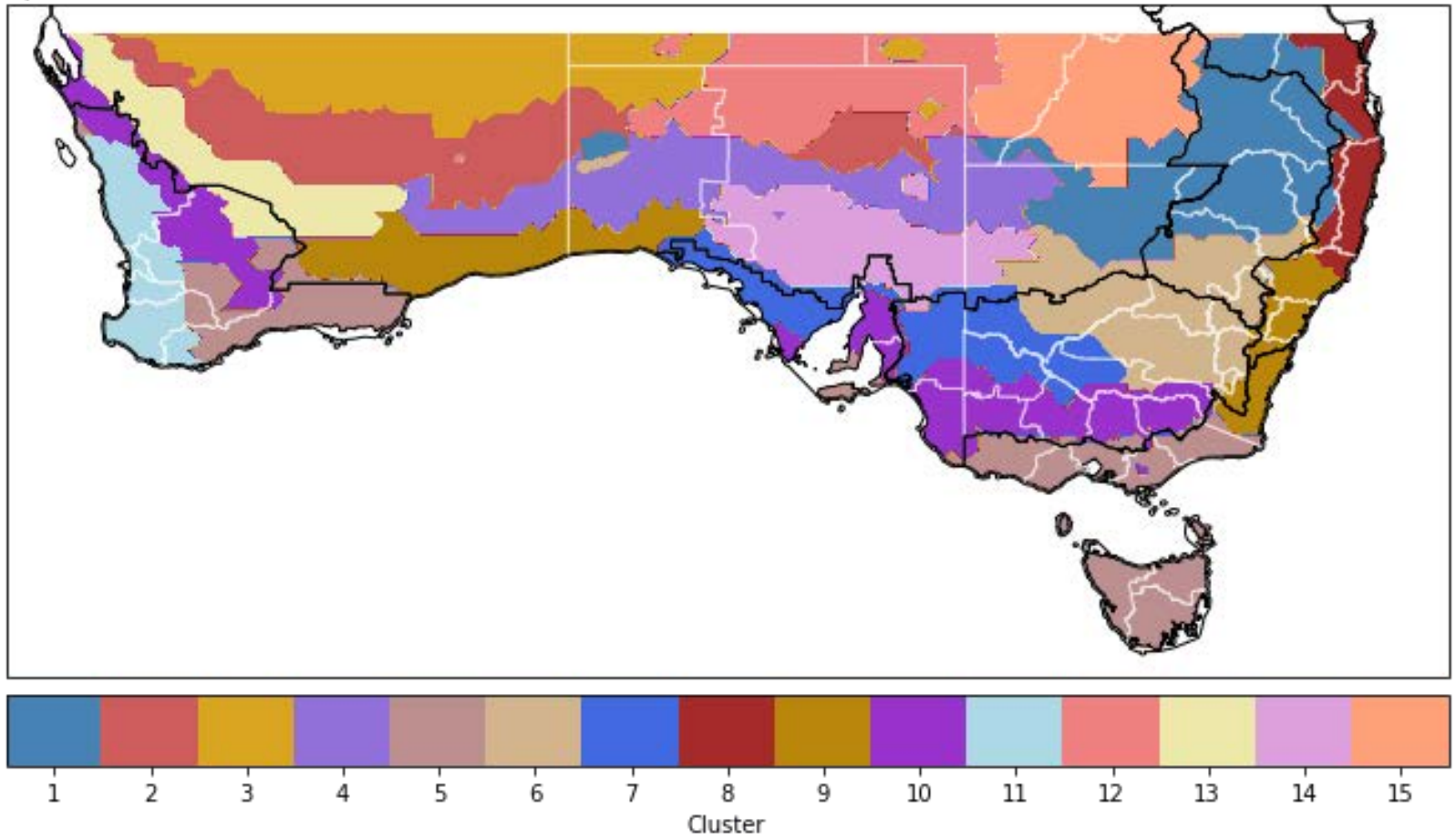
Pros:

- Scales well to very large data sets
- Easy to implement, highly flexible and efficient
- Will always converge
- Observations are not tied to a cluster (i.e can move depending on centroid means).

Cons:

- Does not handle outliers well
- Assumptions of even cluster size & attribute variance
- Depends on initial values (i.e first cluster assignment)

a) Annual clusters



Agglomerative clustering

From Sci-Kit learn: four forms of agglomerative clustering available, each using a different 'linkage' method (ie. the dissimilarity metric they minimize):

- **Ward:** Sum of squares distance (similar to *k*-means)
- **Single:** Maximum distance between observations and pairs of clusters
- **Average**: Average distance between between all observations and pairs of clusters
- **Complete:** distance between closest observations of pairs of clusters

