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Graph Data Science

The world is full of challenges

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The world is full of challenges

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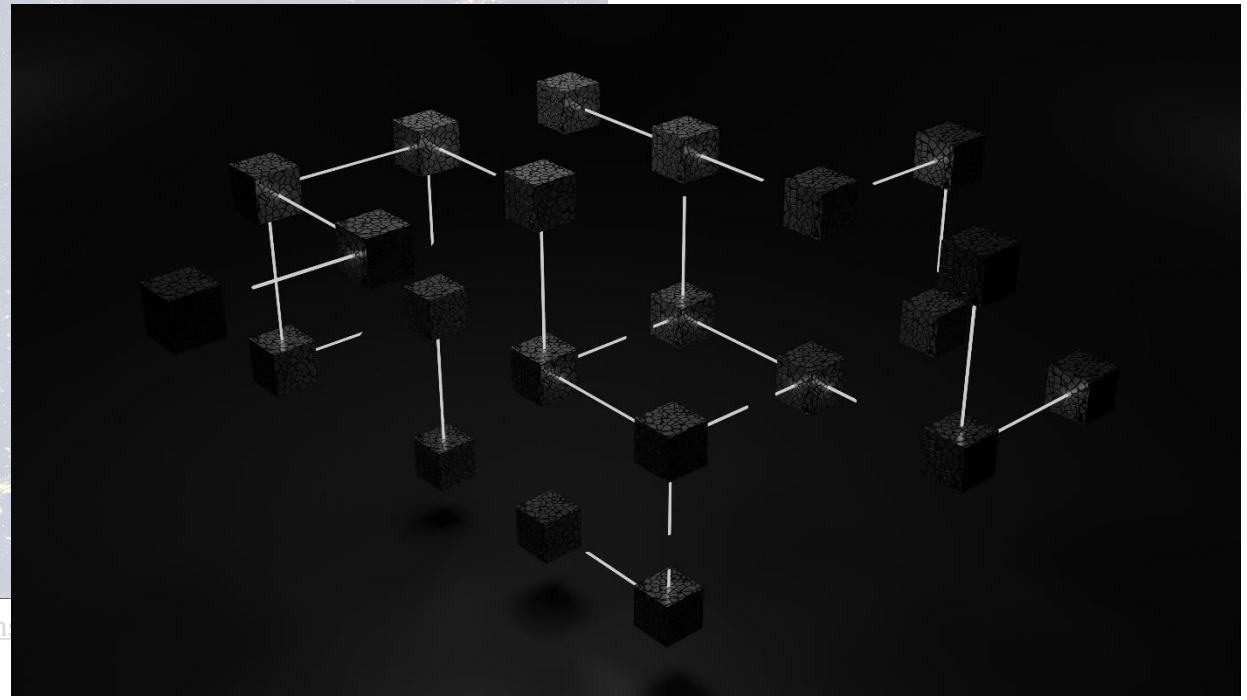

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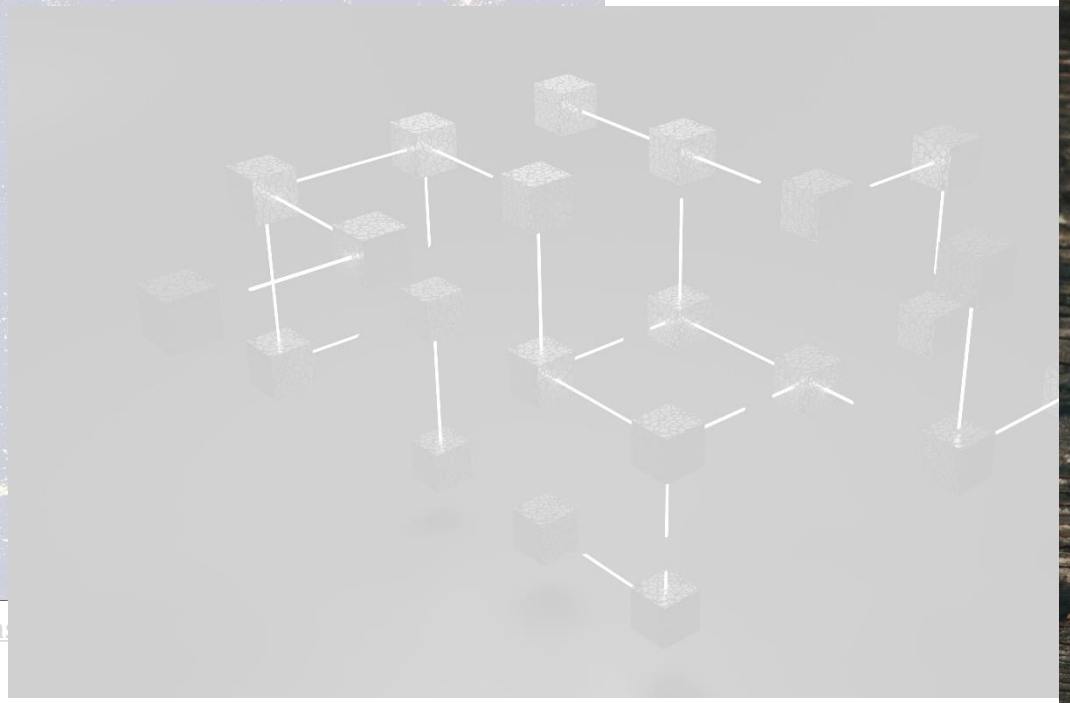

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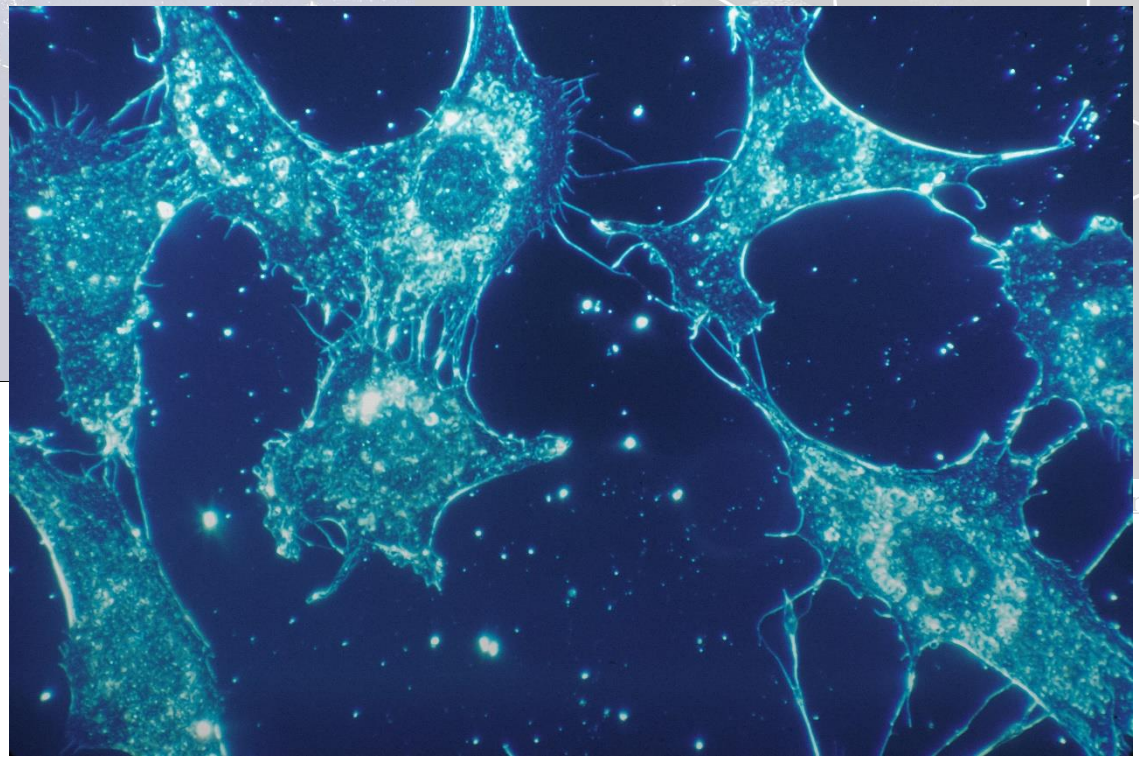

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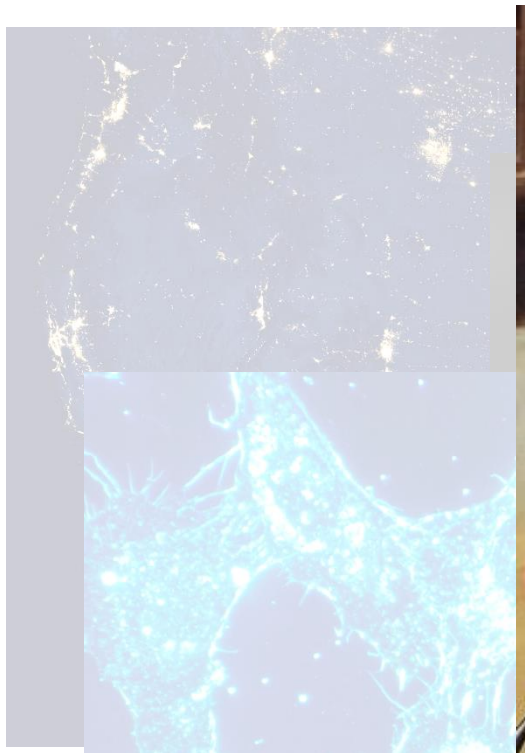

Photo by National Cancer [illegible] Wikimedia (retrieved 2023-05-07)

[illegible] Dumlao on Unsplash (retrieved 2023-05-07)

This course – getting to know each other

About me: Nanotechnology → theoretical physics → complex systems
→ PhD in Computer Science / AI → Sr. Data Scientist at FedEx

My contact: ilja.rausch@pm.me

My LinkedIn: **linkedin.com/in/ilja-rausch/**

Disclaimer: None of the material is linked to FedEx!

