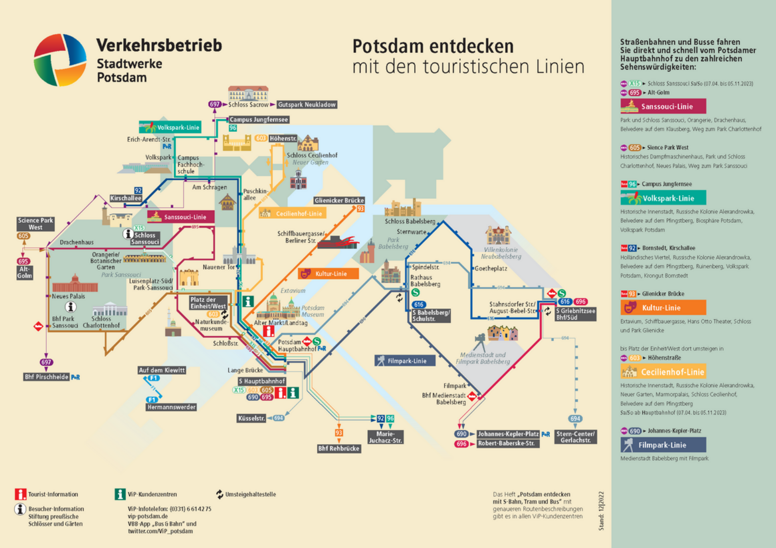


Source: `https://www.swp-potsdam.de/content/verkehr/bilder_6/liniennetz/touristischer_liniennetzplan_screenshot_1280_960.jpg`

Temporal Graphs

Daniel Cermann

January 28, 2025

Hasso Plattner Institute

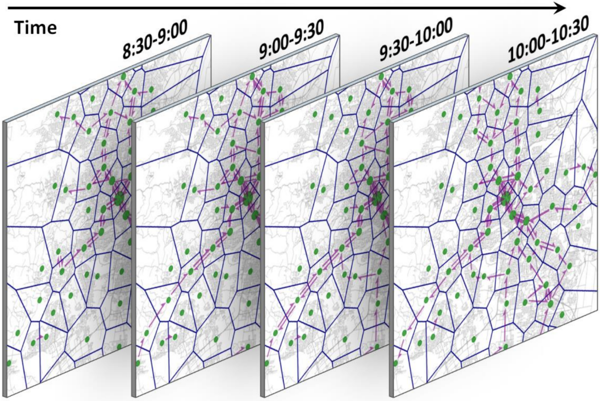
Motivation

Clip: School day

https://youtu.be/BSNJSUkc5-Q?t=996

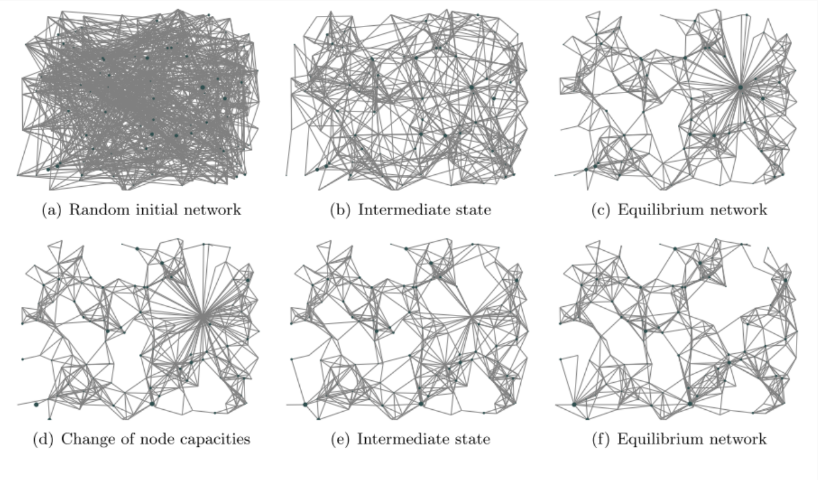
Google Maps

Figure 1: Illustration of a trajectory flow map, a dynamic graph of aggregated traffic flows constructed from trajectory data. The presented example is based on bus passenger trajectories obtained in Brisbane, Australia.



