Topological data analysis

CS524: Big Data Visualization & Analytics

Fabio Miranda

https://fmiranda.me

Topological data analysis

- What is topology?
- Why topological data analysis?
- What is topological data analysis?
- Mathematical background
- Applications
- Scikit-TDA

What is topology?

- Mathematical field that studies properties and relationships that are preserved under continuous transformations.
  - Stretching, twisting: continuous changes.
  - Tearing, gluing: discontinuous changes.
- Study the connectedness of a space.

Topological data analysis

- Approach that uses topology for the analysis of datasets.
- General framework to analyze data that can be:
  - High dimensional
  - Incomplete
  - Noisy
- Study the *shape* of the data.
  - Helps understand relationships between how data varies and its domain.
- General framework for feature extraction from raw data.

Topological data analysis

- Why topological data analysis?
  - Growing interest in academia.
    - 10% of SciVis papers since 2008.
    - ~20% in 2018.
  - Growing interest in companies.

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Ayasdi: A Big Data Start-Up With a Long History

BY STEVE LOHR JANUARY 16, 2013 7:00 AM 1

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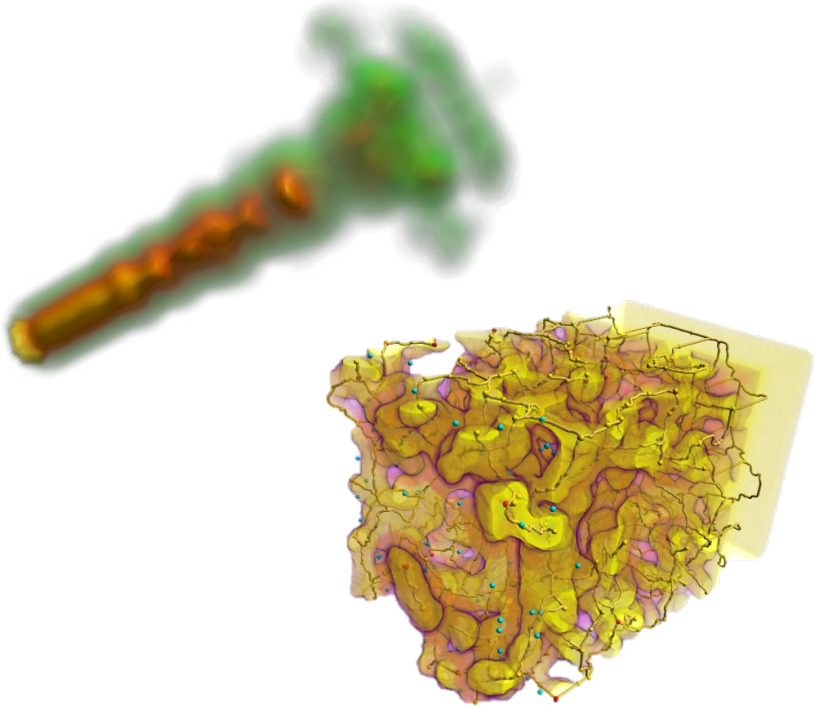
Ayasdi is a data analysis start-up built on the career of one man: Gunnar Carlsson, a professor of mathematics at Stanford.

Government spending for science has helped a lot too. Dr. Carlsson was the principal investigator on research projects that were financed, from 2000 to 2008, with $10 million from the National Science Foundation and the Defense Advanced Research Projects Agency, or Darpa.

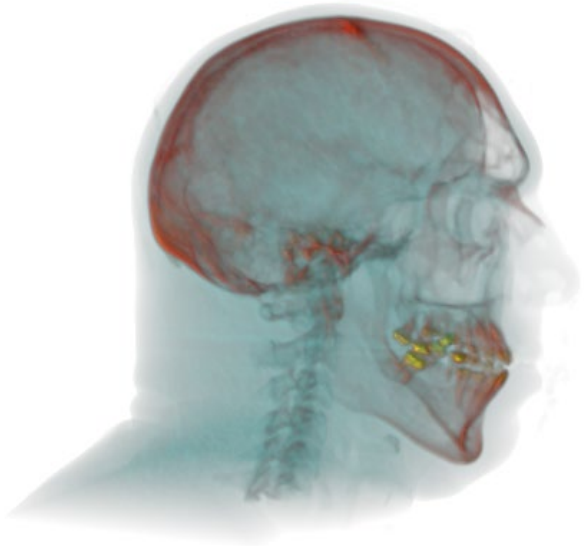
The three founders of Ayasdi, from left, Gurjeet Singh, Gunnar Carlsson and Harlan Sexton. Mark Leet Photography

In 2008, when Dr. Carlsson and his co-founders wanted to try to commercialize the research, it was Darpa and another government organization, IARPA, or Intelligence Advanced Research Projects Activity, that put up $1.25 million in the form of a Small Business Innovation Research grant, for "high-

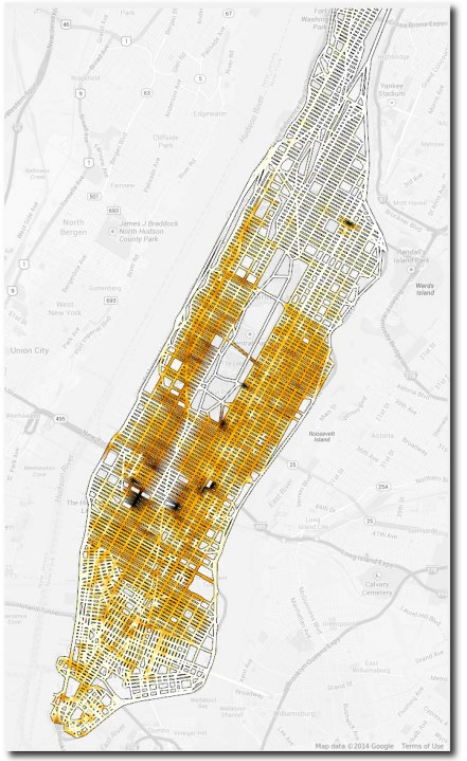
Topological data analysis



Simulation data



Medical data

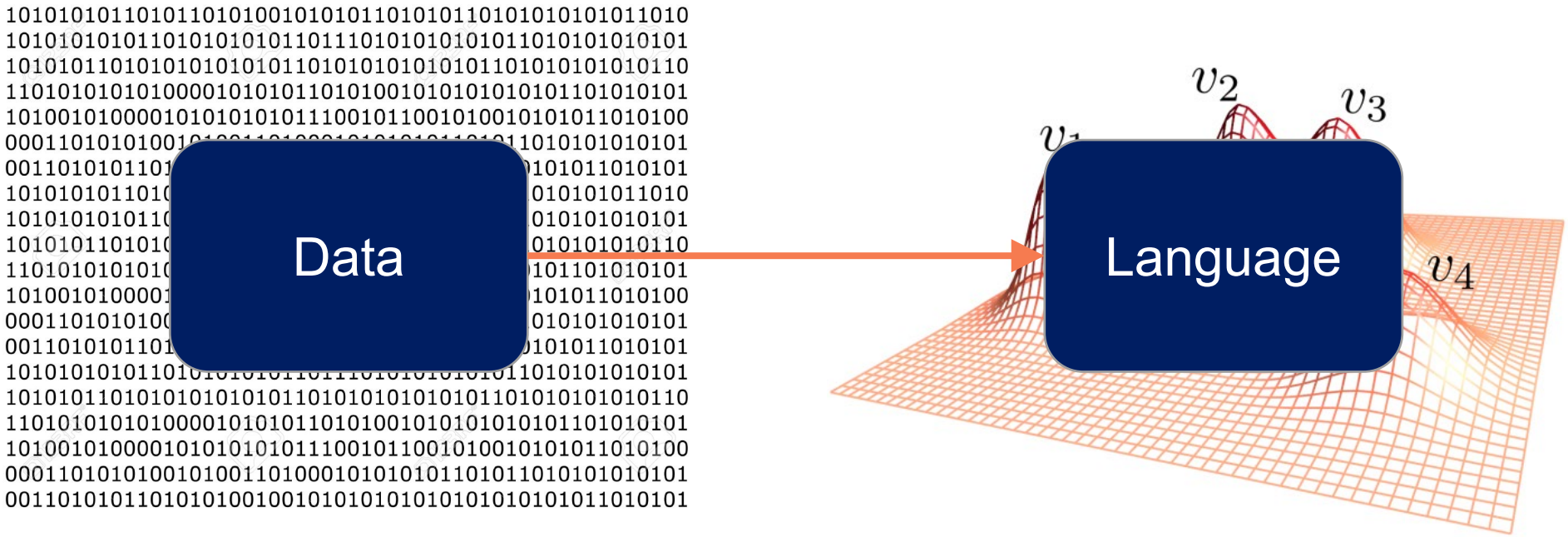


Urban data

Topological data analysis

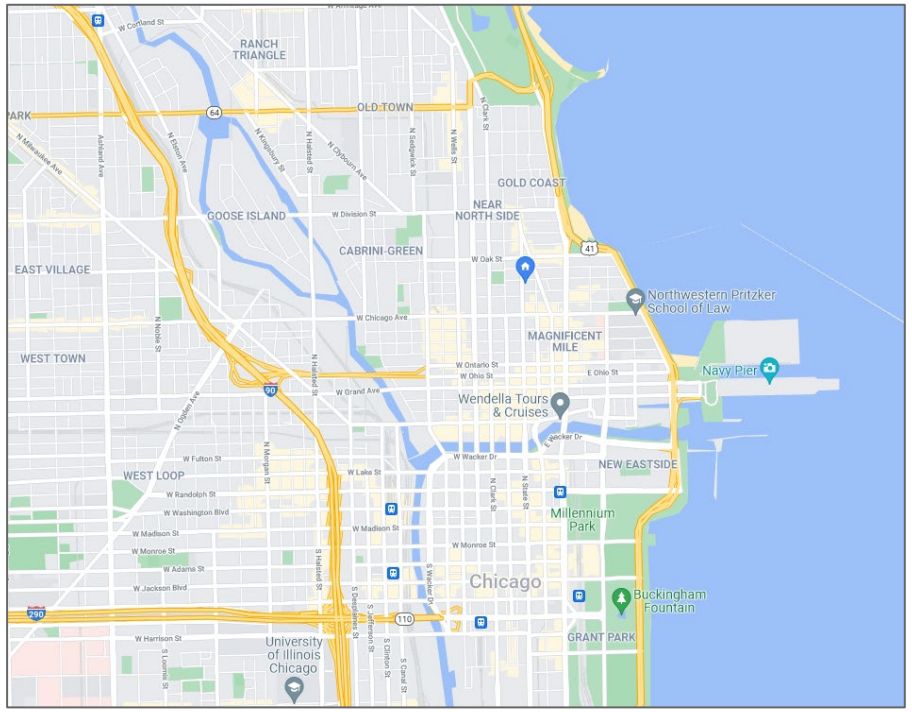
- Data is complex
  - Size
  - Rich features
- Topological data analysis is a framework that summarizes irrelevant stories to get at something interesting.

Topological data analysis



Topological representations

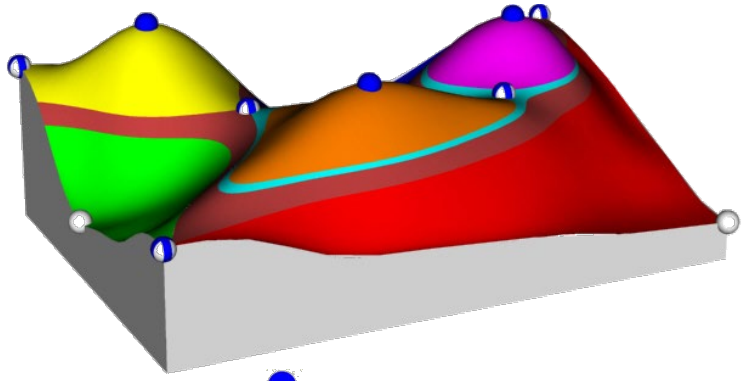
Scalar function

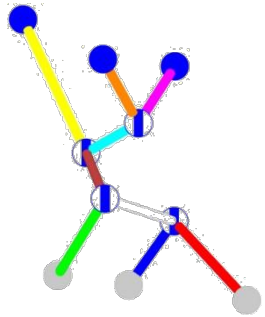


Structural representation

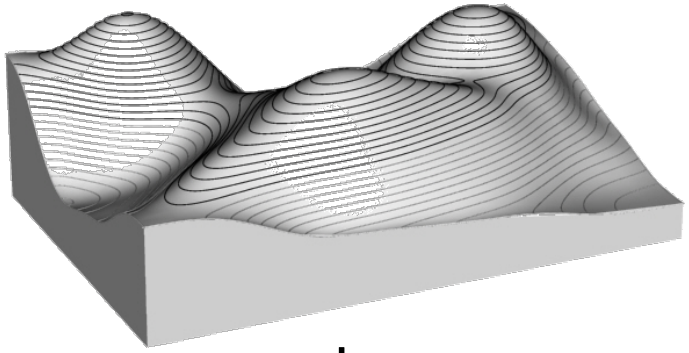
Topological representations

Contour trees
Reeb graphs
Merge trees

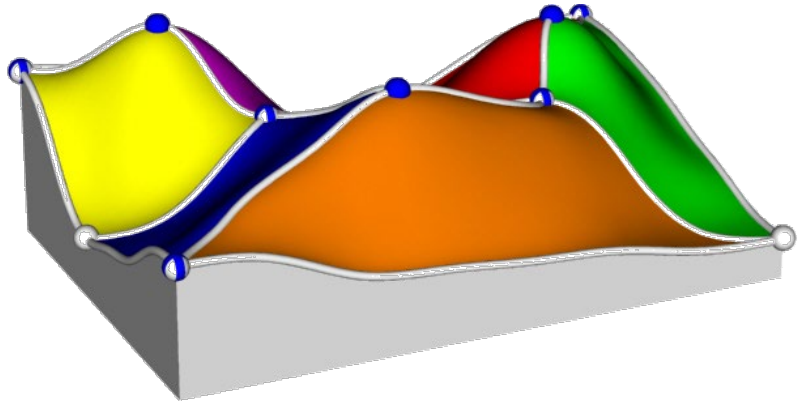


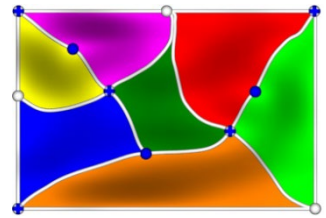


Scalar function



Morse-Smale complexes





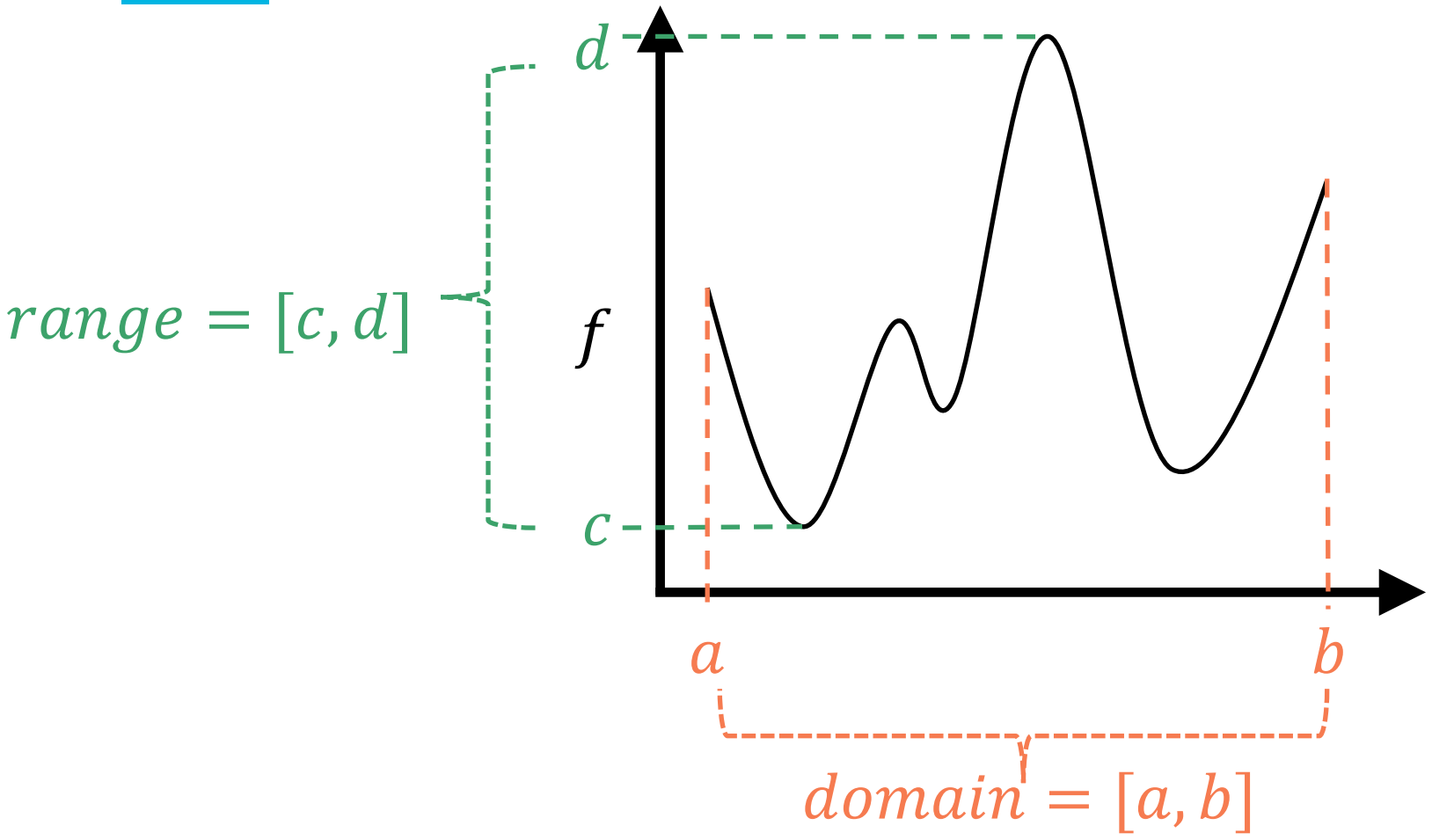
[Gyulassy, VIS 2018]

Topological data analysis

Data has shape, shape has meaning

- How to extract meaning through the shape of the data?
- Shape of the data is related to the topological changes of the data.
- How to extract topological changes?

