Spherical Voronoi Diagrams A PyData London story unfolded

Nikolai Nowaczyk

08/05/2016

Nikolai Nowaczyk Voronoi 08/05/2016 1 / 31

- Planar Voronoi Diagrams
 - Example: Traveling in London
 - Formal description
 - Realization in Python
- Spherical Voronoi Diagrams
 - Example: Traveling around the world
 - Problem description
 - PyData story
 - Realization in Python
 - Applications
- Appendix

2 / 31

Outline

- Planar Voronoi Diagrams
 - Example: Traveling in London
 - Formal description
 - Realization in Python
- Spherical Voronoi Diagrams
 - Example: Traveling around the world
 - Problem description
 - PyData story
 - Realization in Python
 - Applications
- 3 Appendix



Voronoi diagrams in the plane

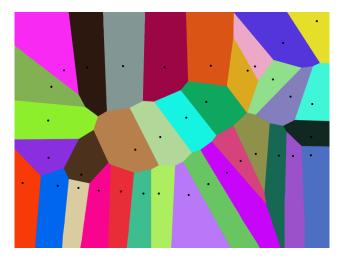
Input: Generator Points

4 / 31

Nikolai Nowaczyk Voronoi 08/05/2016

Voronoi diagrams in the plane

Nikolai Nowaczyk



http://alexbeutel.com/webgl/voronoi.html

Output: Voronoi Regions (coloured)

08/05/2016

4 / 31

Mathematical definition

Definition (Voronoi diagram)

Let (X, d) be a metric space (for instance R^2) and $p = (p_1, \dots, p_K)$ be a finite collection of K distinct points called *generators*.

• For each $1 \le k \le K$, the set

$$R_k := \{x \in X \mid \forall j \neq k : d(x, p_k) \leq d(x, p_j)\}\$$

is the k-th Voronoi region.

② The collection $(R_k)_{1 \le k \le K}$ is the *Voronoi diagram* defined by p.

Mathematical definition

Definition (Voronoi diagram)

Let (X, d) be a metric space (for instance R^2) and $p = (p_1, \dots, p_K)$ be a finite collection of K distinct points called *generators*.

• For each $1 \le k \le K$, the set

$$R_k := \{x \in X \mid \forall j \neq k : d(x, p_k) \leq d(x, p_j)\}\$$

is the k-th Voronoi region.

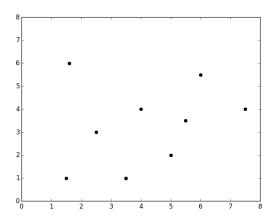
2 The collection $(R_k)_{1 \le k \le K}$ is the *Voronoi diagram* defined by p.

Theorem

If (X, d) is \mathbb{R}^2 with the Euclidean distance function, then every Voronoi region of every Voronoi diagram is a convex polytope.

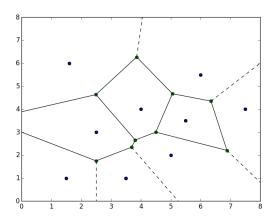
Python: Plotting the generator points

```
points = numpy.array([[1.5, 1.], ...])
import matplotlib.pyplot as plt
plt.plot(points[:, 0], points[:, 1], 'o', color='black')
plt.show()
```



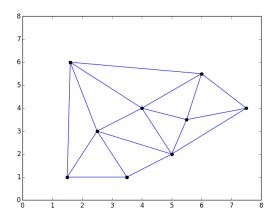
Python: Calculating Voronoi diagram

```
from scipy.spatial import Voronoi, voronoi_plot_2d
vor = Voronoi(points)
voronoi_plot_2d(vor, ax)
plt.show()
```



Python: Delaunay triangulation

```
from scipy.spatial import Delaunay
tri = Delaunay(points)
ax.triplot(points[:,0], points[:,1], tri.simplices.copy(), color='blue')
plt.show()
```



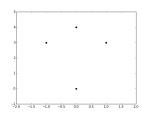
Delaunay triangulation

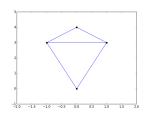
Definition (Delaunay triangulation)

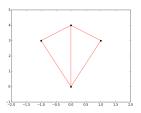
Let P be a set of points in the d-dimensional Euclidean space \mathbb{R}^d . A triangulation T(P) of P is a *Delaunay triangulation* if the circum-hyperspheres of any simplex in T(P) contain no point of P.

Theorem

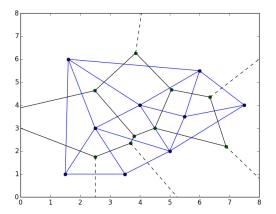
For any discrete set P in \mathbb{R}^d in general position, there exists a unique Delaunay triangulation.