This course – getting to know each other

About you

- Your background and interests
  - Engineering (mechanical, industrial, technology and systems)
  - Innovation and design
  - Cybersecurity

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- Motivation to take this course
  - Fun / curiosity
  - Career development
  - FOMO
  - Other

Course overview - expectations

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    - Wikipedia is acceptable for images but insufficient for information
    - ChatGPT is allowed but be very very careful

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  - strongly invited to do your own literature research
    - Wikipedia is acceptable for images but insufficient for information
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  - cover the core notions about the selected topic + limitations
  - in simplified terms (similar to a technical presentation given to the upper management in business)
  - pack the information into a story (make it a fun story if you want); build an imaginary business case

Course overview - topics for presentations

1. Network centrality (PageRank, Katz)
2. Network controllability and control nodes

3. Trees in ML: random forests and gradient boosting
4. GNNs (GraphSAGE, GIN)
5. Reinforcement learning

6. Word/Text embeddings
7. Clustering and vector similarity in ML
8. Dimensionality reduction (PCA and t-SNE)
9. Data sampling techniques (SMOTE)
10. Bayesian hyperparameter tuning

11. Explainable AI (XAI), Feature importance
12. Recommender Systems
13. Multivariate testing and A/B testing
14. Time Series (ARIMA, drift and temporal networks)
15. Meta-heuristics and Genetic Algorithms/ACO/PSO

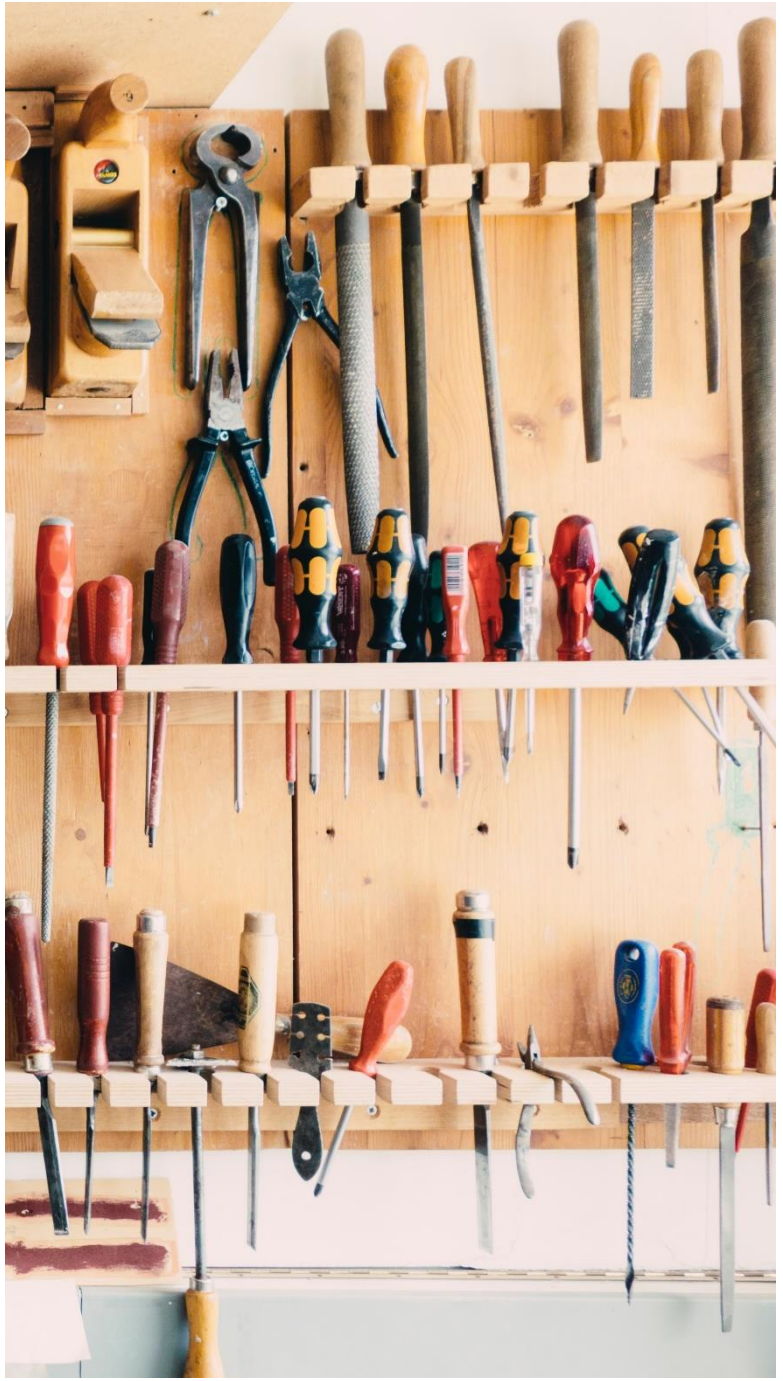
16. Collective foraging/flocking
17. Site-selection + inhibition in bee colonies
18. Simulating signal propagation on networks

19. Qubits

20. Prompt engineering

Course overview - syllabus

	Session #	Description
WEEK 1	1	Introductory lecture, course overview; some useful tools from statistics
	2	Introduction to Network Science
	3	Introduction to Machine Learning
	4	Neural Networks
	5	Deep Learning architectures: CNNs, Attention, Transformers, BERT
WEEK 2	6	Knowledge Graphs and Graph Neural Networks
	7	Data mining; Quantum computing;
	8	Collective intelligence, simulation and agent-based modeling
	9	Practical tips for software and ML development
	10	Practical tips for working in the private sector (business, industry)
WEEK 3	11	Students' presentations I
	12	Students' presentations II
	13	Students' presentations III
	14	Guided hands-on session for creating a simple PoC with GNNs and Python
	15	Last day of class: grading and general feedback



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Course overview – my promise

- The course will widen your horizon
- Provide a broad (but incomplete) overview of Graph Data Science
- Lower the barrier to entry, enabling you to explore beyond
- Some insights useful for business / industry

Image created with Dall-E 2 (created 2023-05-13)

Useful literature and tutorials

- The Art of Statistics book by D. Spiegelhalter
- Statistics course by J. Blitzstein (Harvard)
- Network science book by A.-L. Barabási

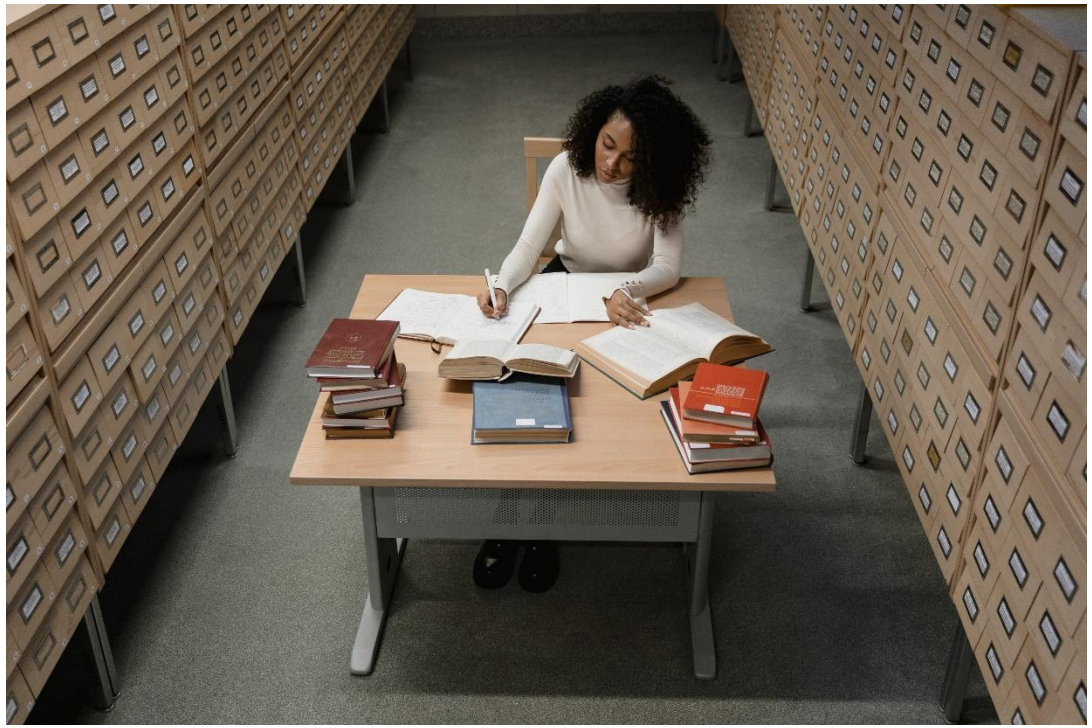
- The Machine and Deep Learning Compendium
- A high-bias, low-variance introduction to Machine Learning for physicists paper by Mehta et al.
- Machine Learning course by Y. Abu-Mostafa

- Neural Networks lecture by F. Marquardt
- Deep Learning course by Andrew Ng
- Attention is all you need publication by Vaswani et al.