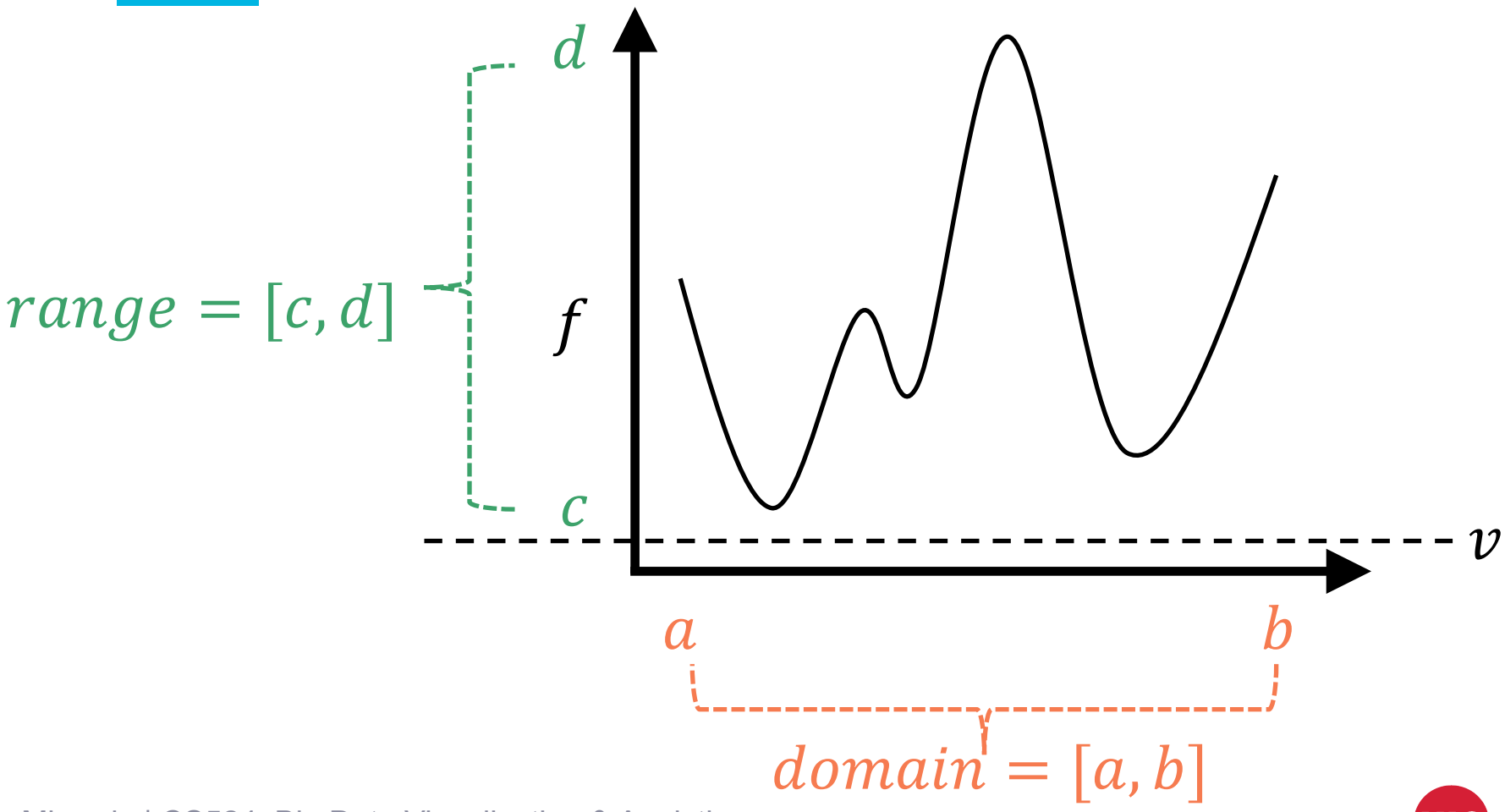
Topological changes



$f: \mathcal{M} \rightarrow \mathbb{R}$

[Gyulassy, VIS 2018]

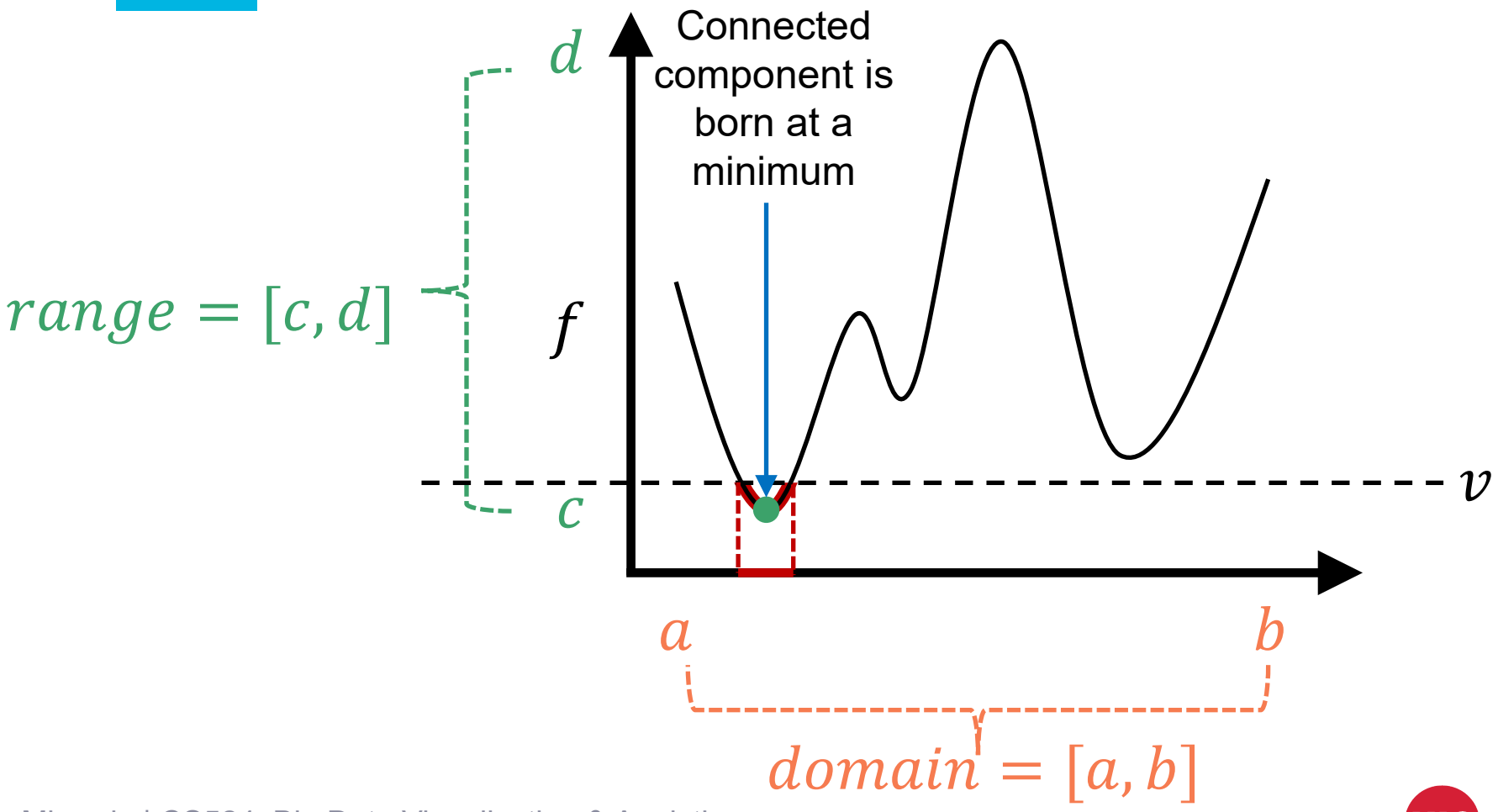
Topological changes



Sweep function from
$v = -\infty \rightarrow \infty$

Topological changes
of subdomain
$f^{-1}((-\infty, v])$

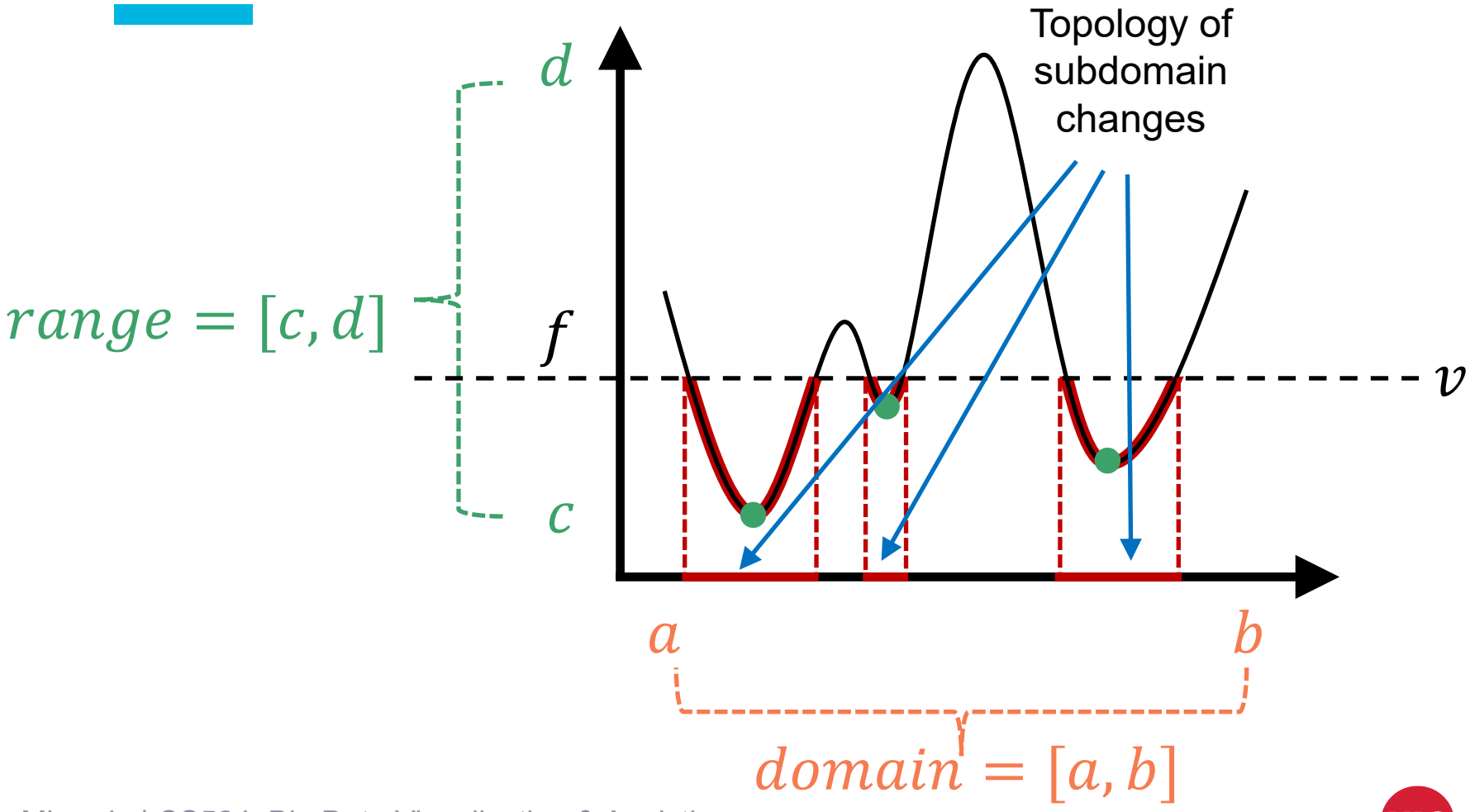
Topological changes



Sweep function from $v = -\infty \rightarrow \infty$

Topological changes of subdomain $f^{-1}((-\infty, v])$

Topological changes



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Topological changes of subdomain $f^{-1}((-\infty, v])$

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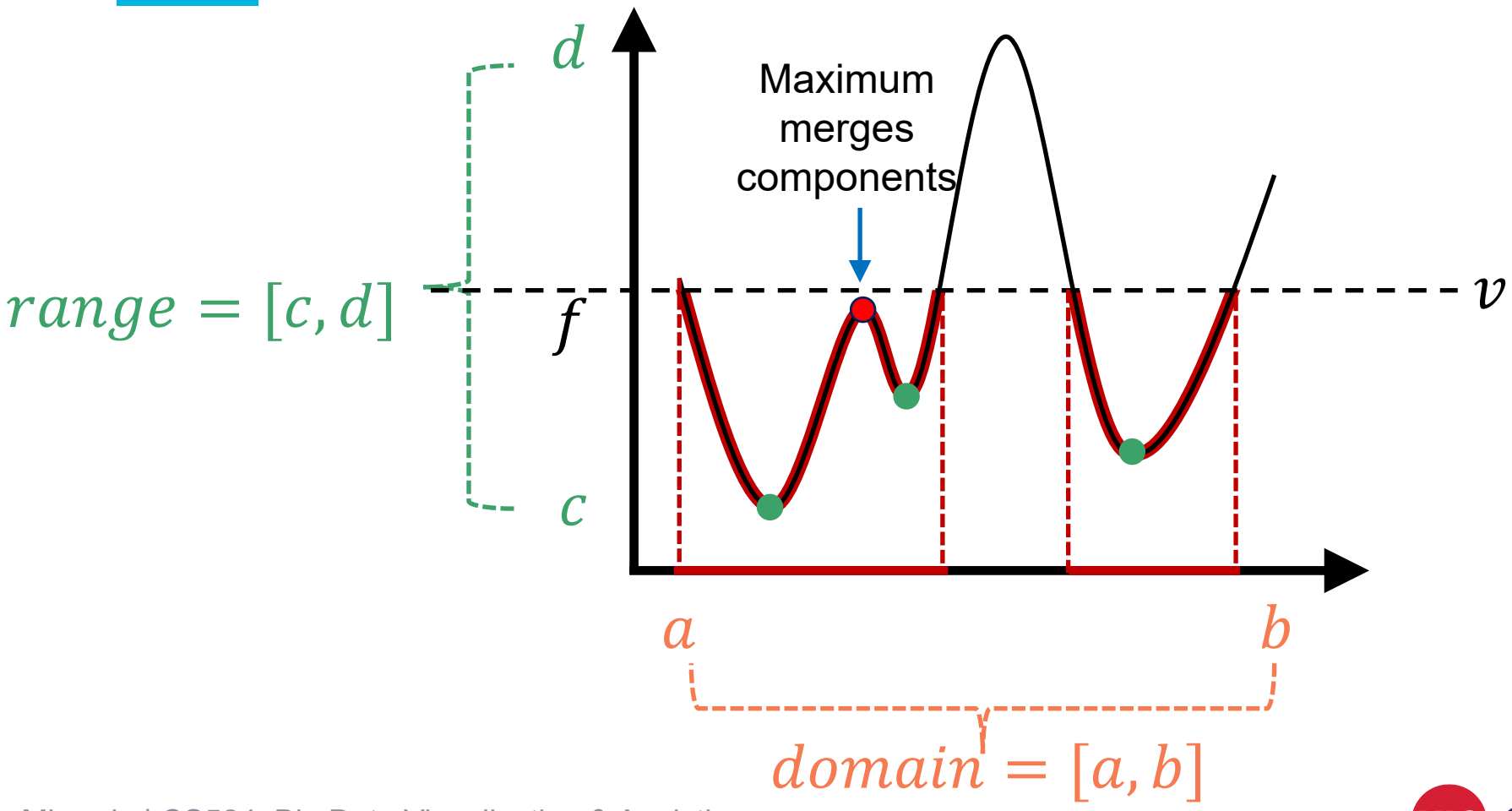

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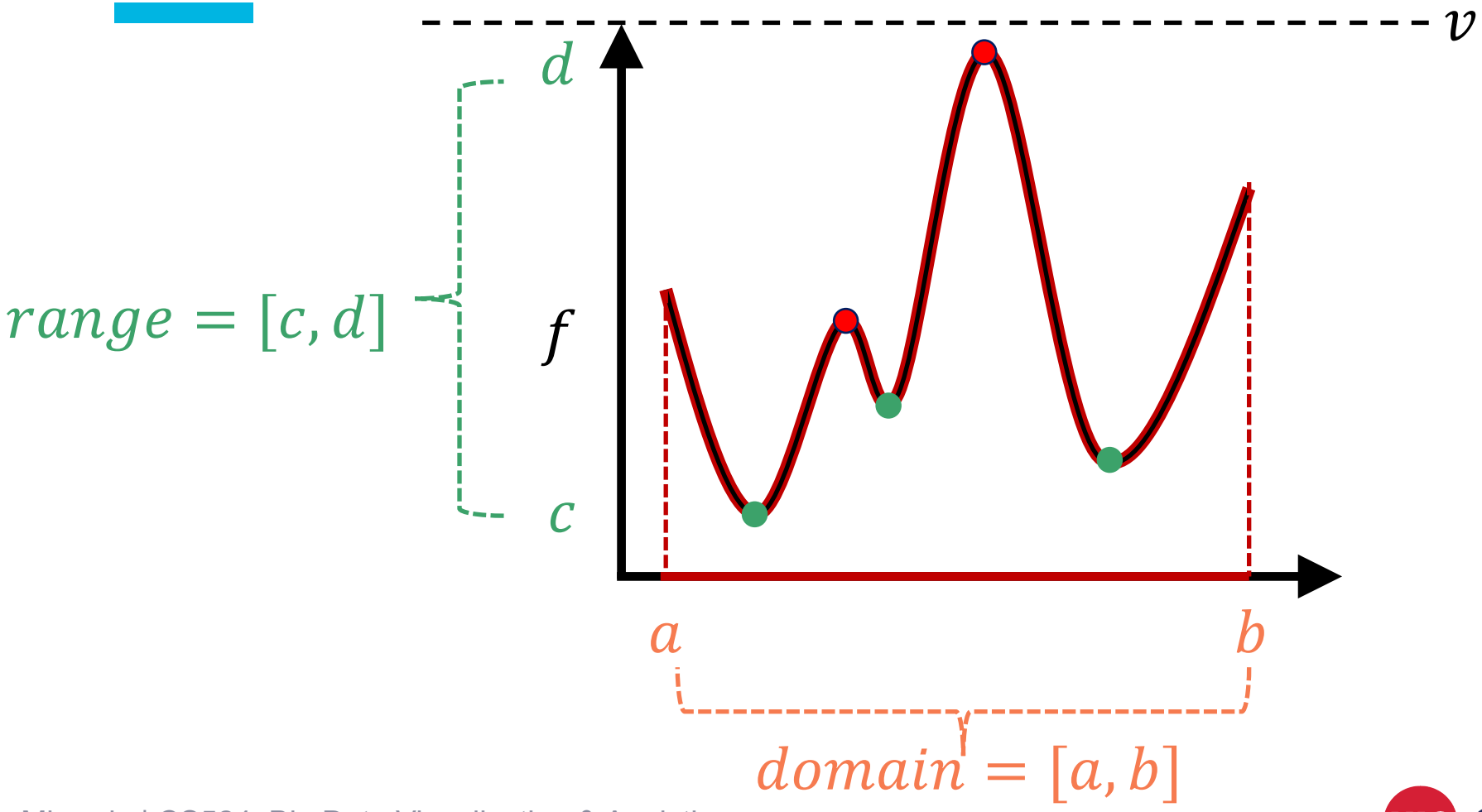
Topological changes of subdomain $f^{-1}((-\infty, v])$

Topological changes



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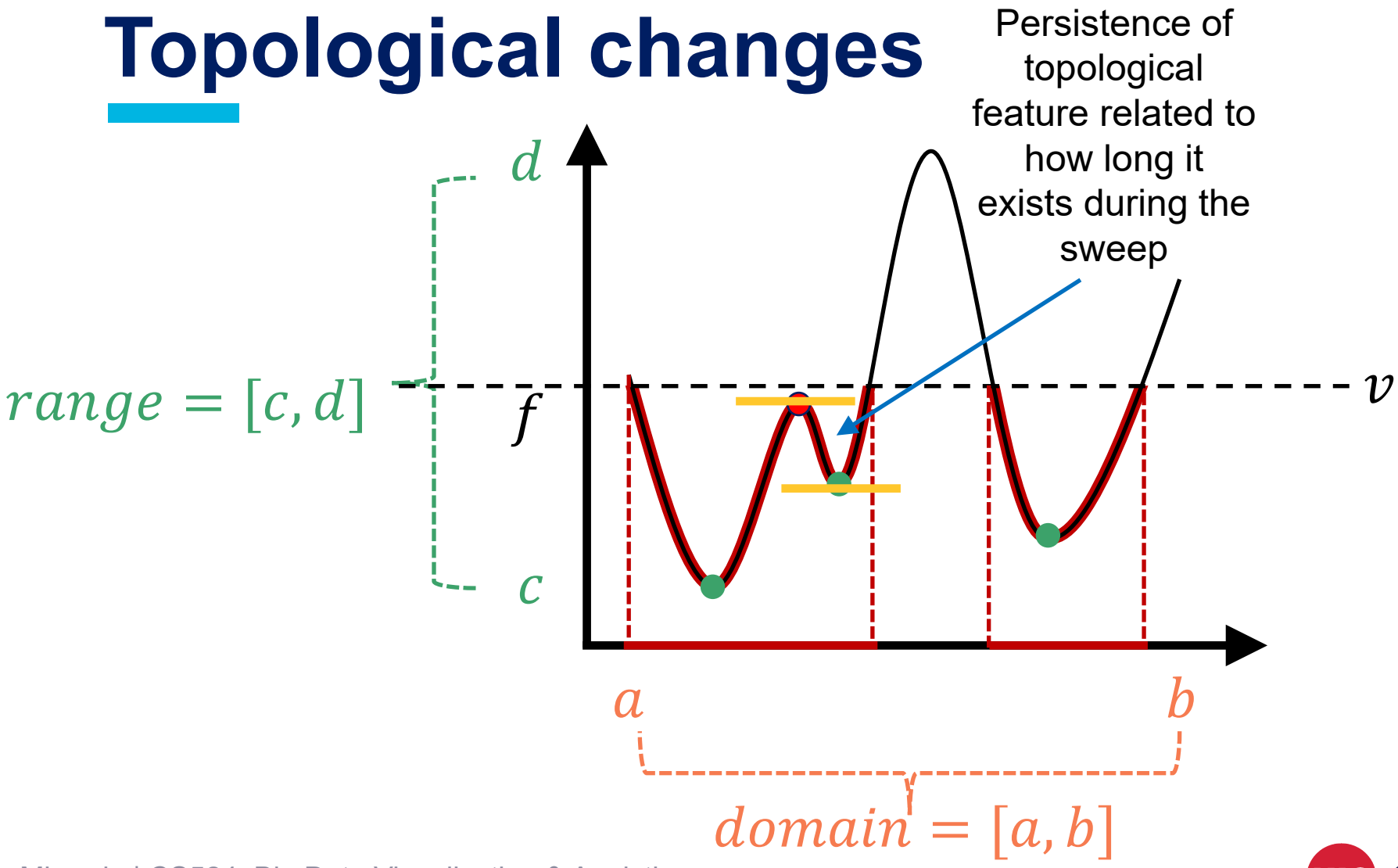
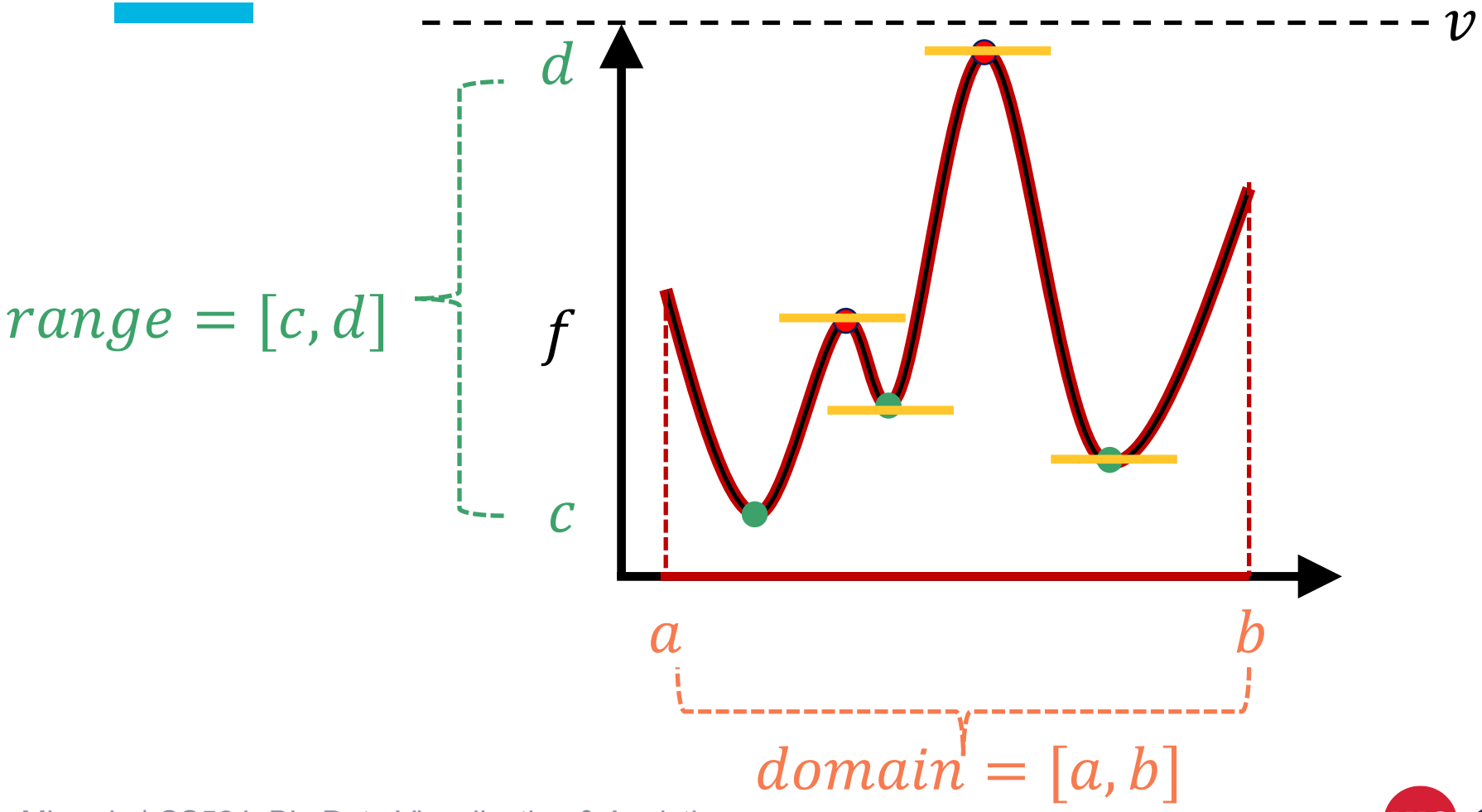