Source: `https://australasiantransportresearchforum.org.au/wp-content/uploads/2022/03/ATRF2016_paper_166.pdf`

Distributed systems



Source: `https://www.sg.ethz.ch/publications/2012/scholtes2012organic-design-of/`

Temporal graphs for physical/chemical models

DATA SCIENCE | May 9, 2023

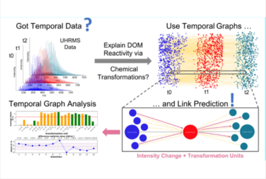
A Temporal Graph Model to Predict Chemical Transformations in Complex Dissolved Organic Matter

Philipp Plamper, Oliver J. Lechtenfeld*, Peter Herzsprung, and Anika Groß*

Open PDF   Supporting Information (1)   ACCESS

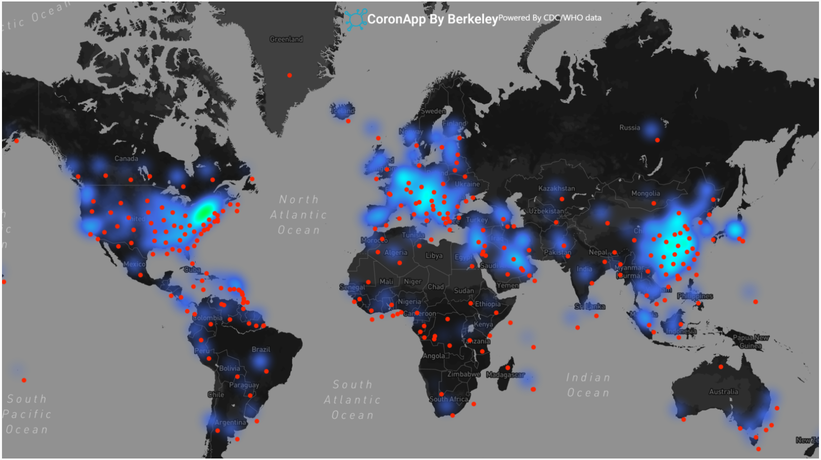
Abstract

Dissolved organic matter (DOM) is a complex mixture of thousands of natural molecules that undergo constant transformation in the environment, such as sunlight induced photochemical reactions. Despite molecular level resolution from ultrahigh resolution mass spectrometry (UHRMS), trends of mass peak intensities are currently the only way to follow photochemically induced molecular changes in DOM. Many real-world relationships and temporal processes can be intuitively modeled using graph data structures (networks). Graphs enhance the potential and value of AI applications by adding context and interconnections allowing the uncovering of hidden or unknown relationships in data sets. We use a temporal graph model and link prediction to identify transformations of DOM molecules in a photo-oxidation experiment. Our link prediction algorithm simultaneously considers educt removal and product formation for molecules linked by predefined transformation units (oxidation, decarboxylation, etc.). The transformations are further weighted by the extent of intensity change and clustered on the graph structure to identify groups of similar reactivity. The temporal graph is capable of identifying relevant molecules subject to similar reactions and enabling to study their time course. Our approach overcomes previous data evaluation limitations for mechanistic studies of DOM and leverages the potential of temporal graphs to study DOM reactivity by UHRMS.



Source: `https://pubs.acs.org/doi/full/10.1021/acs.est.3c00351`

Dissemination processes

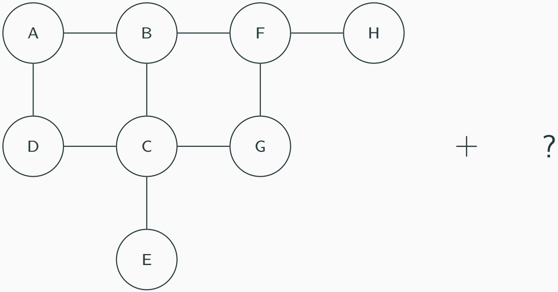


Source: `https://engineering.berkeley.edu/wp-content/uploads/2020/03/CoronApp.png`

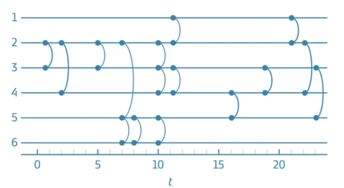
How to model temporal graphs

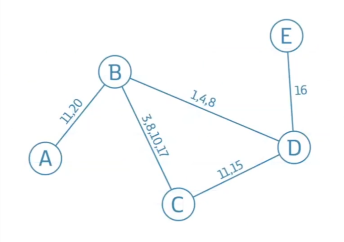
How to represent time in graphs?

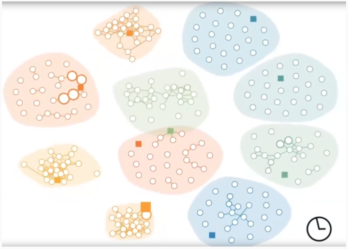
Brainstorm with your neighbor how time can be represented in graphs. Don't think of notation for now, just some visual ways to represent the additional dimension. ≈ 2 min

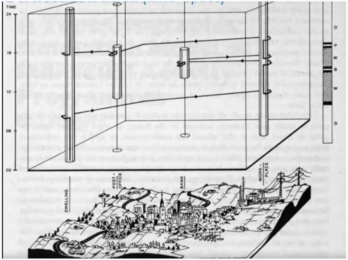


How to represent time in graphs?



