

## Mathematics for Cybersecurity

April 26, 2025 Metro NY MAA Section Meeting

> **Emilie Purvine** Chief Data Scientist

...and a ton of collaborators!



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## **Plan of the talk**

- My path to a nonacademic career
- Cybersecurity 101 (accelerated version!)
- Graphs and hypergraphs via network flow
- Topology via high-dimensional data



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## My path to PNNL



- My path was quite linear. Perhaps too linear...
- Undergrad @ University of Wisconsin
  - Math education  $\rightarrow$  Math
  - Summer math programs for women
  - Study abroad in math program
  - Undergrad research
  - Internship with small gov't contractor
- Grad @ Rutgers
  - Planned to NOT work in academia after graduation
  - Pure math, not applied. That was a choice.
  - Fellowship with DHS → internships at PNNL
- Postdoc @ PNNL started summer 2011







Center for Discrete Mathematics and Theoretical Computer Science Founded as a National Science Foundation Science and Technology Center





## Paul Heideman and I doing undergrad research at UW







## DOE's 17 national laboratories tackle critical scientific challenges





PNNL is advancing scientific frontiers and providing solutions to critical national needs





## **Scientific Discovery** DATA SCIENCE

- Join extreme scale computing and big data
- Deliver advanced visualization technologies and novel algorithms
- Apply artificial intelligence and machine learning to complex computational problems



Search for internship and career opportunities at https://careers.pnnl.gov/



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## Internet of things – how many do you have?





## Where can defenders "see"?





## Pacific Internet communication – behind the scenes Northwest 142.251.33.110 would like to see google.com → C ☆ https://www.google.com I acknowledge your request and will send when you are ready I am ready to receive! Here is the content IP 142.251.33.110 First your browser must find the IP address for google.com via a DNS server Google.com please Then your browser establishes a connection with Flow record the google.com server via a TCP 3-way handshake Source IP Source Port. Each message is broken up into potentially multiple Destination IP packets and reassembled at the destination Destination Port DNS Server Packet count Packets can be aggregated into conversations Byte count called flow (e.g., IPFlow, NetFlow) DATA!! Start time End time









## Aligning data with the cyber kill chain

A Advanced Stealthy, **Sophisticated**  Ρ Persistent Continual, Relentless

T Threat Person(s) with intent and know-how



- The Cyber Kill Chain<sup>®</sup> lays out the steps that an adversary goes through to compromise a system and get what they are looking for
  - This helps us organize how we think about detection – the earlier the better!
- How can we protect our networks?
  - Inspect the data we have to discover:
    - ✓ Known patterns of bad behavior
    - ✓ Unknown anomalies
  - Build in resilience

https://www.lockheedmartin.com/en-us/capabilities/cyber/cyber-kill-chain.html



## **Challenges in Cyber Defense**

- Cyber systems do not have "laws of physics" type rules. Every rule or standard can be broken.
  - They can be broken by benign people that do not realize there is a rule, or by sophisticated adversaries.
- Adversaries are finding and exploiting vulnerabilities faster than defenders can identify them
- Signature-based alerts are still necessary, but threat hunting and anomaly detection are finding traction
  - Caution: An anomaly on one network is perfectly normal on another (e.g., off site backup vs. data exfiltration)







## "OODA loop" – where can mathematicians fit?





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## **Application #1: Host and network data**

time	action- object	host	principal	pid	source IP	dest IP	dest port	protocol	image path
9/24 10:45:00	MESSAGE- FLOW	SysClient0501	bantonio	2192	10.20.5.191	10.20.2.66	5999	UDP	python.exe
9/24 10:45:02	START-FLOW	SysClient0501	bantonio	836	132.197.158.98	202.6.172.98	80	ТСР	powershell.exe
9/24 10:45:25	MESSAGE- FLOW	SysClient0501	bantonio	5100	142.20.57.246	142.20.61.132	80	ТСР	outlook.exe
9/24 10:45:29	START-FLOW	SysClient0501	bantonio	648	142.20.57.246	202.6.172.98	443	TCP	powershell.exe

- Snapshot of data from Operationally Transparent Cyber (OpTC) data set which includes both *host* and *network* events
  - Network data: communications between computers (recorded as "IP addresses"). Records the two computers and metadata about the connection. (See table above.)
  - Host data: processes occurring on individual computers.
- **Questions:** What connection patterns exist? How do they change over time? Can we find unusual patterns or connections? What do they mean?