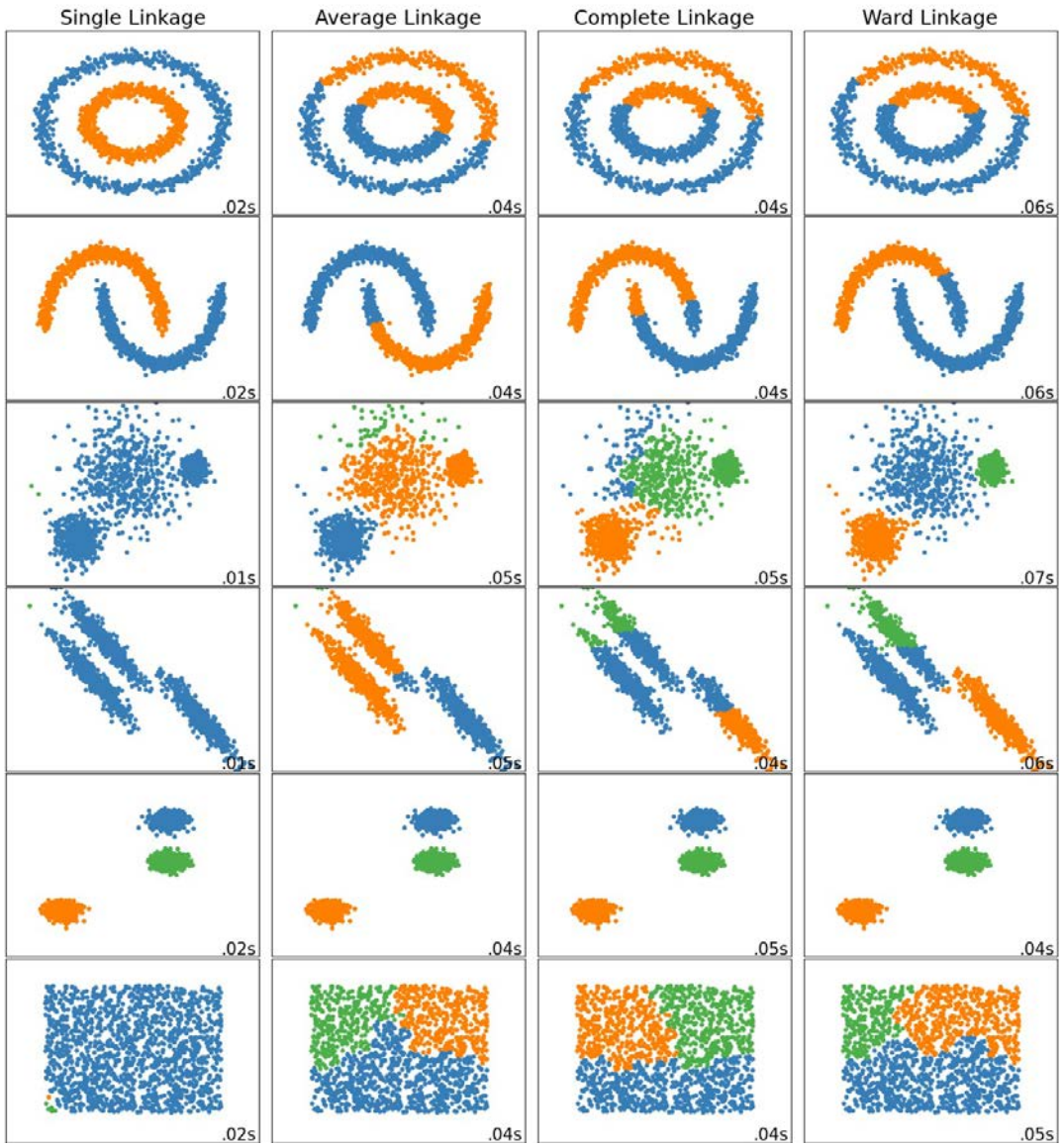


Image: https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html

1. Merge clusters with smallest dissimilarity

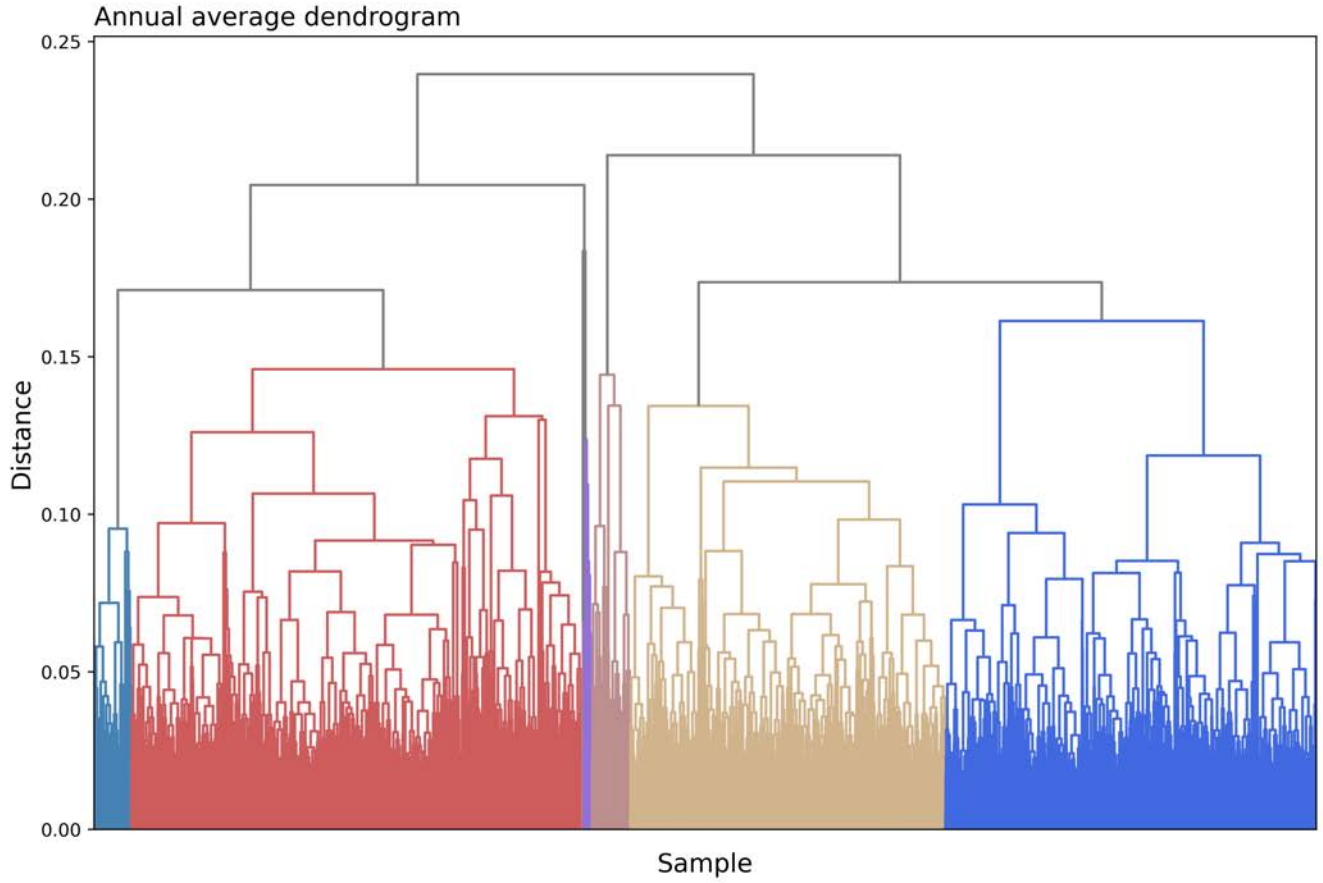
2. Work out new dissimilarities for new clusters*

*** Repeat 1-2 until all observations are merged into a single cluster, or until the desired number of clusters is reached**

Hastie et al. (2009) Elements of statistical learning

Unlike *k*-means, we can gain some idea of the 'structure' of the data before hand

The dendrogram shows us when/how clusters are merged.



Fiddes et al. (2021) Redefining Southern Australia's climate regions and seasons

Pros:

- Scales well to large data sets and large number of clusters
- Does not require clusters to have similar size
- A number of ways to ‘link’ clusters (each with their own pros and cons)
- We can learn about the data structure prior to choosing number of clusters (but ultimately still have to choose number of clusters)

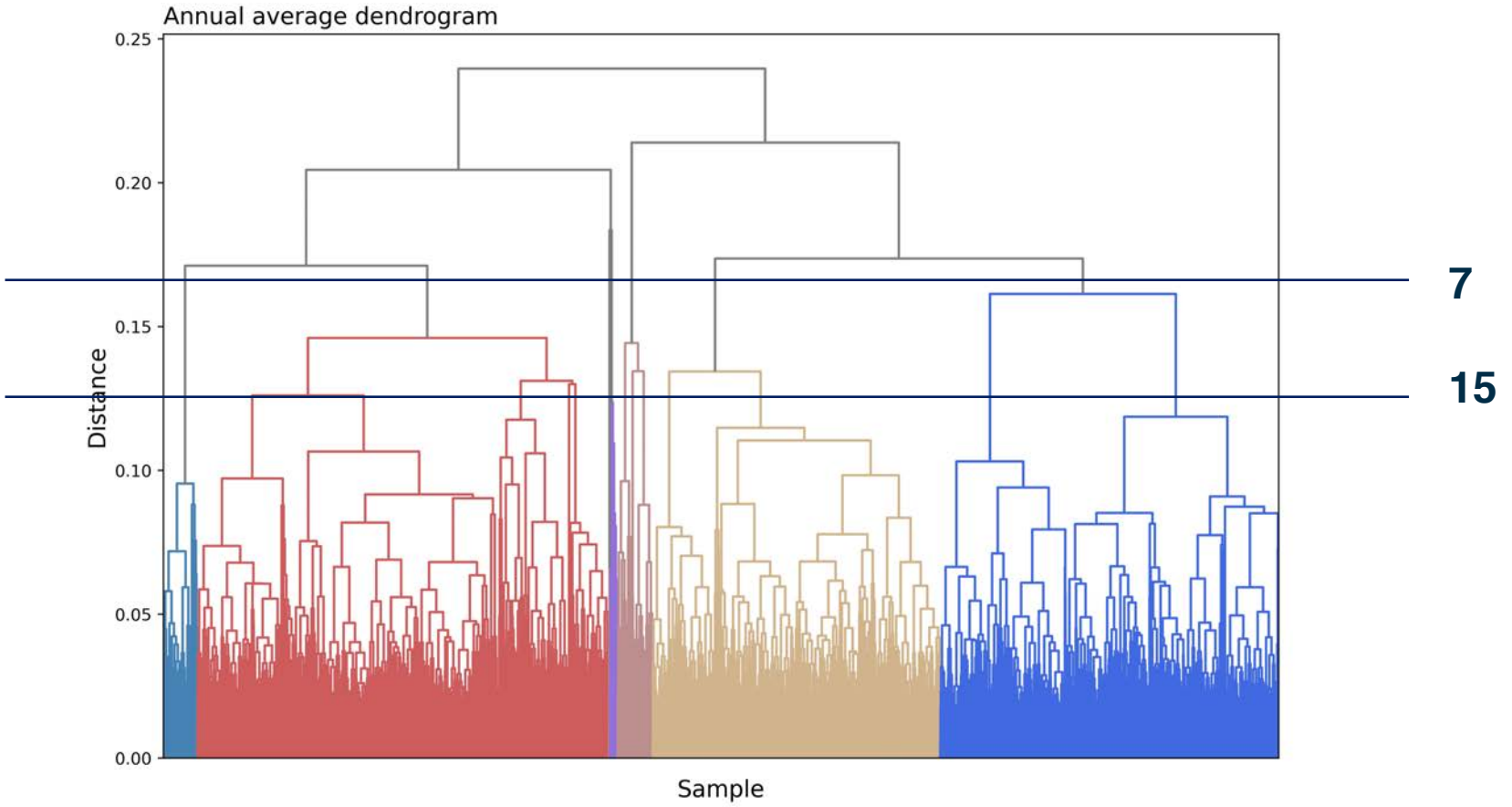
Cons:

- Less flexible, once groups of observations are assigned to a cluster, they will stay in that cluster
- Less efficient

Image: https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html

Average linkage:

We chose 7 and 15 to test, in part based on the dendrogram, and in part due to our knowledge of the system