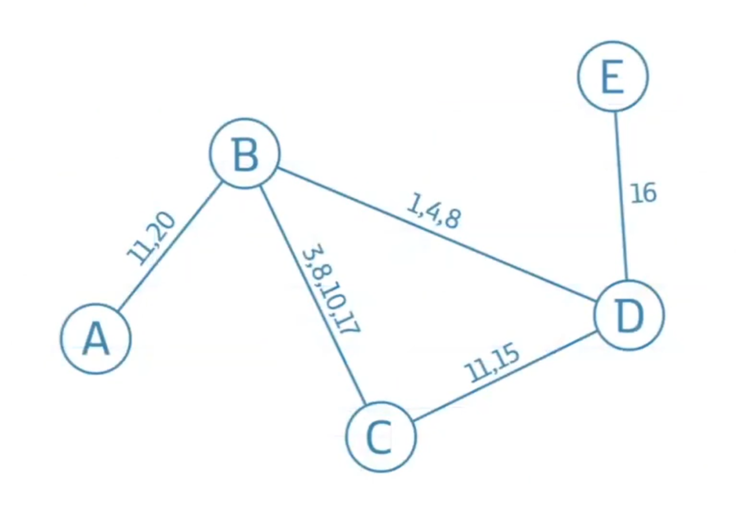






Source: `https://www.youtube.com/watch?v=BSNJSUkc5-Q`

How to model temporal graphs



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Definition labeled and temporal graphs

Definition

A **labeled graph** [1, page 94] is a triple $G = (V, E, \lambda)$ where:

- V, E is a graph
- $\lambda : V \cup E \rightarrow Z$ is a mapping of nodes and edges to a set of labels Z

Definition labeled and temporal graphs

Definition

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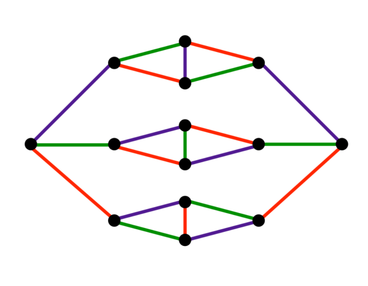
Definition

A **temporal graph** [4, page 243] is is triple $G = (V, E, \lambda)$ where:

- V, E is a graph
- $\lambda : E \to 2^{\mathbb{N}}$ is a mapping edges to a set natural numbers (time steps when this edge is active)

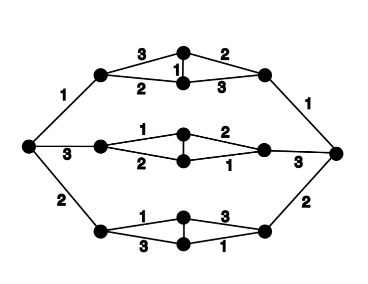
Relationship labeled and temporal graphs



[a]

[a] Source: `https://www.algorist.com/images/figures/edge-coloring-R.png`

$\leftrightarrow$



[a]

[a] Source: `me:)`

Exercise notation

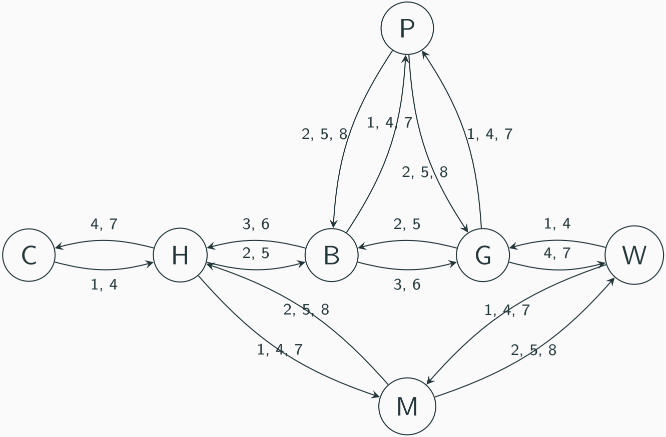
Given the following temporal graph definition $D = (V, E, \lambda)$ draw the visual representation of the temporal graph on the template in the handout! $\approx$ 2 min