## **Mathematical model for communications:** Graph

- **Graphs** provide a mathematical model of data focused on 2-way relationships
  - To ask certain kinds of questions ✓Connectivity of entities
    - ✓ Clustering structure
  - To model certain kinds of interactions
    - ✓ Pairwise relationships

$$G = (V, E), E \subseteq \binom{V}{2}$$

- Network flow graph:
  - $\checkmark$  V = IP addresses / hosts
  - $\checkmark$  E = communications

Data from http://csr.lanl.gov/data/cyber1/

2 minutes of flow in LANL system: |V|=842, |E|=1038









## Network science: methods to study structure of graphs from real data

## **Graph properties**

- Degree (distribution)
- Walk, Path, Diameter
- Connected components
- Centrality
- Clustering coefficient
- Triangle counting









## Network science: methods to study structure of graphs from real data

## **Graph properties**

- Degree (distribution)
- Walk, Path, Diameter
- Connected components
- Centrality measured for each vertex
  - Betweenness: measure of belonging to shortest paths
  - Closeness: measure of average distance to other vertices
  - Eigenvector: Solution to  $Ax = \lambda x$
  - Degree: degree of vertex
  - Harmonic: measure of average distance, ok with disconnected graph
  - Katz: related to number of reachable vertices from, with farther vertices penalized





















By Tapiocozzo - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=3906483



## Network science: methods to study structure of graphs from real data

## **Graph properties**

- Degree (distribution)
- Walk, Path, Diameter
- Connected components
- Centrality
- Clustering coefficient
- Triangle counting



**Recall our questions:** What connection patterns exist? How do they change over time? Can we find unusual patterns or connections? What do they mean?

\* Number of edges, density, average distance, random graph models, link prediction





## **Generative graph models – what and why**

- What are they?
  - Models that create graphs possessing properties we are interested in
- What are they good for?
  - Null model for algorithm testing and experiments
  - Create synthetic graphs on different scales
  - Create surrogate graph to protect anonymity of data
  - Graph generation process may give insight into properties being matched
- What makes them good?
  - Inputs are compact & few
  - Easily measured from real data or generated artificially
  - Generalized and formalized generation process
  - Avoid ad hoc methods/restrictive assumptions on inputs







## **Classic simple generative models**

## **Erdős-Rényi**

- Matches: average degree / density
- **Inputs:** number of vertices (n), edge probability (p)

$$u$$
 ?  $v$  All edges  
 $P(u,v) = p$  independent

## Connected if $p > \log(n)/n$





## Alfred Rényi

## **Chung-Lu** • **Inputs:** degree sequence $\{d_i\}$ where

- Matches: degree distribution
- $d_i$  is desired degree of  $v_i$



## • Typically small-world



Fan Chung



Linyuan Lu<sup>23</sup>



## **Dynamic graphs – background**

- **Graph:** G = (V, E) with vertices V and edges E • **Dynamic graph:**  $\{G_t\}_{t\in T}$  where  $G_t = (V_t, E_t)$  is a graph and T is a set of times
- Dynamic graph considered as a 3-tensor with dimensions  $T \times V \times V$ 
  - Entry at index (t, v, w) if  $(v, w) \in E_t$
- (Static) Random graph models often used as null models Erdos-Renyi, Chung-Lu, other specialized models
- Random *dynamic* graphs:
  - Dynamic Erdos-Renyi <sup>1</sup> missing edges appear with probability α, existing edges disappear with probability β
  - Dynamic Chung-Lu<sup>1</sup> Poisson process, edges added at rate λ, removed at rate μ
  - Dynamic block model <sup>1</sup> Poisson process, rate of addition and removal of edges depends on group membership
  - Additional survey of methods <sup>2</sup>

1 Xiao Zhang, Cristopher Moore, and Mark EJ Newman. "Random graph models for dynamic networks." The European Physical Journal B 90.10 (2017): 200. 2 Holme, Petter, and Jari Saramäki. "Temporal networks." Physics reports 519.3 (2012): 97-125.





