Introduction to spatial data in R for paleontologists

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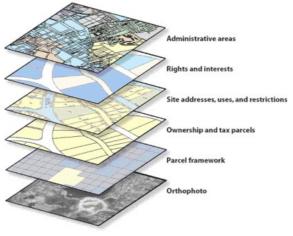
Basic Concepts

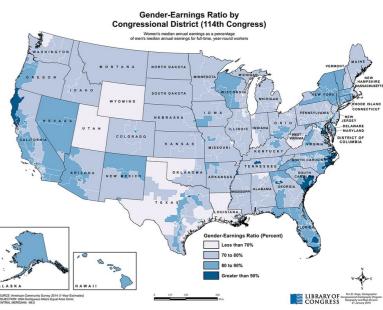
Where, what, why?

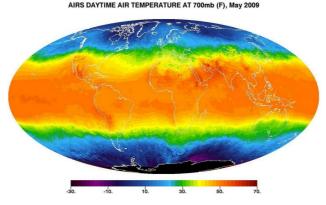
GIS basics

G(eographic) I(nformation) S(ystems/oftware) are everywhere

- Science
- Civil Engineering
- Aeronautics
- Military
- Economics
- etc.









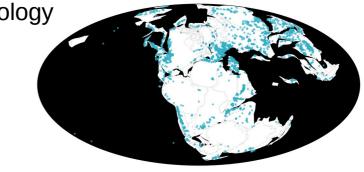
Vital in Earth Sciences

G(eographic) I(nformation) S(ystems) are everywhere

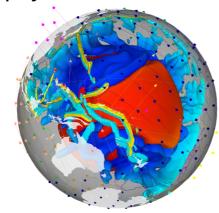
- topography
- geology



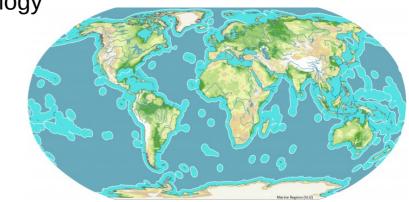
paleontology



- geophysics

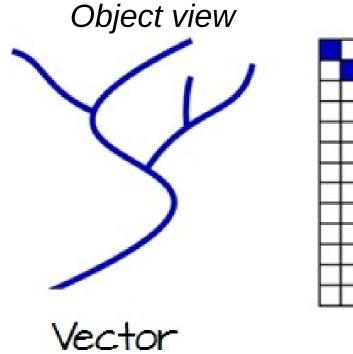


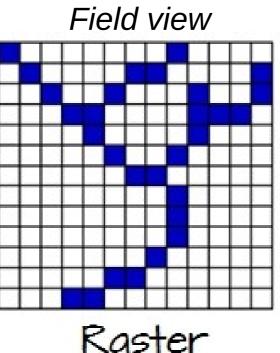
ecology



Basic data types

- Similar to computer graphics
- Sometimes in 3D

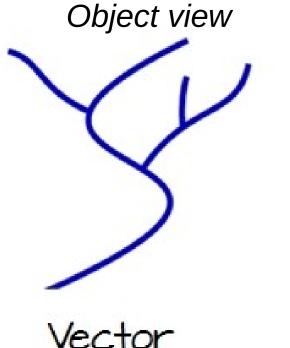


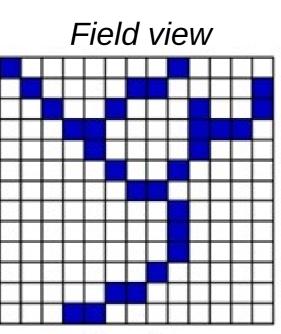


There is one twist:

Basic data types

- Similar to computer graphics
- Sometimes in 3D





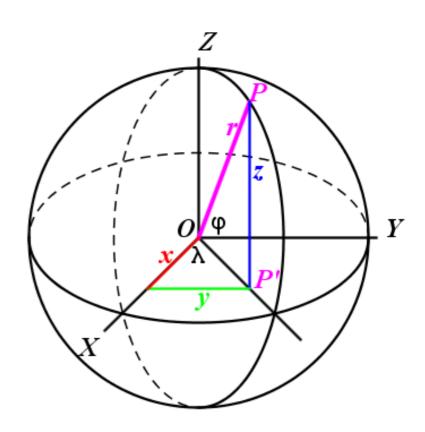


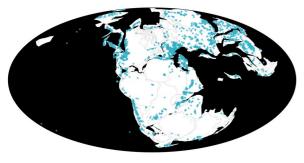


Raster

Vector data

- Structure is defined with points that have coordinates
- Spherical coordinates, Cartesian too, or projection-specific
- Additional attributes are rendered to the entities
- 3 primary kind





Points



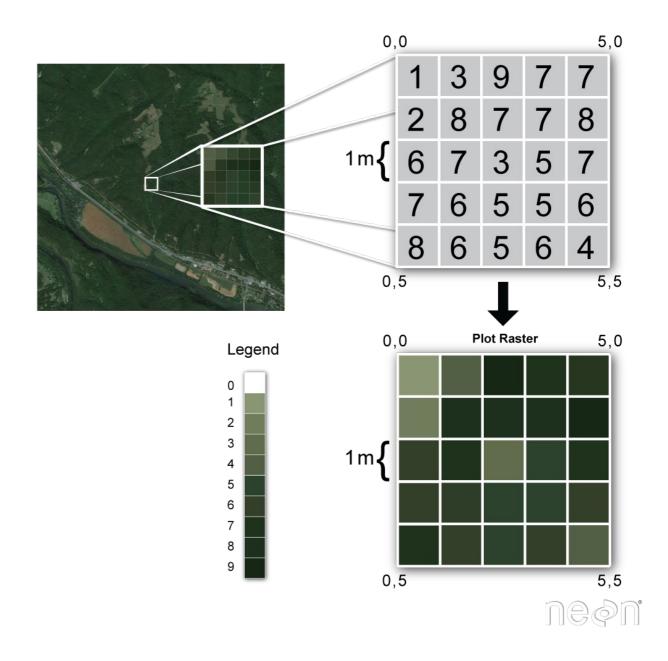
Lines



Polygons (shapes)

Raster data

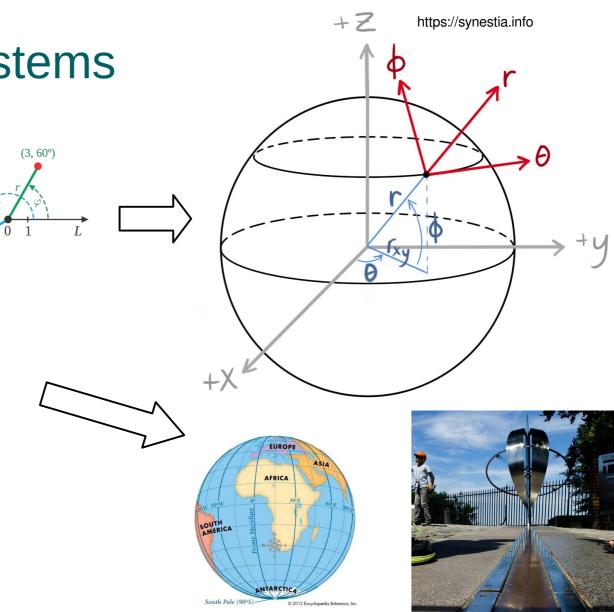
- Structure is defined by a grid, data is a lattice of values
- The field view of Earth
- Similar to raster graphics, but with georeferencing



(4, 210°)

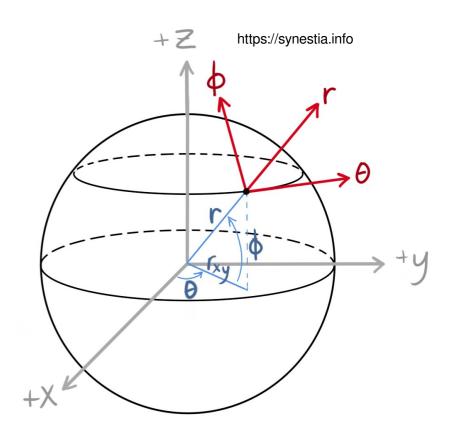
Geographic coordinates

- Based on polar coordinates
- ϕ : latitude
 - ⁻ [-90°, 90°], equator : 0°
- θ: longitude
 - [-180°, 180°], 0°: prime meridian
- r: elevation