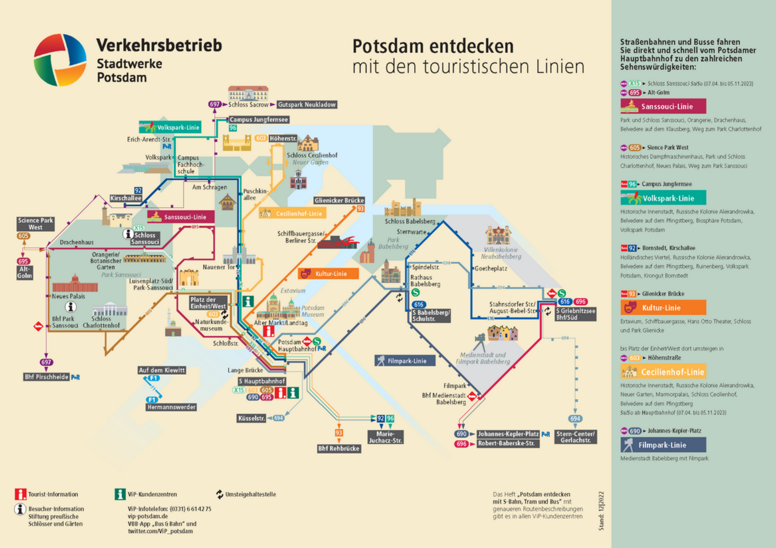
$$V = \{C, H, B, P, M, G, W\}$$

$$E = \{(C, H), (H, B), (B, G), (G, W), (W, P), (H, P), (B, M), (M, G)$$
$$(H, C), (B, H), (G, H), (W, G), (P, W), (P, H), (M, B), (G, M)\}$$

$$\lambda = \{$$
$$(C, H) \mapsto \{1, 4\},$$
$$(H, C) \mapsto \{4, 7\},$$
$$(H, B) \mapsto \{2, 5\},$$
$$(B, H) \mapsto \{3, 6\},$$
$$(B, G) \mapsto \{3, 6\},$$
$$(G, B) \mapsto \{2, 5\},$$
$$(G, W) \mapsto \{4, 7\},$$
$$(W, G) \mapsto \{1, 4\},$$
$$(H, M) \mapsto \{2, 5\},$$
$$(M, H) \mapsto \{3, 6\},$$
$$(M, W) \mapsto \{3, 6\}$$
$$(W, M) \mapsto \{2, 5\}$$
$$(B, P) \mapsto \{1, 4, 7\}$$
$$(P, B) \mapsto \{2, 5, 8\}$$
$$(G, P) \mapsto \{2, 5, 8\}$$
$$(P, G) \mapsto \{1, 4, 7\}$$
$$\}$$

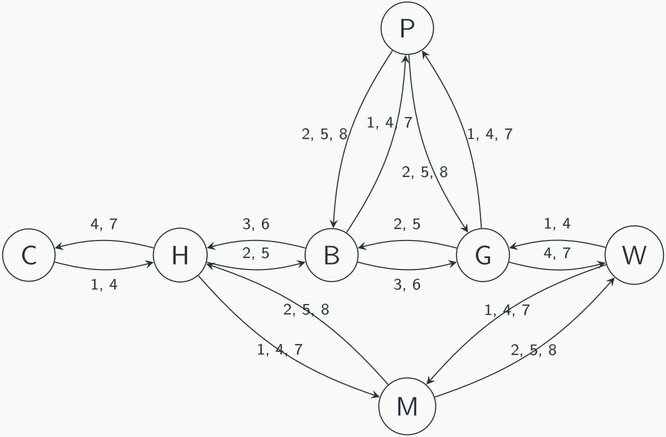
Solution





Source: `https://www.swp-potsdam.de/content/verkehr/bilder_6/liniennetz/touristischer_liniennetzplan_screenshot_1280_960.jpg`

Solution



Notation for convenience $\rightarrow$ [4, p. 243ff]

- $\lambda(G)$ - temporal graph with respect to G
- $\lambda(E)$ - multiset of all labels
- $|\lambda| = \sum_{e \in E} |\lambda(e)|$
- $\lambda_{min} = min\{l \in \lambda(E)\}$
- $\lambda_{max} = max\{l \in \lambda(E)\}$
- $\alpha(\lambda) = \lambda_{max} - \lambda_{min} + 1$ - lifetime of a temporal graph $\lambda(G)$

Transitivity of reachability in static graphs

Reachability in a static graph is transitive

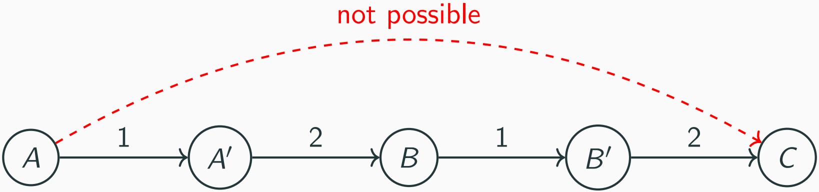
Given A static graph $G = (V, E)$, for all nodes $A, B, C \in V$ we have: If B is reachable by A and C is reachable by B, then C is reachable by A.

$$A \longrightarrow B \longrightarrow C$$

Transitivity of reachability in static graphs

Is reachability in a temporal graph transitive?

Time matters!