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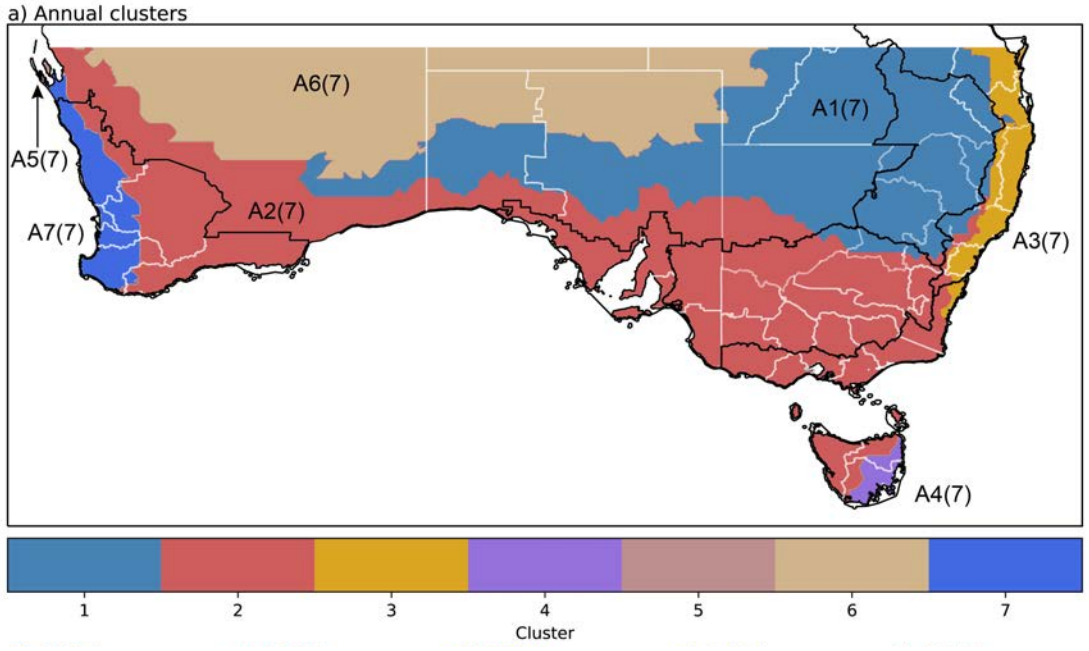
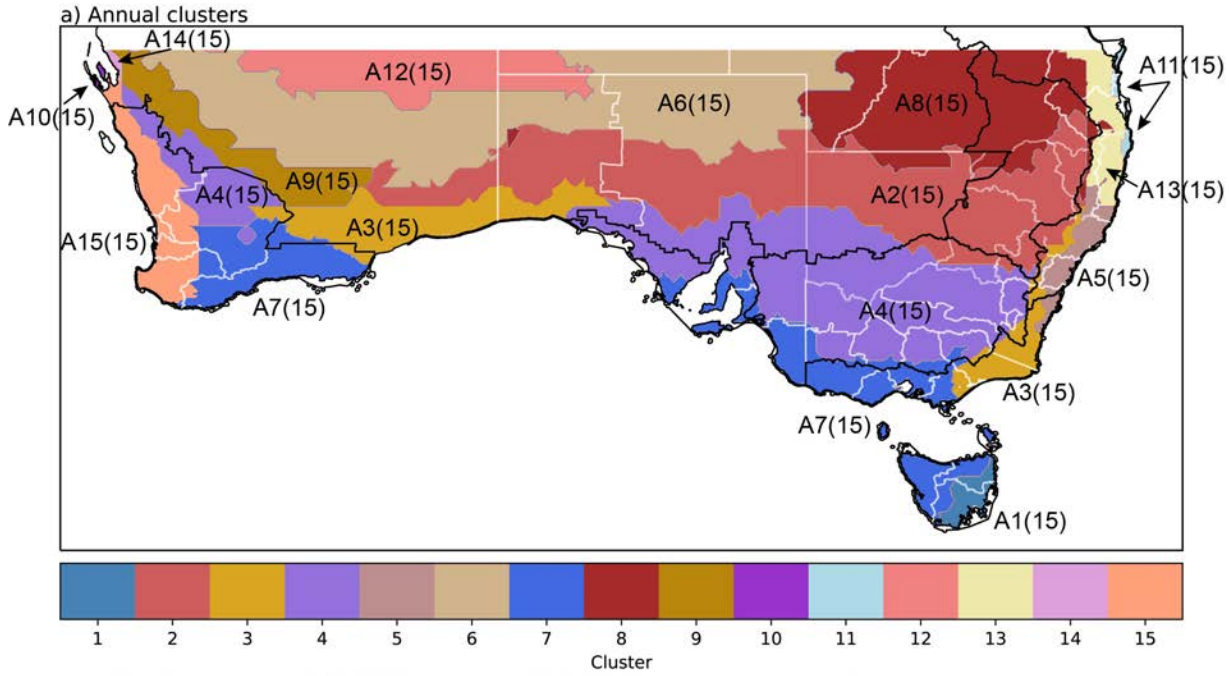
Average linkage:

Seven clusters didn't capture the differentiations were were after in SE Aus, so 15 clusters were. also produced.





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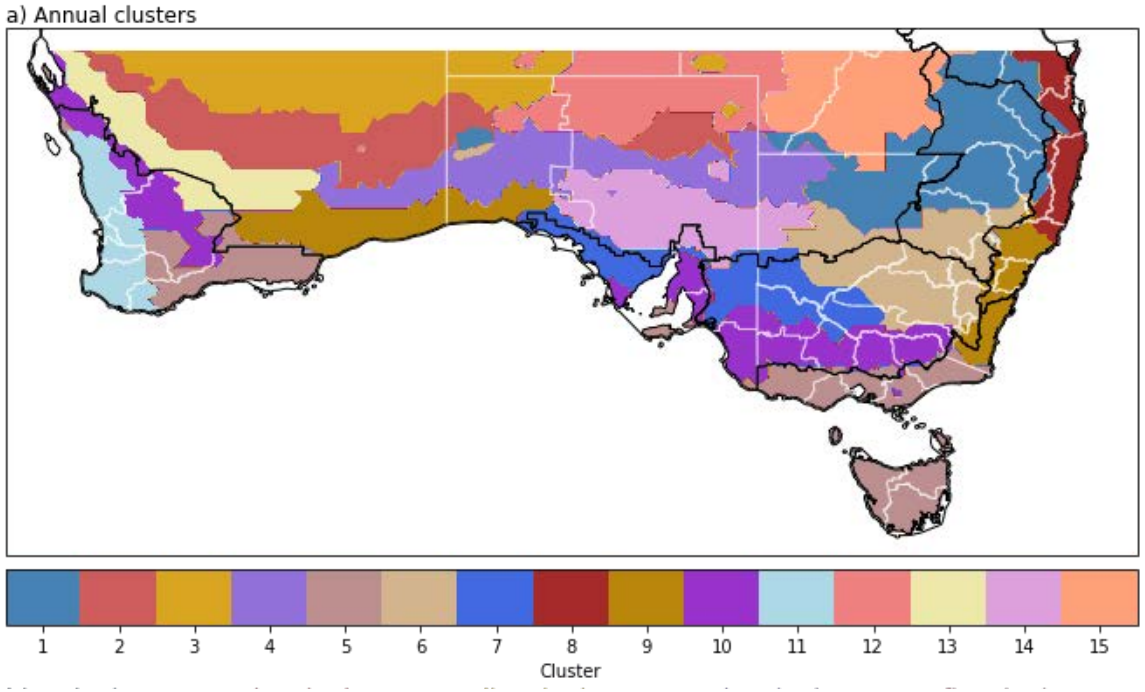
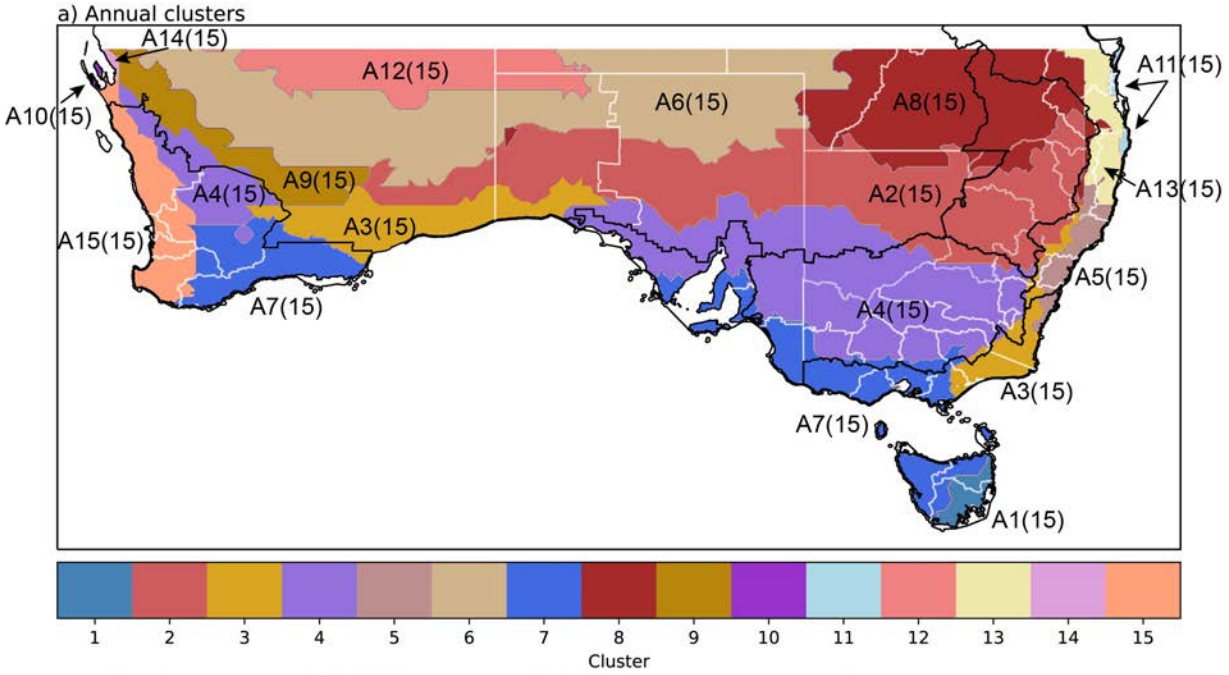
K-means