- Gentle introduction to GNNs web article by Sanchez-Lengeling et al.
- Machine Learning with Graphs by J. Leskovec (Stanford)

- Collective Motion paper by Viscek et al.
- Corey Shafer YouTube channel
- Scaled Agile Framework material

What is Graph Data Science?



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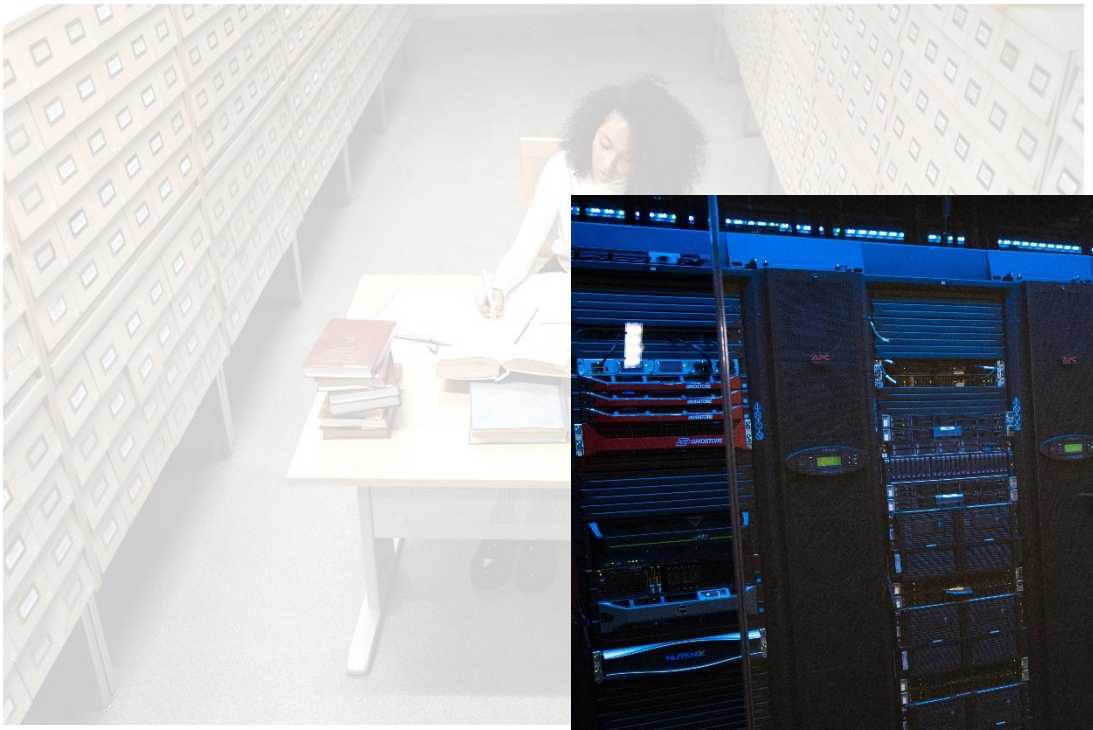

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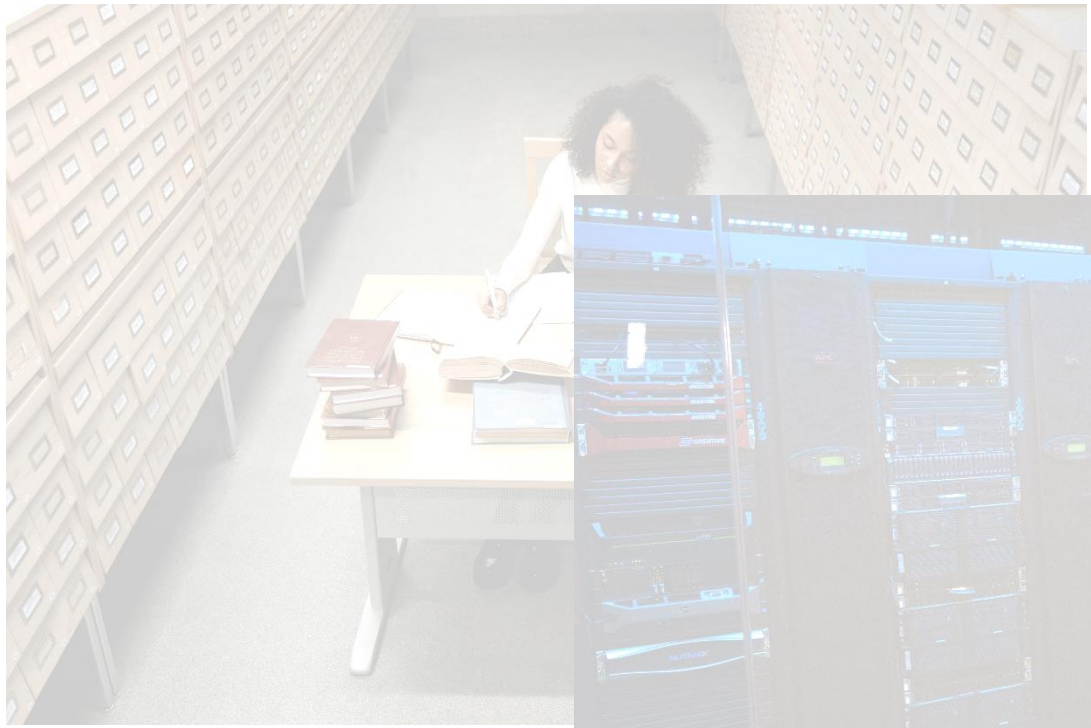

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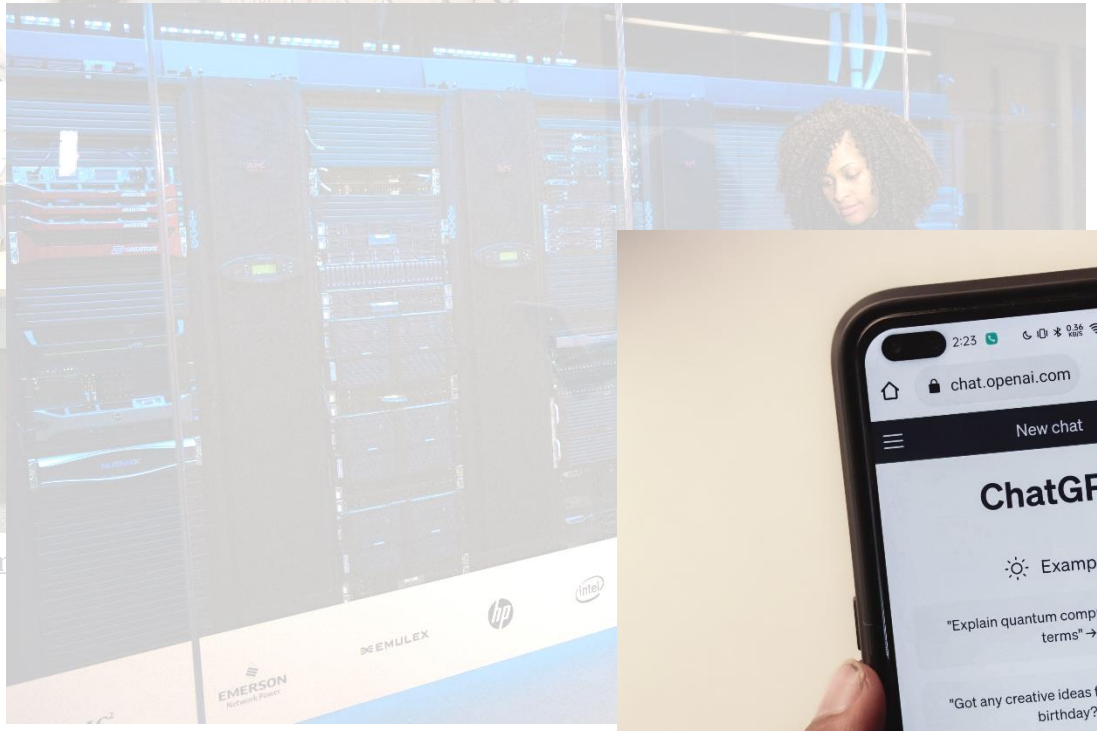