Sweep function from $v = -\infty \rightarrow \infty$

Topological changes of subdomain $f^{-1}((-\infty, v])$

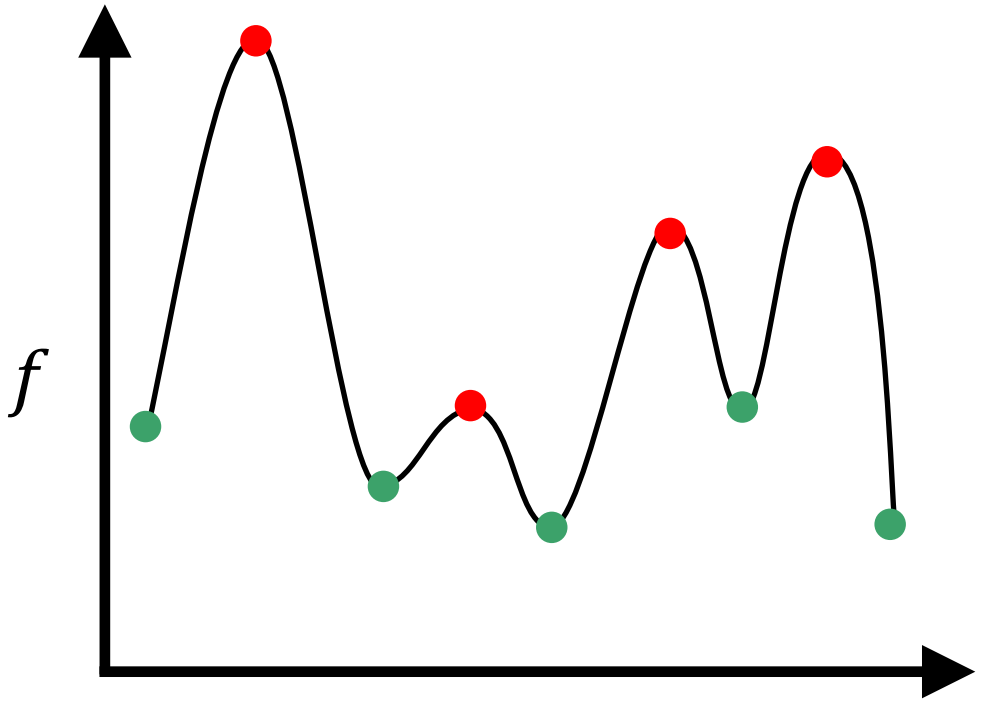
Topological changes



Sweep function from
$v = -\infty \rightarrow \infty$

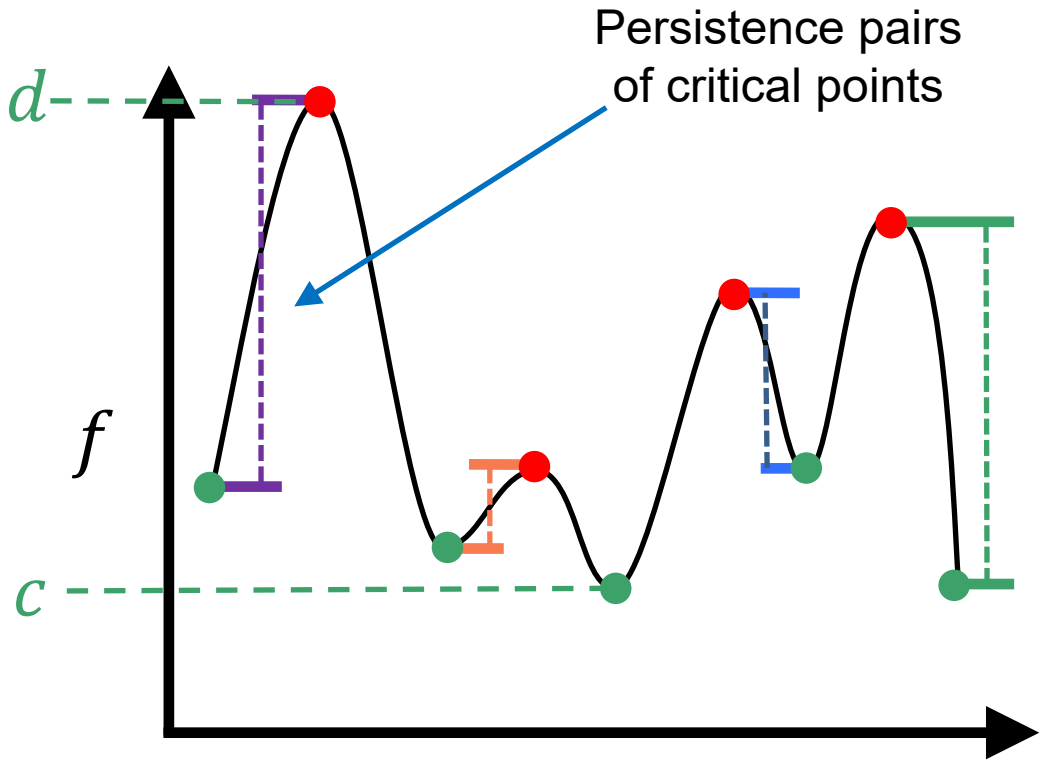
Topological changes
of subdomain
$f^{-1}((-\infty, v])$

Features of a 1-dimensional function

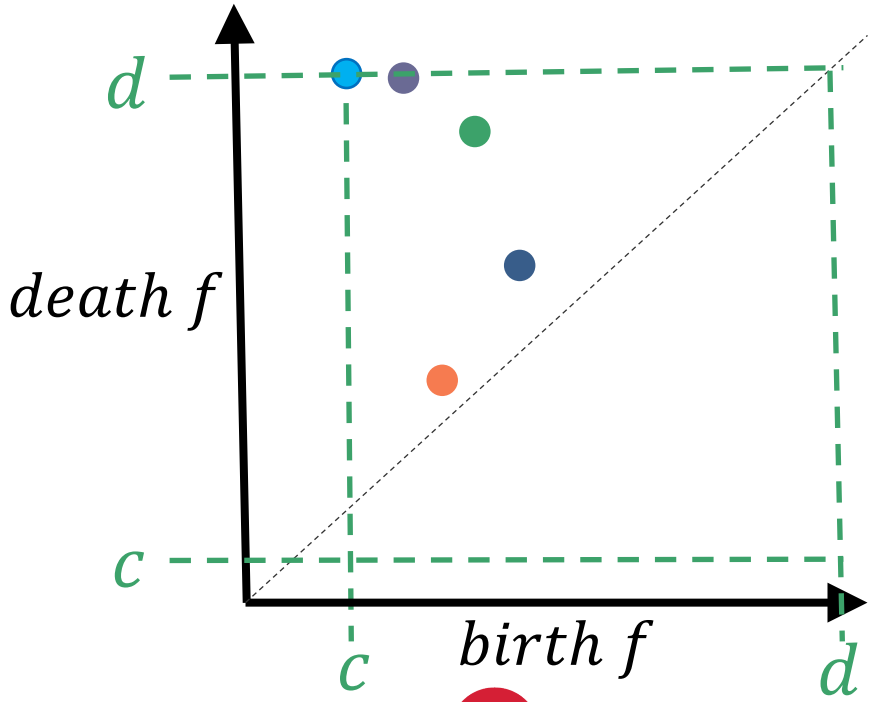


- Critical points where $\nabla f = 0$

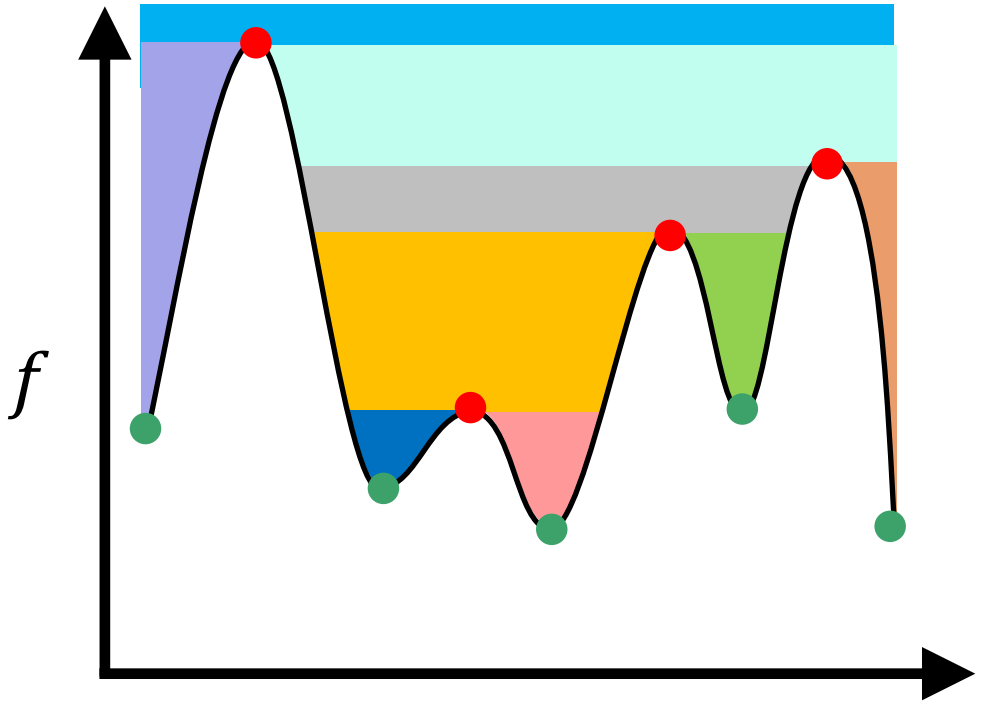
Features of a 1-dimensional function



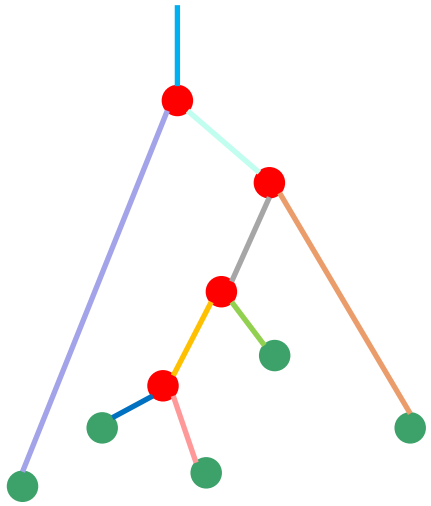
- Critical points where $\nabla f = 0$
- Persistence diagram