Geocentric coordinates

- x, y, z, Earth-Centered Coordinate System
- Based on center of mass, equator and PM
- Used for satellite tracking and navigation (e.g. GPS)
- WGS84 datum

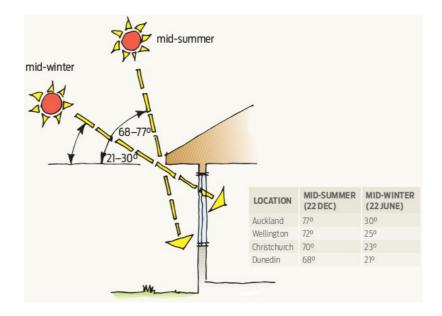




Projection based coordinate systems

- Surface: a 2-dimensional map
- Traditionally: Cartography
- Especially nautical applications



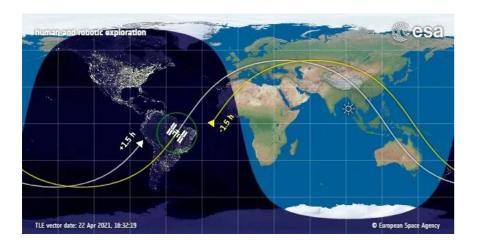


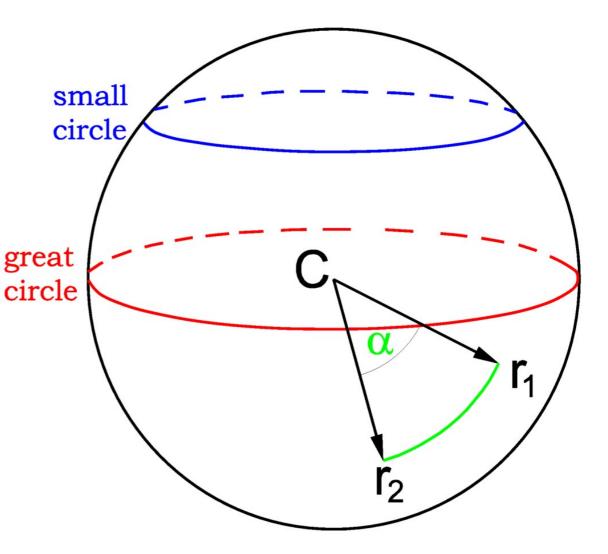




Spheres and Circles

- There are no straight lines
- All points are connected by arcs, either along a great or small circles

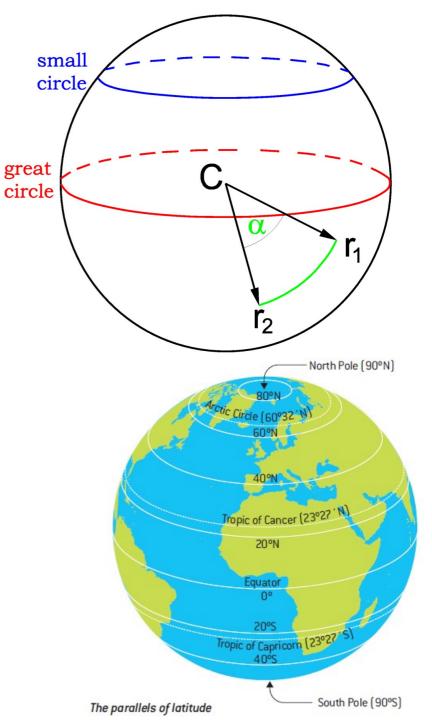




Path of the ISS

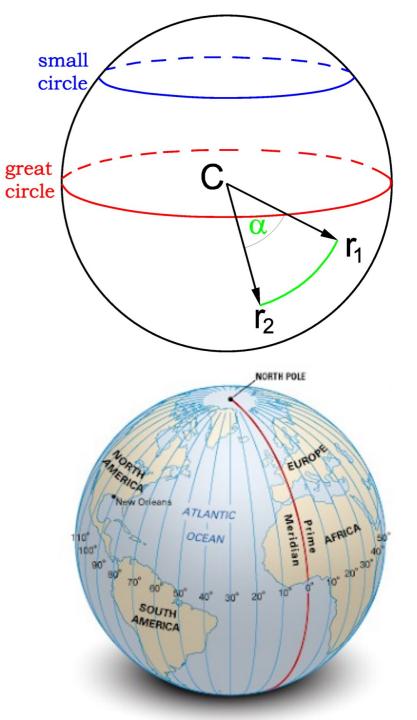
Latitude [-90-90°]

- Latitudinal circles: parallels
- The only great circle is the equator!
- Length decrease with a cosine function of latitude
- 10° wide **zone** has different area at different latitudes
- Direction: zonal (u)
- Notable circles:



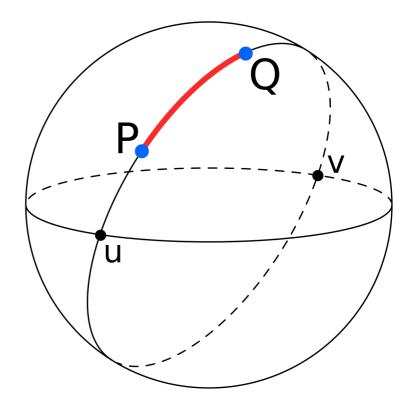
Longitude [-90-90°]

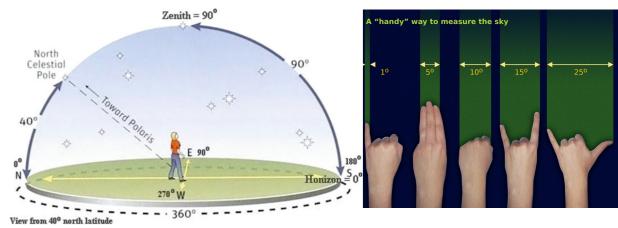
- Latitudinal circles: meridians
- All of them are great circles!
- Their distance decreases at the poles
- Direction: meridional (v)
- Notable circle:



Distances

- Two points define a great circle
- Shortest distance between them is a great circle arc (Great Circle Distance)
- Distance on a surface of a sphere is simplest in angles (degrees)
- For practicality we give this in distance:
- 1° (longitude) = 1 nautical mile \sim 111.1 km



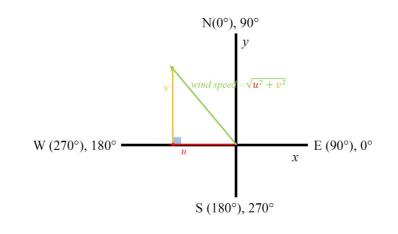


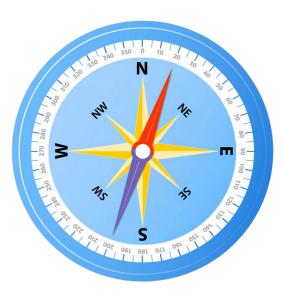
Directions

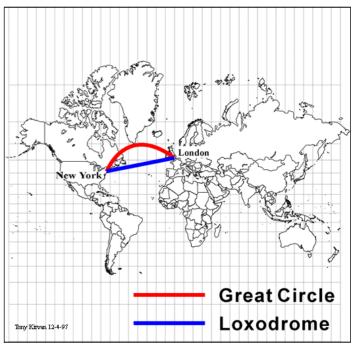
- Heading: angular distance to north
- Going straight: great circle
- Constant change of heading! (even without the true vs. magnetic difference)

Vectors

 Given with a) initial heading and magnitude or b) as zonal and meridional components