## Hagberg-Lemons-Misra (HLM)<sup>3</sup> **Model**

<sup>3</sup>A. Hagberg, N. Lemons, and S. Misra, Temporal reachability in dynamic networks, in Dynamic Networks and Cyber-Security, WORLD SCIENTIFIC (EUROPE), Mar 2016, pp. 181-208.

Desired degree sequence:  $w_1, w_2, \ldots, w_n$  $G_1$  is Chung-Lu graph with this deg. sequence

Parameter  $\alpha \in [0, 1]$  controls extent to which  $G_{i+1}$  depends on  $G_i$ 

- HLM was created to mimic network traffic
- Each  $G_i$  is Chung-Lu •
- over time.



## Cannot capture density changes

Note: can generalize to arbitrary edge probability matrix P and alphas for each edge



## **Temporal HLM = THeLMa** Model

Desired degree sequence:  $w_1, w_2, \ldots, w_n$ Temporal parameter:  $\tau_1, \tau_2, \ldots, \tau_n$  $G_1$  is Chung-Lu graph with this deg. sequence times  $\tau_1$ 

THeLMa: Include density parameter in evolution

of presence of  $\tau$  parameters

Parameter  $\alpha \in [0, 1]$  controls extent to which  $G_{i+1}$  depends on  $G_i$ Pairs (u, v) in M with prob.  $\alpha$  $w_u w_v$  $\tau_{i+1}$  $w_u w_v$ Joint with Sinan Aksoy, Helen Jenne, Stephen Young

# G<sub>i</sub> no longer Chung-Lu because





## THeLMa as a flexible network baseline model

- Assumption: anomalies are sparse in network data
- *Measure* simple parameters from observed data
  - Average degree sequence across time = average degree for each vertex
  - $\tau$  = Number of edges for each time step
  - $\alpha$ ... it's not so simple, but it's possible (MLE estimator) [paper in progress]
- Generate a THeLMa sequence using the measured parameters
- Use the generated dynamic graph as a baseline for:
  - Anomaly detection
  - Background identification/subtraction
  - Anomaly injection for algorithm testing



## **Case study: synthetic LANL data**

Two days of network flow<sup>4</sup> in 3-minute time windows



<sup>4</sup> <u>https://csr.lanl.gov/data/cyber1/</u>

Pacific

Northwest

NATIONAL LABORATOR



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## Graph structure is only part of the story...

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9/24 10:45:29	START-FLOW	SysClient0501	bantonio	648	142.20.57.246	202.6.172.98	443	TCP	powershell.exe

- Network flow has so much more information than just pairs of IPs!
  - Ports can be surrogates for type of communication
  - Protocols dictate the format of communication
  - Host, principal (not always present in network flow) indicate who on the computer is connected to the communication
  - Image path and PID (also not always present) tie the communication to a specific process
- How do we incorporate this information in a structural way?





## Mathematical model for group relationships: Hypergraph

- Hypergraphs provide a mathematical model of data focused on multi-way relationships
  - To ask certain kinds of questions
    - ✓ Connectivity of entities
    - ✓ Clustering structure
  - To model certain kinds of interactions ✓ Multi-way relationships
    - $H = (V, E), E \subseteq 2^V$
  - Cyber hypergraph:
    - $\checkmark$  Vertices = IPs, ports, users, executables, ...
    - $\checkmark$  Hyperedges = "behaviors"



"Vertex"

IF.Com



IPs (vertices) grouped into website domains (hyperedges)



## What kind of data generate Hypergraphs?

Imagine your tabular data:

• Attributes: Entities (rows) are indicated as having specific attributes or properties (columns)

	svchost.exe	powershell.exe	lsass.exe	firefox.exe
Host01	0	1	0	0
Host02	0	0	1	1
Host03	1	1	1	1
Host04	0	0	1	0
Host05	1	0	1	1

- Joint relationships: Entities jointly participate in some relationship or activity
- Numeric data: consider thresholding the data e.g., cell value > 1

	camcountry.com	crowr	nedicine.	com sony	/musicnas	hville.com	elvisthemusic.com
10.16.236.100	1			1		1	
10.16.237.100	1			1		0	
10.16.238.100	1			1		1	
10.16.235.100	0			1		1	
			Port 80	Port 443	Port 22	Port 3389	_
	10.20.	.30.40	10.262	0.869	0.619	0.989	
	10.20.	.30.41	0.312	14.609	0.106	17.427	
	10.20.	.30.42	7.401	0.674	4.977	0.831	
	10.20.	.30.43	0.282	17.785	8.053	0.195	
	10.20.	30.44	18.484	14.705	0.028	16.451	

ľ	y.com	crowr	medicine.	com sony	musicnas	hville.com	elvisthemusic.com
	1			1		1	0
	1			1		0	1
	1			1		1	1
	0			1		1	1
			Port 80	Port 443	Port 22	Port 3389	
	10.20.	30.40	10.262	0.869	0.619	0.989	
	10.20.	30.41	0.312	14.609	0.106	17.427	
	10.20.	30.42	7.401	0.674	4.977	0.831	
	10.20.	30.43	0.282	17.785	8.053	0.195	
	10.20.	30.44	18.484	14.705	0.028	16.451	3



## What kind of data generate Hypergraphs?



3.7

Pacific

Northwest

	svchost.exe	powershell.exe	lsass.exe	firefox.exe
Host01	0	1	0	0
Host02	0	0	1	1
Host03	1	1	1	1
Host04	0	0	1	0
Host05	1	0	1	1

	camcountry.com	crowmedicine.	com sony	vmusicnas	hville.com	elvisthemusic.com
10.16.236.100	1		1		1	0
10.16.237.100	1		1		0	1
10.16.238.100	1		1		1	1
10.16.235.100	0		1		1	1
		Port 80	Port 443	Port 22	Port 3389	
	10.20	<b>.30.40</b> 1	0	0	0	
	10.20	<b>.30.41</b> 0	1	0	1	
	10.20	<b>.30.42</b> 1	0	1	0	
	10.20	<b>.30.43</b> 0	1	1	0	
	10.20	<b>.30.44</b> 1	1	0	1	3

ry.com	crowr	nedicine.	com sony	musicnas	hville.com	elvisthemusic.cor	n
1			1		1		0
1			1		0		1
1			1		1		1
0			1		1		1
		Port 80	Port 443	Port 22	Port 3389	_	
10.20.3	30.40	1	0	0	0		
10.20.3	30.41	0	1	0	1		
10.20.3	30.42	1	0	1	0		
10.20.3	30.43	0	1	1	0		
10.20.3	30.44	1	1	0	1		3





## Hypernetwork science



## Hypergraph properties

- Degree (distribution)
- Edge size (distribution)
- s-Walk, s-Path, s-Diameter
- s-Connected components
- s-Centrality

. . .

- Clustering coefficient?
- Triangle counting?

Vertex or edge?



## Walks on edges or vertices?

- For graphs, essentially the same.
  - Each pair of vertices in G belong to at most 1 edge, so:



• Each pair of edges in G intersect in at most 1 vertex, so:

 $\underbrace{e_1, e_2}_{\text{incident}}, \dots, \underbrace{e_{k-1}, e_k}_{\text{incident}} \xrightarrow{\rightarrow} \underbrace{v_0}_{e_1 \setminus e_2}, \underbrace{v_1}_{e_1 \cap e_2}, \dots, \underbrace{v_{k-1}}_{e_{k-1} \cap e_k}, \underbrace{v_k}_{e_k \setminus e_{k-1}}$ 

- For hypergraphs, not the same.
  - Each pair of vertices can belong to many edges.
  - Each pair of edges can intersect at many vertices.