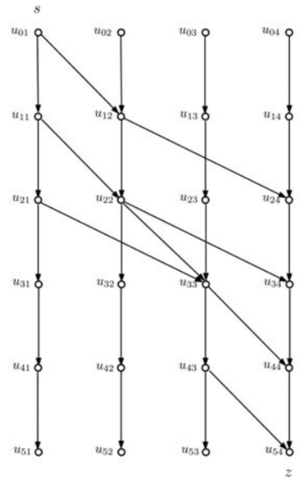


$\Longrightarrow$ Deep implications for complexity of temporal graphs

Notation #2

- A temporal graph D is an ordered set of disjoint sets (V, A)
- $A \subseteq V^2 \times \mathbb{N}$ - 'time edges'
- $A(t) = \{e|(e, t) \in A\}$ - set of edges at time t
- $D(t) = (V, A(t))$ - snapshot of graph D at time t

Static expansion of a temporal graph



(a)

[4, page 318]

Static expansion of a temporal graph

Definition: static expansion of a graph

The static expansion of a temporal graph $D = (V, A)$ with $V = \{u_1, u_2, ..., u_n\}$ is a DAG $H = (S, E)$ with:

$$S = \{u_{ij} | \lambda_{min} - 1 \leq i \leq \lambda_{max}, 1 \leq j \leq n\}$$

and

$$E = \{(u_{(i-1)j}, u_{ij'}) | \lambda_{min} \leq i \leq \lambda_{max} \wedge$$

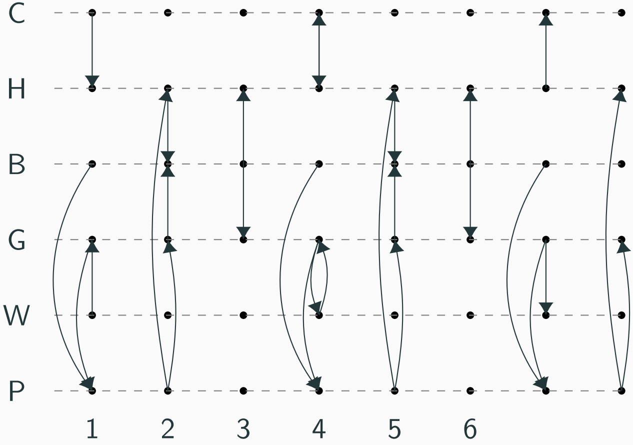
$$1 \leq j, j' \leq n \wedge (j = j' \vee (u_j, u_{j'}) \in A(i))\}$$

Exercise: Static expansion of a temporal graph

Turn the Potsdam-Map temporal graph into its static expansion using the template given on the handout (we leave out M(edienstadt Babelsberg) for simplicity sake here) !

$\approx$ 3 min

Solution: Static expansion of a temporal graph



Repetition - walks and paths in static graphs

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- A **walk** is a finite or infinite sequence of edges which joins a sequence of vertices.

Repetition - walks and paths in static graphs

- A **walk** is a finite or infinite sequence of edges which joins a sequence of vertices.
- A **path** is a walk where all vertices are distinct.

Definition: temporal/time respecting walk

A **temporal** or **time-respecting walk** W of a temporal graph $D = (V, A)$ is an alternating sequence of of nodes and times $(u_1, t_1, u_2, t_2, ..., u_{k-1}, t_{k-1}, u_k)$ where

- $\forall 1 \leq i \leq k-1 : ((u_i, u_{i+1}), t_i) \in A$ and
- $1 \leq i \leq k-2 : t_i < t_{i+1}$

- t_1 - departure time
- t_{k-1} arrival time
- $t_{k-1} - t_1 + 1$ - duration/temporal length

Definition: Journey

A **journey** is a is a temporal walk with pairwise distinct nodes $\hat{=}$ a journey of D is a path of the underlying static graph of D that uses strictly increasing edge-labels.

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Definition: Foremost Journey

A u-v journey J is called foremost from time $t \in \mathbb{N}$ if it departs after time t and its arrival time is minimized.

Definition: Temporal distance

The **temporal distance** from a node u to at time t to a node v is defined as the duration of a foremost journey from u to v that departs at time t.

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Definition: Temporal diameter d

The minimum integer d such that there exists a foremost journey from every node $(u, t) \in V \times \{0, 1, ..., \alpha - d\}$ to every node $v \in V$ with duration at most d.

Computing foremost journeys - Problem formulation

Given a source node $s \in V$ and a start time t_{start} compute the foremost $s - w$ journey for all $w \in V \backslash \{s\}$

Sidenote - offline vs. online algorithms

offline algorithms

takes whole temporal graph D as input

online algorithms

temporal graph is revealed to algorithm over time

Source: `https://encrypted-tbn0.gstatic.com/images?q=tbn:ANd9GcQbpwyZnBM48yDEHLT9Sww1J8AJrgs4lj-VLi2EkxpIoKMeI6-stF-R9uAsLl5K4gXFBts&usqp=CAU`

Computing foremost journeys - Algorithm

Algorithm 1: Computing earliest-arrival time

Input : A temporal graph $G = (V, E)$ in its edge stream representation, source vertex x, time interval $[t_\alpha, t_\omega]$