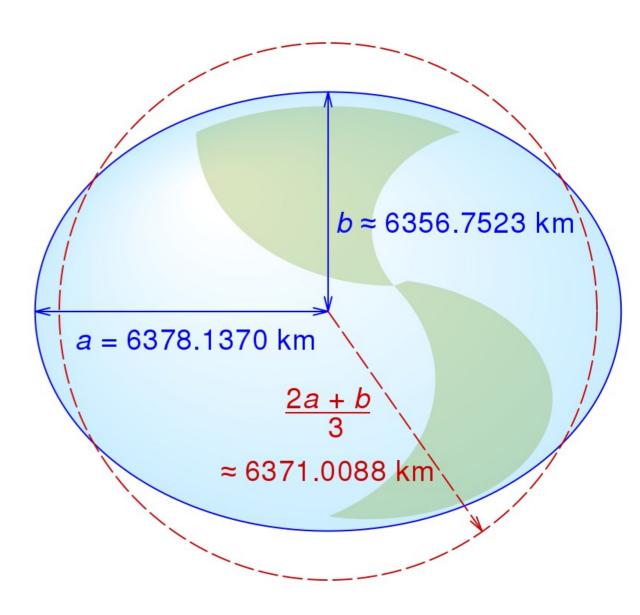




Mercator projection

The reference ellipsoid

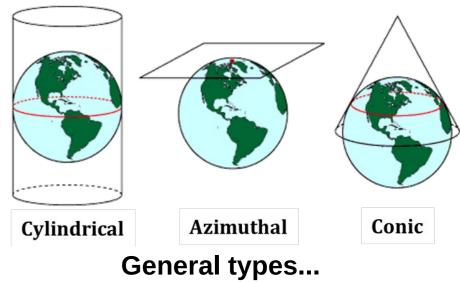
- Approximates the geoid
- Flattened rotational ellipsoid
- Used as a basis for elevation



Map projections

- There is dozens of them
- Complex transformations of spherical coordinates
- They all distort the globe in some sense:
 - conserve area and distort angles *(equal-area projection)*
 - distort area and conserve angles (conformal projection)
 - distort both area and angles

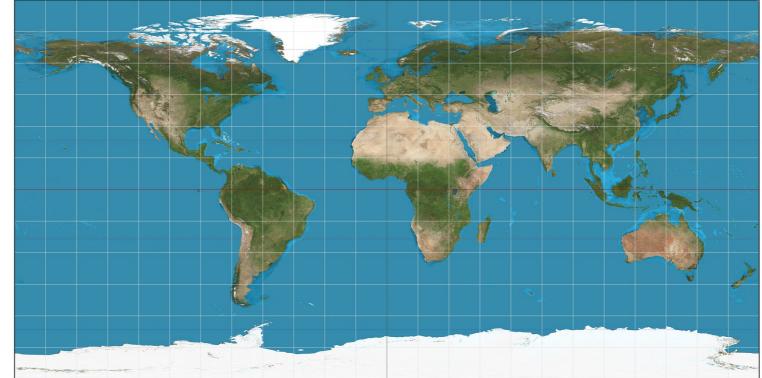
Types of Map Projections



The True size of.. : https://www.thetruesize.com

e.g. Equirectangular Projection

- Longitude (x) Latitude (y)
- Centered around (0, 0)
- Plate Carée
- Most frequently used for visualization of global-scale data
- Distorts everything



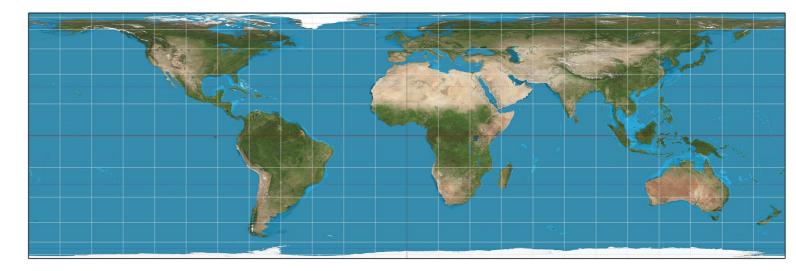
e.g. Mercator projection

- Conformal
- (nautical use)
- Highly distorts areas
- Cannot represent poles
- Variant: Google Earth



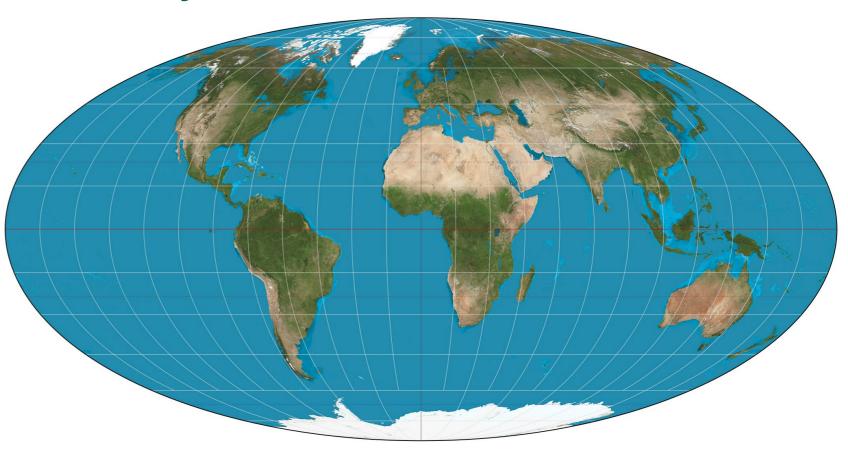
e.g. Lambert's Cylindrical EA Projection

- Equal-area
- Highly distorts angles latitudinally



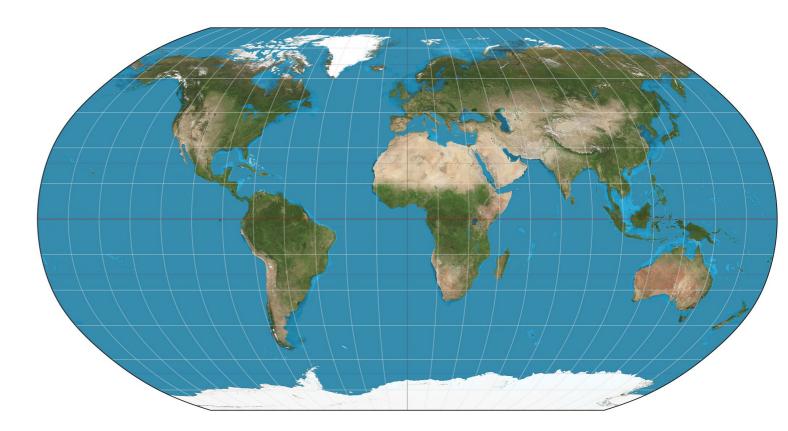
e.g. Mollweide Projection

- Equal-area
- Highly distorts angles longitudinally



e.g. Robinson Projection

- Distorts both angles and areas
- Relatively representative
- Promoted by NatGeo and now used by IPCC



Representation

- Older: PROJ.4 string: "+proj=moll"
- Well known text WKT2 string

```
PROJCS["World_Mollweide",
GEOGCS["WGS 84",
DATUM["WGS_1984",
SPHEROID["WGS 84",6378137,298.257223563]],
PRIMEM["Greenwich",0],
UNIT["Degree",0.0174532925199433]],
PROJECTION["Mollweide"],
PARAMETER["central_meridian",0],
PARAMETER["false_easting",0],
PARAMETER["false_northing",0],
UNIT["metre",1],
AXIS["Easting",EAST],
AXIS["Northing",NORTH],
AUTHORITY["ESRI","54009"]]
```

• EPSG registry ID (epsg.io) : ESRI:54009



EPSG

GEODETIC PARAMETER DATASET

Managed by IOGP's Geomatics Committee

Implementation

Where, what, why?

GIS tools: Why R?