Walks between edges: sequence of successively intersecting edges Walks between vertices: sequence of successively adjacent vertices







## Hypergraph walks have width

- s-Walk: sequence of edges  $e_1, \ldots, e_k$  such that  $|e_i \cap e_{i+1}| \ge s$
- Walks/paths in hypergraphs have width in addition to length:



• **s-Path** = s-Walk where edges are not repeated





Hypergraph properties

- Degree (distribution)
- Edge size (distribution)
- s-Walk, s-Path, s-Diameter
- s-Connected components
- s-Centrality
- Clustering coefficient?
- Triangle counting?
- . . .

Vertex or edge?



## Hypergraph construction from multi-column data

hostname	principal	pid	src_ip	dest_ip	dest_port	l4protocol	image_path
SysClient0201.systemia.com	NT AUTHORITY\SYSTEM	4	142.20.56.198	142.20.59.255	138	UDP	System
SysClient0201.systemia.com	NT AUTHORITY\NETWORK SERVICE	864	10.20.4.125	224.0.0.252	5355	UDP	svchost.exe
SysClient0201.systemia.com	NT AUTHORITY\NETWORK SERVICE	864	142.20.59.255	224.0.0.252	5355	UDP	svchost.exe
SysClient0201.systemia.com	SYSTEMIACOM\zleazer	636	142.20.56.198	222.206.244.5	443	TCP	firefox.exe
SysClient0201.systemia.com	NT AUTHORITY\SYSTEM	4	142.20.59.149	142.20.59.255	138	UDP	System
SysClient0201.systemia.com	NT AUTHORITY\NETWORK SERVICE	864	142.20.59.149	224.0.0.252	5355	UDP	svchost.exe

- Multi-dimensional data set: nD-array, n-column data frame
- Specify column set for hyperedges (yellow)
  - Unique combinations: (142.20.59.255, 138), (224.0.0.252, 5355), (222.206.244.5, 443)
- Specify disjoint column set for vertices (blue)
  - Unique vertices: 142.20.59.149, 10.20.4.125, 142.20.59.255, 142.20.56.198
- A vertex is contained in a hyperedge if there is a record with that combination in the data. Think "hyperedges = common behaviors"





## Identifying anomalies via simple dynamic hypergraph measures

- "Do the simple thing first"
- Sometimes just counting things (vertices, edges, degrees, edge sizes) and looking for temporal changes gives you insight.
  - A. Network simulation startup activity
  - B. Actual red team activity – "Deathstar" to scan domain
- But there's much more to find in this data...

Joint with Helen Jenne









Number of edges and maximum degree, Day 2 V: (source IP, hostname), E: (dest port, dest IP)



Jenne, H., Aksoy, S.G., Best, D., Bittner, A., Henselman-Petrusek, G., Joslyn, C., Kay, B., Myers, A., Seppala, G., Warley, J., Young, S.J., and Purvine, E. Stepping Out of Flatland: Discovering behavior patterns as topological structures in Cyber hypergraphs. The Next Wave, 25(1), 2024.



## **Finding complex patterns** of connectivity



• While adversaries try to fly below the radar they still operate within the network and likely do things that are abnormal. Their activities may create unusual patterns of connectivity.

(DC1, WMI)

Edge containment

structures

Red singleton edge represents 335 identical edges containing vertex for Sysclient0501 (DC2, WMI) (C2A, HTTPS)

bantonio rsantilli (DC1, LDAP) (C2B, HTTP)





This structure is not always tied to malicious activity, but it is rare in this data and thus potentially of interest.