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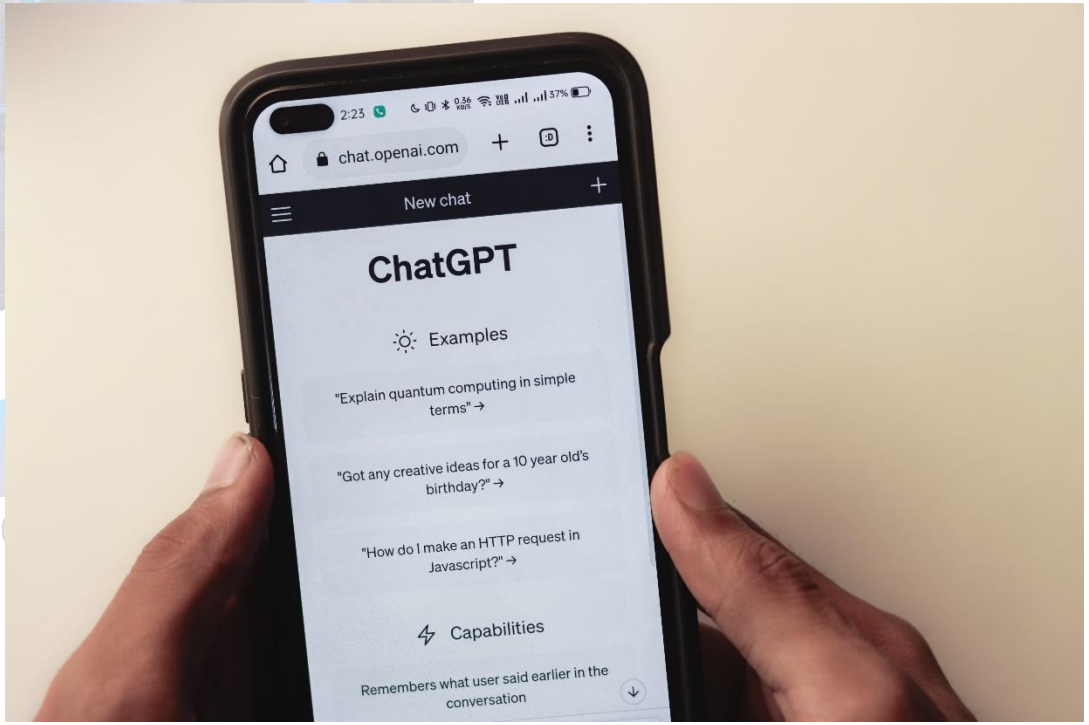

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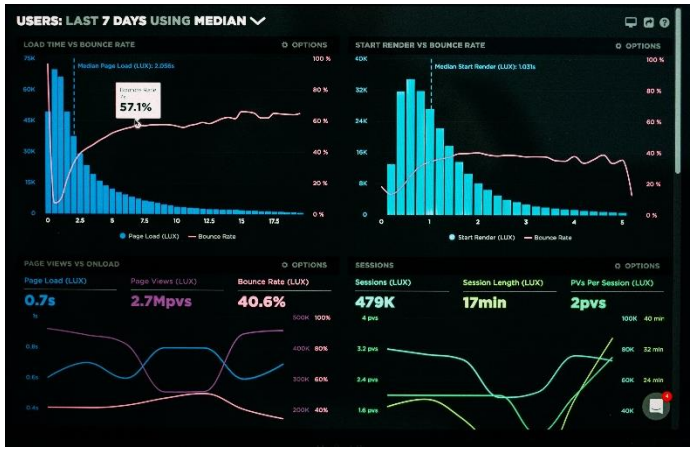
What is Graph Data Science?

Data analysis



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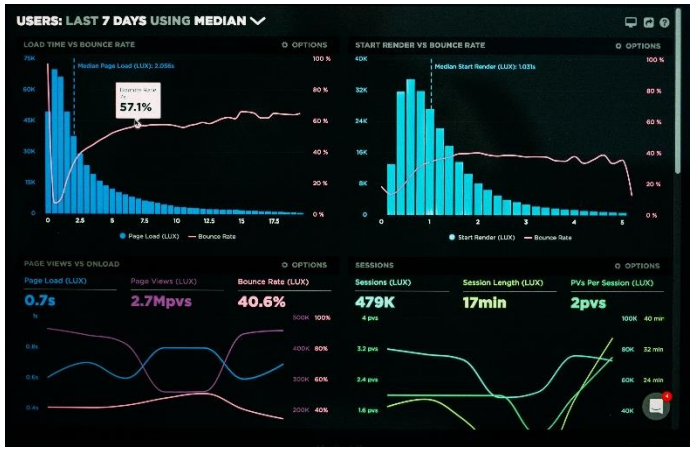

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Data bases & DevOps

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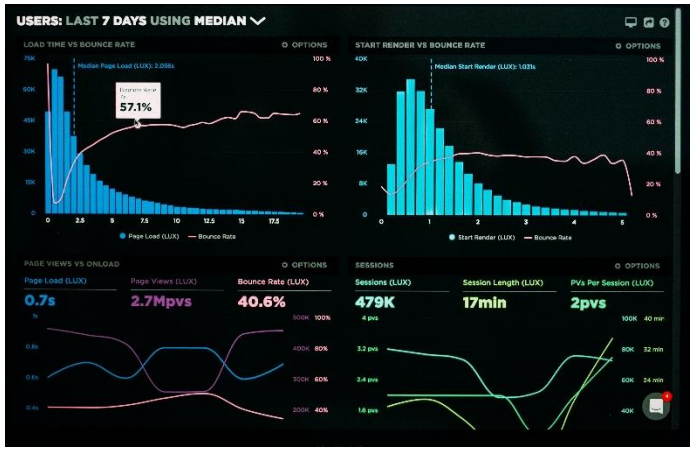

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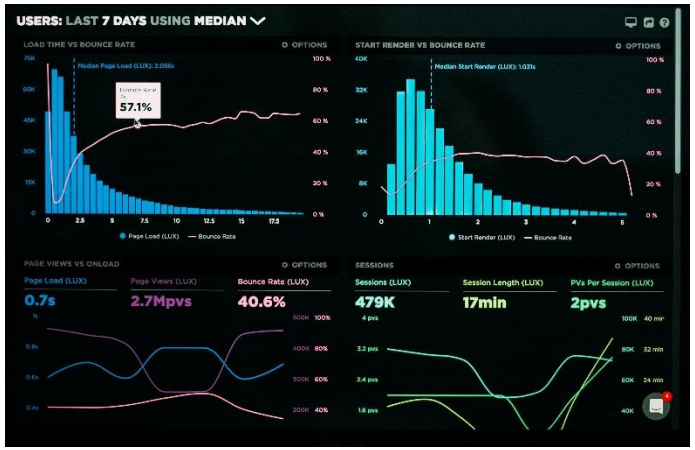

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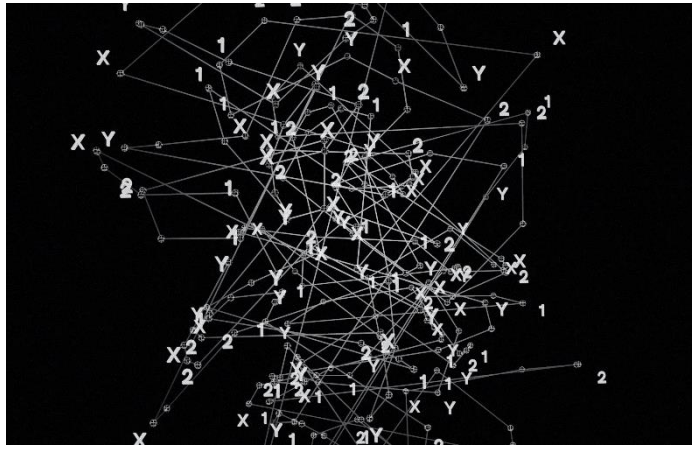
Graphs / Networks



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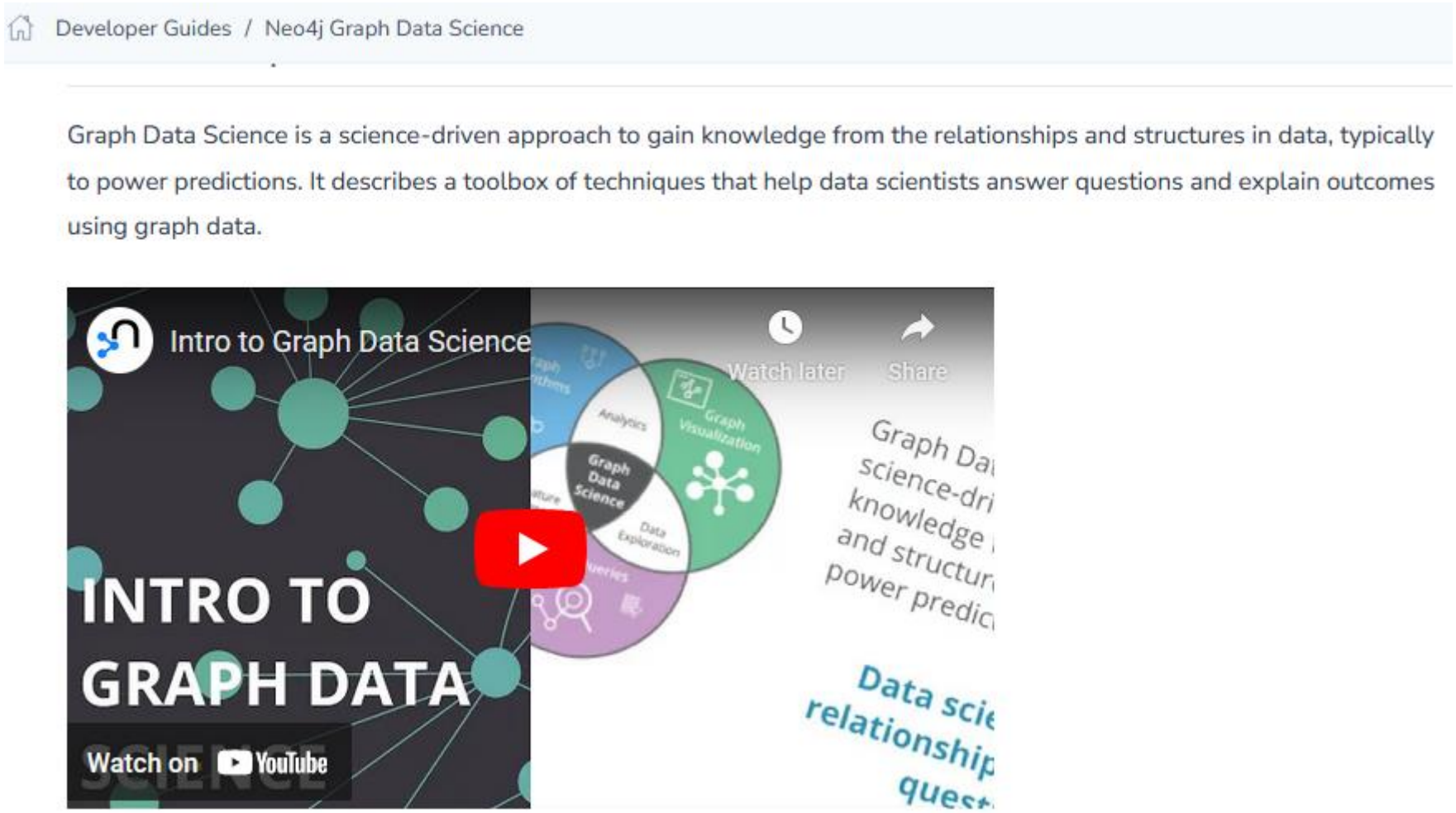
What is Graph Data Science?