Average

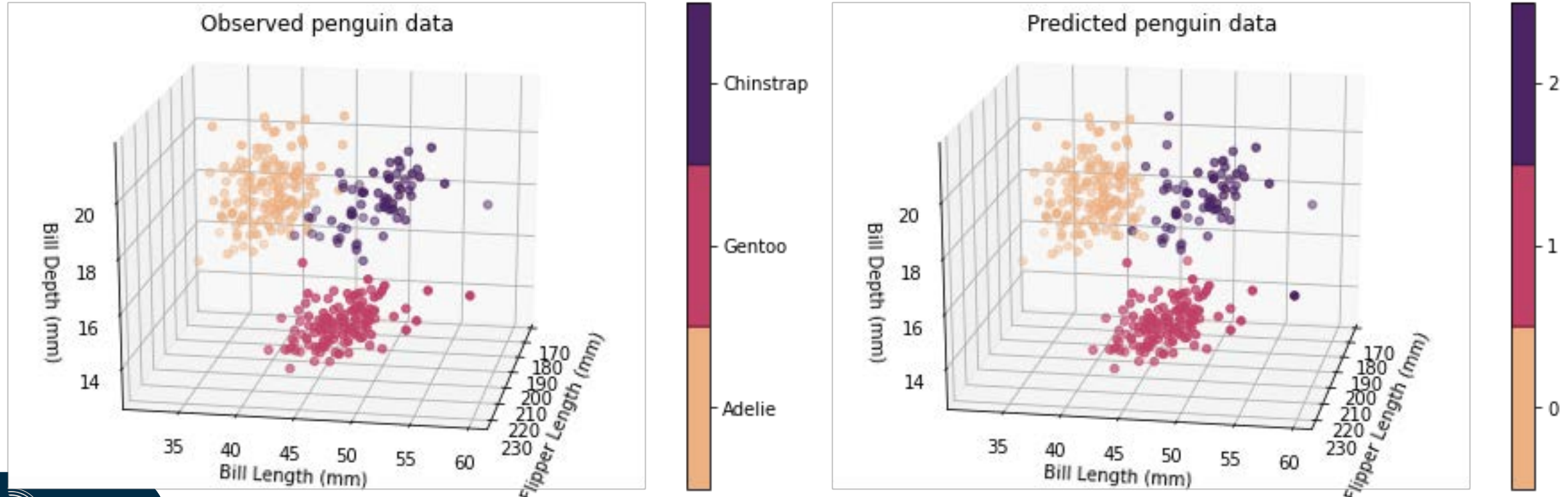


Tutorial

https://github.com/sfiddes/teaching/blob/main/2021_08_ML_workshop/Clustering101.ipynb

Use the Palmer Penguins data set and SK-Learn to perform k-means and agglomerative clustering.

Note in this instance, we already know the structure of our data, so our lives are *a lot* easier.



Clustering with big data sets

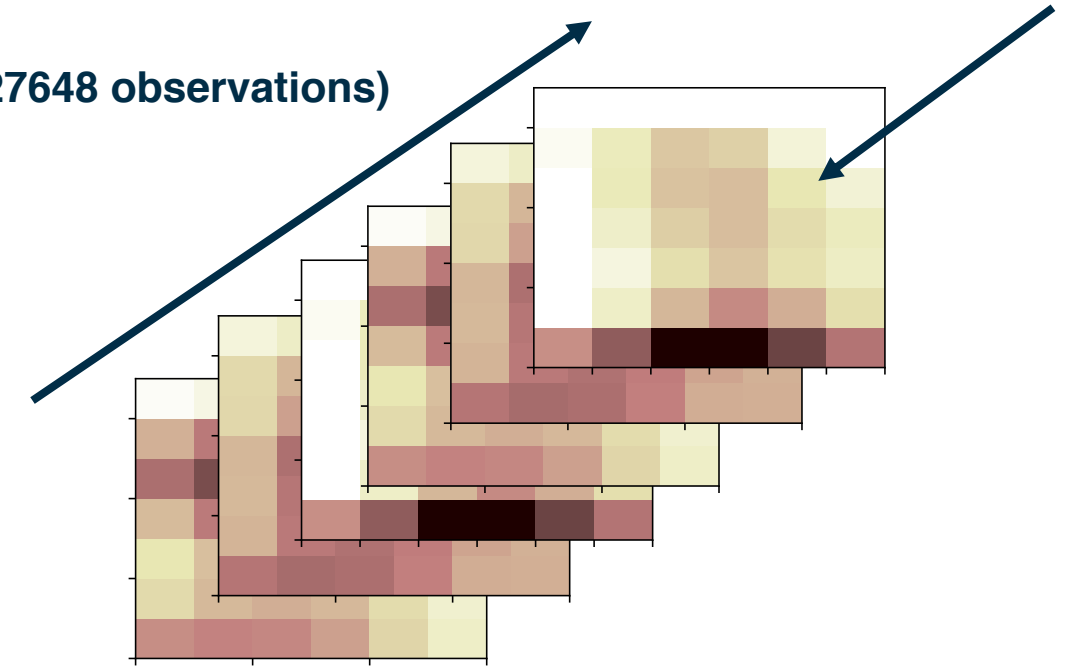
In many instances in climate science, you are using gridded data over time and space

This adds up quickly

In my current work: using histograms of cloud optical depth vs cloud top pressure (the attributes) for global gridded data, over 4 years.

Attributes (42 grid points)

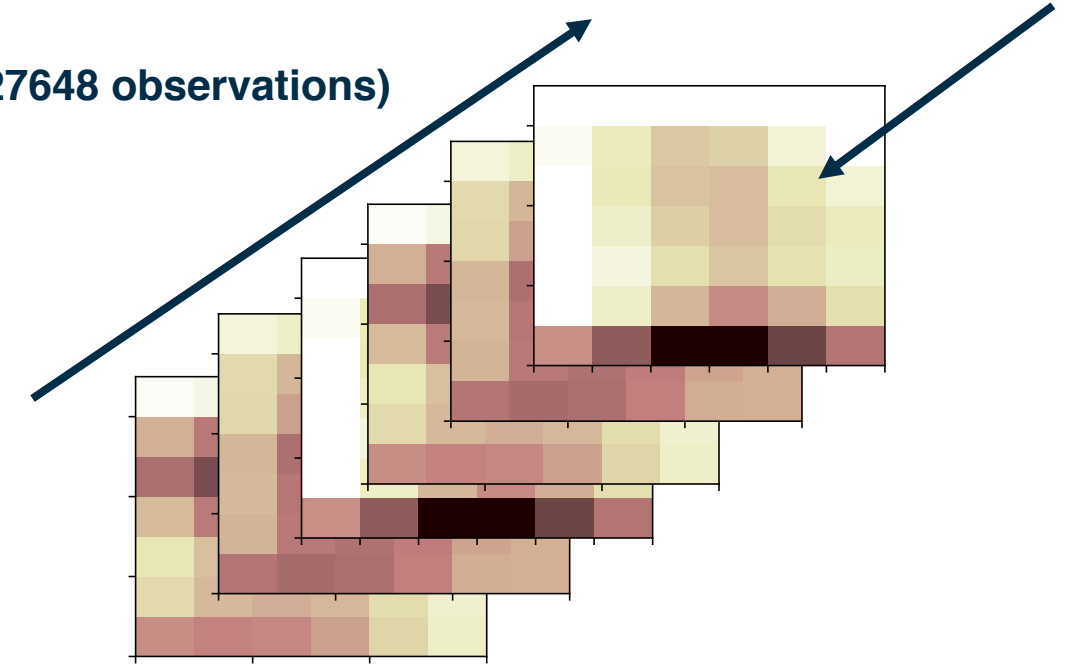
Time X Space (1461 x 27648 observations)