Features of a 1-dimensional function

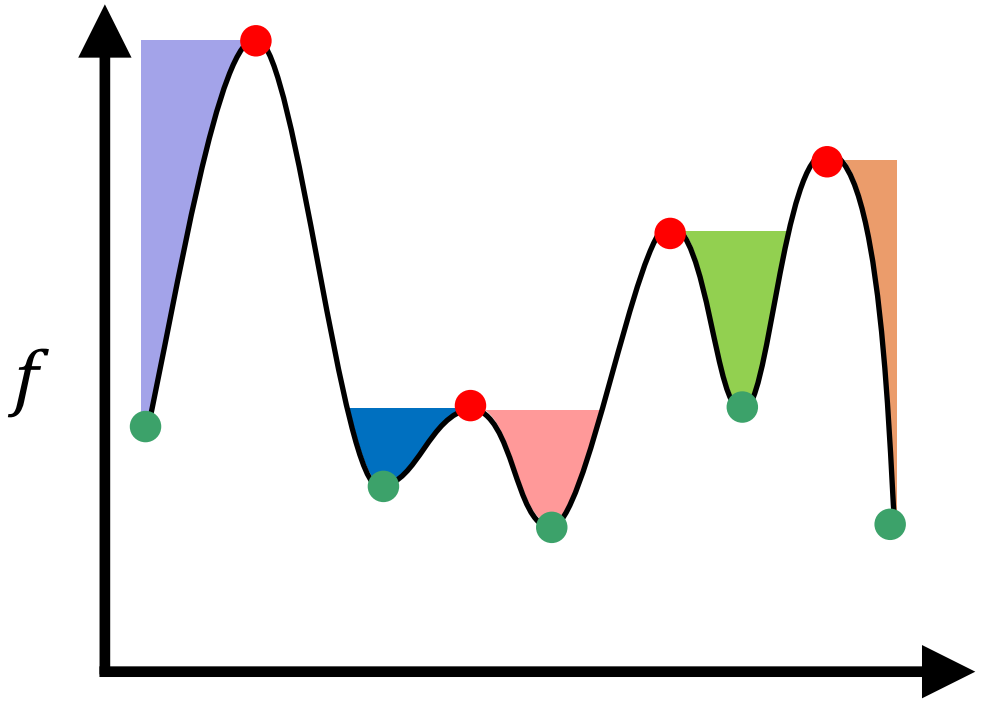


- Critical points where $\nabla f = 0$
- Components through sweep

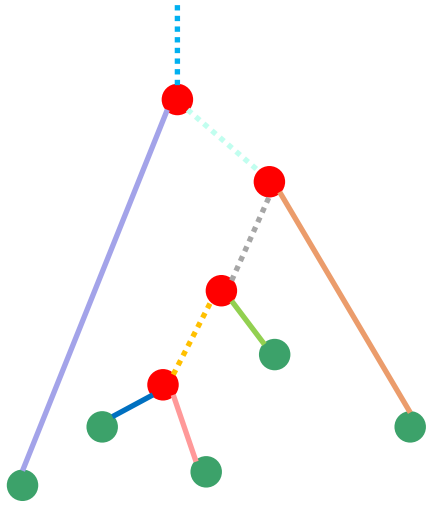


Join tree

Features of a 1-dimensional function

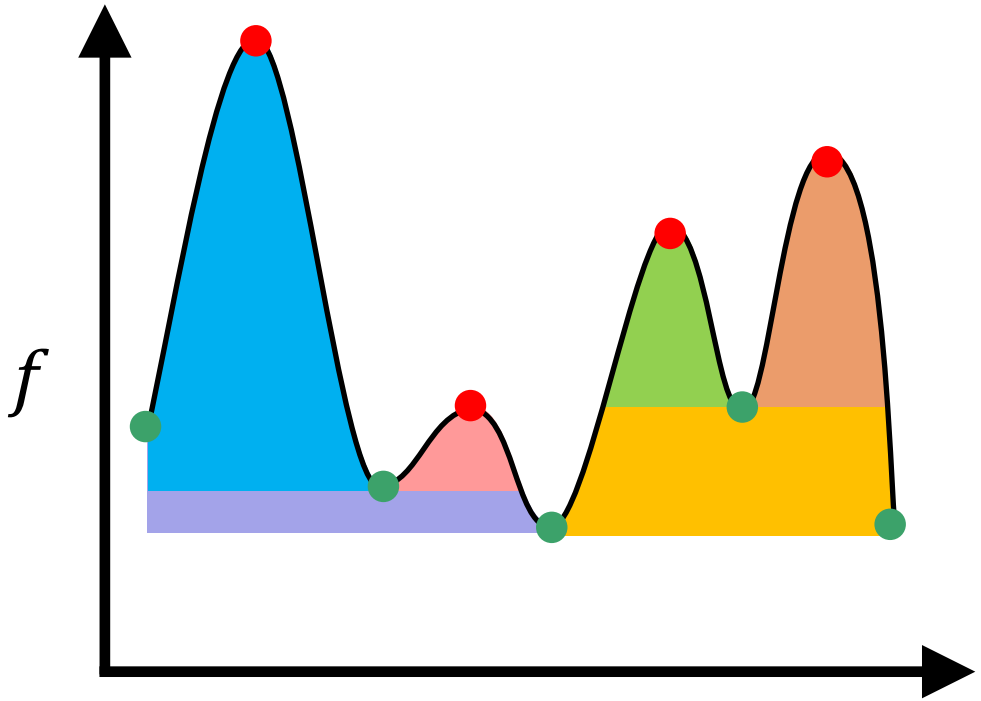


- Critical points where $\nabla f = 0$
- Components through sweep

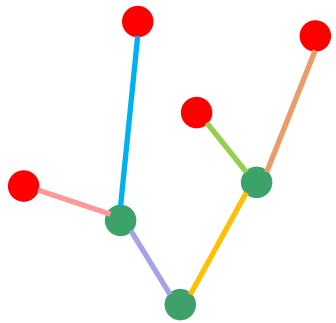


Join tree

Features of a 1-dimensional function

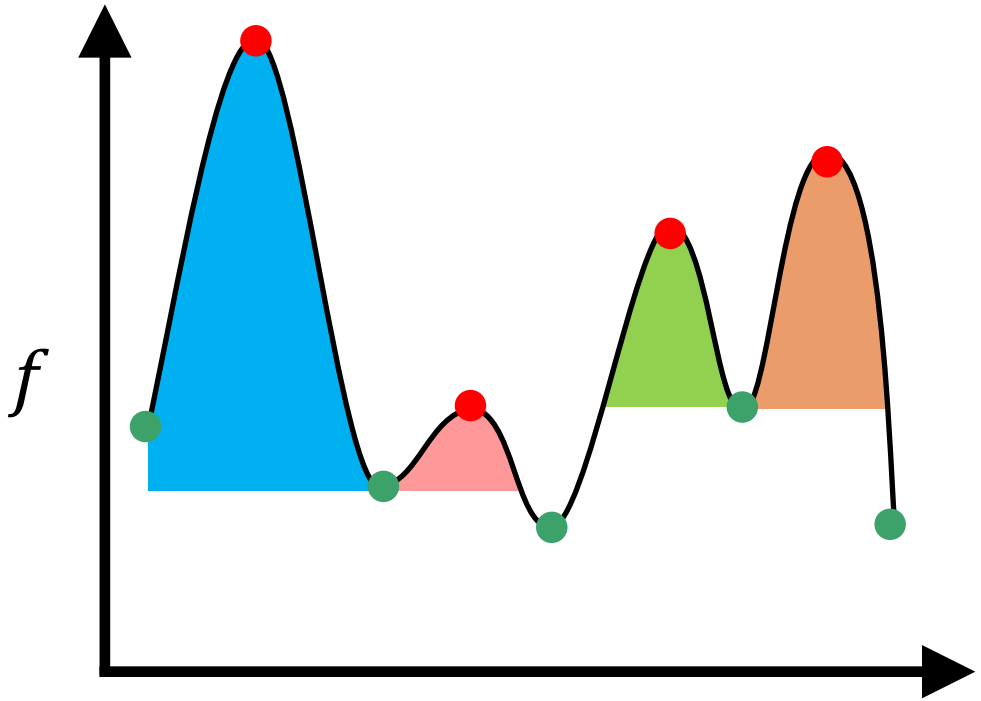


- Critical points where $\nabla f = 0$
- Components through sweep

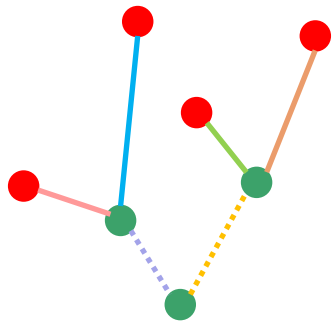


Merge tree

Features of a 1-dimensional function



- Critical points where $\nabla f = 0$
- Components through sweep

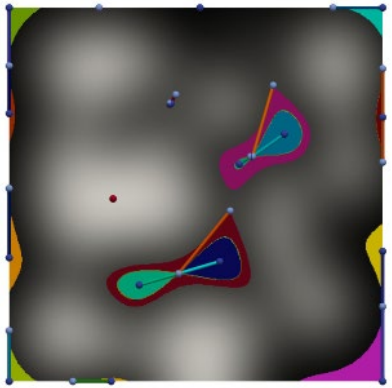


Merge tree

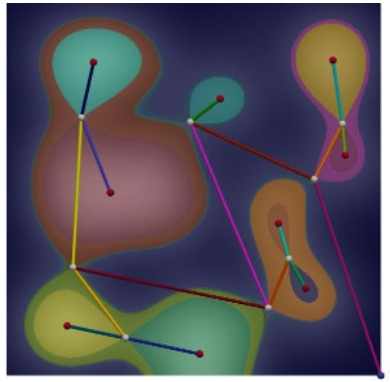
Features of a 2-dimensional function

Scalar function

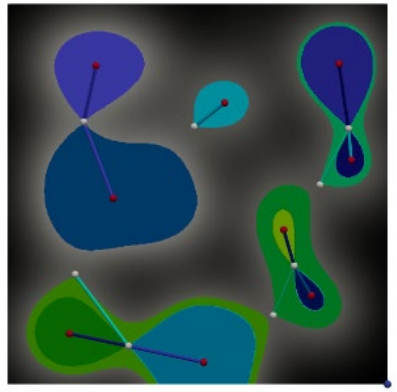
Join tree



Local valleys



Split tree

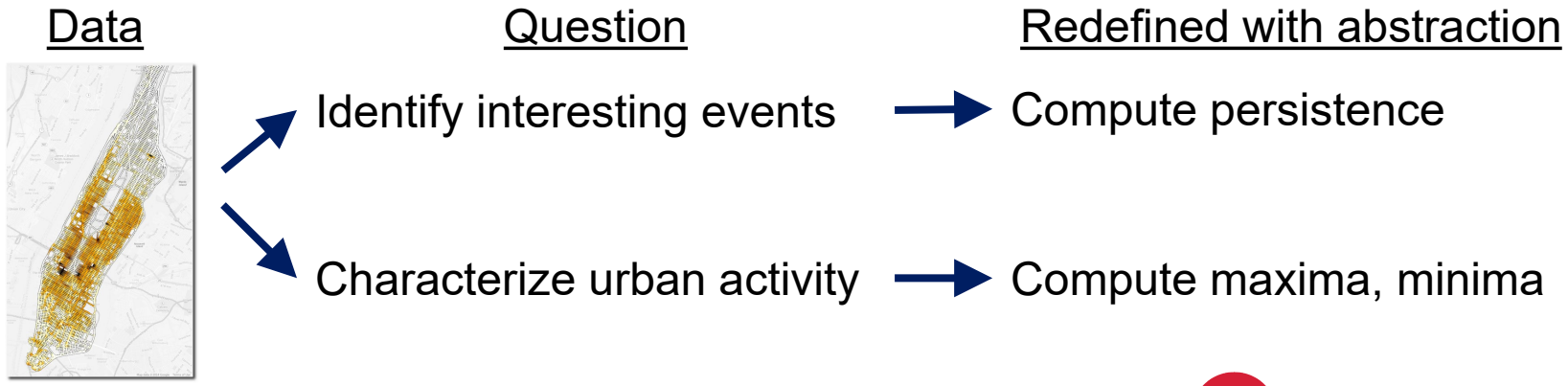


Local peaks

[Gyulassy, VIS 2018]

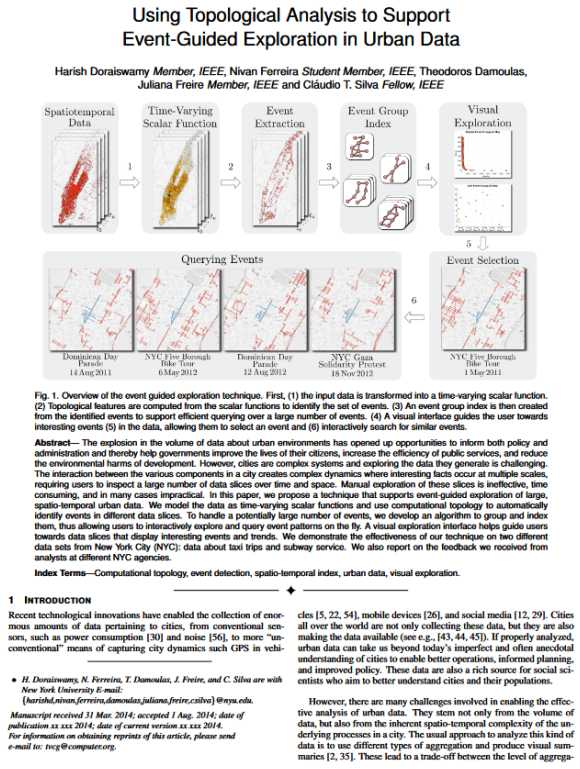
Topological data analysis

- Analysis workflow:
  1. Generate data
  2. Pick an abstraction
  3. Define the features
  4. Vis: evaluate features
- Create hypotheses for topological features:



Applications

1. Taxi patterns: finding interesting events on spatiotemporal data.
   - *"Using Topological Analysis to Support Event-Guided Exploration in Urban Data"* [TVCG 2014]
2. Urban Pulse: characterizing urban activity with spatiotemporal data.
   - "*Urban Pulse: Capturing the Rhythm of Cities*" [TVCG 2016]



Using Topological Analysis to Support Event-Guided Exploration in Urban Data

Harish Doraiswamy *Member, IEEE*, Nivan Ferreira *Student Member, IEEE*, Theodoros Damoulas, Juliana Freire *Member, IEEE* and Cláudio T. Silva *Fellow, IEEE*

Fig. 1. Overview of the event guided exploration technique. First, (1) the input data is transformed into a time-varying scalar function. (2) Topological features are computed from the scalar functions to identify the set of events. (3) An event group index is then created from the identified events to support efficient querying over a large number of events. (4) A visual interface guides the user towards interesting events (5) in the data, allowing them to select an event and (6) interactively search for similar events.

Abstract— The explosion in the volume of data about urban environments has opened up opportunities to inform both policy and administration and thereby help governments improve the lives of their citizens, increase the efficiency of public services, and reduce the environmental harms of development. However, cities are complex systems and exploring the data they generate is challenging. The interaction between the various components in a city creates complex dynamics where interesting facts occur at multiple scales, requiring users to inspect a large number of data slices over time and space. Manual exploration of these slices is ineffective, time consuming, and in many cases impractical. In this paper, we propose a technique that supports event-guided exploration of large, spatio-temporal urban data. We model the data as time-varying scalar functions and use computational topology to automatically identify events in different data slices. To handle a potentially large number of events, we develop an algorithm to group and index them, thus allowing users to interactively explore and query event patterns on the fly. A visual exploration interface helps guide users towards data slices that display interesting events and trends. We demonstrate the effectiveness of our technique on two different data sets from New York City (NYC): data about taxi trips and subway service. We also report on the feedback we received from analysts at different NYC agencies.

Index Terms—Computational topology, event detection, spatio-temporal index, urban data, visual exploration.

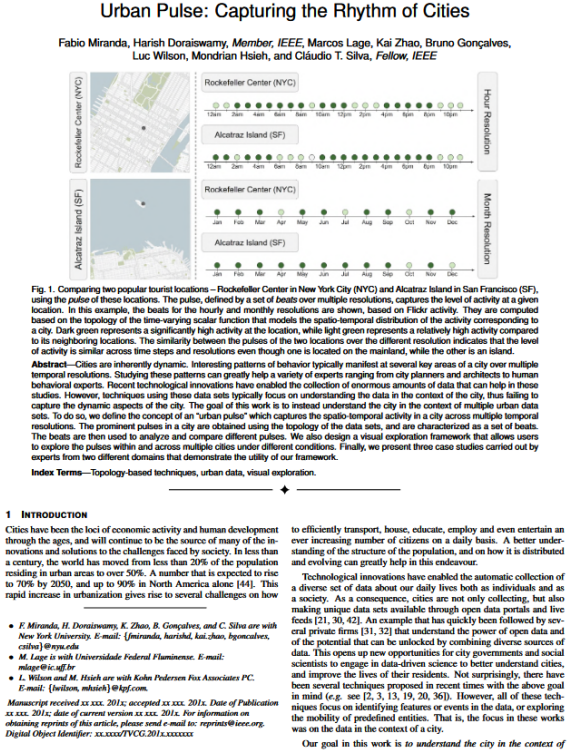
1 Introduction

Recent technological innovations have enabled the collection of enormous amounts of data pertaining to cities, from conventional sensors, such as power consumption [30] and noise [56], to more "unconventional" means of capturing city dynamics such GPS in vehicles [5, 22, 54], mobile devices [26], and social media [12, 29]. Cities all over the world are not only collecting these data, but they are also making the data available (see e.g., [43, 44, 45]). If properly analyzed, urban data can take us beyond today's imperfect and often anecdotal understanding of cities to enable better operations, informed planning, and improved policy. These data are also a rich source for social scientists who aim to better understand cities and their populations.

However, there are many challenges involved in enabling the effective analysis of urban data. They stem not only from the volume of data, but also from the inherent spatio-temporal complexity of the underlying processes in a city. The usual approach to analyze this kind of data is to use different types of aggregation and produce visual summaries [2, 35]. These lead to a trade-off between the level of aggrega-

• *H. Doraiswamy, N. Ferreira, T. Damoulas, J. Freire, and C. Silva are with New York University. E-mail: {harishd,nivan.ferreira,damoulas,juliana.freire,csilva}@nyu.edu.*

Manuscript received 31 Mar. 2014; accepted 1 Aug. 2014; date of publication xx xxx 2014; date of current version xx xxx 2014. For information on obtaining reprints of this article, please send e-mail to: tvcg@computer.org.



Urban Pulse: Capturing the Rhythm of Cities

Fabio Miranda, Harish Doraiswamy, *Member, IEEE*, Marcos Lage, Kai Zhao, Bruno Gonçalves, Luc Wilson, Mondrian Hsieh, and Cláudio T. Silva, *Fellow, IEEE*

Fig. 1. Comparing two popular tourist locations – Rockefeller Center in New York City (NYC) and Alcatraz Island in San Francisco (SF), using the *pulse* of these locations. The pulse, defined by a set of *beats* over multiple resolutions, captures the level of activity at a given location. In this example, the beats for the hourly and monthly resolutions are shown, based on Flickr activity. They are computed based on the topology of the time-varying scalar function that models the spatio-temporal distribution of the activity corresponding to a city. Dark green represents a significantly high activity at the location, while light green represents a relatively high activity compared to its neighboring locations. The similarity between the pulses of the two locations over the different resolution indicates that the level of activity is similar across time steps and resolutions even though one is located on the mainland, while the other is an island.

Abstract—Cities are inherently dynamic. Interesting patterns of behavior typically manifest at several key areas of a city over multiple temporal resolutions. Studying these patterns can greatly help a variety of experts ranging from city planners and architects to human behavioral experts. Recent technological innovations have enabled the collection of enormous amounts of data that can help in these studies. However, techniques using these data sets typically focus on understanding the data in the context of the city, thus failing to capture the dynamic aspects of the city. The goal of this work is to instead understand the city in the context of multiple urban data sets. To do so, we define the concept of an "urban pulse" which captures the spatio-temporal activity in a city across multiple temporal resolutions. The prominent pulses in a city are obtained using the topology of the data sets, and are characterized as a set of beats. The beats are then used to analyze and compare different pulses. We also design a visual exploration framework that allows users to explore the pulses within and across multiple cities under different conditions. Finally, we present three case studies carried out by experts from two different domains that demonstrate the utility of our framework.

Index Terms—Topology-based techniques, urban data, visual exploration.

1 Introduction

Cities have been the loci of economic activity and human development through the ages, and will continue to be the source of many of the innovations and solutions to the challenges faced by society. In less than a century, the world has moved from less than 20% of the population residing in urban areas to over 50%. A number that is expected to rise to 70% by 2050, and up to 90% in North America alone [44]. This rapid increase in urbanization gives rise to several challenges on how to efficiently transport, house, educate, employ and even entertain an ever increasing number of citizens on a daily basis. A better understanding of the structure of the population, and on how it is distributed and evolving can greatly help in this endeavour.

Technological innovations have enabled the automatic collection of a diverse set of data about our daily lives both as individuals and as a society. As a consequence, cities are not only collecting, but also making unique data sets available through open data portals and live feeds [21, 30, 42]. An example that has quickly been followed by several private firms [31, 32] that understand the power of open data and of the potential that can be unlocked by combining diverse sources of data. This opens up new opportunities for city governments and social scientists to engage in data-driven science to better understand cities, and improve the lives of their residents. Not surprisingly, there have been several techniques proposed in recent times with the above goal in mind (e.g. see [2, 3, 13, 19, 20, 36]). However, all of these techniques focus on identifying features or events in the data, or exploring the mobility of predefined entities. That is, the focus in these works was on the data in the context of a city.

Our goal in this work is *to understand the city in the context of*

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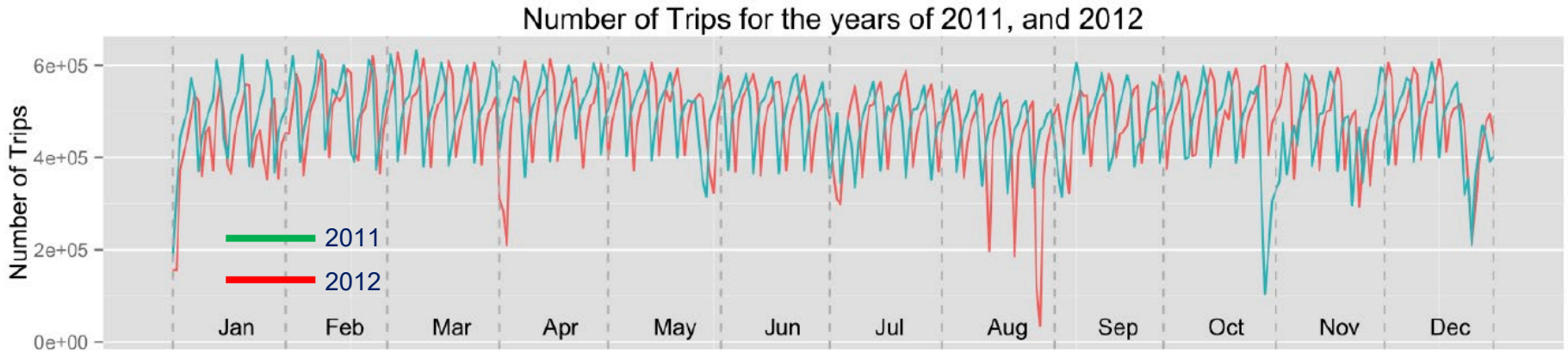
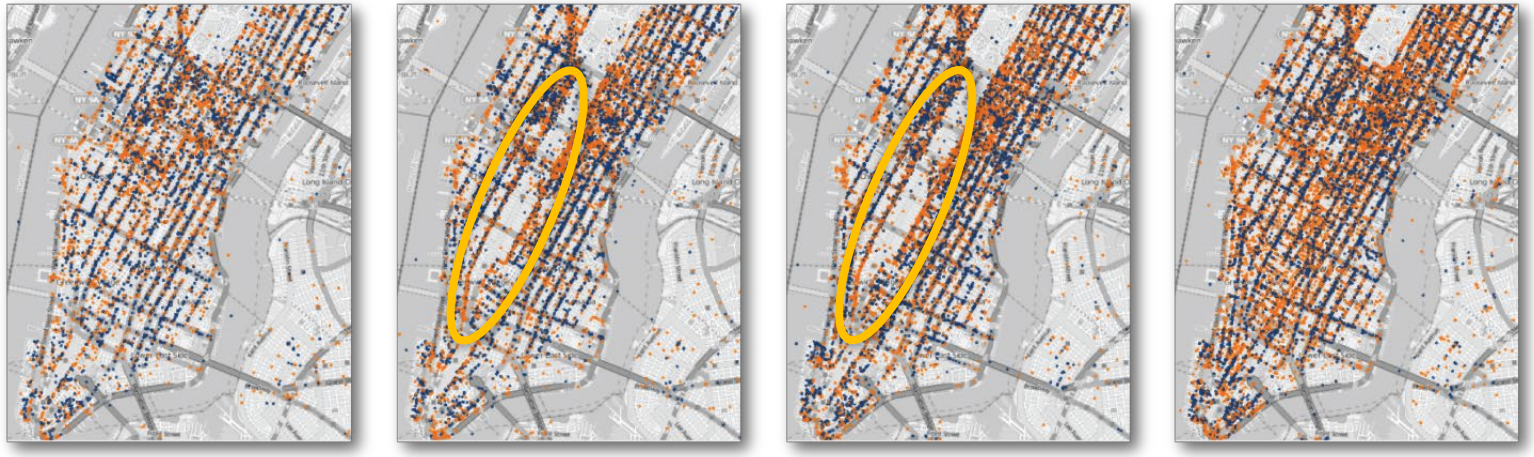
Applications: taxi patterns

- NYC taxi data:
  - ~175 million trips / year
  - Spatiotemporal
  - Other attributes:
    - Fare, tip
    - Distance
    - Duration
    - …

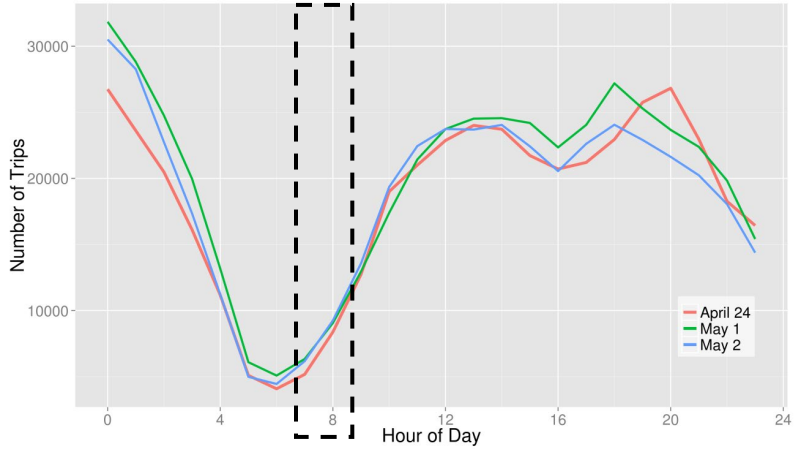
Taxi data slices

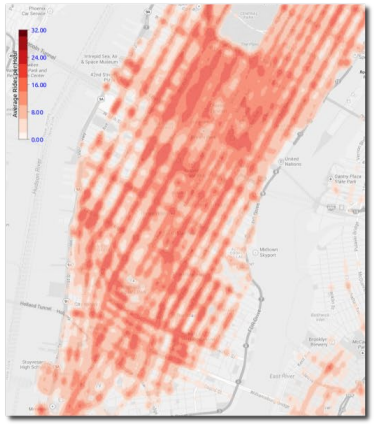




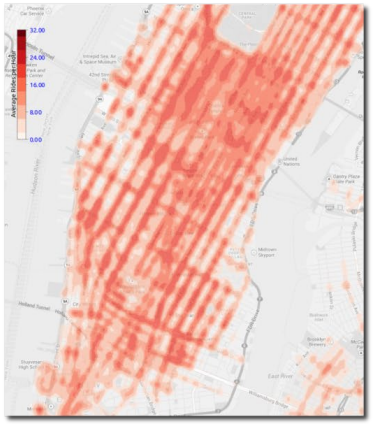
7am - 8am | 8am - 9am | 9am - 10am | 10am - 11am