- Automatized manipulation and extraction of data
- Larger quantity of work then with a GUI
- Python is much more powerful
- Integration with other analyses
- Statistical analyses



The Spatial ecosystem

- Multiple R extension packages form the backbone
- The heart: Open Source Geospatial Foundation
- Recipe:
 - Open source libraries for calculations + R interface

- R packages hook on the APIs of these libraries
- + extra calculations in compiled code (C, C++, Fortran)



Open Source Libraries/Projects

GDAL: Geodetic Data Abstraction Library

- Definitions of data formats
- Translation between data formats
- https://gdal.org/



Open Source Libraries/Projects

PROJ

- Coordinate transformation
- Definition of Coordinate Reference Systems (CRS) and translation
- Current version is 9.2.1 (June 2023)
- R packages rely on older versions (PROJ4 or PROJ6)



Open Source Libraries/Projects

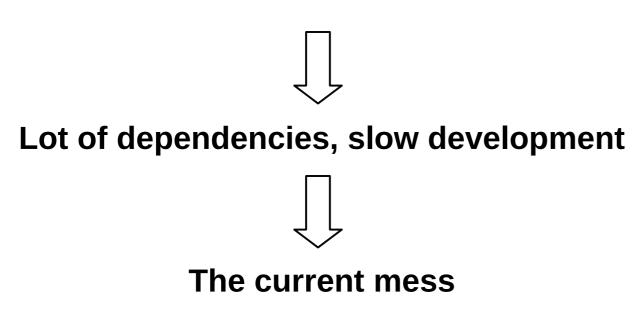
GEOS: Geometry Open Source

- Computational geometry especially towards the manipulation of spatial data
- http://libgeos.org/



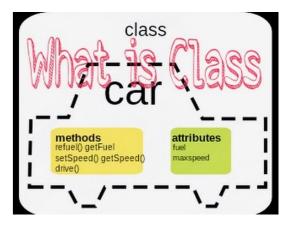
The R packages

- Only some are essential, they are on the CRAN
- They are using the libraries
- Class definitions and basic methods
- Lots of packages build on these...

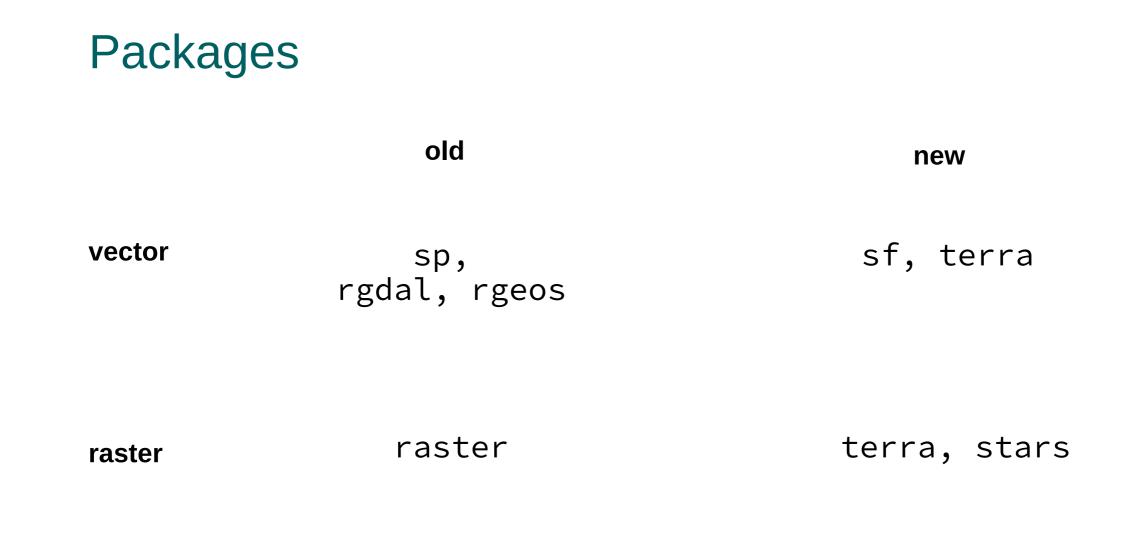




What is a class?



https://www.youtube.com/watch?v=XqrkcO42DI8



+ others: e.g. geosphere

Installing all of them

Focus on the new but...

- On Windows this is trivial, you can get all from the CRAN with install.packages()
- On Mac (and Linux), it is recommended to install them one at a time. They will a) either tell you what libraries need to be installed so they can function properly, 2) only indicate errors and then we have to google :)
- The list, again:

sp raster rgdal rgeos terra sf (stars) geosphere



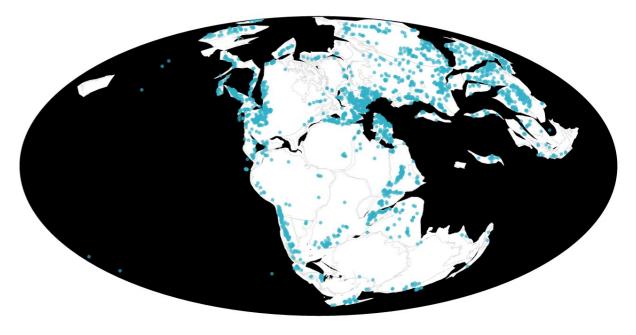
Vector data

with sf (and sp, rgdal, and rgeos)

Data concepts

Feature types: points

- A feature is a thing everything is a feature, that can be combined to form sets.
 - **Geometry**: It has coordinates and a CRS
 - Attributes: every point has data such as age, name, id etc..
- Features can be combined into sets, e.g. Multipoint



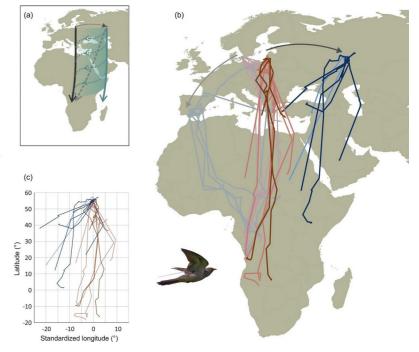
Fossil occurrences in the PBDB

Data concepts

Feature types: line

- Made up of sequence of points
 - One line: path, GPS track
 - Multiline: multiple paths combined that represent one thing
- Both a single line and a multiline can have attributes



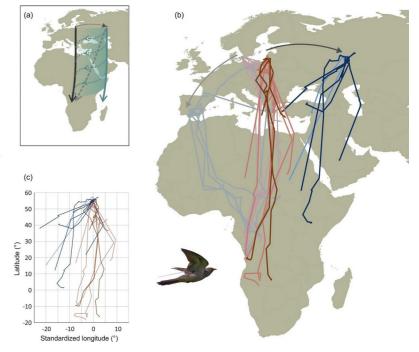


Thorup et al. 2020 Sci. Rep.

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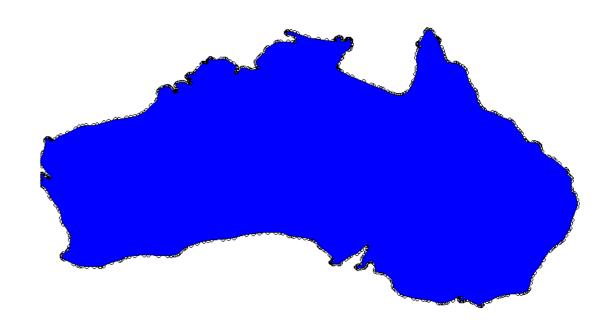




Thorup et al. 2020 Sci. Rep.