Python: Delaunay triangulation and Voronoi diagram

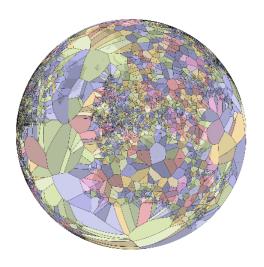


Outline

- Planar Voronoi Diagrams
 - Example: Traveling in London
 - Formal description
 - Realization in Python
- Spherical Voronoi Diagrams
 - Example: Traveling around the world
 - Problem description
 - PyData story
 - Realization in Python
 - Applications
- 3 Appendix



World Aiport Map



https://www.jasondavies.com/maps/voronoi/airports/

Nikolai Nowaczyk Voronoi 08/05/2016 12 / 31

A long time ago (PyData London 2015)...



https://www.youtube.com/watch?v=gxNa9BD5CnQ

Nikolai Nowaczyk Voronoi 08/05/2016 13 / 31

Spherical Voronoi Diagrams

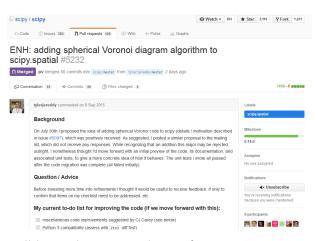
- Exactly the same problem as planar Voronoi diagram, just on a sphere instead of a plane.
- Many theoretical papers exist.
- Found no ready-to-go implementation in Python.

PyData London 2015 initiated quite a collaboration between...

- Tyler Reddy,
- Nikolai Nowaczyk,
- Ross Hemsley,
- Edd Edmondson,
- Joe Pitt-Francis,
- Mark Sansom,
- Ralf Gommers,
- Pauli Virtanen,
- Juan Luis Cano Rodríguez,
- CJ Carey,
- ...

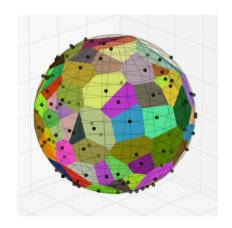
Result of PyData 2015: scipy.spatial.SphericalVoronoi

https://github.com/scipy/scipy/pull/5232



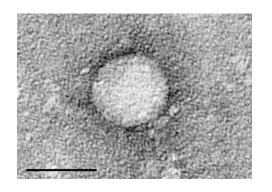
Will be in the 0.18.0 release of scipy.

PyData London 2016: scipy.spatial.SphericalVoronoi



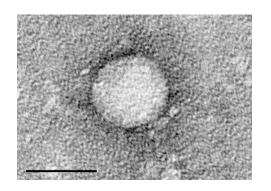
```
>>> points = np.array([...])
>>> from scipy.spatial import
    SphericalVoronoi
>>> sv = SphericalVoronoi(points)
```

Possible Application: Hepatitis C



- 200mio people infected worldwide
- can cause liver disease, cirrhosis, liver cancer
- 350.000 deaths per year
- new medication available (more successful, but expensive)

Possible Application: Hepatitis C



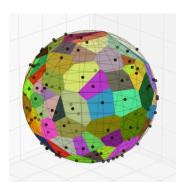
- 200mio people infected worldwide
- can cause liver disease, cirrhosis, liver cancer
- 350.000 deaths per year
- new medication available (more successful, but expensive)

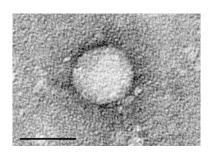
no vaccine

Nikolai Nowaczyk Voronoi 0

18 / 31

Modelling Hepatitis C





Hepatitis C virus

This could be a virus!

- Computational virology tries to understand a virus through computer simulations.
- Calculating spherical Voronoi diagrams is an important tool.

Nikolai Nowaczyk Voronoi 08/05/2016 19 / 31

Maybe more collaboration coming up...



- Help with plotting: https://github.com/matplotlib/matplotlib/issues/5294
- Help with surface area: https://github.com/scipy/scipy/issues/6069

Questions, Comments? Get in touch!

- Nikolai Nowaczyk
 - mail@nikno.de
 - https://github.com/niknow
- Tyler Reddy
 - tyler.reddy@bioch.ox.ac.uk
 - https://github.com/tylerjereddy
- How to further improve scipy.spatial.SphericalVoronoi?
- Other applications of spherical Voronoi diagrams?
- Get the code examples: https://github.com/niknow/pydata-london-2016-voronoi

Questions, Comments? Get in touch!