Taxi data slices

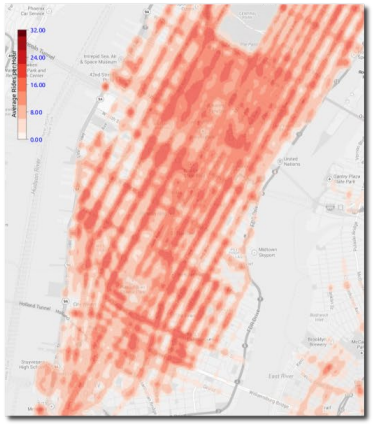




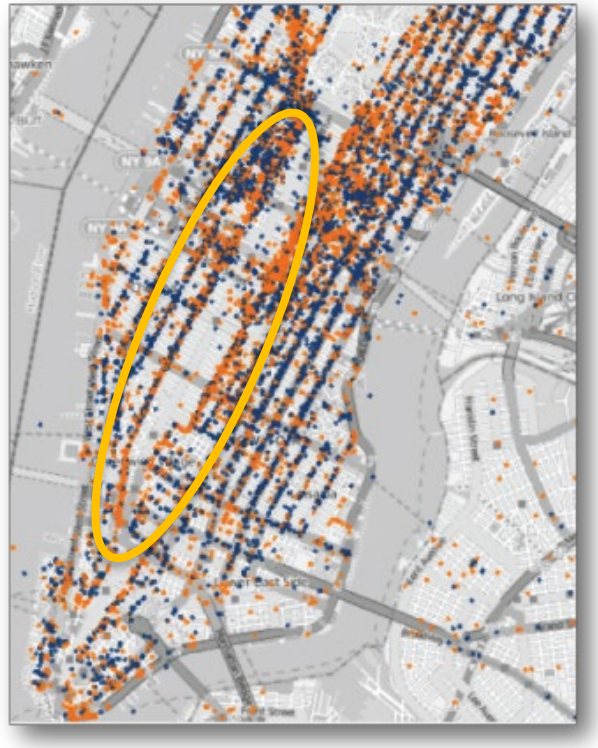
April 24



May 1

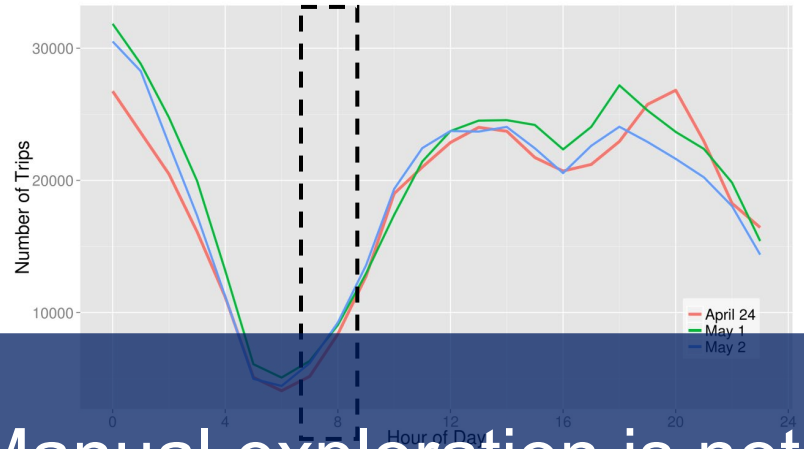


May 8

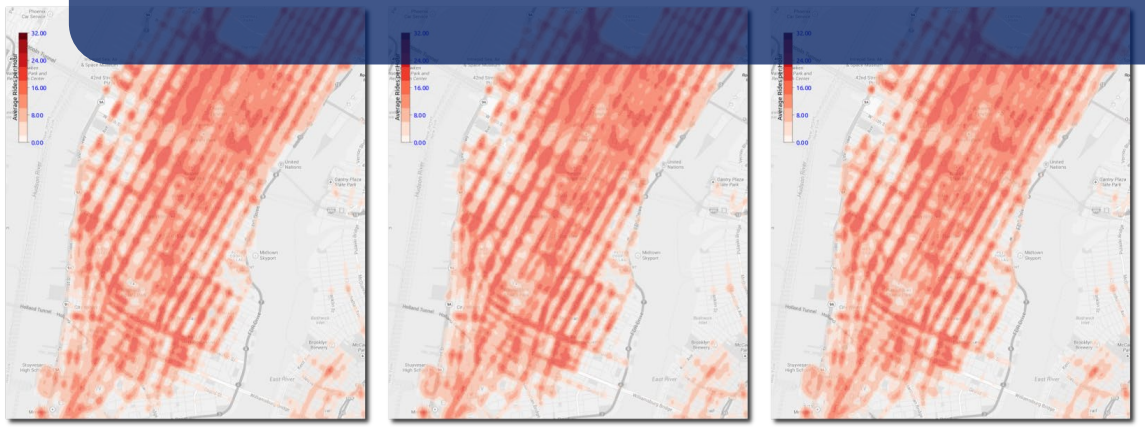


8am - 9am

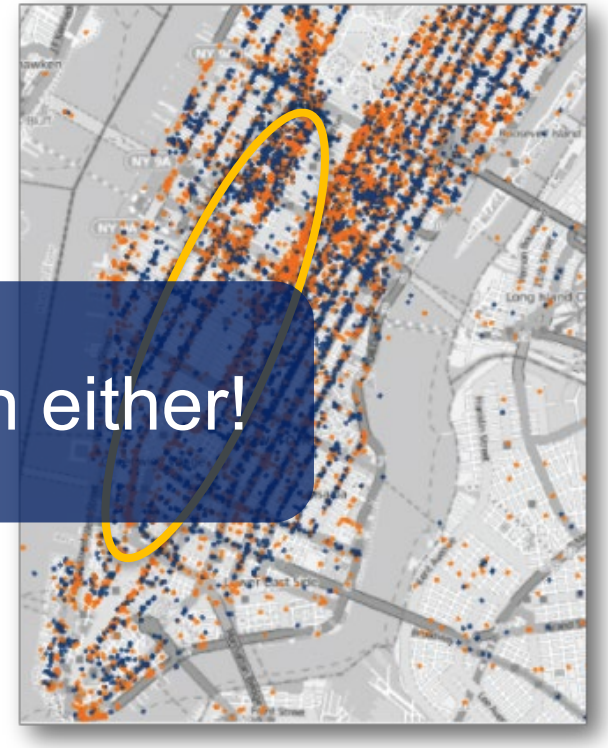
Taxi data slices



Manual exploration is not an option either!



April 24 May 1 May 8

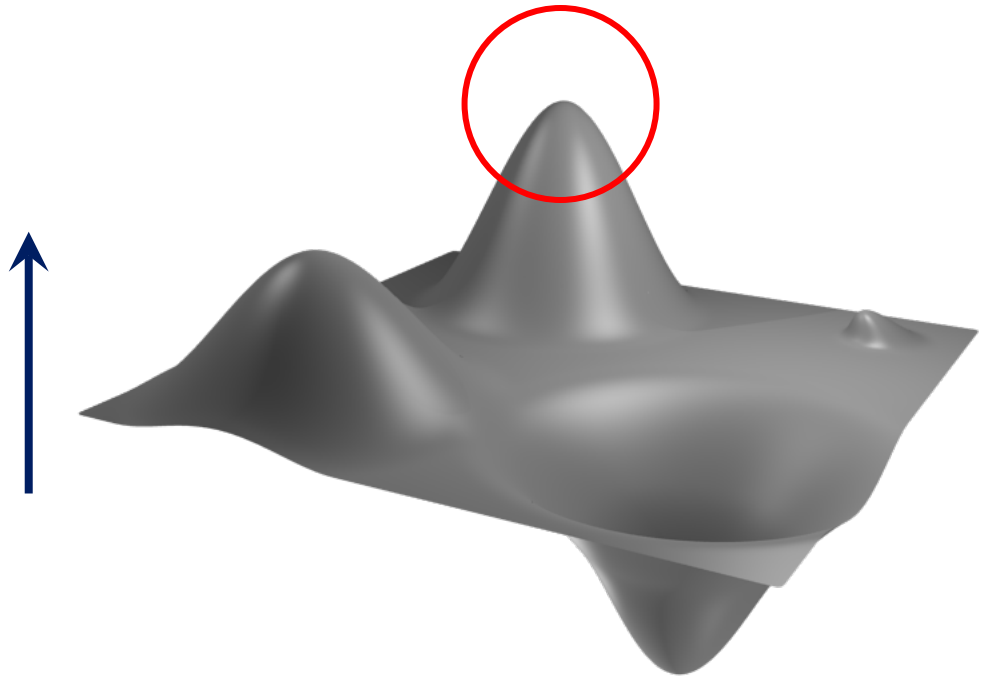


8am - 9am

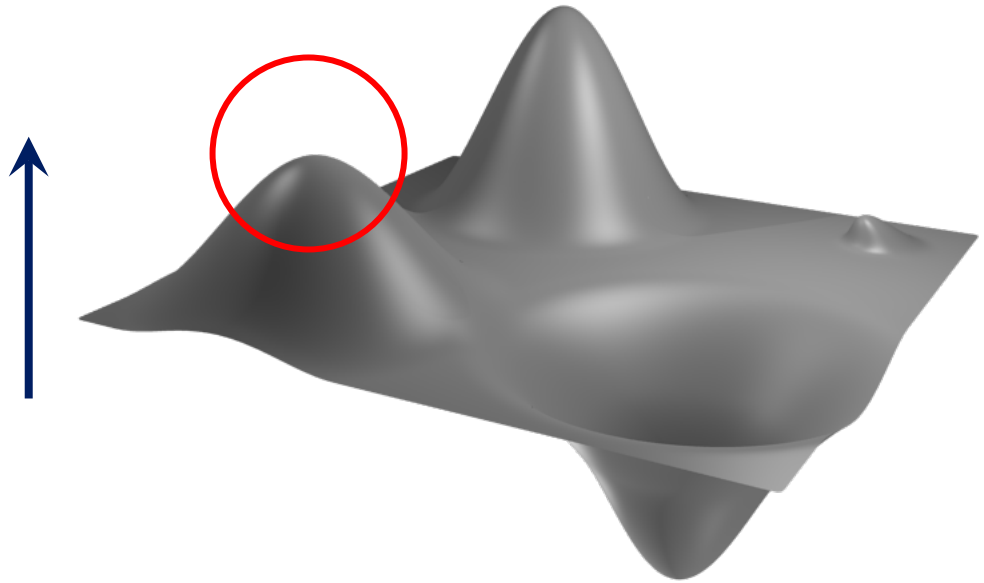
Taxi patterns: goals

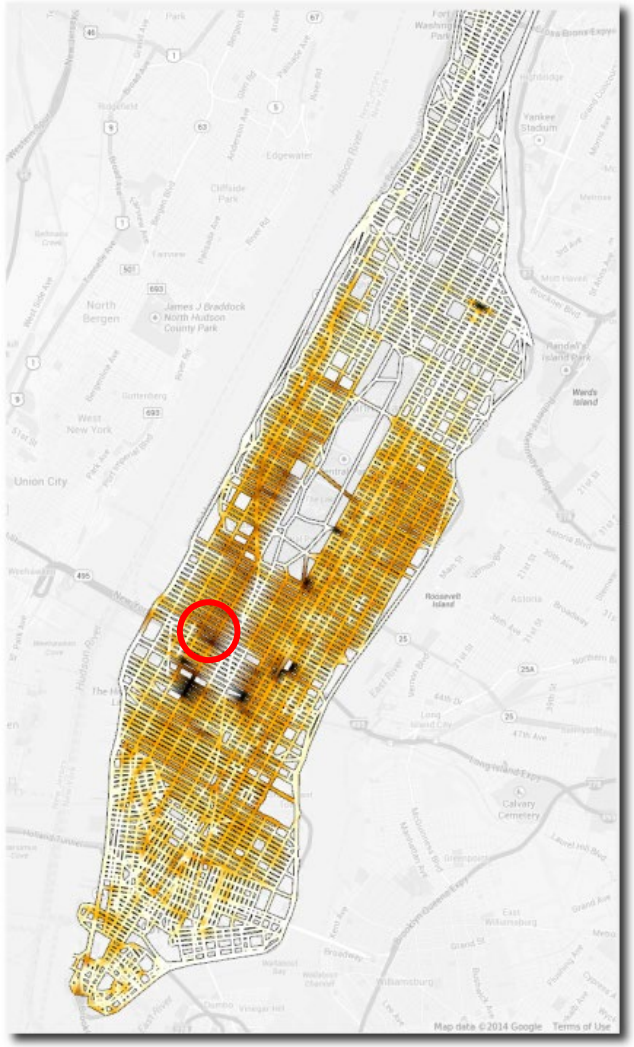
- Guide users towards potentially interesting slices
- What is an interesting data slice?
  - Contains an “event”
- Flexible definition of events:
  - Arbitrary spatial structure.
  - Different types of events.
  - Multiple temporal scales.
- Efficient search for similar event patterns.

Topology of the data

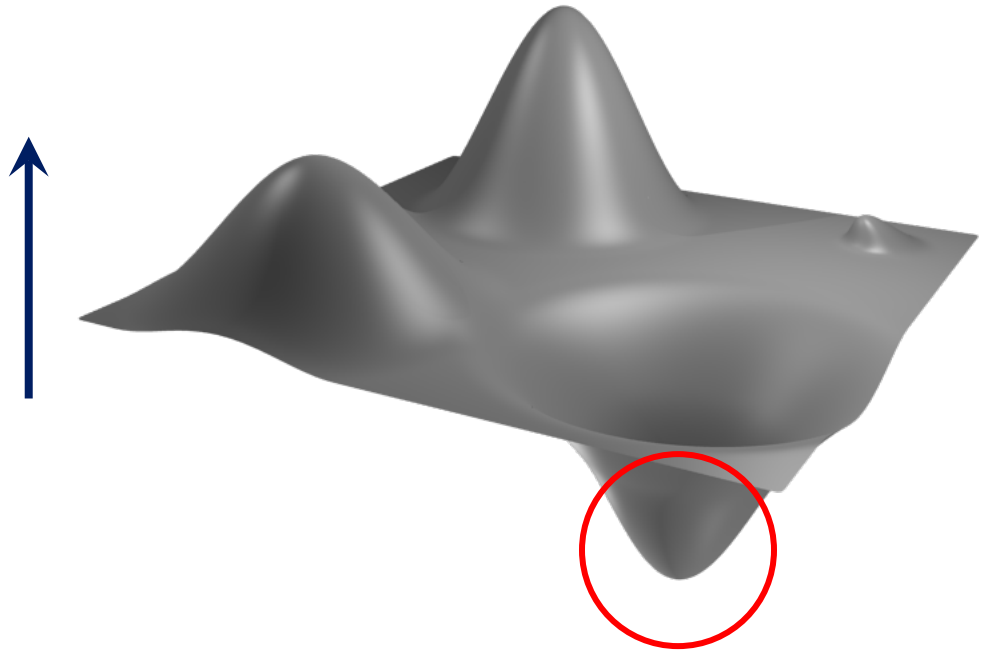


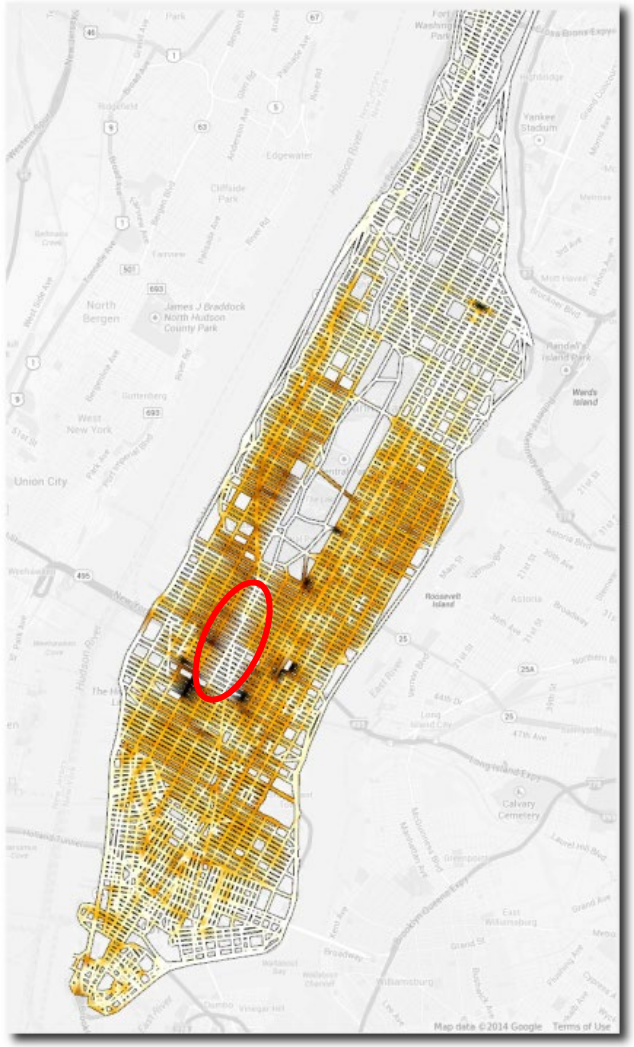
Topology of the data



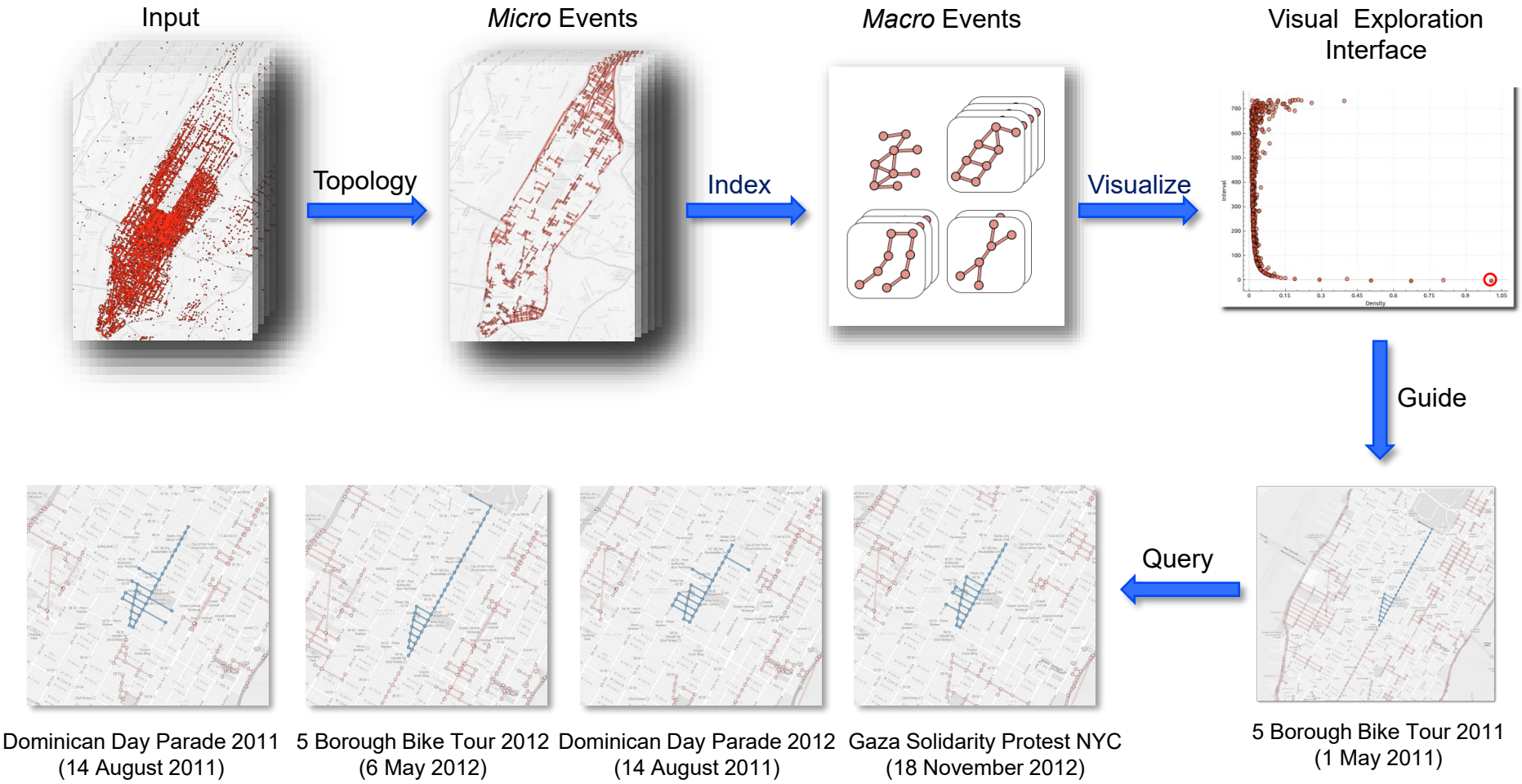


Topology of the data



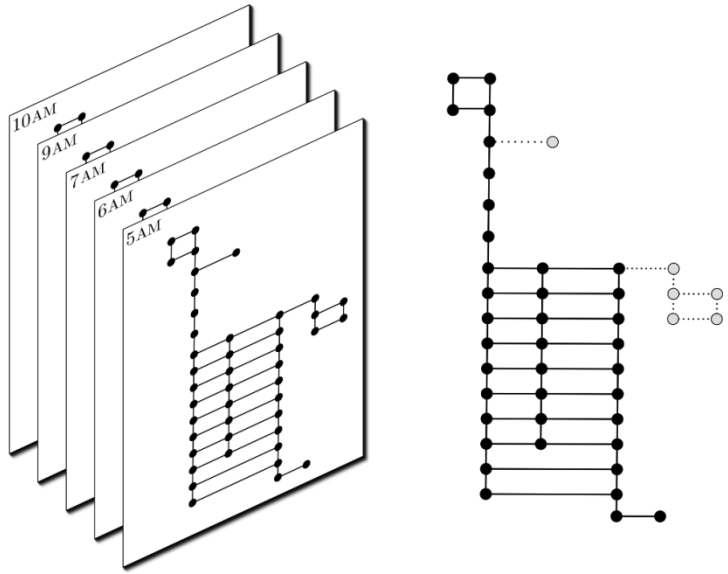


Topology framework



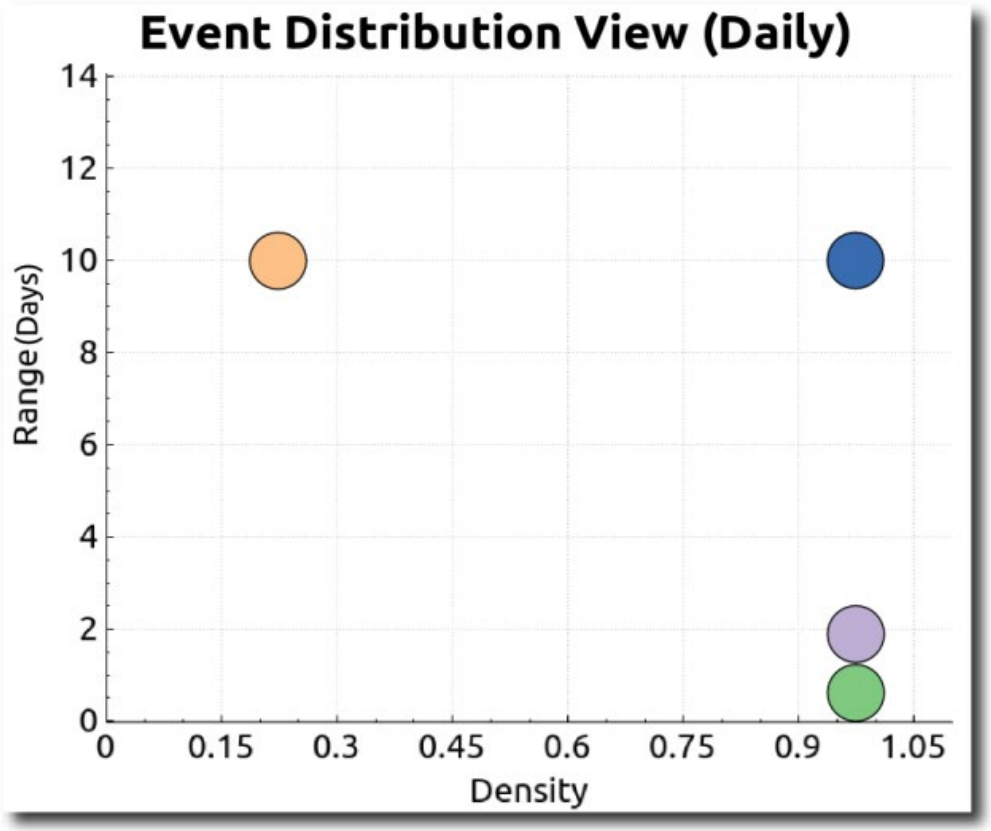
Exploring topological features

- Several features per time step.
- Group similar features within a larger time interval.
  - Represents “macro” events.