Graph Data Science term coined / promoted by Neo4j



Screenshot from Neo4J.com (retrieved 2023-05-13)

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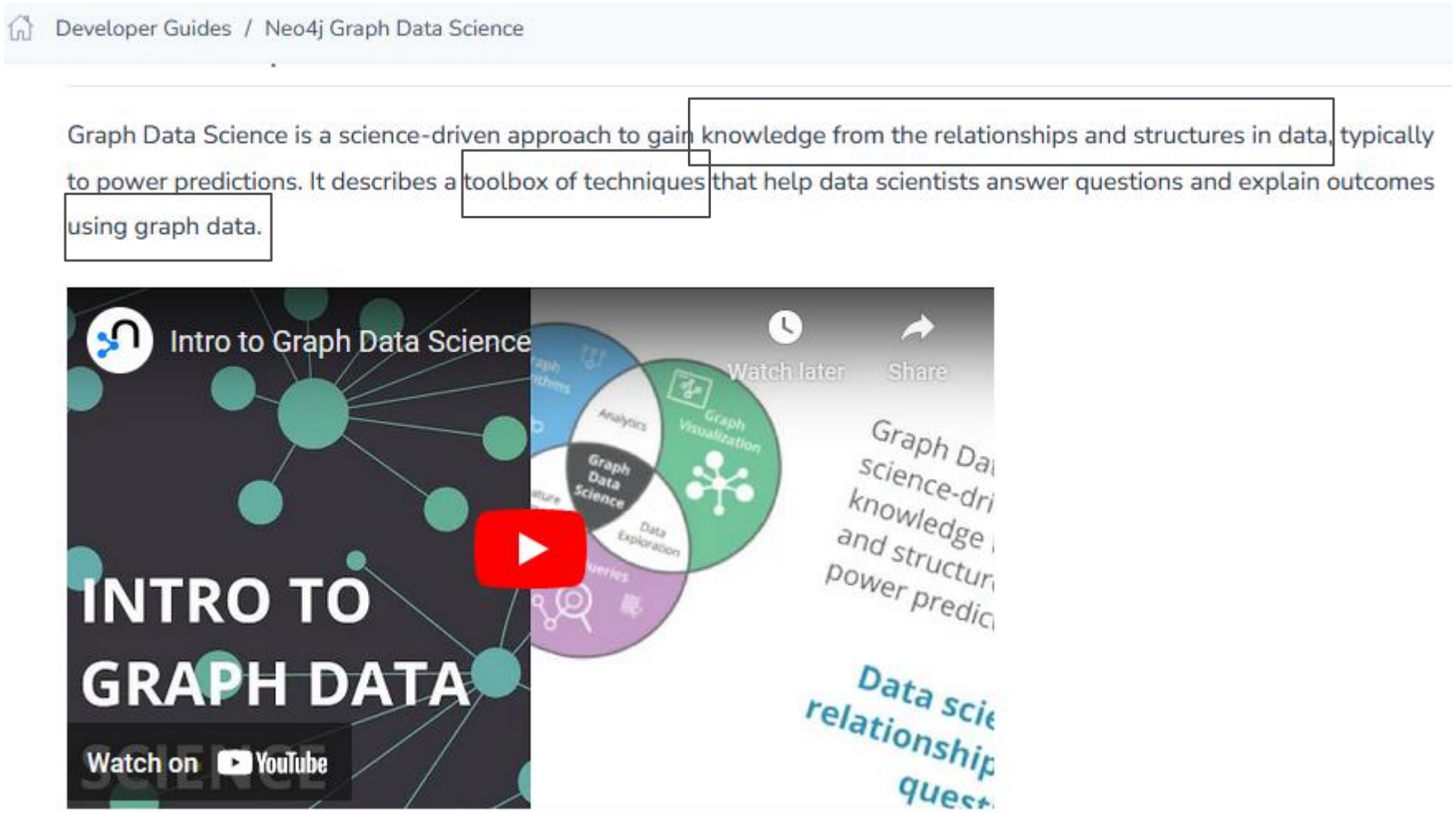

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What is Graph Data Science?

"Traditional Data Science"

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"Traditional Data Science"

structured data

	a1	a2	a3	a4
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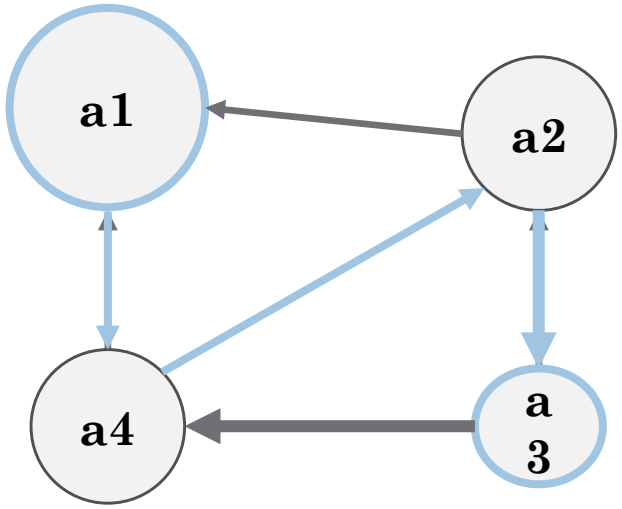
r2	1	0	1	0
r3	0	1	0	1
r4	1	1	0	0

"Graph Data Science"

graph-structured data



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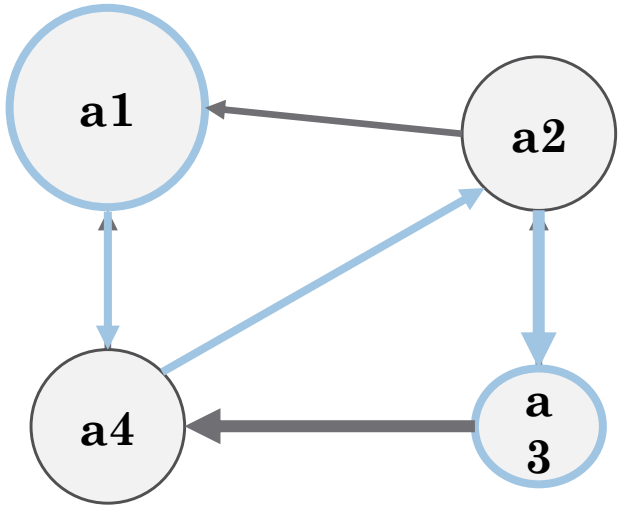

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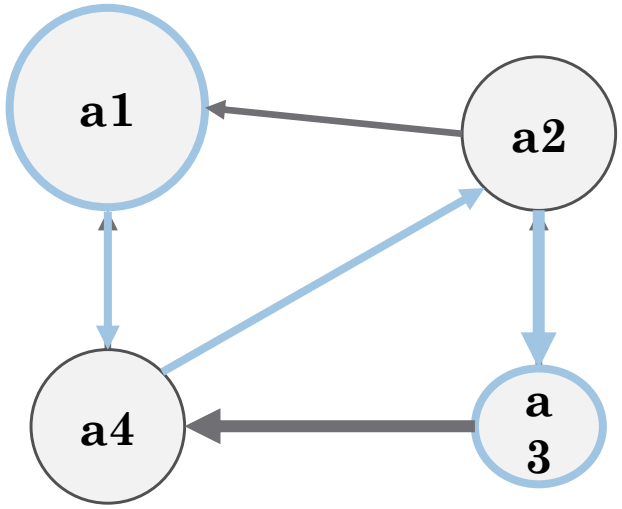

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GDS = Data Science enriched with complex data relations