Feature types: Single Polygons

- Made up of sequence of points
- Closed to separate inside from outside
- Every polygon has attributes
- E.g. every island/landmass is by definition one polygon



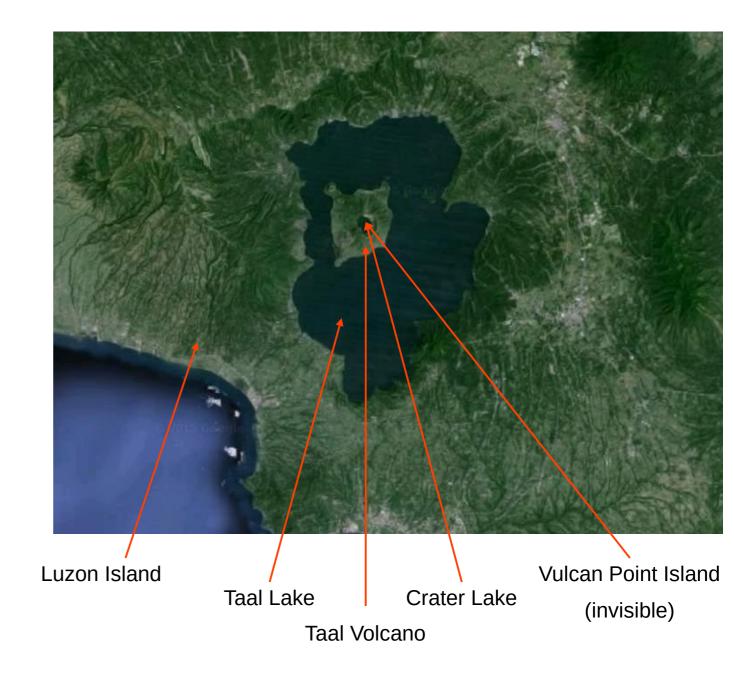
Feature types: Multiple polygons

- Polygons can be combined to represent single entities
- One thing is represented by multiple polygons, e.g. a country



Feature types: Multiple polygons

- Polygons can have holes
- Holes are also polygons that are inside other polygons
- The direction of points defines whether something is a hole or not



Registering complex data in R

- For GIS, 2 column matrices can do the job for points, lines and polygons
- You can create lists of Polygons and lists of that, but it quickly becomes a mess...
- S3 and S4 classes

	long	lat
1	142.3752	-10.99448
2	142.5119	-11.01241
3	142.6009	-11.05538
4	142.6376	-11.08747
5	142.7468	-11.26374
6	142.9131	-11.68280
7	142.9775	-11.80399
8	143.0637	-11.90817
9	143.0800	-11.90902
10	143.0876	-11.88224
11	143.1104	-11.88547
12	143.1691	-11.92764
13	143.2208	-11.98907
14	143.2265	-12.05601
15	143.1904	-12.18825
16	143.1972	-12.27063
17	143.3962	-12.80673
18	143.4831	-13.10462
19	143.5455	-13.38480
20	143.5754	-13.67029
21	143.6182	-13.85430
22	143.6887	-14.04426

S3 Objects

- Informal classes, which is based on a label: the class attribute
- They are often just lists: access elements with \$ or [[]]
- Example the "lm" class produced by lm()
- Methods dispatch works based on function names:
 - predict.lm() is called when predict() is used on an object that comes from this class
- There is no constraint on the object structure!
- Example in spatial: sf



S4 Objects

- Formal classes, with a pre-defined structure
- The object has slots, that can have only specific types and they must have them!
- Slots can be accessed with the @ operator
- Methods are written more explicitly for the argument classes (with setMethod())
- Most spatial objects use this framework!

> str(spp)
Formal class 'SpatialPolygons' [package "sp"] with 4 slots
\$:Formal class 'Polygons' [package "sp"] with 5 slots
@labpt : num [1:2] 134.4 -25.6
@area : num 685
attr(*, "dimnames")=List of 2
Second class 'Polygon' [package "sp"] with 5 slots
<pre>@ area : num [1:2] 63.8 36.8</pre>
attr(*, "dimnames")=List of 2
[10] [10] [10] [10] [10] [10] [10] [112] "V1" "V2"
@labpt : num [1:2] 63.8 36.8
@area : num 9569
@ bbox : num [1:2, 1:2] -17.4 -39 180.4 77.7
<pre> attr(*, "dimnames")=List of 2</pre>
\$: chr [1:2] "min" "max"
@ proj4string:Formal class 'CRS' [package "sp"] with 1 slot

An object from the old sp package

Package sp: Classes and Methods for Spatial Data

- Primarily by Edzer Pebesma and Roger Bivand
- From 2005
- The structures to represent the data in R
- S4 classes and how to interact with them
- Primarily used for vector data also some raster
 - SpatialPoints(DataFrame)
 - SpatialLines(DataFrame)
 - SpatialPolygons(DataFrame)

Vector File formats

ESRI Shapefiles

- Multiple files represent the data
 - .shx: Index file, where is what
 - .shp: Main file, geometries
 - .dbf: Attribute information (dBASE)
 - .prj, .sbn, etc..





Vector File formats

Keyhole Markup Language

- .kml or .kmz file (z for zipped)
- Standard for the web



Google Earth uses .kml



Vector File formats

GeoJSON

- .js .json also for the web
- Human readable

```
"type": "Feature",
"geometry": {
   "type": "Point",
   "coordinates": [125.6, 10.1]
},
"properties": {
   "name": "Dinagat Islands"
}
```

PostGIS

• Database-oriented (PostgreSQL)

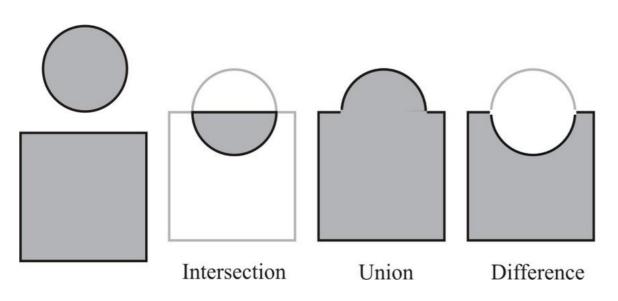
Package rgdal: Bindings for the 'Geospatial' Data Abstraction Library

- Primarily by Roger Bivand
- Interface to GDAL and PROJ<6
- Accessing data (I/O) and executing projections



Package rgeos: Interface to Geometry Engine - Open Source ('GEOS')

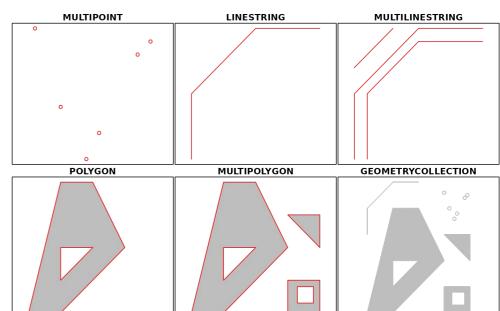
- Primarily by Roger Bivand
- Interface to GEOS
- Geometric calculations in the same CRS (e.g. Area)
- Boolean operations with shapes





Package sf: Simple Features for R

- Primarily by Edzer Pebesma
- From 2017
- Integrates with GDAL, GEOS and PROJ
- Uses the simple feature standard
- Good tidyverse integration







- Coastlines Natural Earth
- Plotting a world map!



Natural Earth is a public domain map dataset available at 1:10m, 1:50m, and 1:110 million scales. Featuring tightly integrated vector and raster data, with Natural Earth you can make a variety of visually pleasing, well-crafted maps with cartography or GIS software.

Natural Earth was built through a collaboration of many volunteers and is supported by NACIS (North American Cartographic Information Society), and is free for use in any type of project (see our Terms of Use page for more information).

Get the Data



Convenience

Natural Earth solves a problem: finding suitable data for making small-scale maps. In a time when the web is awash in geospatial data, cartographers are forced to waste time sifting through confusing tangles of poorly attributed data to make clean, legible maps. Because your time is valuable, Natural Earth data comes readyto-use.

0	RRP	7
	Sacramento	≪ B
San Francisco	an A ETA	/

Neatness Counts

The carefully generalized linework maintains consistent, recognizable geographic shapes at 1:10m, 1:50m, and 1:110m scales. Natural Earth was built from the ground up so you will find that all data layers align precisely with one another. For example, where rivers and country borders are one and the same, the lines are coincident.