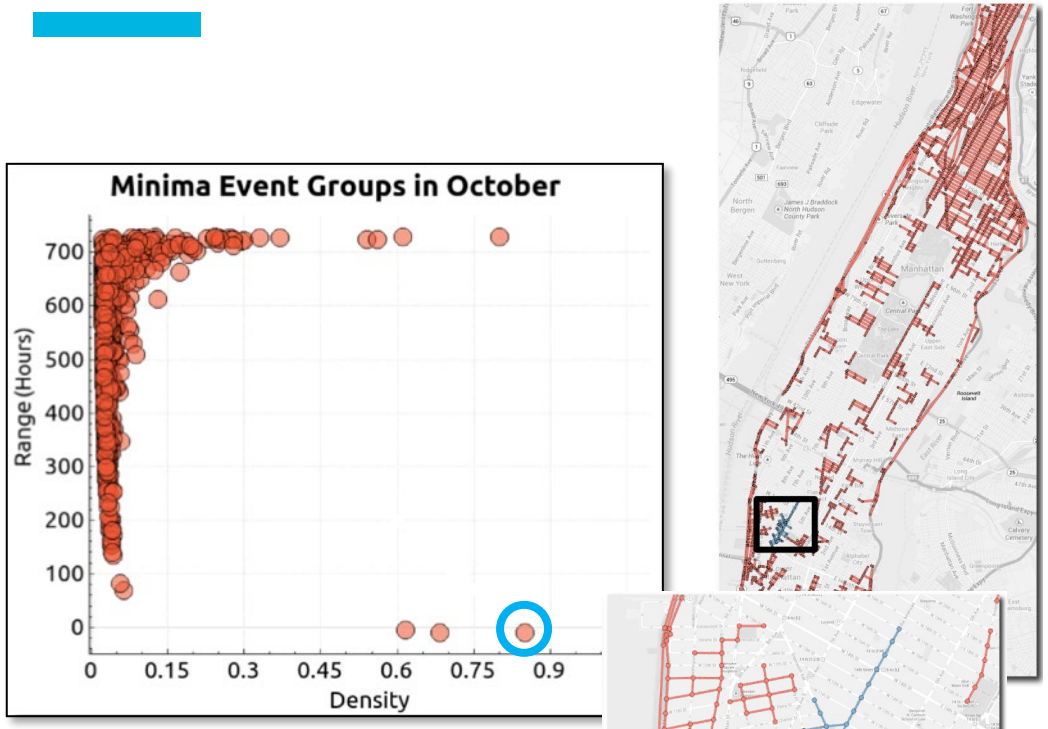


Event distribution view

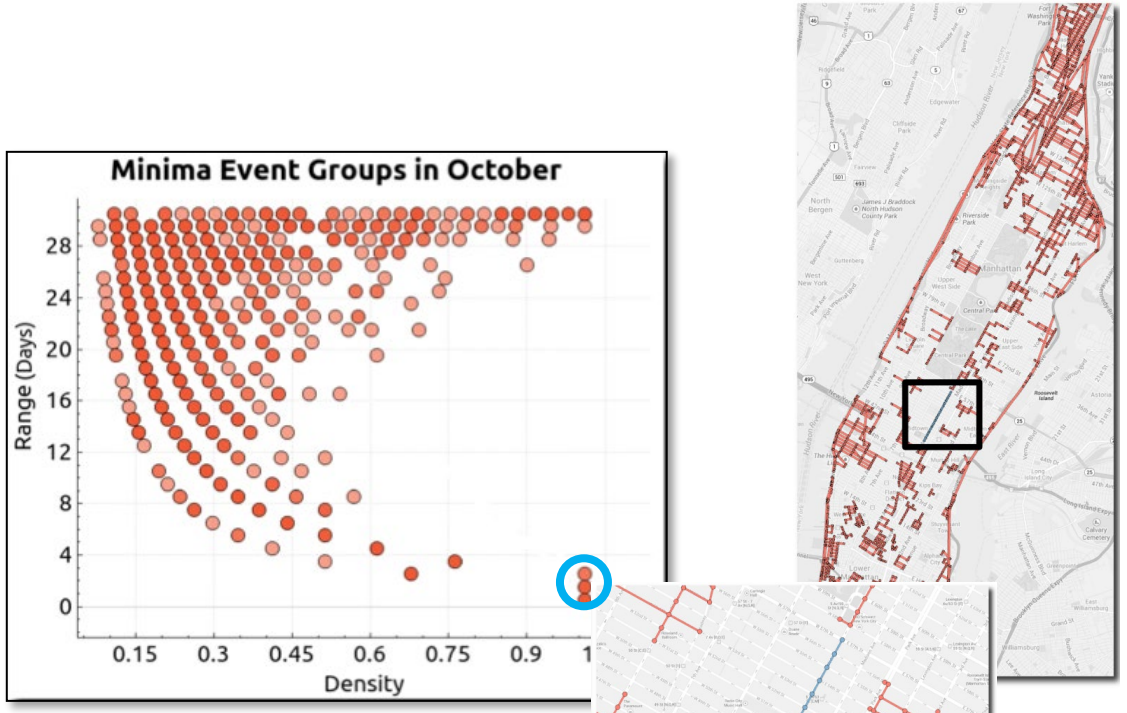
- Event group properties:
  - Range: time span of the group
    - Hours, days, weeks
  - Density: time span / no. of events
    - Frequency of events within a group



Rare events



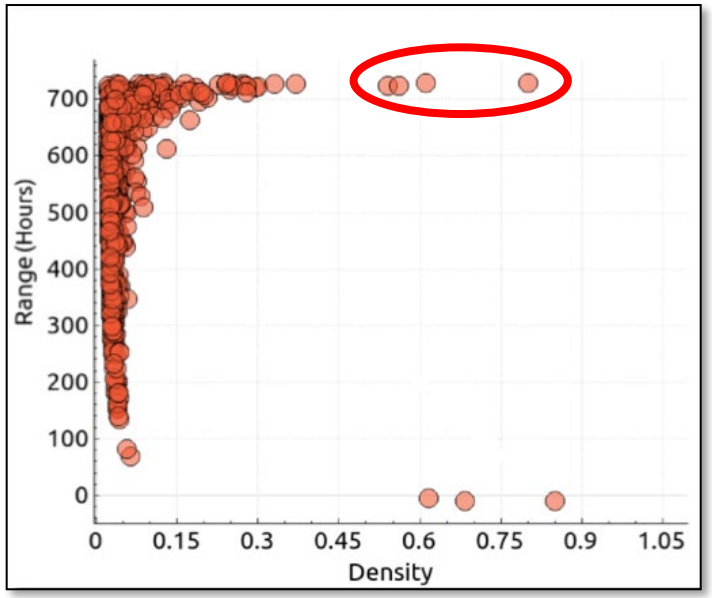
Hourly: Halloween parade



Daily: halloween parade

Frequent events

Maxima: taxi hotspots



Nighttime trends

Applications: Urban Pulse

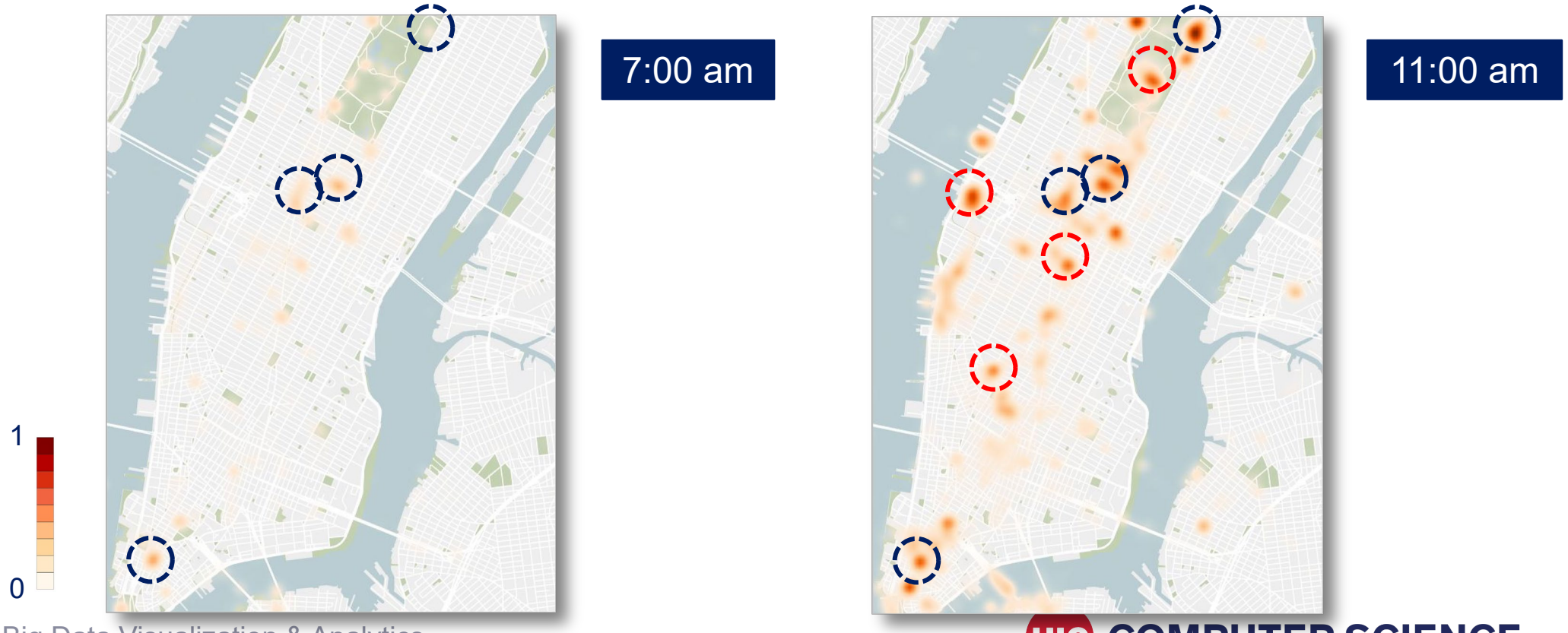
flickr

twitter

Infrastructure Environment Social media

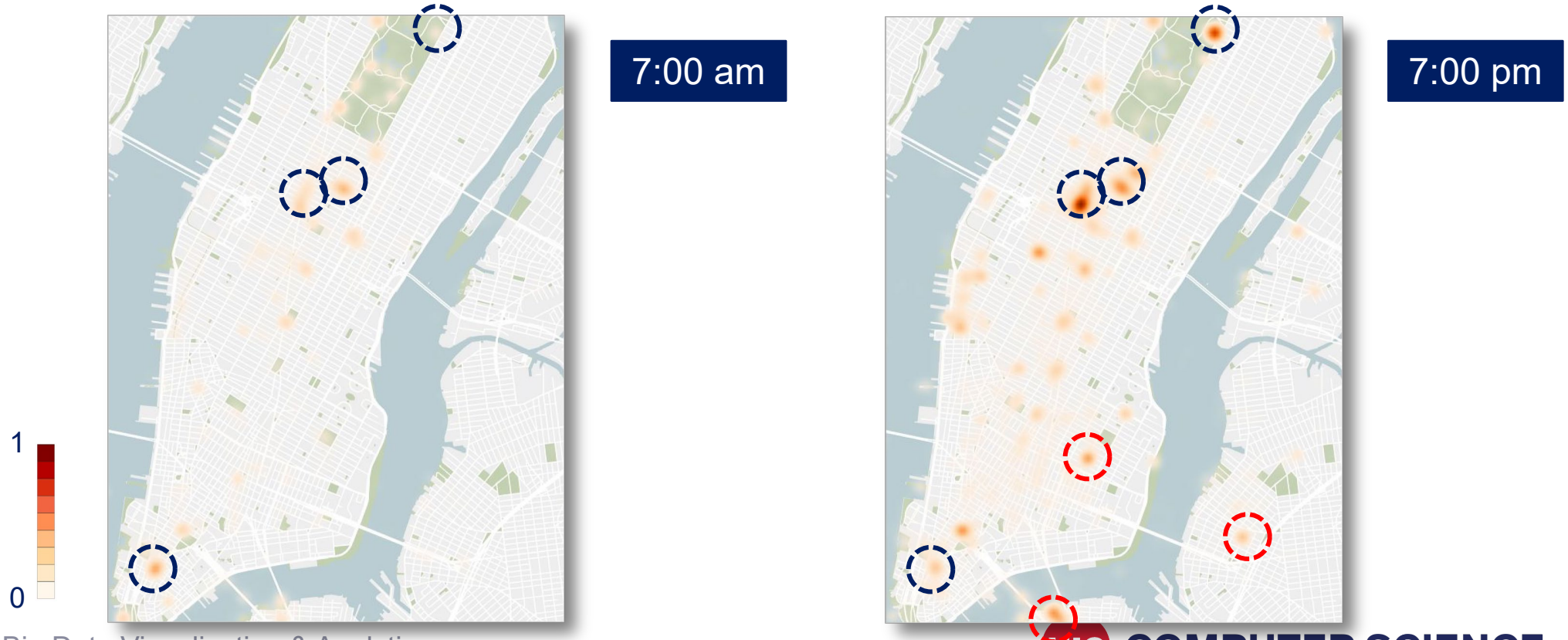
Urban Pulse

Flickr activity in New York City



Urban Pulse

Flickr activity in New York City

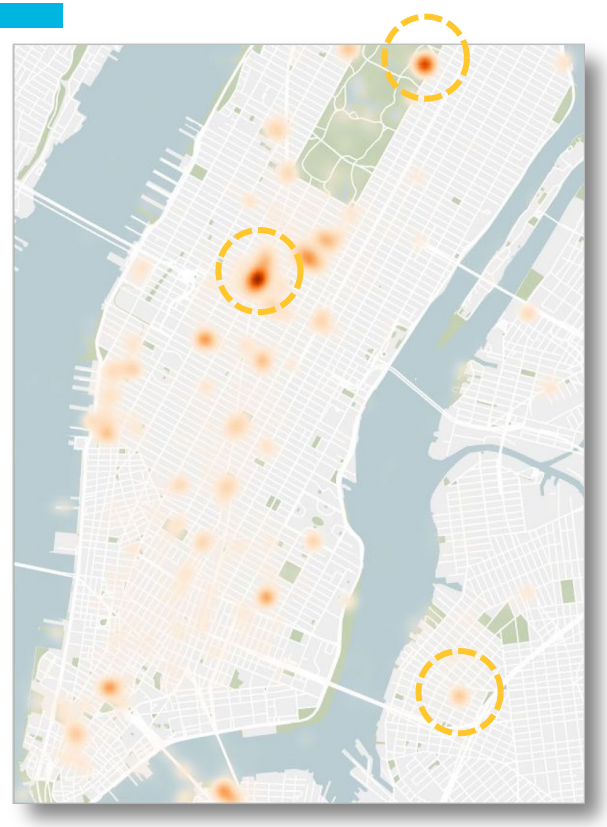


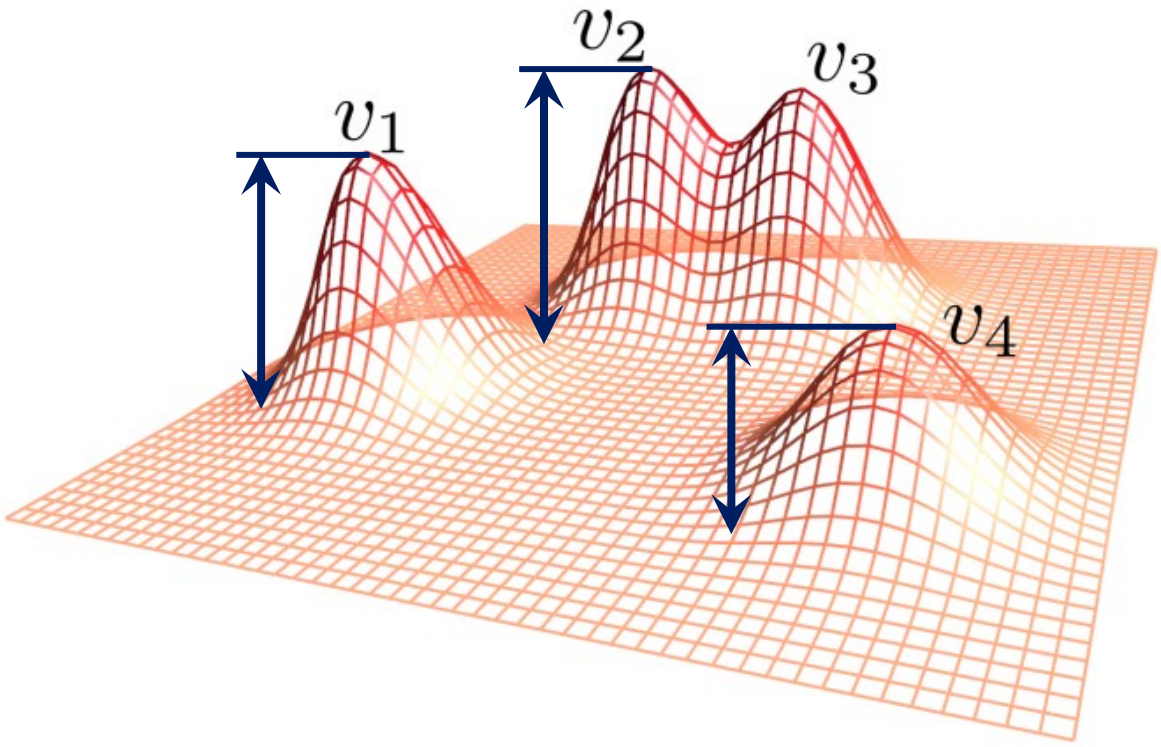
Urban Pulse: desiderate

- Capture locations where the pulse is “interesting”
- Quantify the pulse
  - Track “activity”
- Temporal resolutions