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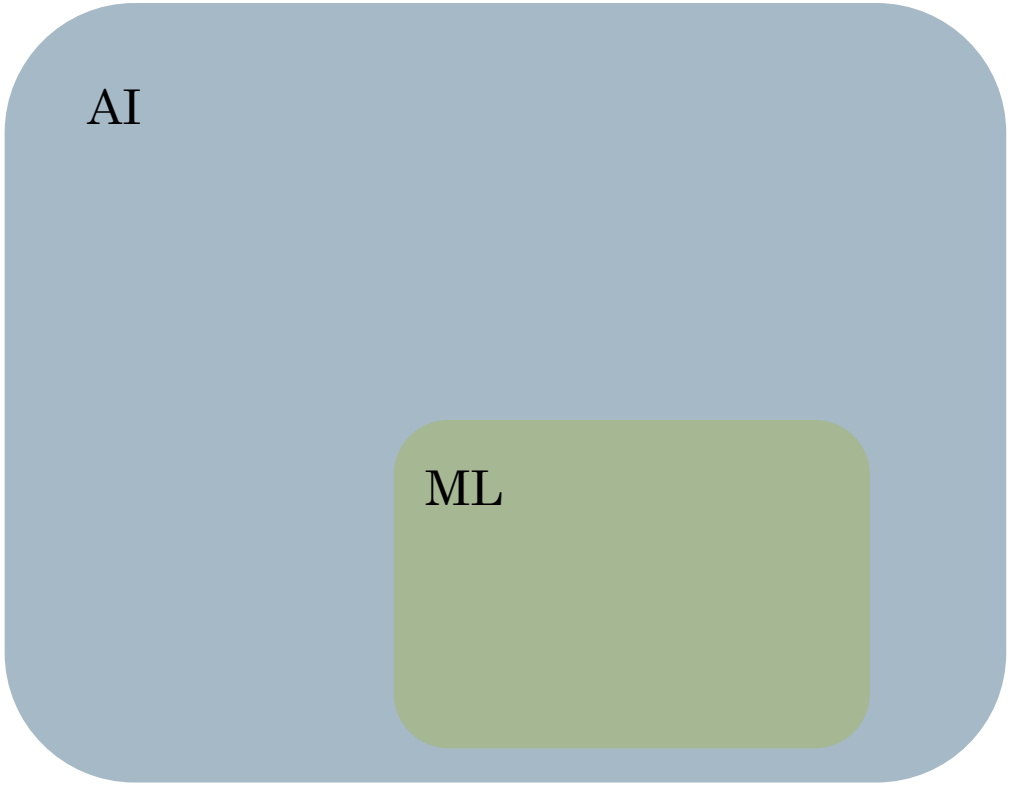

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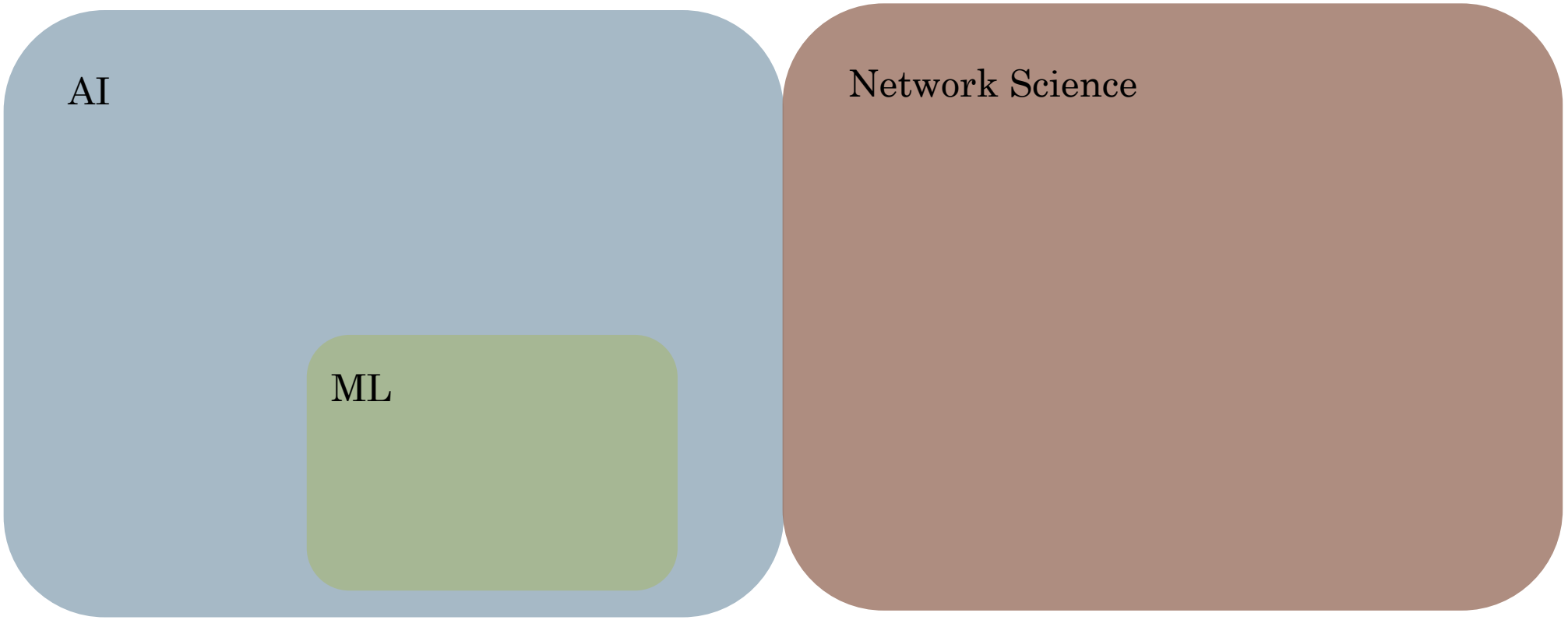

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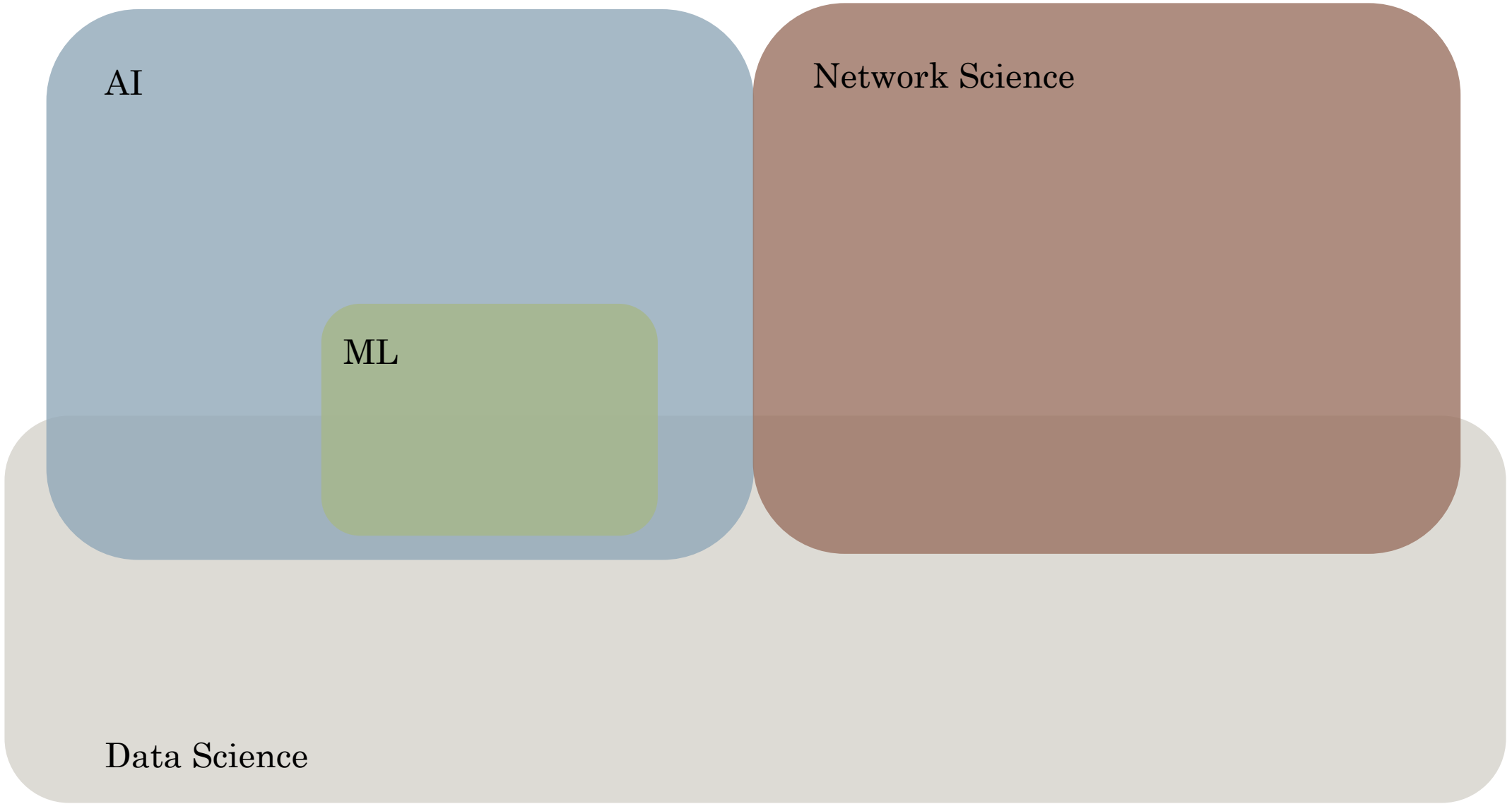