S COUNTRYNAM	R SCALERANK T	S FEATURECLA	S SOVE
Afghanistan	1.00000000000	Countries	Afghani
Aland	3.00000000000	Countries	Finland
Albania	1.00000000000	Countries	Albania
Algeria	1.00000000000	Countries	Algeria

GIS Attributes

Natural Earth, however, is more than just a collection of pretty lines. The data attributes are equally important for mapmaking. Most data contain embedded feature names, which are ranked by relative importance. Other attributes facilitate faster map production, such as width attributes assigned to river segments for creating tapers.

https://www.naturalearthdata.com/downloads/110m-physical-vectors/

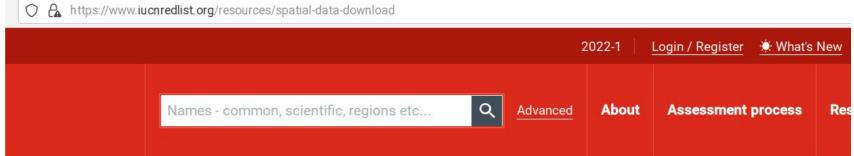
• World Administrative Boundaries

World Administrative Boundaries - Countries and Territories

 Information 	🌐 Table 🛛 🎯 Map 🔄 Lul Analyze 🎿 Export 🗱 API
This dataset display	s level 0 world administrative boundaries. It contains countries as well as non-sovereign territories (like, for instance, French overseas).
Dataset Identi	er world-administrative-boundaries
Downloa	ds 33,342
Then Keywo Licer Langua Modif Publis Referer	 United Nation, ISO-3 code, Countries, Territories, Shape, Boundaries Open Government Licence v3.0 English April 26, 2019 11:09 AM World Food Programme (UN agency)
Territ	ry • world
Last process	ng May 15, 2019 9:49 AM (metadata) May 15, 2019 9:49 AM (data)

- Range data from the IUCN
- Freely available for academic use





SPATIAL DATA & MAPPING RESOURCES

Spatial Data Download



Raster data

With terra (and raster)

Package raster: Geographic Data Analysis and Modeling

- Primarily by Robert Hijmans
- Since 2010
- Standard for raster processing for a long time
- Most ecological packages depend on this
- Integration of WorldClim data

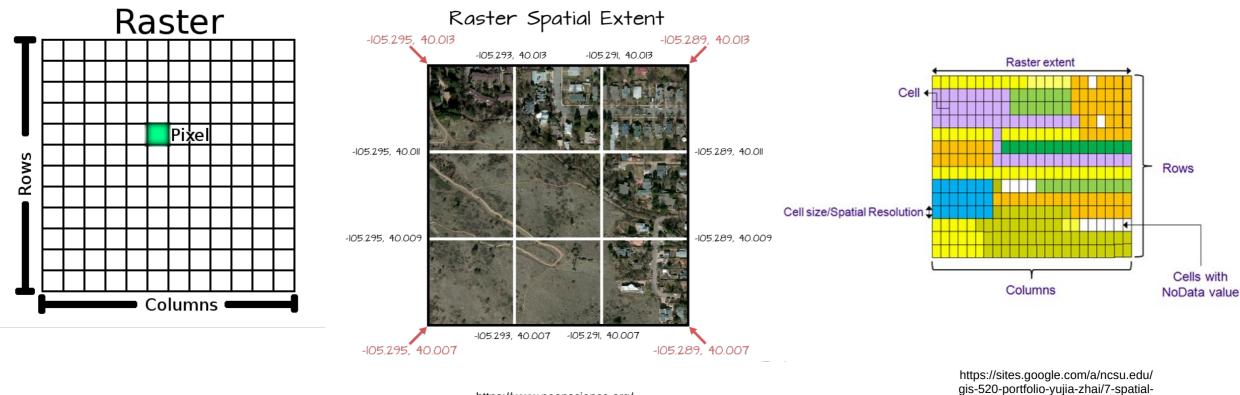


Package terra: Spatial Data Analysis

- Primarily by Robert Hijmans
- Interface to GEOS
- Almost the same as raster, this is the easier transition.



Raster properties

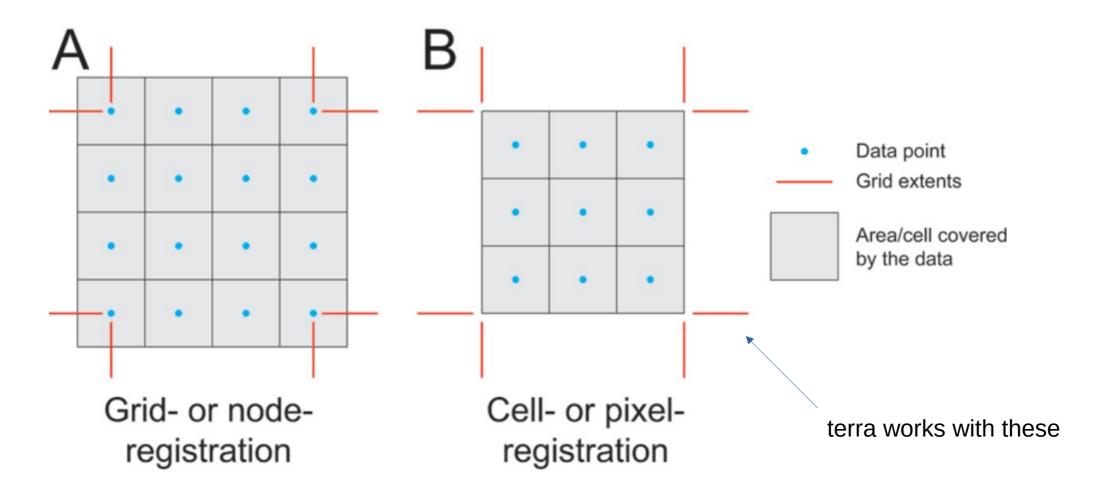


analysis-with-raster-data/1-basics-of-

raster-data

https://www.neonscience.org/ resources/learning-hub/tutorials/ raster-res-extent-pixels-r

Grid vs. cell registered rasters



https://www.ncei.noaa.gov/products/grid-cell-registration

Raster File formats

CSV

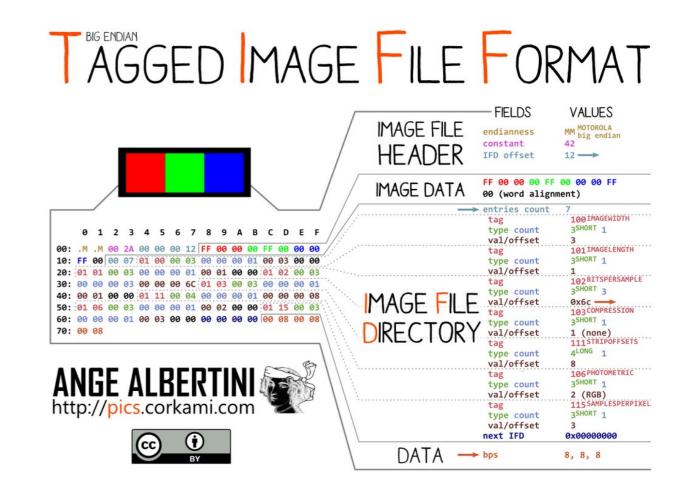
- Single uncompressed layer, a table of values
- Not properly georeferenced
- Column and row names might help