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## **Application #2: High-dimensional data (generally)**

Lorem ipsum dolor sit amet. elit, sed do eiusmod tempor dolore magna nostrud exe **88 com** ente

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learn.readthedocs.io/en/latest/document\_embedding.html



PID	Src IP	Dst IP	Dst Port	Protocol	Image pa
4	142.20.56.198	142.20.59.255	138	UDP	System
864	10.20.4.125	224.0.0.252	5355	UDP	svchost.ex
864	142.20.59.255	224.0.0.252	5355	UDP	svchost.ex
636	142.20.56.198	222.206.244.5	443	TCP	firefox.ex
4	142.20.59.149	142.20.59.255	138	UDP	System
864	142.20.59.149	224.0.0.252	5355	UDP	svchost.ex





## Creating high dimensional data from cyber logs: **Feature engineering**

- For a given time-window of data we can create a feature vector
- Hand-crafted features:
  - Count of unique values in a column
  - Count occurrences of specific values in a column
  - Numerical aggregations min, max, mean, median, sum
  - Max degree of a graph of the data
  - . . .
- Machine learned features
  - Train an autoencoder or LLM on log lines, aggregate all encoded lines in a window

PID	$\operatorname{Src}\operatorname{IP}$	Dst IP	Dst Port	Protocol	Image path				
4	142.20.56.198	142.20.59.255	138	UDP	System				
864	10.20.4.125	224.0.0.252	5355	UDP	svchost.exe				
864	142.20.59.255	224.0.0.252	5355	UDP	svchost.exe				
636	142.20.56.198	222.206.244.5	443	$\mathrm{TCP}$	firefox.exe				
4	142.20.59.149	142.20.59.255	138	UDP	System				
864	142.20.59.149	224.0.0.252	5355	UDP	svchost.exe				
Feature									

Count of Src IPs

Count of Dst Port = 443

Count of Image path = svchos

Max in-degree in Src IP -> Ds

Max out-degree in Src IP -> D



142.20.59.149

10.20.4.125

	4
	1
st.exe	3
t IP graph	3
st IP graph	2





## **Temporal anomaly detection** from feature point clouds

- **Main assumption:** Behavior varies smoothly from set of recent small time windows to the next window
- Method:
  - Partition data into time intervals, create a single vector for each
  - Baseline contains many time intervals many vectors current time interval is single vector
  - How, and how much, does adding the single vector change the structure of the collection of baseline vectors?







## Structure = Topology

- Geometry without distance; stretchy geometry
- Properties (= holes) of geometric objects preserved under "continuous deformation" – stretching and twisting are ok but tearing and gluing are not
- Abstract an object into a simpler version that preserves certain properties – "topological invariants"



1736 Leonhard Euler, Seven Bridges of Königsberg



## Donut? Coffee cup?

Lucas Vieira, Public domain, via Wikimedia Commons



## **Persistent Homology**

- Given a point cloud we want to understand its coarse topological structure
- Connect points at increasing distance thresholds
- Track birth and death threshold for topological features ("holes")



Image credit: Sarah Tymochko





Joint with Helen Jenne, Dan Best, Paul Bruillard, Alyson Gauthier, Greg Henselman-Petrusek, Cliff Joslyn, Bill Kay, Audun Myers, Kathleen Nowak, Garret Seppala, Stephen J. Young



## **Use case example: BitTorrent Detection**

- Network flow for a single building was captured
  - BitTorrent traffic added after the fact by node 6893 during windows 278-301
- Feature vectors came from counts of small graph patterns
- Our pipeline was able to detect an anomaly from 6893 during the correct time windows



Christopher R. Harshaw, Robert A. Bridges, Michael D. lannacone, Joel W. Reed, and John R. Goodall. 2016. GraphPrints: Towards a Graph Analytic Method for Network Anomaly Detection. In Proceedings of the 11th Annual Cyber and Information Security Research Conference (CISRC '16).



## **Plan End of the talk**

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Topology captures global features in data sets

Graphs model pairwise interactions. Random models can generate realistic data sets to help explore properties consistent with real systems.

hypergraph model can capture more information and sometimes identify additional structure.





## Thank you

Check out our internships and jobs! <u>https://careers.pnnl.gov/</u>

Contact me with questions! <u>Emilie.Purvine@pnnl.gov</u>





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