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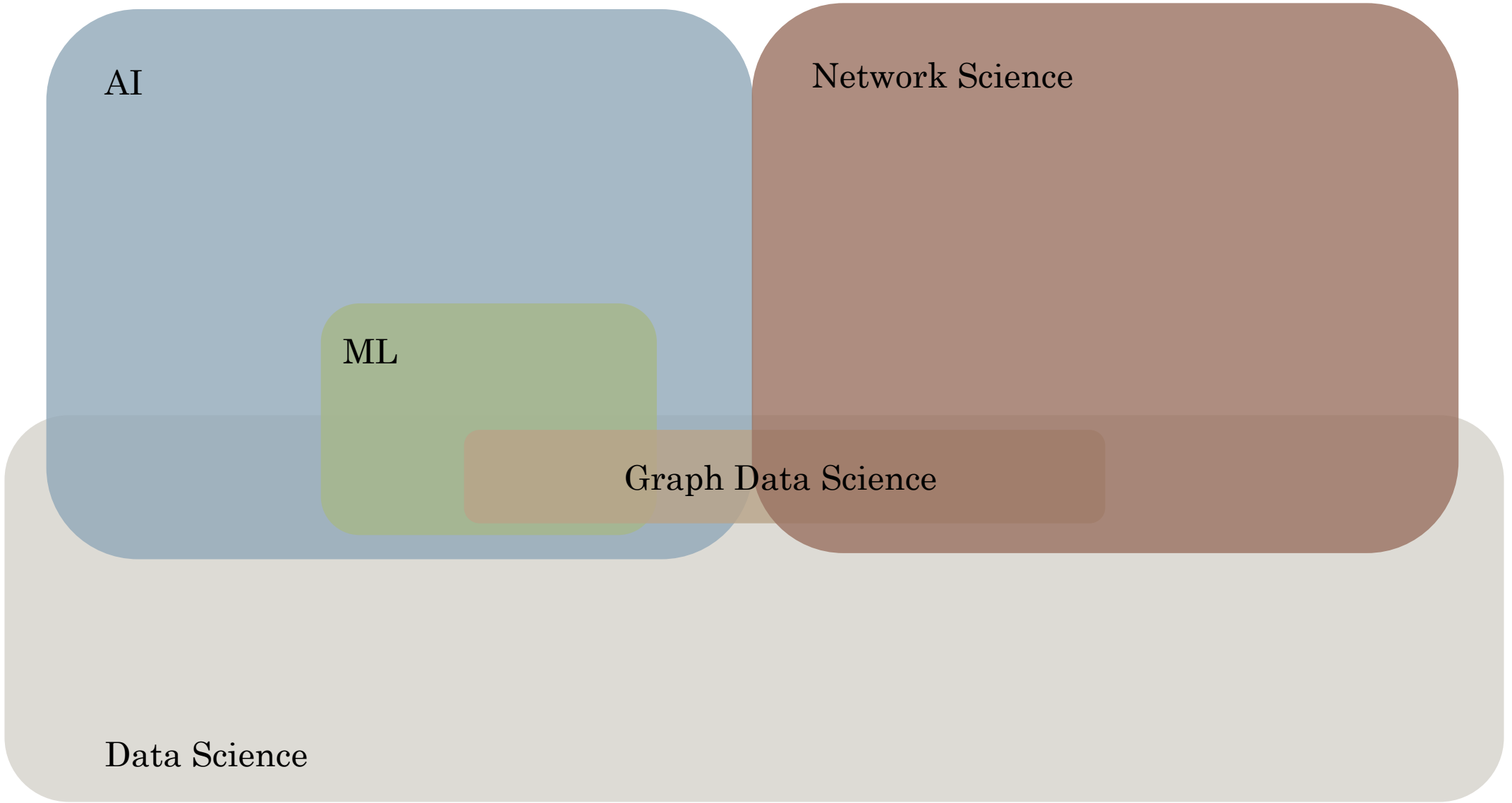

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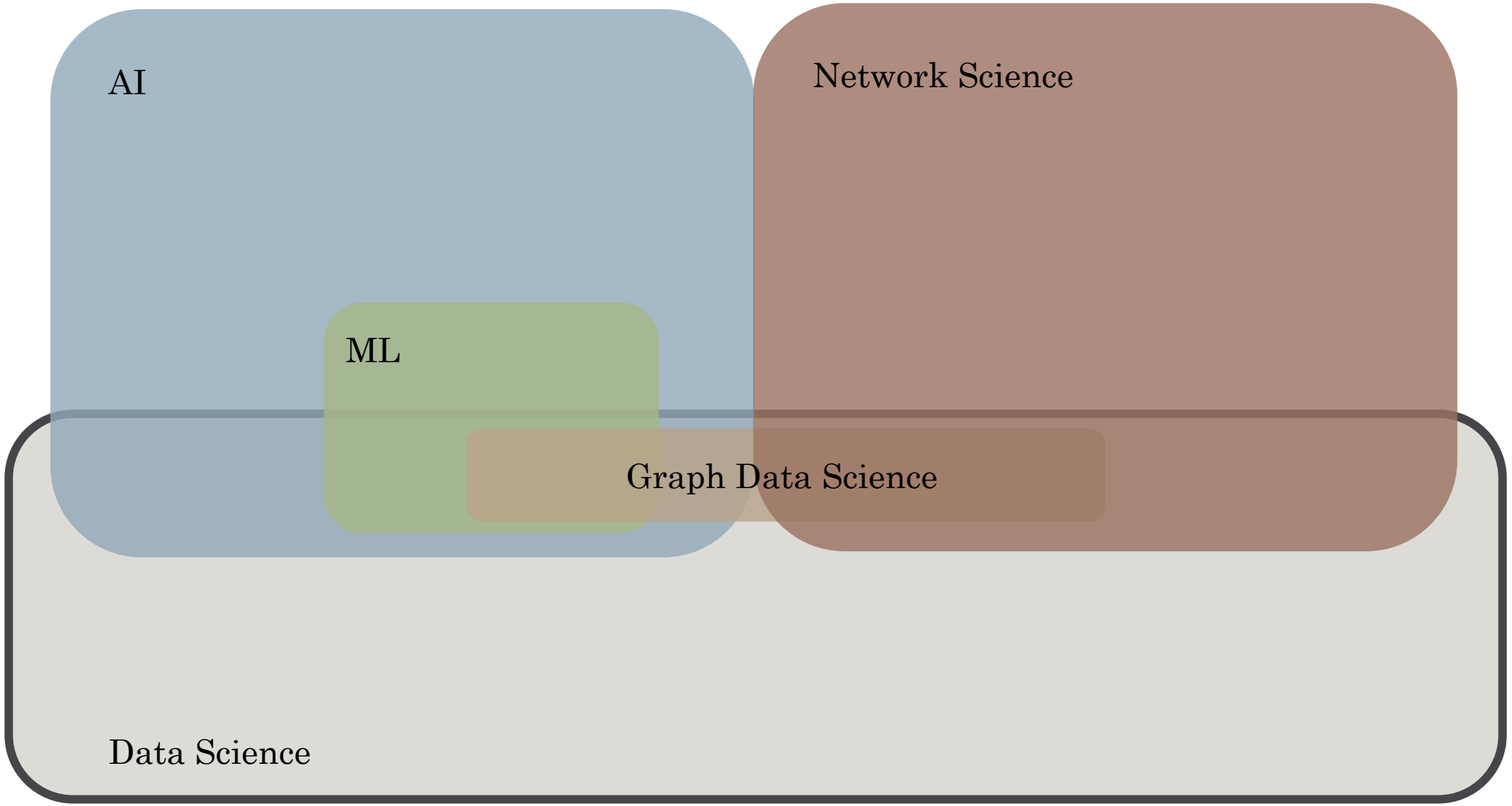

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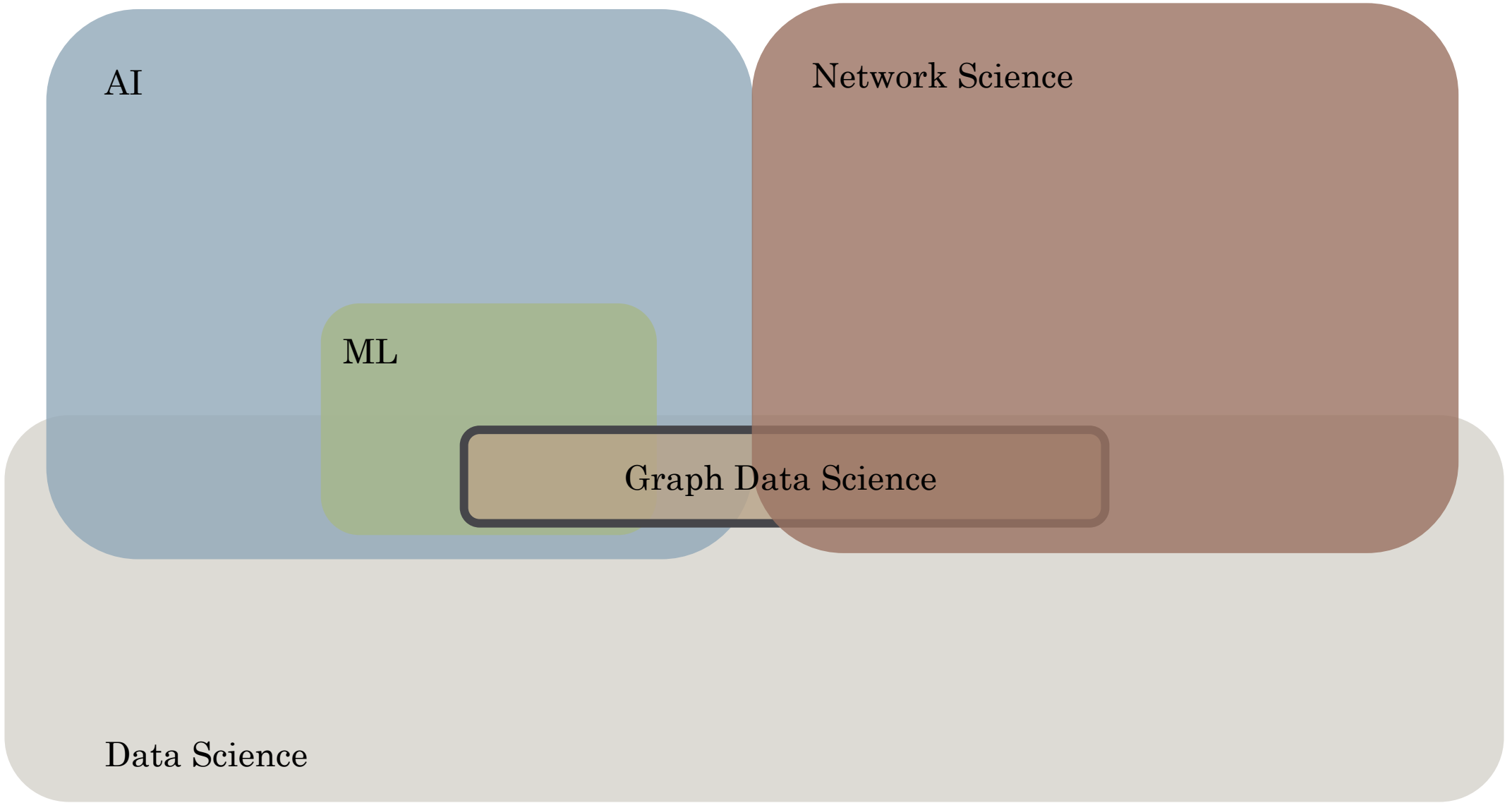