- Nikolai Nowaczyk
 - mail@nikno.de
 - https://github.com/niknow
- Tyler Reddy
 - tyler.reddy@bioch.ox.ac.uk
 - https://github.com/tylerjereddy
- How to further improve scipy.spatial.SphericalVoronoi?
- Other applications of spherical Voronoi diagrams?
- Get the code examples: https://github.com/niknow/pydata-london-2016-voronoi

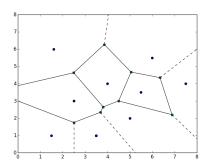
THANK YOU!

Outline

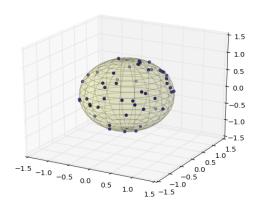
- 🕕 Planar Voronoi Diagrams
 - Example: Traveling in London
 - Formal description
 - Realization in Python
- Spherical Voronoi Diagrams
 - Example: Traveling around the world
 - Problem description
 - PyData story
 - Realization in Python
 - Applications
- Appendix



Python: A closer look at the data structures



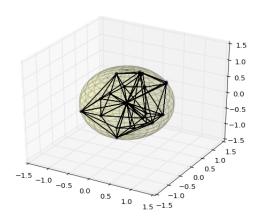
```
>>> points
[[1.5, 1.0], [3.5, 1.0], [5.0,
     2.0], [2.5, 3.0], [3.5, 1.0],
      [4.0, 4.0], [5.5, 3.5],
     [6.0, 5.5], [7.5, 4], [1.6,
     6.011
>>> points.shape
(10L, 2L)
vor = Voronoi(points)
>>> vor.vertices
[[-1.11, 3.55], [2.49, 4.63],
     [3.81, 2.65625], [3.86,
     6.27], [6.87, 2.20], [4.5,
     3.], [ 6.35, 4.35], [5.06,
     4.67], [2.5, 1.75], [3.69,
     2.34]]
>>> vor.vertices.shape
(10L, 2L)
>>> vor.regions
[[-1, 0, 1, 3], [7, 5, 4, 6], [7,
     3, 1, 2, 5], [7, 3, -1, 6],
     [9, -1, 8], [], [-1, 4, 6],
     [9, 2, 5, 4, -1], [8, 0, -1],
      [9, 2, 1, 0, 8]]
# list of tuples of integers. The
     tuple at the k-th position
     contains the indices of the
     Voronoi vertices of the
     Voronoi region surrounding
     the k-th generator.
        イロト 不倒り イヨト イヨト
```



Generator points



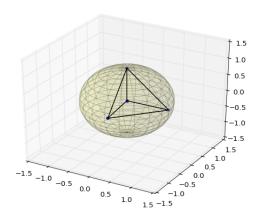
Nikolai Nowaczyk Voronoi 08/05/2016 24 / 31



Calculate triangulation

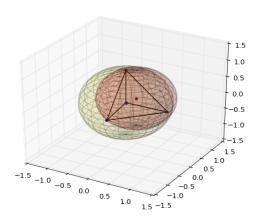


Nikolai Nowaczyk Voronoi 08/05/2016 25 / 31



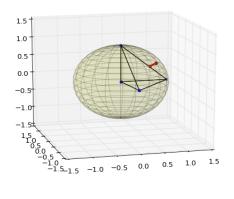
For each tetrahedron in the triangulation...

◆ロト ◆個 ト ◆ 差 ト ◆ 差 ・ 夕 へ で 。



...compute circumcenter of circumsphere.

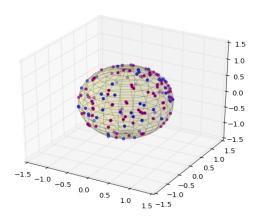
◆ロト ◆個ト ◆恵ト ◆恵ト ・恵 ・ からで



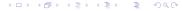
...and project onto sphere.



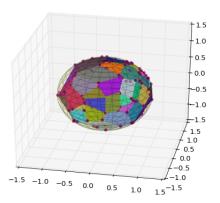
Nikolai Nowaczyk Voronoi 08/05/2016 28 / 31



Get lots of points on the sphere.



Nikolai Nowaczyk Voronoi 08/05/2016 29 / 31



These points are the Voronoi vertices!



Nikolai Nowaczyk Voronoi 08/05/2016 30 / 31

SphericalVoronoi Algorithm: Summary

- Calculate 3D Delaunay triangulation of the generator points.
- Add the center of the sphere to the triangulation and get a tetrahedralization.
- Solution
 Calculate the circumcenter of the circumsphere of each tetahedron.
- Projet circumcenters to the sphere to get the Voronoi vertices.
- Use the neighbourhood information from the triangulation to infer, which vertices belong to which region.

31 / 31