102,102,103,103,103,103,103,102,102,102,102,103,103,104,104,104,104,105,106,105,104,104,105,106,107,108,110,11 103,103,104,104,104,104,104,103,103,103,103,104,104,104,105,105,106,107,106,106,106,107,108,110,111,114,117 104,104,105,105,105,105,105,105,104,104,103,104,104,105,105,105,105,106,107,108,108,108,109,110,112,114,115,118,121,122, 105,105,105,106,106,106,106,105,105,104,104,105,105,106,106,107,109,110,110,112,113,115,116,118,119,121,124,126, 107,108,108,109,109,109,109,108,108,107,108,108,110,111,113,116,118,120,123,125,127,129,130,132,134,135,137,139, ,108,109,109,110,110,110,110,109,109,108,110,110,113,116,118,120,122,125,127,129,133,136,138,140,141,142 ,110,110,111,113,112,111,113,112,112,114,116,119,121,124,127,129,133,138,143,146,149,149,151,153,154,157,159,160 ,110,111,113,115,114,113,114,114,115,117,119,121,124,126,129,133,140,145,150,154,155,155,157,159,161,162,164,165 ,111,113,115,117,116,115,116,117,117,119,121,124,126,128,132,137,143,151,156,161,161,162,163,165,166,167,168,170 ,114,115,117,117,117,118,119,119,120,121,124,126,128,131,137,143,150,156,160,163,165,168,170,171,172,173,174,175 ,116,118,118,118,120,121,121,122,122,123,125,128,130,134,141,147,152,156,160,165,168,170,174,176,179,180, ,118,120,120,121,122,123,124,124,125,126,127,129,132,135,142,149,153,157,161,166,170,174,178,180,182,183,184,184 ,120,121,122,123,124,125,126,127,127,128,130,132,134,137,142,151,155,158,162,169,172,176,181,183,184,186,187,188 ,120,122,125,126,126,127,128,129,130,130,132,134,136,139,145,152,157,160,167,172,175,178,181,185,186,188,190,191 ,121,124,126,128,129,129,130,131,132,133,135,137,139,143,150,154,159,164,170,173,176,179,184,186,189,190,191,192 <u>,122,125,127,130,130,131,133</u>,134,135,136,137,140,143,147,154,158,162,166,171,174,177,181,186,189,190,190,191,192 ,122,125,128,130,132,133,135,136,137,139,140,143,147,152,157,161,164,168,172,175,179,182,186,190,190,190, ,123,126,129,131,133,135,137,138,139,141,143,147,150,156,161,164,167,170,173,177,181,184,187,188,190,189,187,185 ,124,127,130,132,135,137,138,140,142,144,147,149,154,157,161,165,168,171,175,178,181,184,186,187,187,184,184,181 ,123,128,131,133,136,138,140,142,144,146,149,151,154,157,160,164,168,172,175,178,181,183,184,184,185,183,180,177 ,123,127,131,134,136,138,140,142,144,147,149,151,154,157,160,164,168,171,174,178,180,181,181,182,183,181,178,173 ,120,124,128,131,134,137,139,142,144,146,149,151,153,156,160,163,167,171,174,178,180,180,180,180,180,180,175,171 ,118,121,125,129,132,134,137,140,142,145,147,149,151,155,159,163,166,169,173,177,179,180,180,180,180,179 ,117,120,121,125,129,132,135,138,140,143,145,147,149,153,157,160,163,166,171,174,177,179,180,180,180,179,172,168 ,115,118,120,122,126,130,133,136,138,141,143,145,148,151,154,157,160,163,168,171,174,177,179,179,179,176,171,167 ,114,116,118,120,122,127,131,133,136,138,141,143,146,148,151,154,157,160,164,168,171,174,178,178,179,177,173,169 ,115,114,116,118,120,122,127,129,132,136,139,141,143,146,148,151,153,156,160,164,167,172,174,176,177,176,173,170

Raster File formats

GeoTIFF

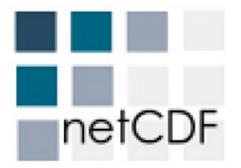
- Single uncompressed layer
- Completely open source
- TIFF image + georeferencing

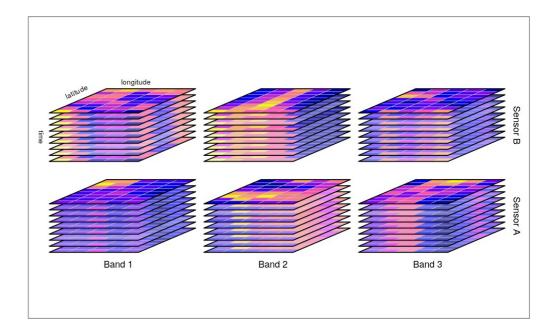


Raster File formats

NetCDF

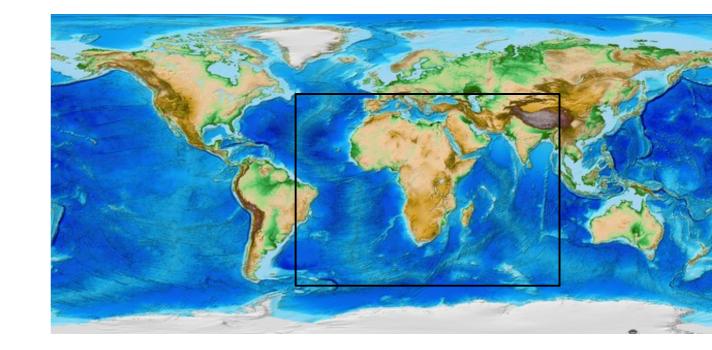
- Binary data cubes, lots of dimensions can be included
- Data registered in bands
- Requires the presence of ncdf4 in R!





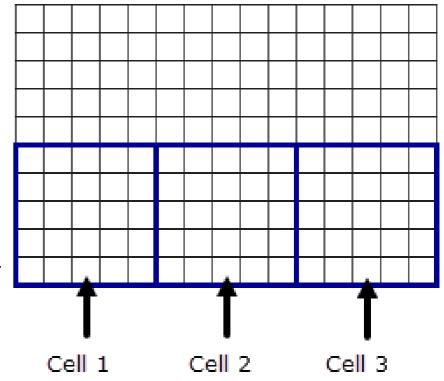
Cropping

• Changes the extent of a raster



Aggregation / Disaggregation

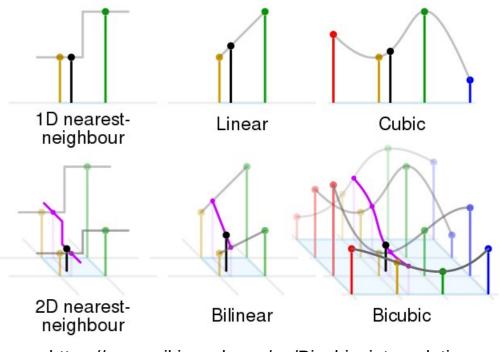
- Change resolution without changing cell boundaries
- Iteration of a function for data that belongs in a new cell



https://desktop.arcgis.com/en/arcmap/latest/tools/spatial-analyst-toolbox/ how-aggregate-works.htm

Resampling

- Change resolution to any resolution
- Often relies on interpolation

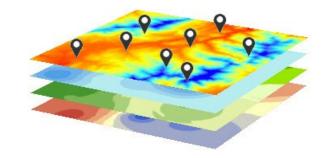


https://www.wikiwand.com/en/Bicubic_interpolation

Extraction

- Getting data out of a raster at given coordinates/locations
- Basic operation for species distribution modelling

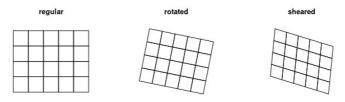




esri.com

Package stars: Spatiotemporal Arrays, Raster and Vector Data Cubes

- Primarily by Edzer Pebesma
- Somewhat more complex than terra



rectilinea

curvilinear







• The ETOPO1 Topography (1° by 1°)

SINCAA NATIONAL CENTERS FOR ENVIRONMENTAL INFORMATION

AA > NESDIS > NCEI (formerly NGDC) > Marin All Bathy/Relief	e Geology and Geophysics > Bathymetry & F Coastal DEMs	Relief Fishing	Global	Lakes	Multibeam
	ETOPO1 Global Relief Model				
Extract Custom Grid Metric Data			integrates land to regional data sets Greenland ice sh ETOPO1 Global I	co-minute global relief model of Earl pography and ocean bathymetry. B s, it is available in "Ice Surface" (top pets) and "Bedrock" (base of the ice Relief Model is used to calculate the and to derive a Hypsographic Curve 0.7289/V5C8276M	uilt from global and o of Antarctic and e sheets). e Volumes of the
ETOPO1 Report: Procedures, Data Sources & Analysis					
Frequently Asked Questions	Grid Versions				
Color Images	• ETOPO1 Ice Surface: Grid of Earth's surface depicting the top of the Antarctic and Greenland ice sheets.				
Posters	 grid-registered: netCDF, georeferenced tiff 				
KMZ Images	 cell-registere 	ed: netCDF, georeferenced tiff			
Web Services					
	ETOPO1 Bedrock:	Grid of Earth's surface depicting the bee	drock underneath the ice sheets.		
	 grid-registered 	ed: netCDF, georeferenced tiff			
Global Grids:	 cell-registere 	ed: netCDF, georeferenced tiff			

ETOPO2 (deprecated) ETOPO5 (deprecated) GLOBE Topography

View Metadata, Relief for the rest of the world is the same in both versions.