Output : The earliest-arrival time from x to every vertex $v \in V$ within $[t_\alpha, t_\omega]$

1 Initialize $t[x] = t_\alpha$, and $t[v] = \infty$ for all $v \in V \setminus \{x\}$;

2 **foreach** *incoming edge* $e = (u, v, t, \lambda)$ *in the edge stream* **do**

3   **if** $t + \lambda \leq t_\omega$ *and* $t \geq t[u]$ **then**

4   **if** $t + \lambda < t[v]$ **then**

5             $t[v] \leftarrow t + \lambda$;

6   **else if** $t \geq t_\omega$ **then**

7   Break the for-loop and go to Line 8;

8 **return** $t[v]$ for each $v \in V$;

[5, page 724]

Computing foremost journeys - Proof of correctness

Computing foremost journeys - Running time

Reachability

Definition: Reachability

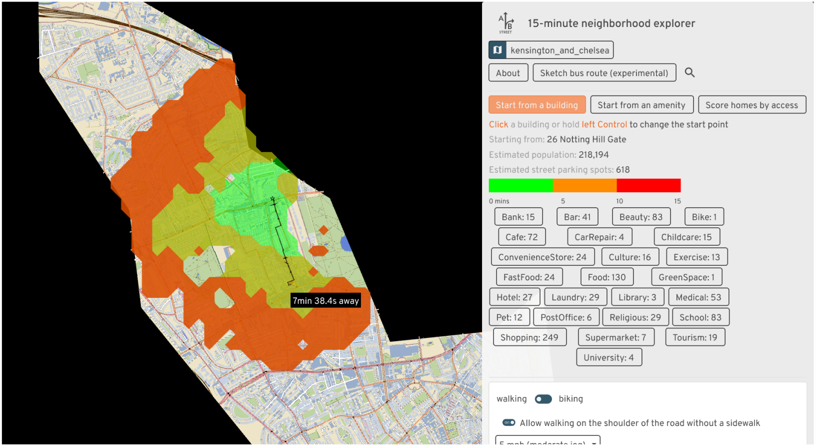
A vertex v is **reachable** from a vertex u at time t if there exists a foremost journey from u to v that departs at time t.

The government has been lying to us

Figure 2: You-are-here-maps are wrong!

Source: `https://commons.wikimedia.org/wiki/File:Notting_Hill_Royal_Borough_Of_K%26C_Council_Map_Outlining_the_Official_Area_of_Notting_Hill_and_the_Surrounding_Areas_2018.jpg`

15 min walk



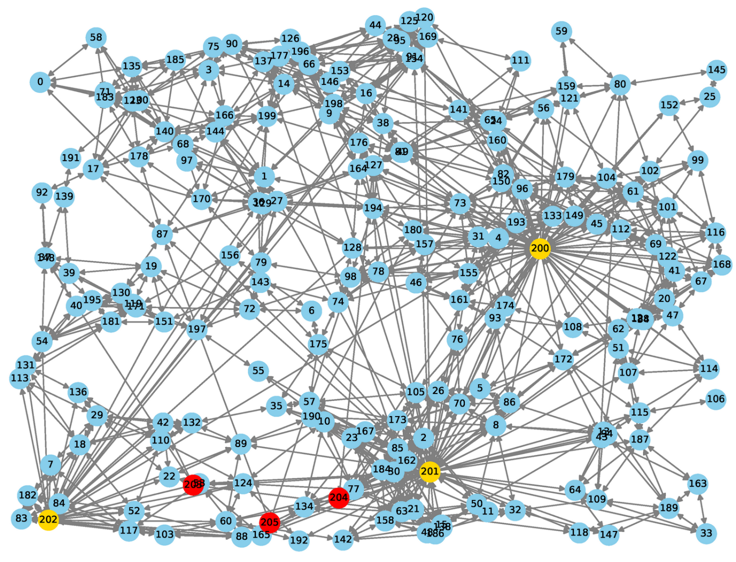
Source: `https://play.abstreet.org/0.3.49/fifteen_min.html`

Temporal graphs for modeling dissemination processes

A natural application domain of temporal graphs is that of *gossiping*

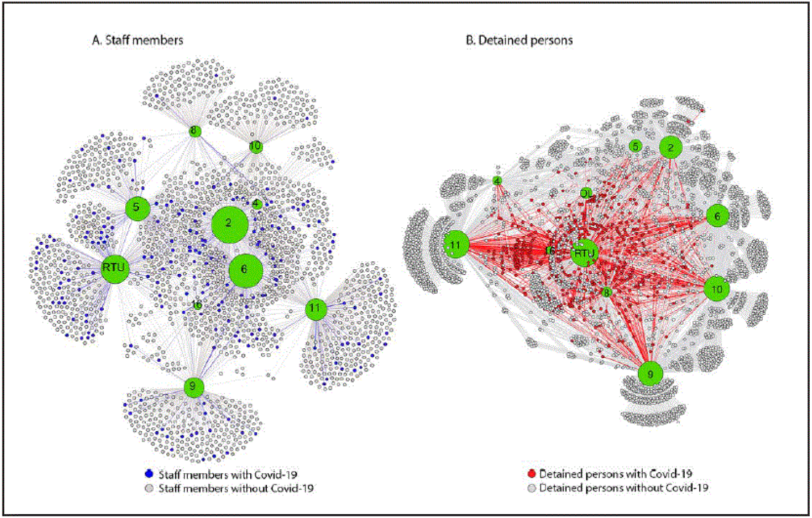
~ [4]

What are dissemination processes?