To perform the clustering, I either need heaps of memory (less feasible) or to distribute the computations across a number of cores

Attributes (42 grid points)

Time X Space (1461 x 27648 observations)



Dask ML

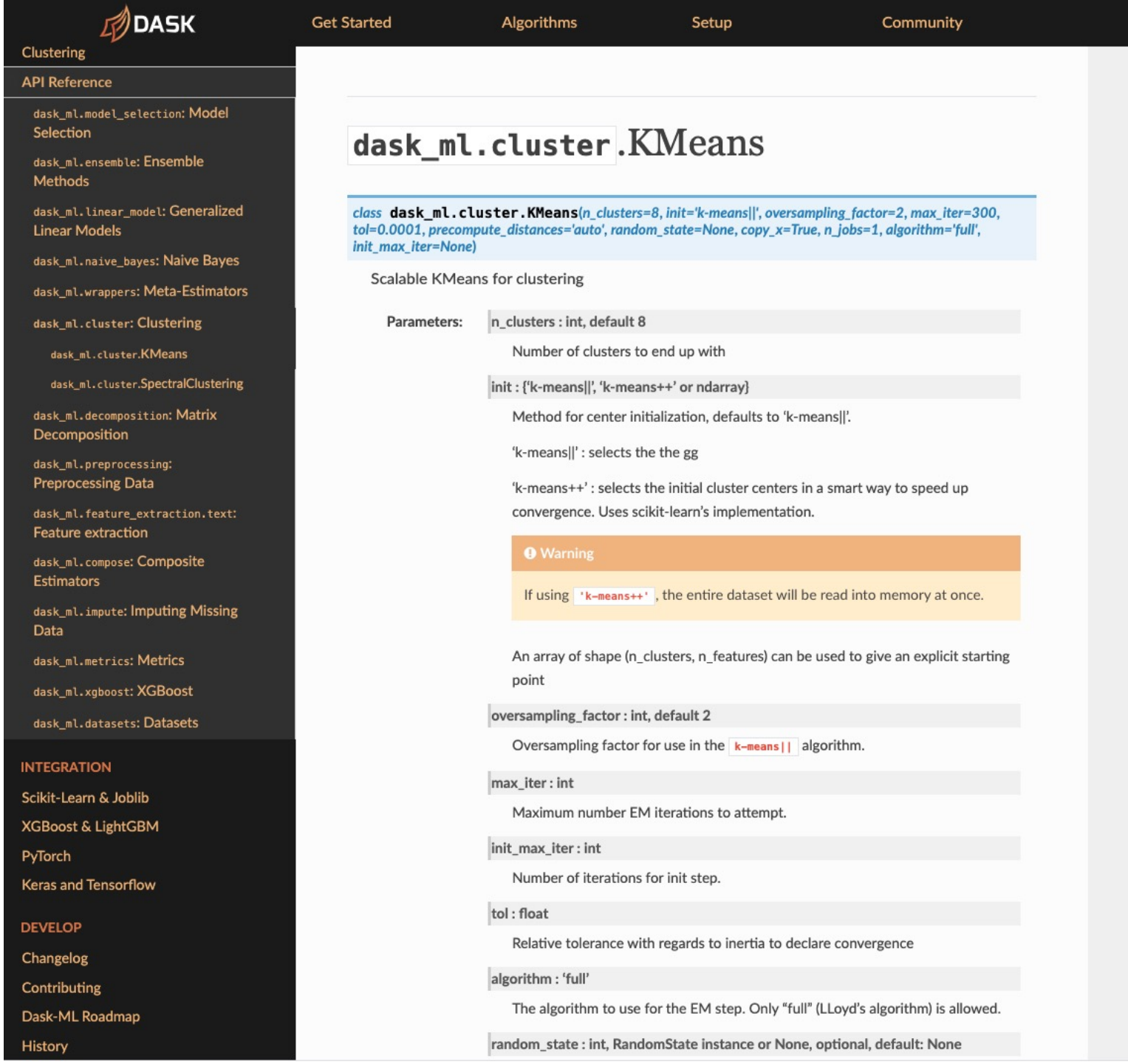
Fiddes et al. (2021) Redefining Southern Australia's climate regions and seasons

Thankfully, Dask – Machine Learning, can do this for you, if you are using *k*-means.

Set up for *k*-means very similar to SK-Learn, super easy to implement

Dask handles the distribution for you

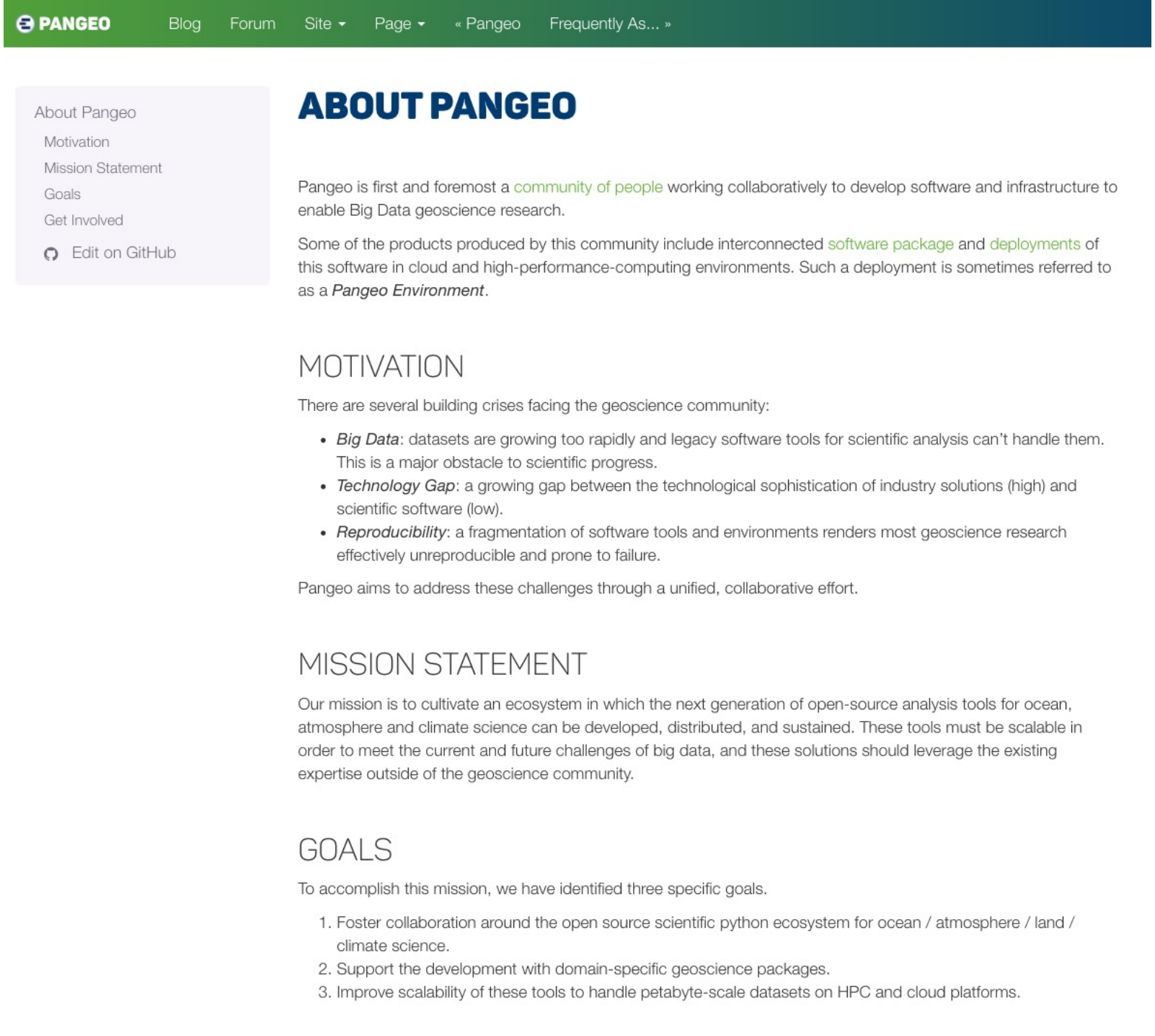
https://ml.dask.org/modules/generated/dask_ml.cluster.KMeans.html