Step 1: identify pulse locations

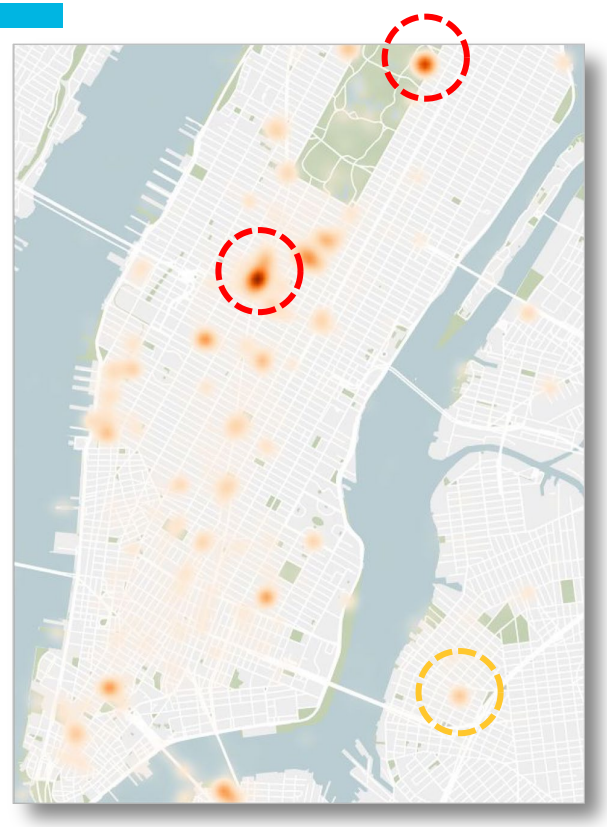
1. Identify Locations
2. Quantify Pulse

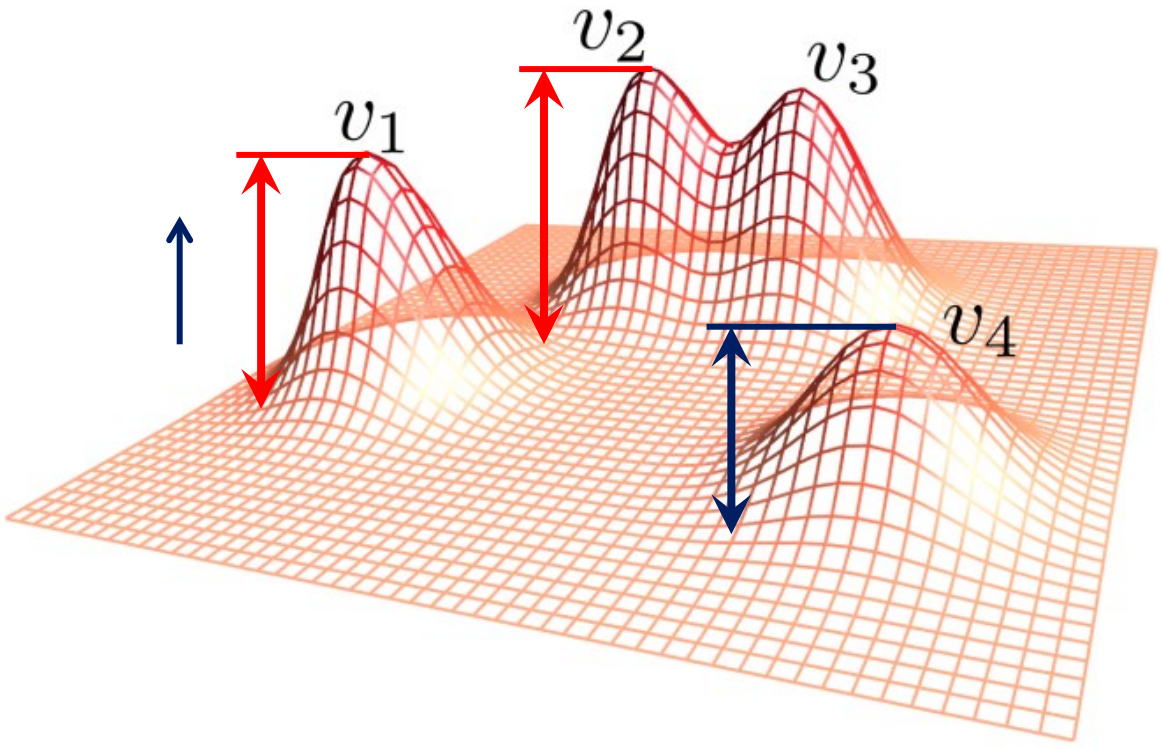




Step 1: identify pulse locations

1. Identify Locations
2. Quantify Pulse

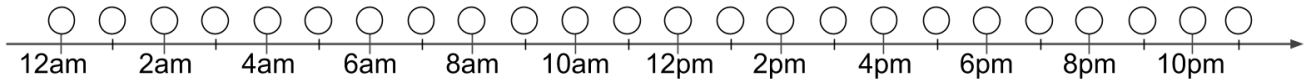




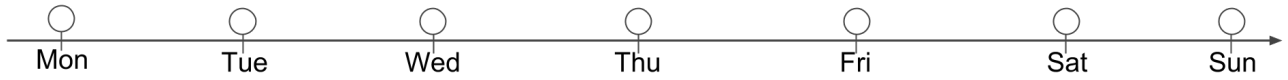
Handling temporal resolutions

Assume functions are defined along 3 resolutions (group by operations)

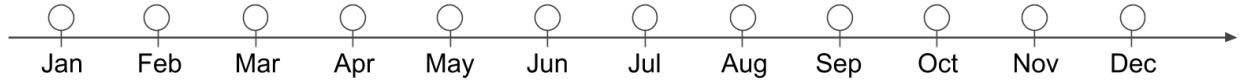
Time of Day



Day of Week



Month of Year



Step 1: identify pulse locations

1. Identify Locations
2. Quantify Pulse

- Set of scalar functions over time
  - Density functions as Gaussian weighted sum:

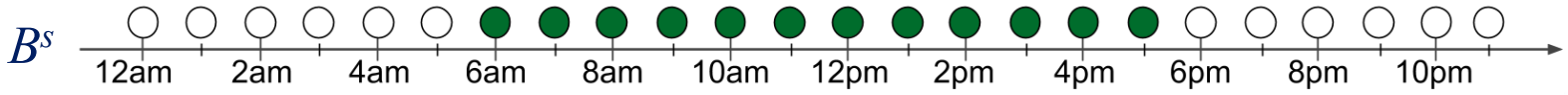
$$\sum_{x_i \in N(p)} e^{\frac{-d(p,x_i)^2}{\varepsilon^2}}$$

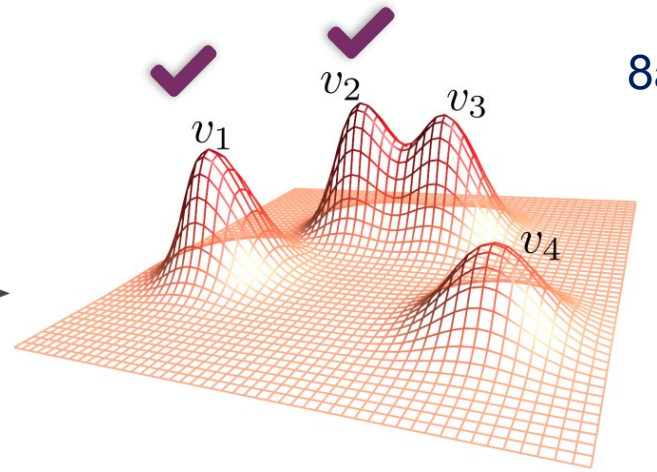
- Identify all maxima
- Location of **prominent** pulses:
  - is a high persistent maxima in at least one timestep
  - is a high persistent maxima in at least one resolution

Step 2: quantifying pulse

1. Identify Locations
2. Quantify Pulse

- 3 **Beats** to quantify the pulse at each location
- Significant Beats B^s
  - Pulse is a high persistent maximum



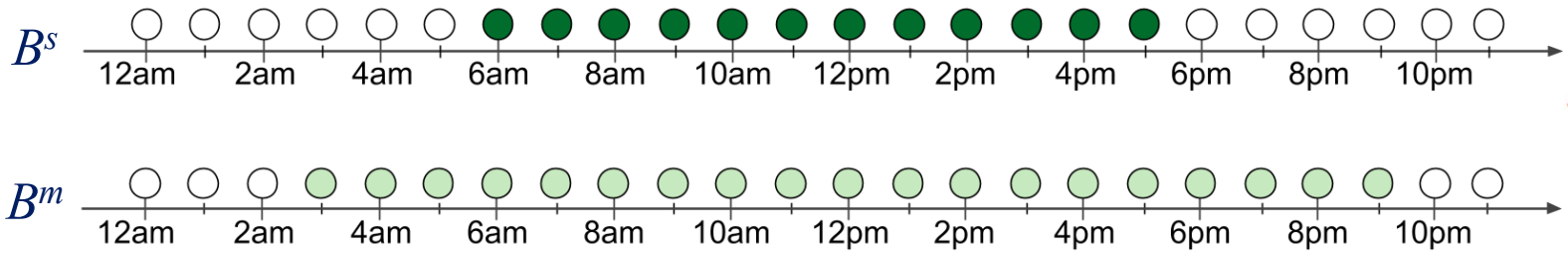


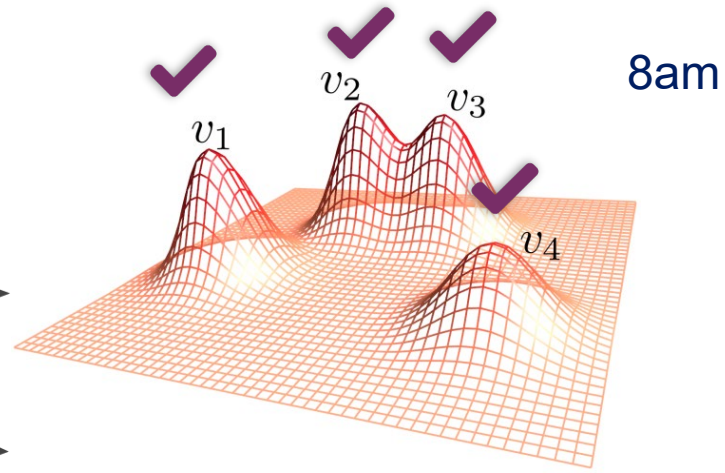
8am

Step 2: quantifying pulse

1. Identify Locations
2. Quantify Pulse

- 3 **Beats** to quantify the pulse at each location
- Maxima Beats B^m
  - Pulse is a maximum

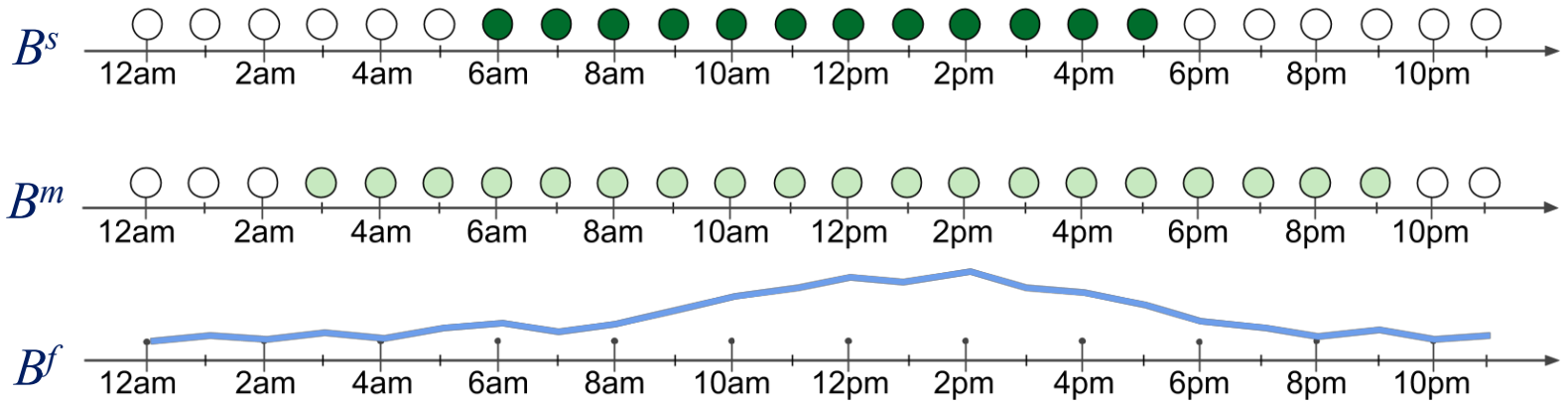




Step 2: quantifying pulse

1. Identify Locations
2. Quantify Pulse

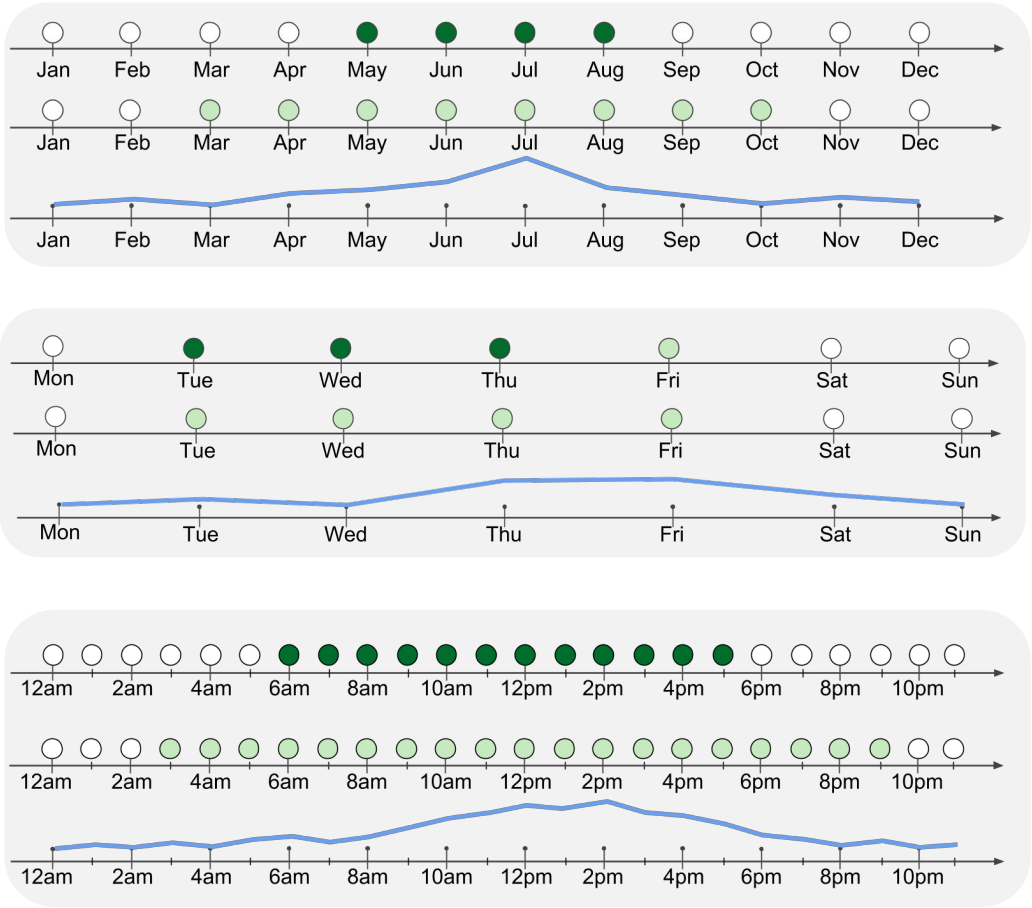
- 3 **Beats** to quantify the pulse at each location
- Function Beats B^f
  - Variation of the function values



Step 2: quantifying pulse

1. Identify Locations
2. Quantify Pulse

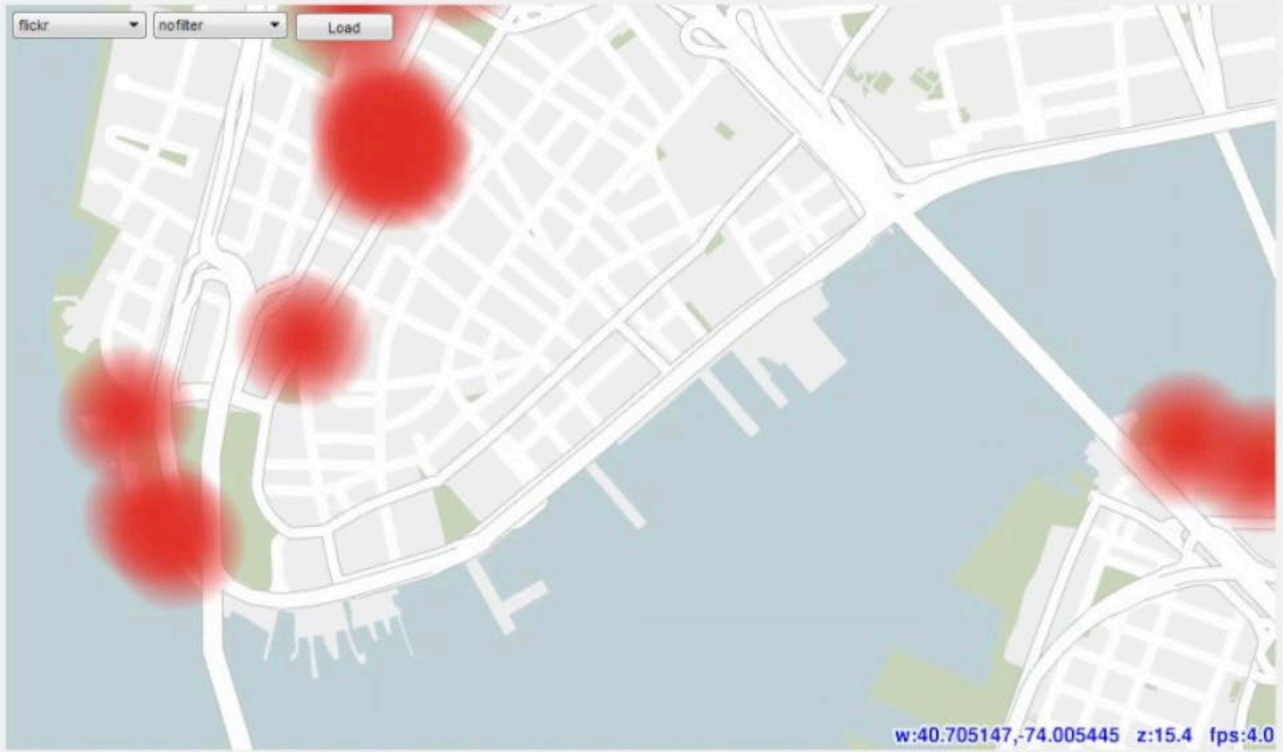
$$B_1, B_2, B_3, B_4, B_5, B_6, B_7, B_8, B_9$$



Signature

Data Oblivious

Rank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nofilter
Load
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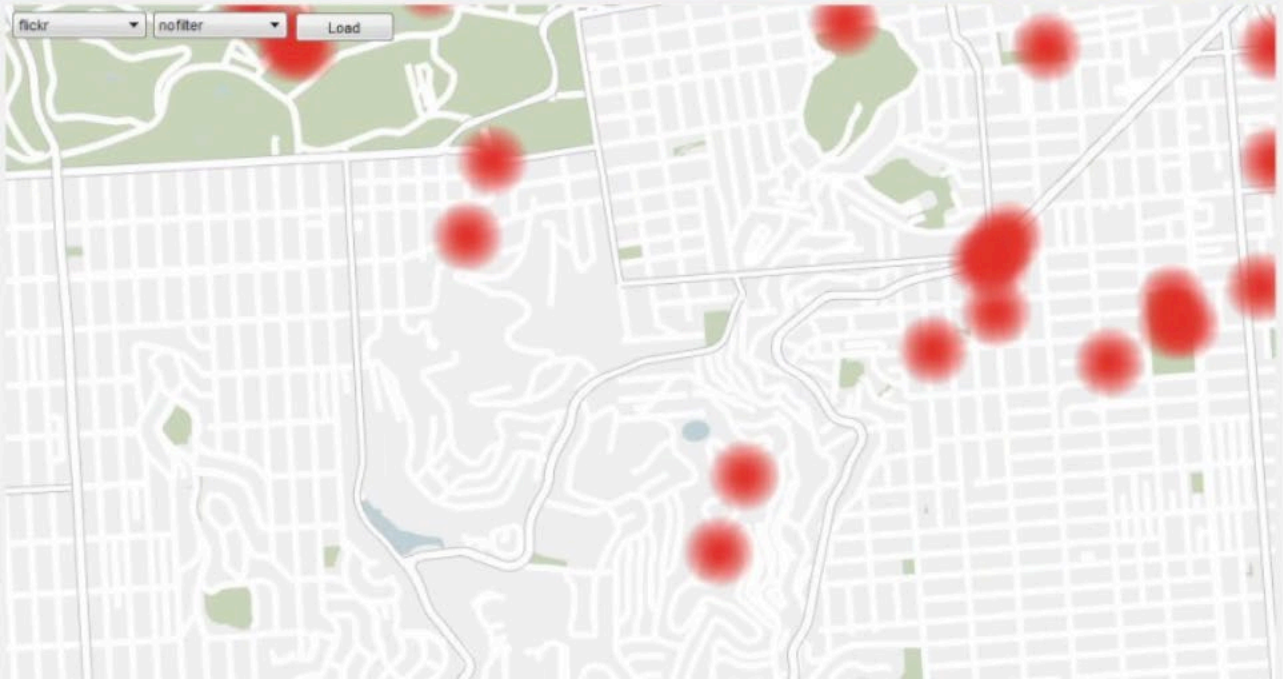
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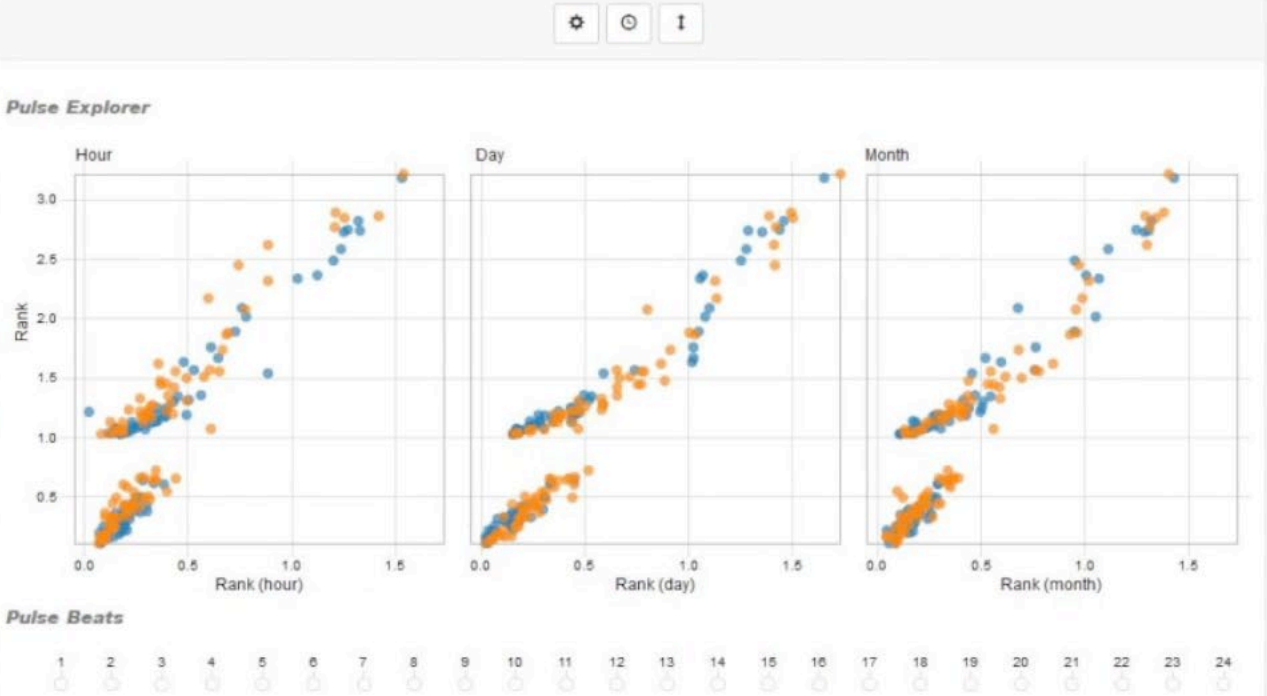