[3]

What are dissemination processes?



Source: `https://www.cdc.gov/mmwr/volumes/69/wr/figures/mm6944a3-F1.gif?_=06726`

Vaccination Problem

Definition: The vaccination problem involves optimizing the allocation and timing of vaccines to control the spread of infectious diseases.

Key Questions:

- Who should be vaccinated first?
- How can we minimize the spread of the disease?
- What role does timing play in vaccination strategies?

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Herd immunity

Herd immunity occurs when a large enough fraction f of a community is immune to a disease, thus limiting its ability to spread.

$\Rightarrow$ lower f by vaccinating people in risk

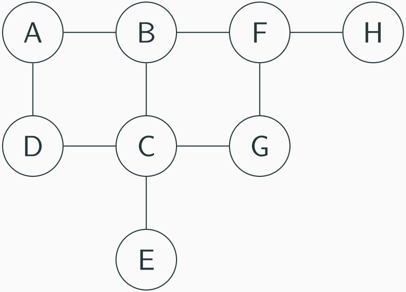
Vaccination Problem - technical problem statement

How can we optimally chooose a fraction f of a population to vaccinate using only local information?

Vaccination Problem on static graphs

Neighbourhood Vacination protocol

choose a person at random among all persons that have been involved in at least one contact at time t*, ask her to name someone she met, vaccinate this other person, and repeat until a desired fraction of the vertices are vaccinated



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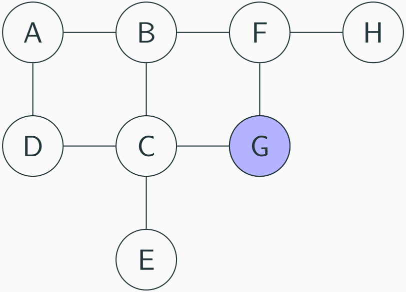

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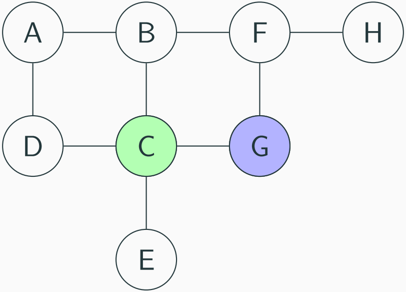

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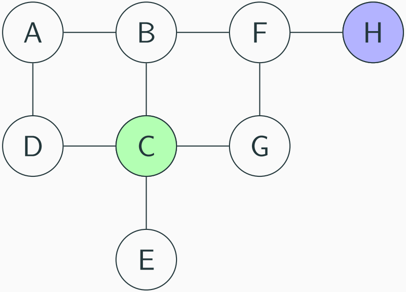

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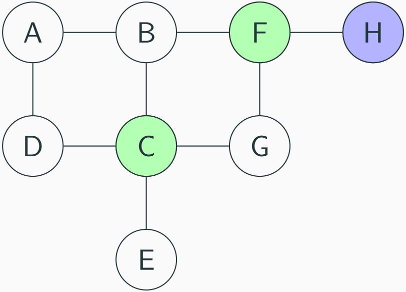

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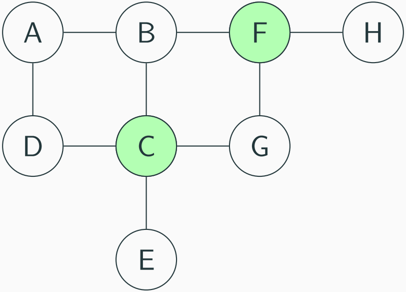

Modelling dissemination processes

- Nodes represent individuals/groups/organizations
- Edges represent interactions
- Time labels represent the time of interaction