Pangeo

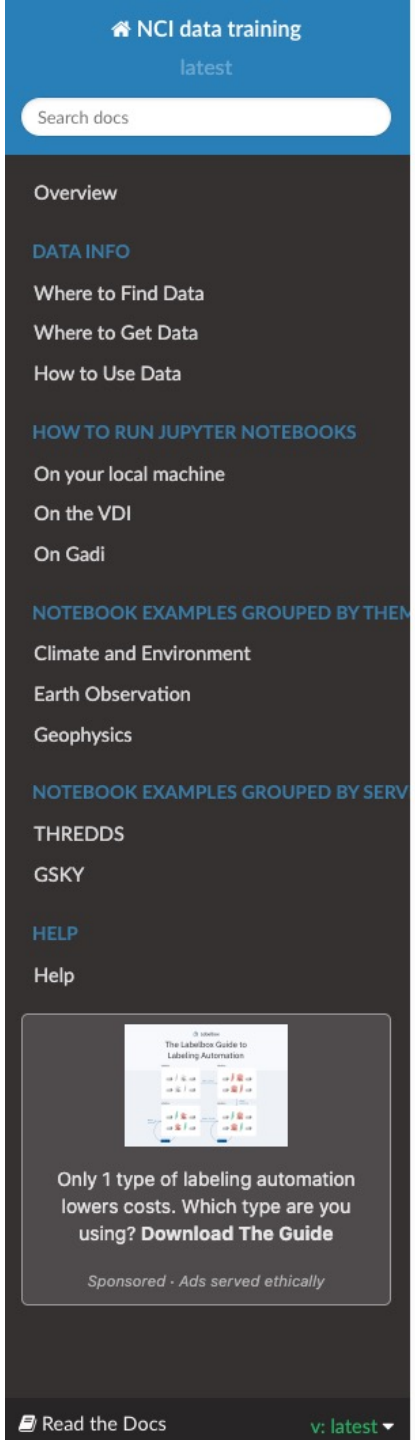
To make your life even easier, the NCI have now set up a Pangeo environment specifically for these types of tasks, using JupyterLab

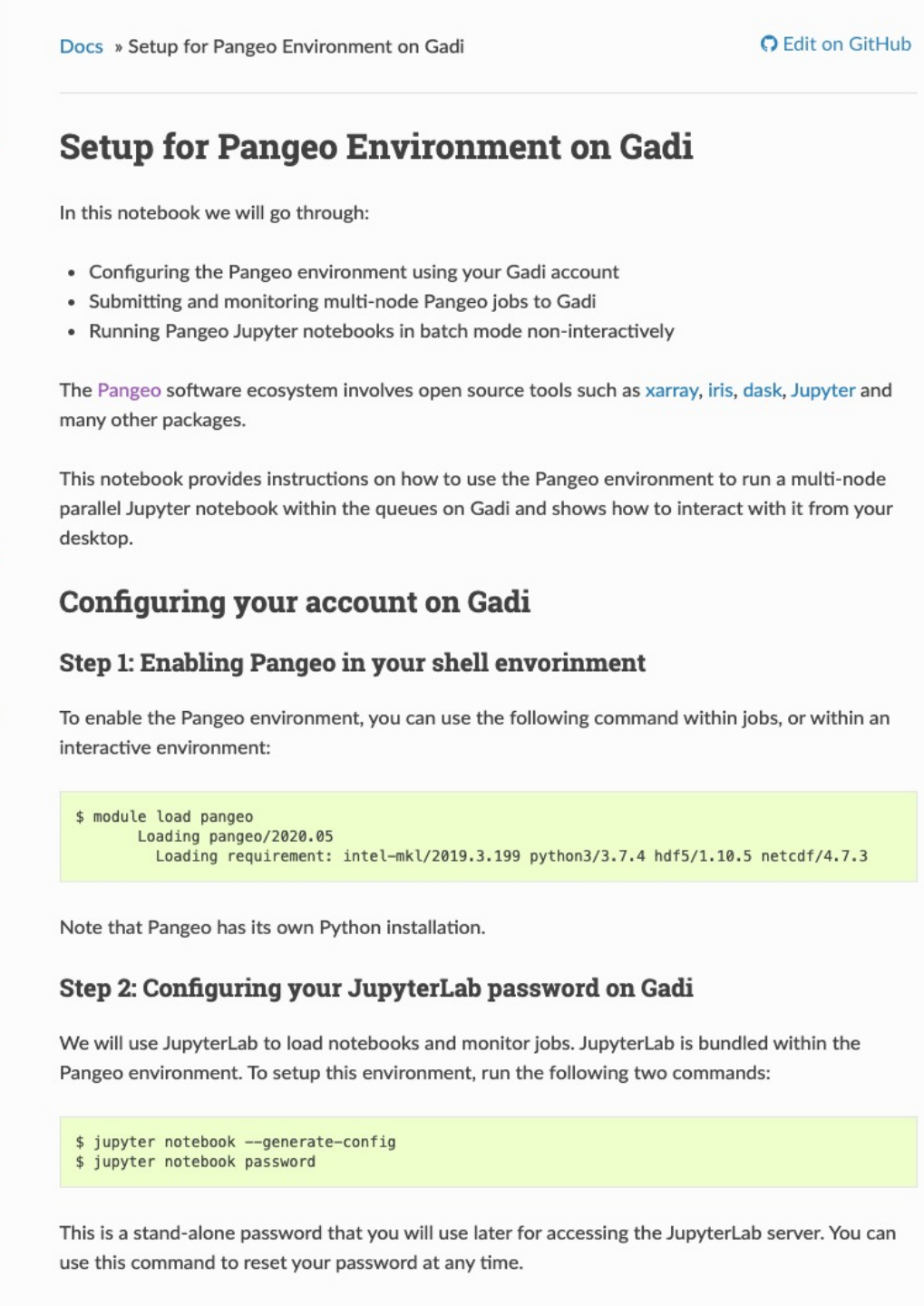
https://pangeo.io/



The NCI have clear instructions for setting a Pangeo environment, which included standard python packages needed for this type of application (xarray, dask, Jupyter and more!)

https://nci-data-training.readthedocs.io/en/latest/_notebook/prep/Setup_Pangeo_environment_Gadi.html





NCI also have a range of example notebooks using Dask and a Pangeo environment (including one for clustering!):

https://github.com/NCI-data-analysis-platform/examples-dask

https://opus.nci.org.au/display/Help/examples-dask

jupyter nbviewer

JUPYTER FAQ

examples-dask / Dask_18_machine_learning.ipynb

Dask for Machine Learning

- Scaling problems
- Distributed training
- Train larger-than-memory datasets

- Authors: NCI Virtual Research Environment Team
- Keywords: Machine Learning, Dask-ML, Training, Scaling
- Creation Date: 2020-Sep
- Lineage/Reference: This tutorial is referenced to dask tutorial.

Set up

Choose from the following two options to create a client:

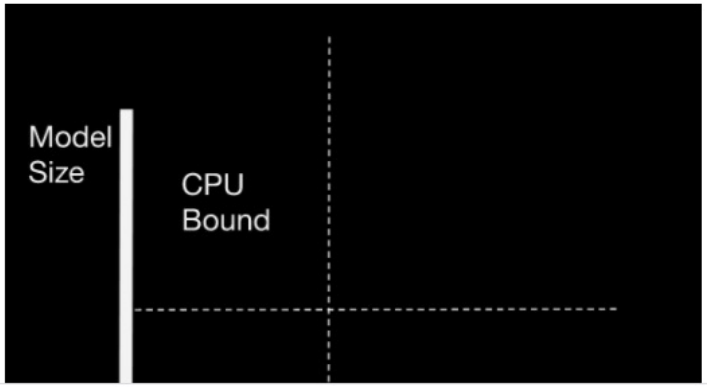
In [ ]:
```
# If you run this notebook on your local computer or NCI's VDI instance, you can create cluster
from dask.distributed import Client, progress
client = Client()
client
```

In [ ]:
```
# If you run this notebook on Gadi under pangeo environment, you can create cluster using scheduler.json file
from dask.distributed import Client, LocalCluster
client = Client(scheduler_file='scheduler.json')
print(client)
```

Types of Scaling

There are a couple of distinct scaling problems you might face. The scaling strategy depends on which problem you're facing.