Registrations

WorldClim

WorldClim Maps, graphs, tables, and data of the global climate Download

Example +

♦ https://interactive-atlas.ipcc.ch

 $\leftarrow \rightarrow C$

climate change

• IPCC AR6 Atlas



IPCC WGI Interactive Atlas

A novel tool for flexible spatial and temporal analyses of much of the observed and projected climate change information underpinning the Working Group I contribution to the Sixth Assessment Report, including regional synthesis for Climatic Impact-Drivers (CIDs).

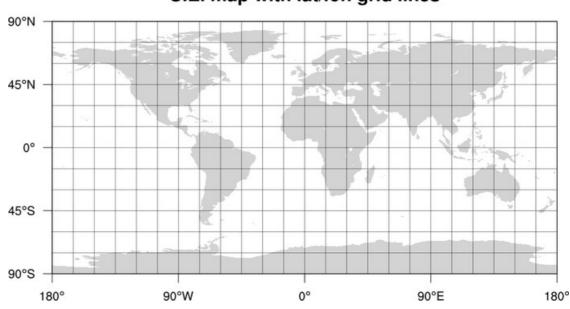
Participate in the user testing survey \mathscr{O}	Errata and problem reporting O	License and citation 4	Contact 🖂



3

The advantage of rectangles

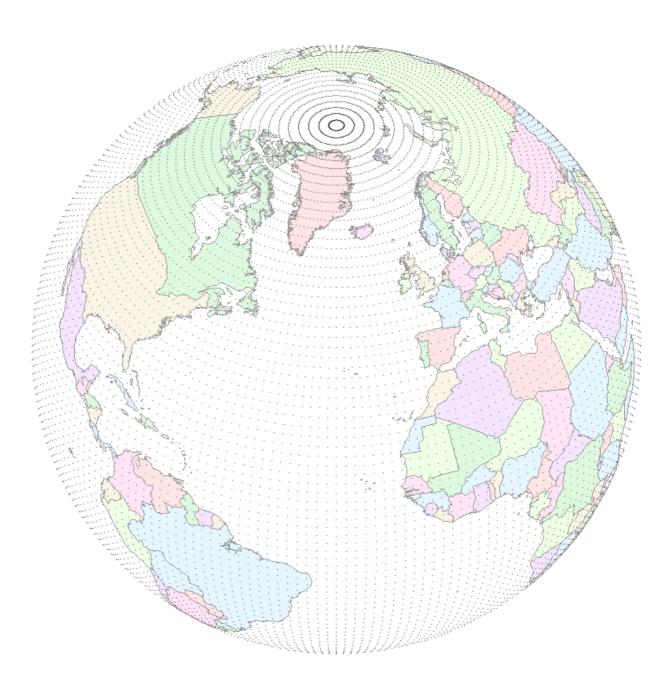
- Structure is easy to define
- Very easy to store in the memory
- Look natural in projections



C.E. map with lat/lon grid lines

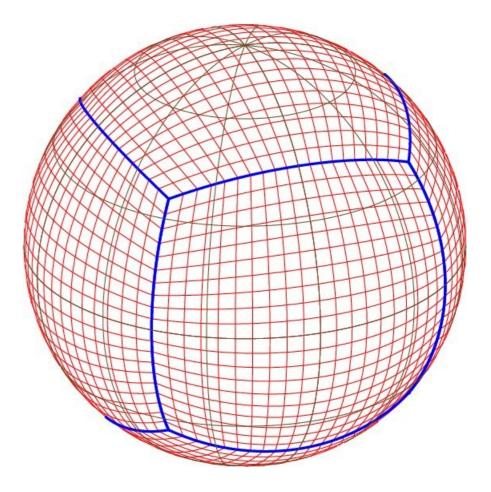
The disadvantage

- long-lat grids are Gaussian
- Non-uniform on a sphere
 - Increased density towards the poles
 - Cell sizes decrease towards the poles
- Spatial binning will be biased!



Common solution: cubed-sphere grid

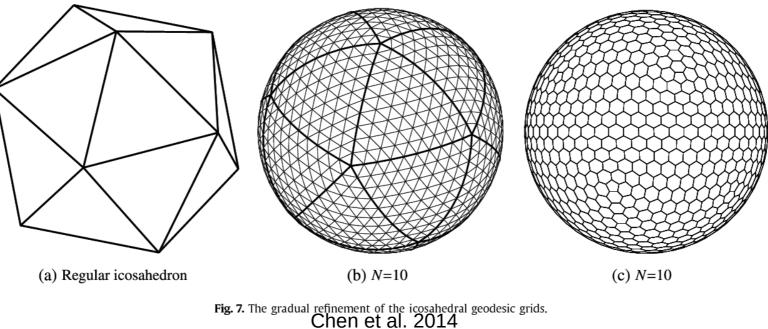
- Still quadrilateral
- Some climate models rely on this



Purser and Tong, 2017

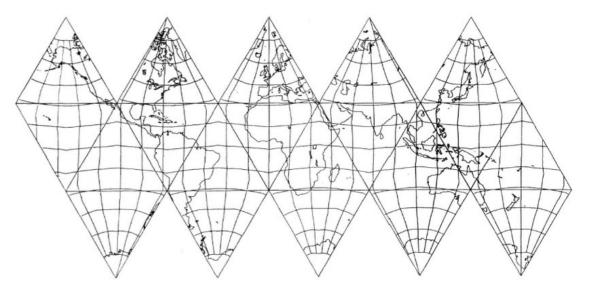
Most common solution: polyhedra

- Trianglular or Penta-Hexagonal grids
- Also in some climate models



Package ddgridR: Discrete Global Grids for R

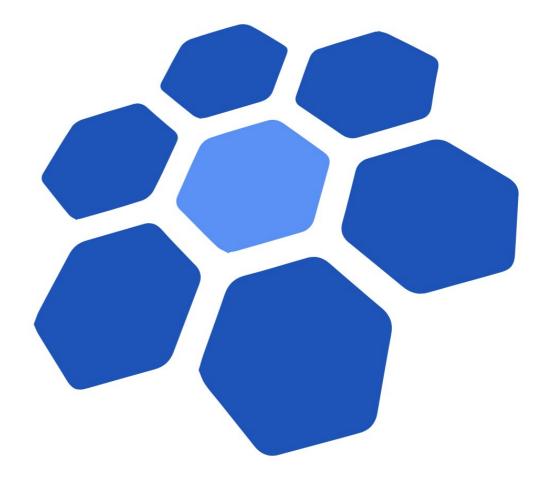
- by Richard Barnes
- Based on an program by Kevin Sahr
- Not on CRAN! https://github.com/rbarnes/dggridR
- Based on a Snyder projection
- Very high resolution, and well-known mathematical properties



Package h3jsr: Access to H3 (via javascript)

R library for the H3 system (https://h3geo.org/)

- Developed For Uber
- Hierarchical system (fine scale)
- https://cran.r-project.org/package=h3js



Package icosa: Coarse grids based on tessellated icosahedra

- Adam wrote this (first package)
- More scalable for global scale
- Interface to sf
- 3D model
- The mathematical properties are partially explored
- https://adamkocsis.github.io/icosa/