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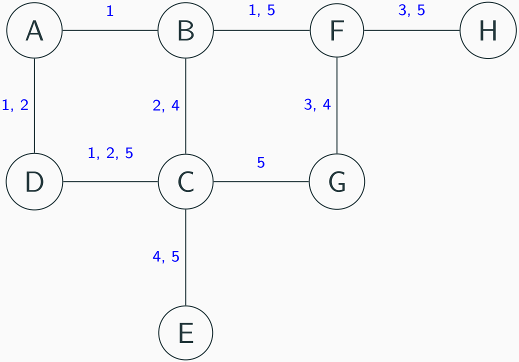
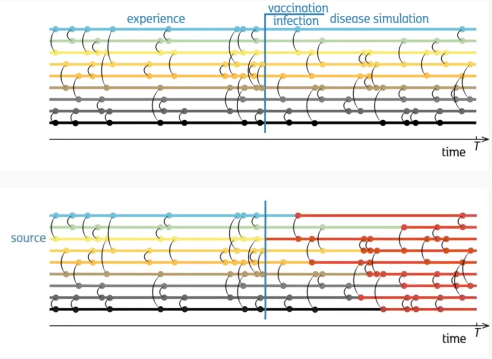


The infection process



[2]

Protocols for vaccination in temporal graphs

Brainstorm protocols that could be used to vaccinate individuals in a temporal graph.
Use the neighbourhood vaccination protocol from static graphs as inspiration.

4 min

Protocols for vaccination in temporal graphs

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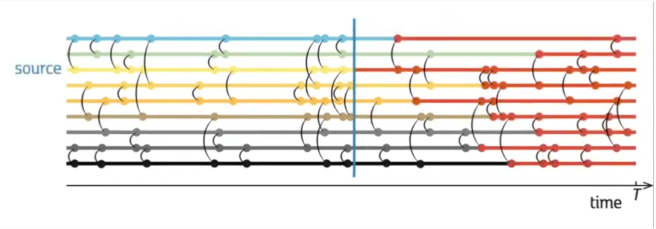


4 min

Protocols for vaccination in temporal graphs

Recent protocol

iteratively ask a random individual I to name the most recent contact and vaccinated this person

Weight protocol

iteratively asked a random individual I to name its most frequent contact since some time t in the past

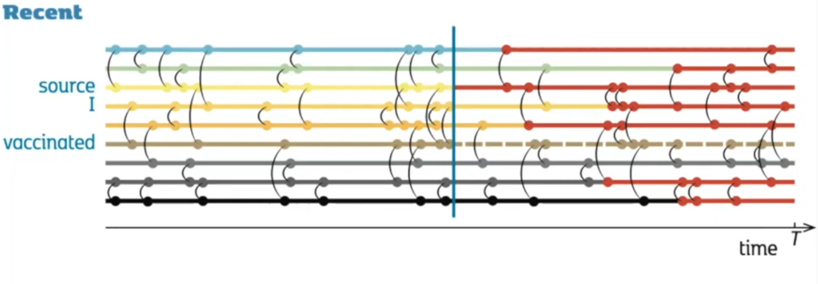
Protocols for vaccination in temporal graphs

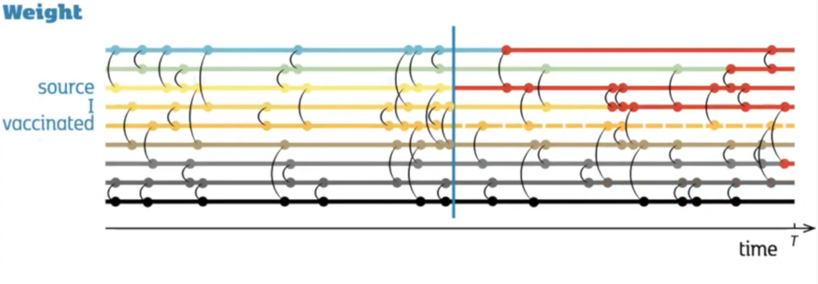
Recent protocol
iteratively ask a random individual I to name the most recent contact and vaccinated this person

Weight protocol
iteratively asked a random individual I to name its most frequent contact since some time t in the past

Apply those two protocols to the given temporal graphs on your handout. Then, discuss how the performance of the protocols might scale in real-world data (e.g. contacts in hospital, on a dating website, ...). *6min*

Solution


Recent
source
I
vaccinated
time
T


Weight
source
I
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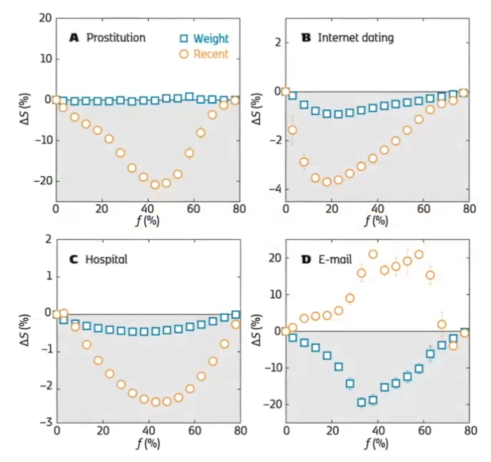
Performance on bigger datasets



[2]

Teasers

Centrality of nodes in a temporal graph

Temporal Graph Neural Networks

Sources i

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