1. CPU-Bound: Data fits in RAM, but training takes too long. Many hyperparameter combinations, a large ensemble of many models, etc.
2. Memory-bound: Data is larger than RAM, and sampling isn't an option.



Example

- Read in the data I need
- Organise it into the dimensions I need
- Flatten the attributes (so instead of 6x7, it is 1x42) and the observations (1461x144x192 to 40,393,728x1)
- Normalise
- Ready to be passed to *k*-means

Prep the MODIS data

Rename dims and merge first two tau bins, flatten and normalise. Then save out.

```
fdir = '/g/data/p66/slf563/OBS/MCD06COSP_D3_MODIS/'
modis = xr.open_mfdataset(fdir+'MCD06COSP_D3_MODIS.201*PCL_CL.nc', parallel=True,combine='by_coords').astype('float32')
modis = modis.drop_vars(('longitude','latitude','Mean','Standard_Deviation','Sum','Pixel_Counts','Sum_Squares'))
modis = modis.rename_dims({'jhisto_cloud_optical_thickness_total_7':'tau',
                           'jhisto_cloud_top_pressure_7':'pressure',
                           'lat':'latitude',
                           'lon':'longitude'})
modis = modis.rename_vars({'JHisto_vs_Cloud_Top_Pressure':'histo',
                           'lat':'latitude',
                           'lon':'longitude'})
modis = modis.transpose('tau','pressure','time','latitude','longitude',)

data2 = modis.histo[1:,:,:]
data2[0,:,:].values = data2[0,:,:].values + modis.histo[0,:,:].values
modis = data2.fillna(0)

dataout = modis.stack(x = ('time','longitude','latitude'),
                      y = ('tau','pressure')).reset_index(dims_or_levels=['x','y'])
dataout = dataout/dataout.sum(dim='y')
a = np.where(dataout.sum(dim='y').values!=0)[0]
dataout = dataout.chunk(841536,1)

dataout.to_netcdf('/g/data/jk72/slf563/ACCESS/output/bx400/modis_clustering_data.nc')
del dataout
```

```
modis
```

Show/Hide data repr Show/Hide attributes

xarray.DataArray

'histo'

- tau: 6
- pressure: 7
- time: 1461
- latitude: 144
- longitude: 192

You can see the actual running of *k*-means is the same!

I then re-shape the data back into its original form (ie, 6x7 attributes and 1461x144x192 observations)

K-means:

We have worked out the optimum number of clusters previously.

[8]:
```
nclus = 12
```

[9]:
```
model = KMeans(n_clusters=nclus,random_state=0).fit(data)
```

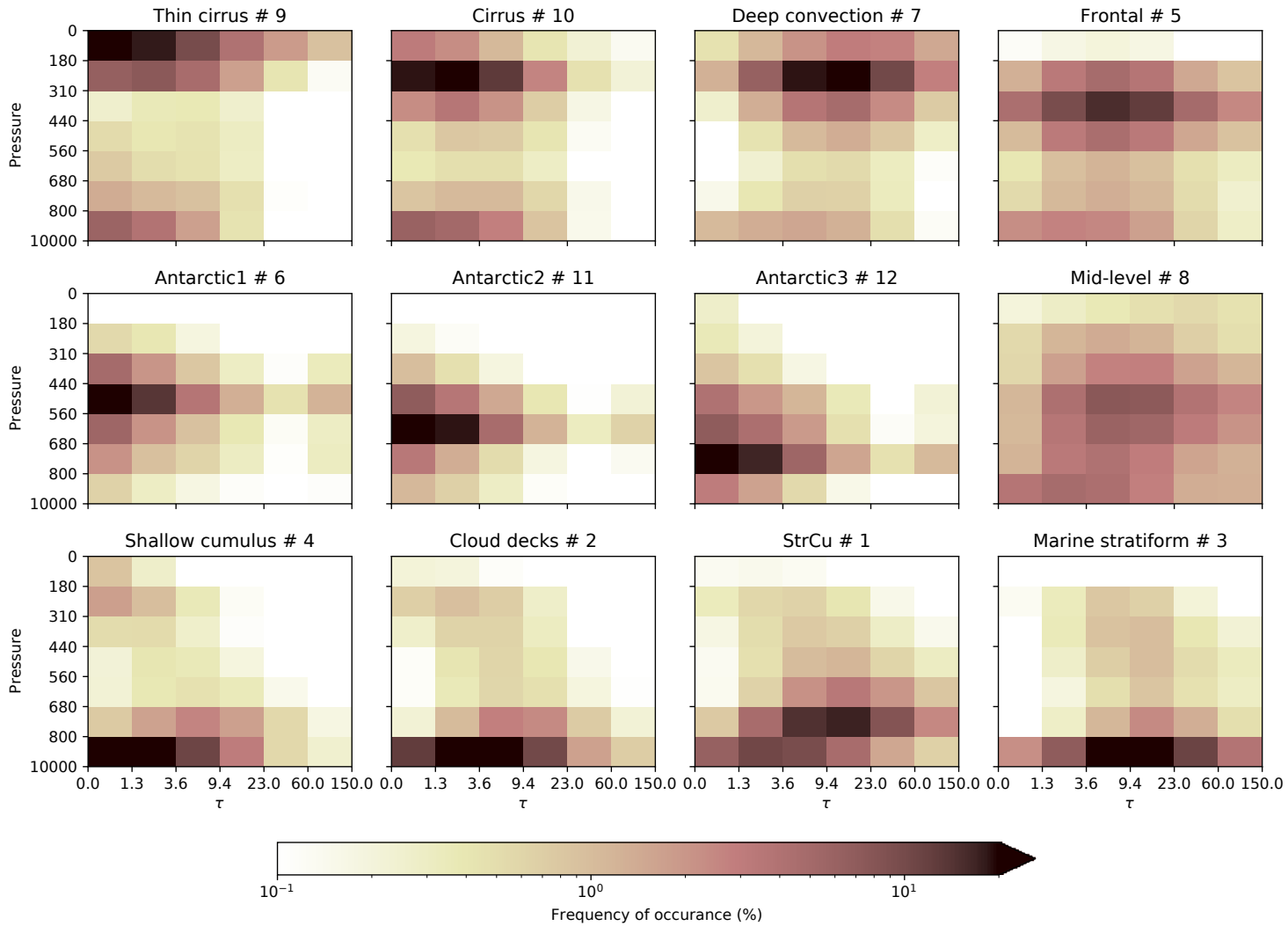
```
/g/data/dk92/apps/anaconda3/2020.12/envs/NCI-data-analysis_2021.03/lib/python3.7/site-packages/distribu
  ("('open_dataset-f0ea9dcd1d35bd78f322e113ff995e34h ... , None, None)))
Consider scattering large objects ahead of time
with client.scatter to reduce scheduler burden and
keep data on workers

    future = client.submit(func, big_data)    # bad

    big_future = client.scatter(big_data)     # good
    future = client.submit(func, big_future)  # good
  % (format_bytes(len(b)), s)
```

[10]:
```
clusters = model.cluster_centers_
centers = clusters.reshape(nclus,6,7)
```