Pulse Explorer
Hour
Day
Month
Rank
Rank (hour)
Rank (day)
Rank (month)
Pulse Beats

Use cases

- Provided the interface to domain experts
- Architects from Kohn Pedersen Fox
  - Better understand design precedents
- Human behavioral expert
  - Try to understand the cohabitation between cultural communities
  - Twitter as proxy for cultural communities

Understanding Public Spaces

Rockefeller Center

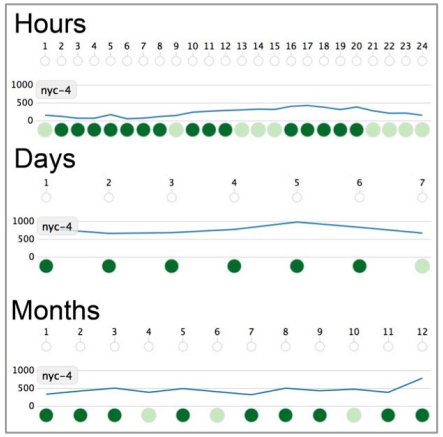
Union Square

Bryant Park

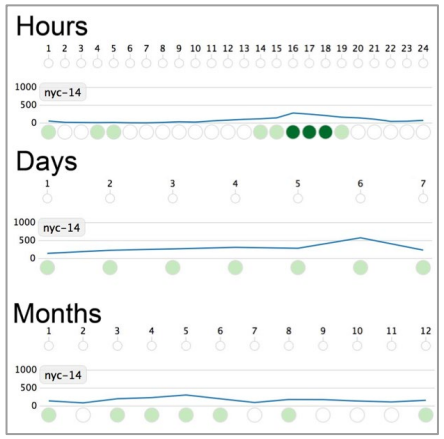
Typically classified together as being similar

Understanding public spaces

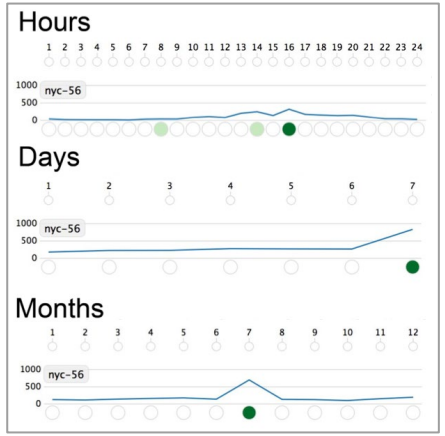
Rockefeller Center



Union Square

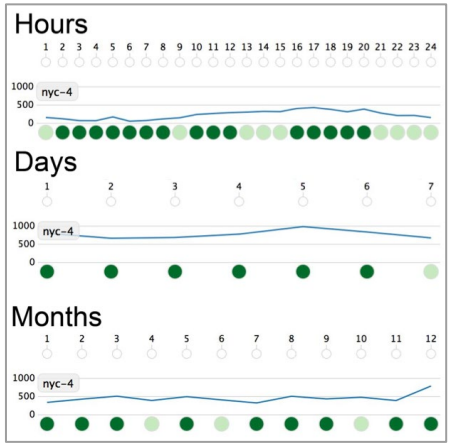


Bryant Park



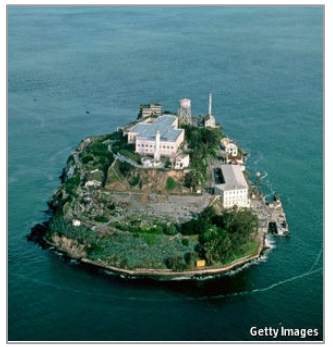
Understanding public spaces

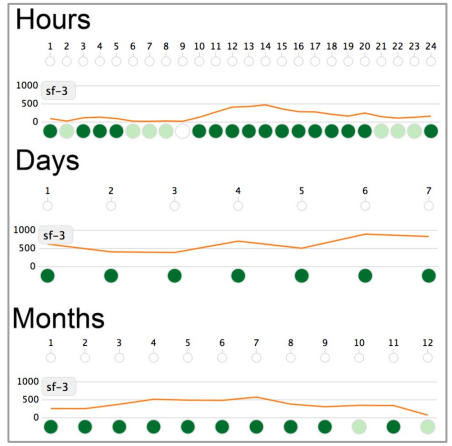
Rockefeller Center

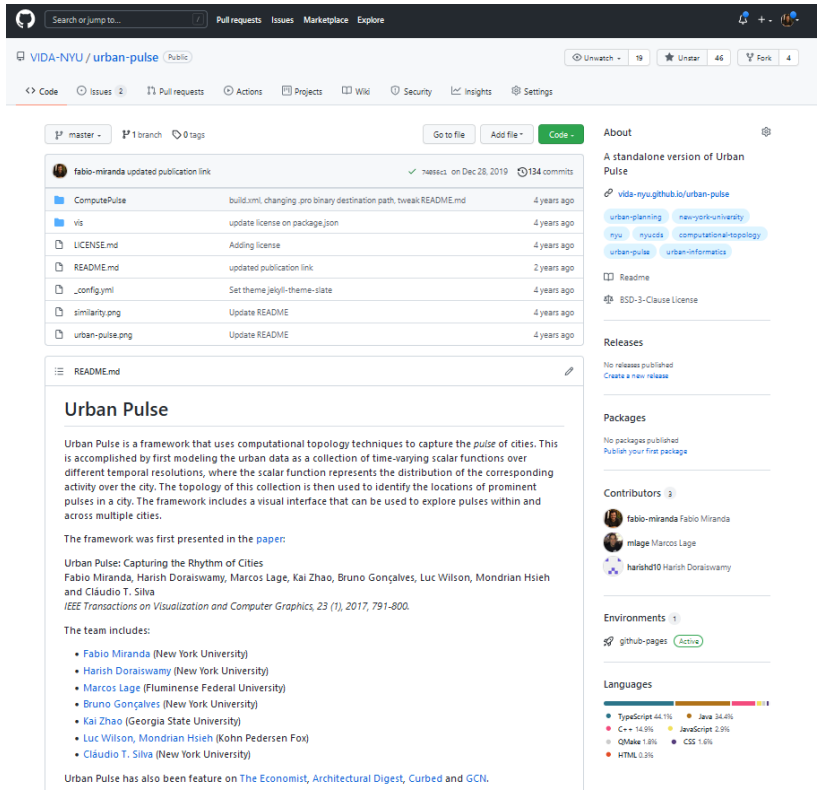


San Francisco

Alcatraz

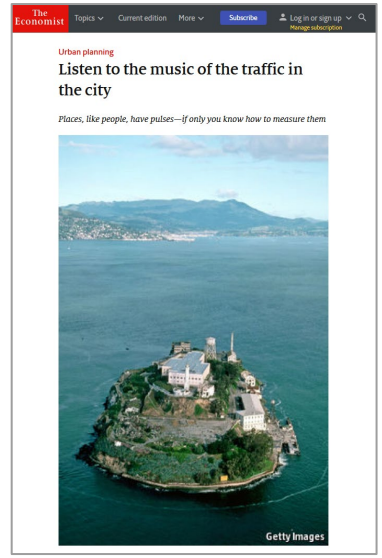






Curbed

Architectural Digest



The Economist

https://github.com/VIDA-NYU/urban-pulse

Topological data analysis

- Naturally captures interesting features.
- Features can have arbitrary shapes.
- Very efficient.
- Robust to noise.
- Works on data in any dimension.

Scikit-TDA

- Python libraries for topological data analysis.

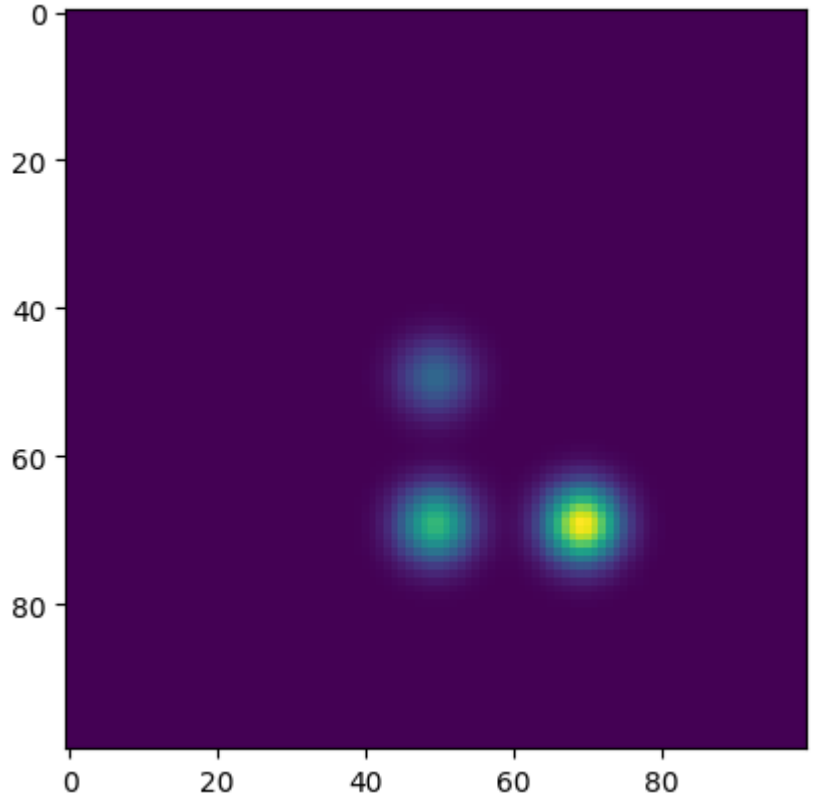
```
user@DESKTOP MINGW64 ~/
$ pip install scikit-tda
```

https://scikit-tda.org/

Scikit-TDA: synthetic data example

Creating 2D synthetic data:

```
ts = np.linspace(-1, 1, 100)
x1 = np.exp(-ts**2/(0.1**2))
ts -= 0.4
x2 = np.exp(-ts**2/(0.1**2))
scalar = x1[None, :]*x1[:, None] + 2*x1[None, :]*x2[
:, None] + 3*x2[None, :]*x2[:, None]
plt.imshow(scalar)
plt.show()
```

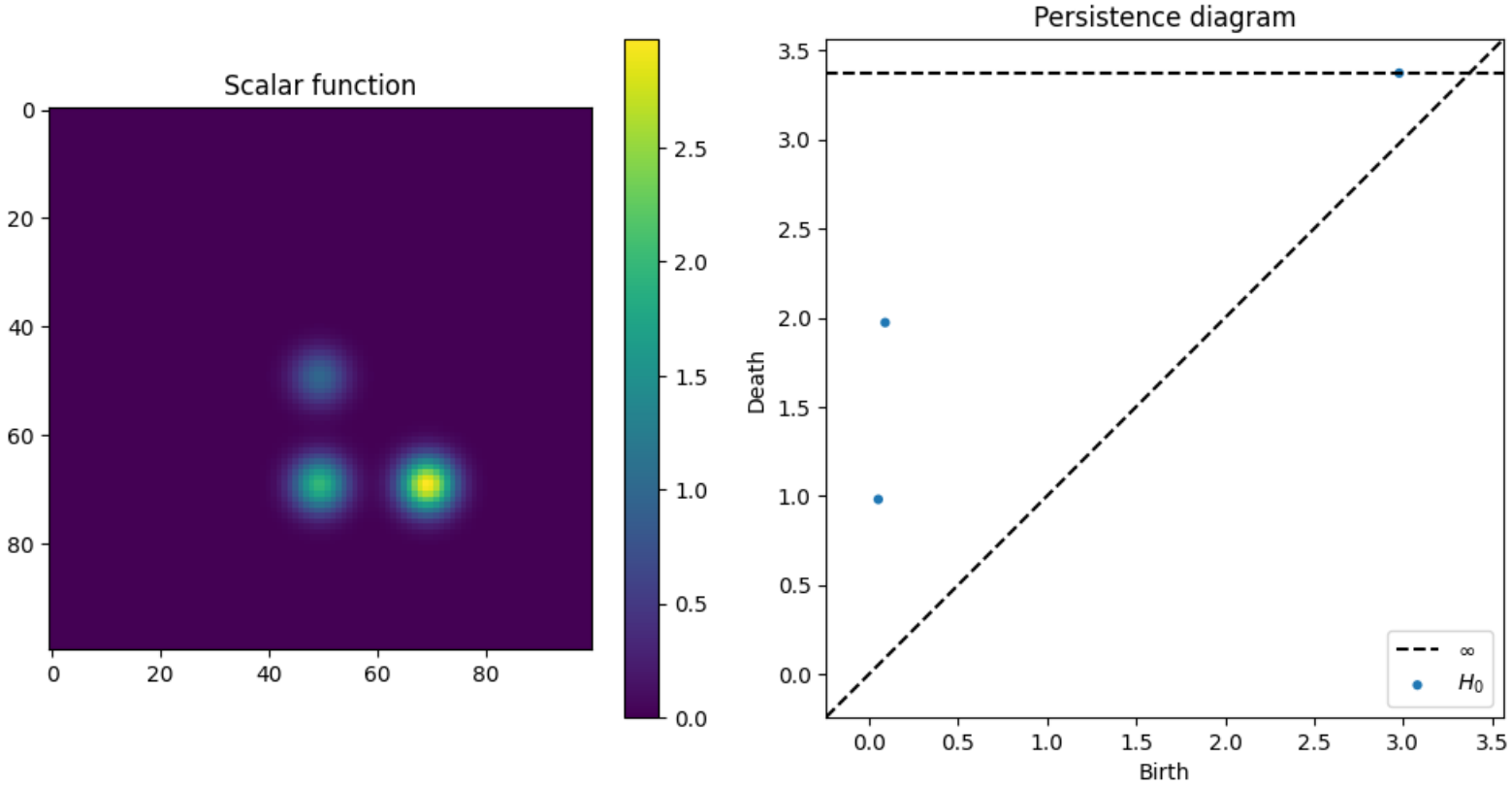


Scikit-TDA: synthetic data example

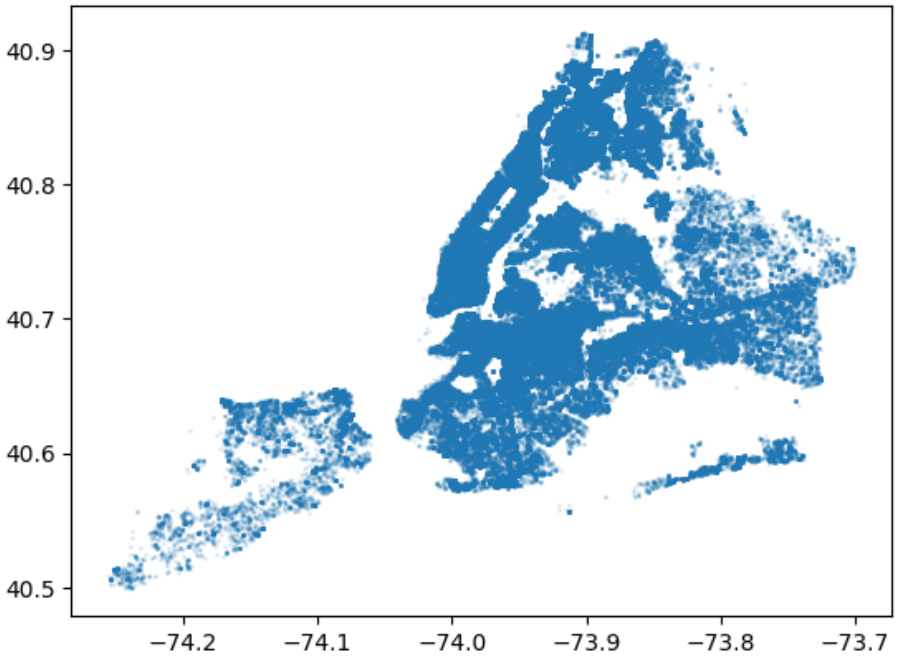
Computing persistence diagram:

```
dgm = lower_star_img(-scalar)
dgm[~np.isinf(dgm)] = -dgm[~np.isinf(dgm)]
dgm[~np.isinf(dgm).any(axis=1)] = np.flip(dgm[~np.isinf(dgm).any(axis=1)])

plt.figure(figsize=(10, 5))
plt.subplot(121)
plt.imshow(img)
plt.colorbar()
plt.title("Scalar function")
plt.subplot(122)
plot_diagrams(dgm)
plt.title("Persistence diagram")
plt.tight_layout()
plt.show()
```

Scikit-TDA: synthetic data example



Scikit-TDA: spatiotemporal data example



Spatiotemporal dataset with 311 noise complaints

Scikit-TDA: spatiotemporal data example

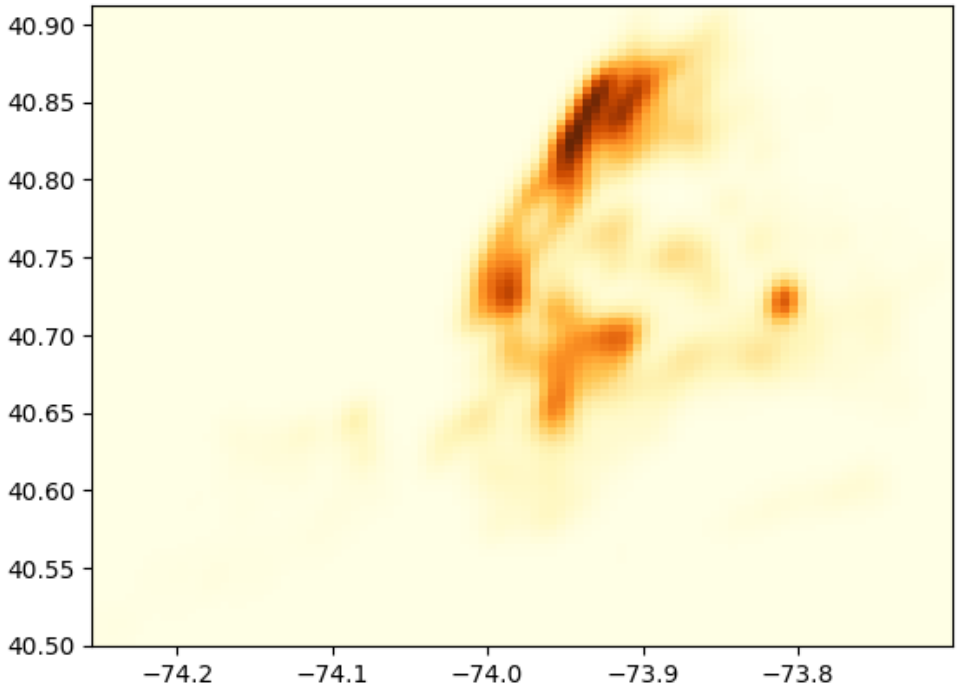
Creating 2D scalar function with KDE:

```
df = pd.read_pickle('data/311_2019.pkl.gz')

m1 = df[['latitude','longitude']].to_numpy()[:,1]
m2 = df[['latitude','longitude']].to_numpy()[:,0]
xmin = m1.min()
xmax = m1.max()
ymin = m2.min()
ymax = m2.max()

X, Y = np.mgrid[xmin:xmax:100j, ymin:ymax:100j]
positions = np.vstack([X.ravel(), Y.ravel()])
values = np.vstack([m1, m2])
kernel = stats.gaussian_kde(values)
Z = np.reshape(kernel(positions).T, X.shape)
```

Scikit-TDA: spatiotemporal data example

Plotting 2D scalar function:

```
fig, ax = plt.subplots()
ax.imshow(np.rot90(Z), cmap=plt.cm.YlOrBr, extent=[x
min, xmax, ymin, ymax])
ax.set_xlim([xmin, xmax])
ax.set_ylim([ymin, ymax])
plt.show()
```



Scikit-TDA: spatiotemporal data example

Computing persistence diagram:

```
dgm = lower_star_img(-Z)
dgm[~np.isinf(dgm)] = -dgm[~np.isinf(dgm)]
dgm[~np.isinf(dgm).any(axis=1)] = np.flip(dgm[~np.isinf(dgm).any(axis=1)])

plt.figure(figsize=(10, 5))
plt.subplot(121)
plt.imshow(np.rot90(Z), cmap=plt.cm.YlOrBr, extent=[xmin, xmax, ymin, ymax])
plt.colorbar()
plt.title("Scalar function")
plt.subplot(122)
plot_diagrams(dgm)
plt.title("Persistence diagram")
plt.tight_layout()
plt.show()
```

Scikit-TDA: spatiotemporal data example