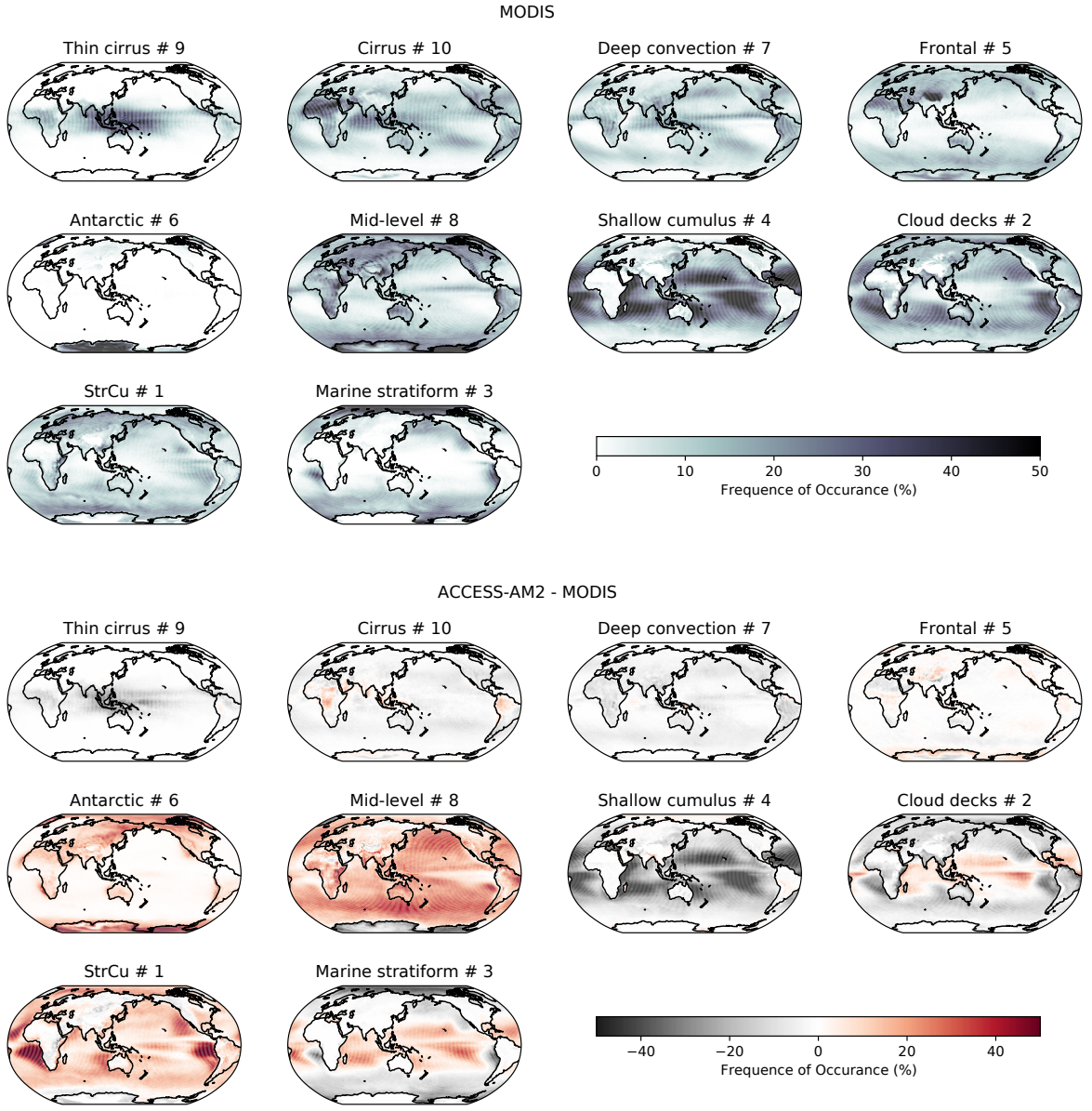
[11]:
```
centers = xr.DataArray(dims=['k','Tau','Pressure'],
                       coords={'k':np.arange(1,nclus+1),'Tau':np.arange(0,6),'Pressure':np.arange(0,7)
                       attrs={'Cloud top pressure':plevs,'Cloud optical depth':tau})
centers[:] = clusters.reshape(nclus,6,7)
centers = centers.transpose('k','Pressure','Tau')
centers = centers.reindex(Pressure=list(reversed(centers.Pressure)))
```

[12]:
```
labels = model.labels_
C = xr.DataArray(dims=['time','latitude','longitude'],
                 coords={'time':modis.time,
                         'latitude':modis.latitude,
                         'longitude':modis.longitude}))
C = C.stack(x = ('time','longitude','latitude'))
C[a] = labels
C = C.unstack('x')
```

I end up with 12 cloud regimes based on cloud top pressure (y-axis) and cloud optical depth (x-axis).



I can then use this to evaluate the ACCESS climate model by fitting the learnt *k*-means centroids to the equivalent model data.



Resources:

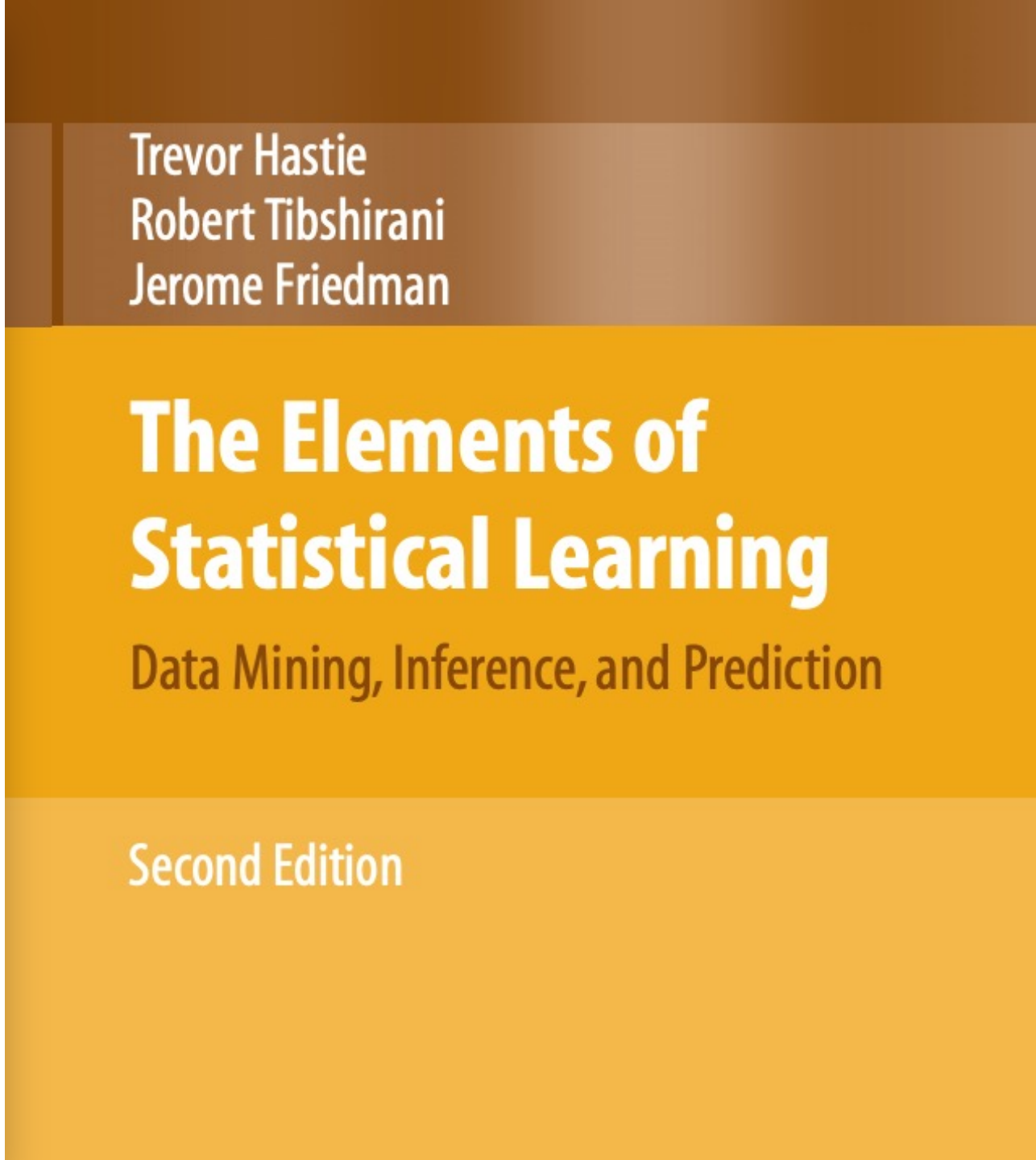
Hastie, T., Friedman, J., and Tibshirani, R. (2009). The Elements of Statistical Learning. Springer Series in Statistics. (Springer: New York, NY.) **Chapter 14.3**

Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J.,Passos, A., Cournapeau, D., Brucher, M., Perrot, M., and Duchesnay, E. (2011). Scikit-learn: Machine Learning in Python. J. Mach. Learn. Res.12(12), 2825–2830

https://nci-data-training.readthedocs.io/en/latest/_notebook/prep/Setup_Pangeo_environment_Gadi.html

https://opus.nci.org.au/display/Help/examples-dask

Fiddes, S., Pepler, A., Saunders, K., & Hope, P. (2021). Redefining southern Australia's climatic regions and seasons. *Journal of Southern Hemisphere Earth Systems Science*. https://doi.org/10.1071/ES20003



THANK YOU

Any questions?

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