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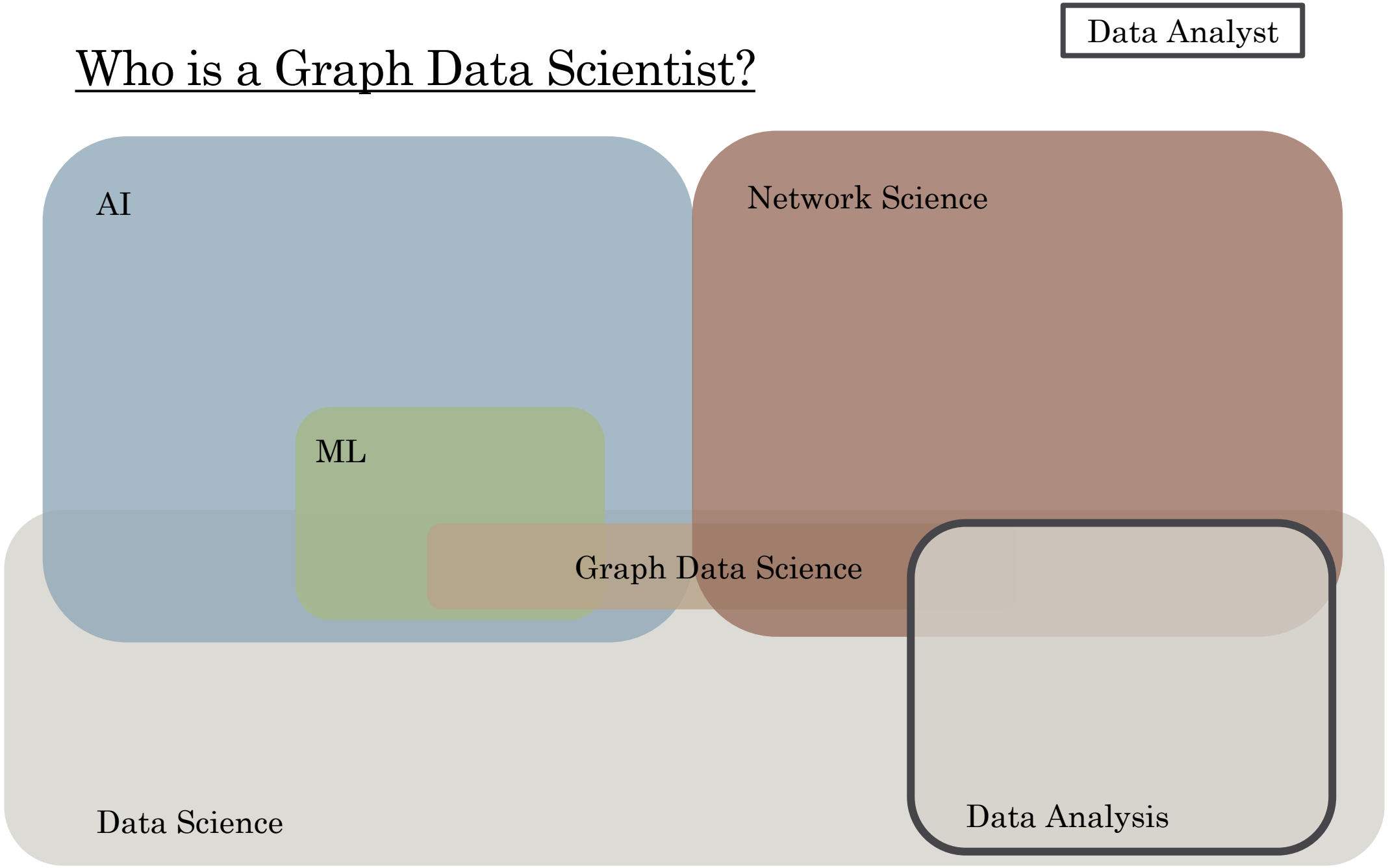

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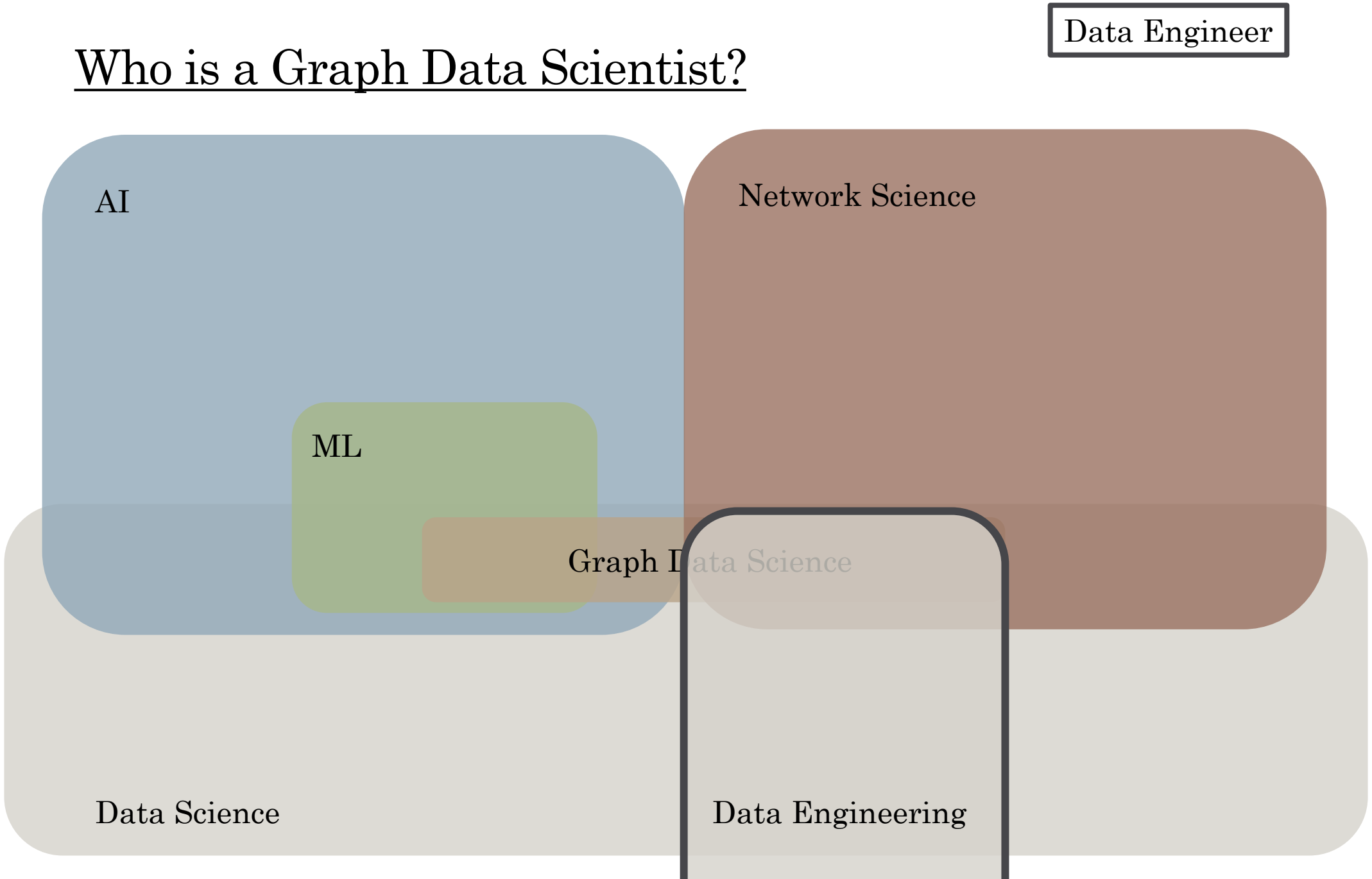

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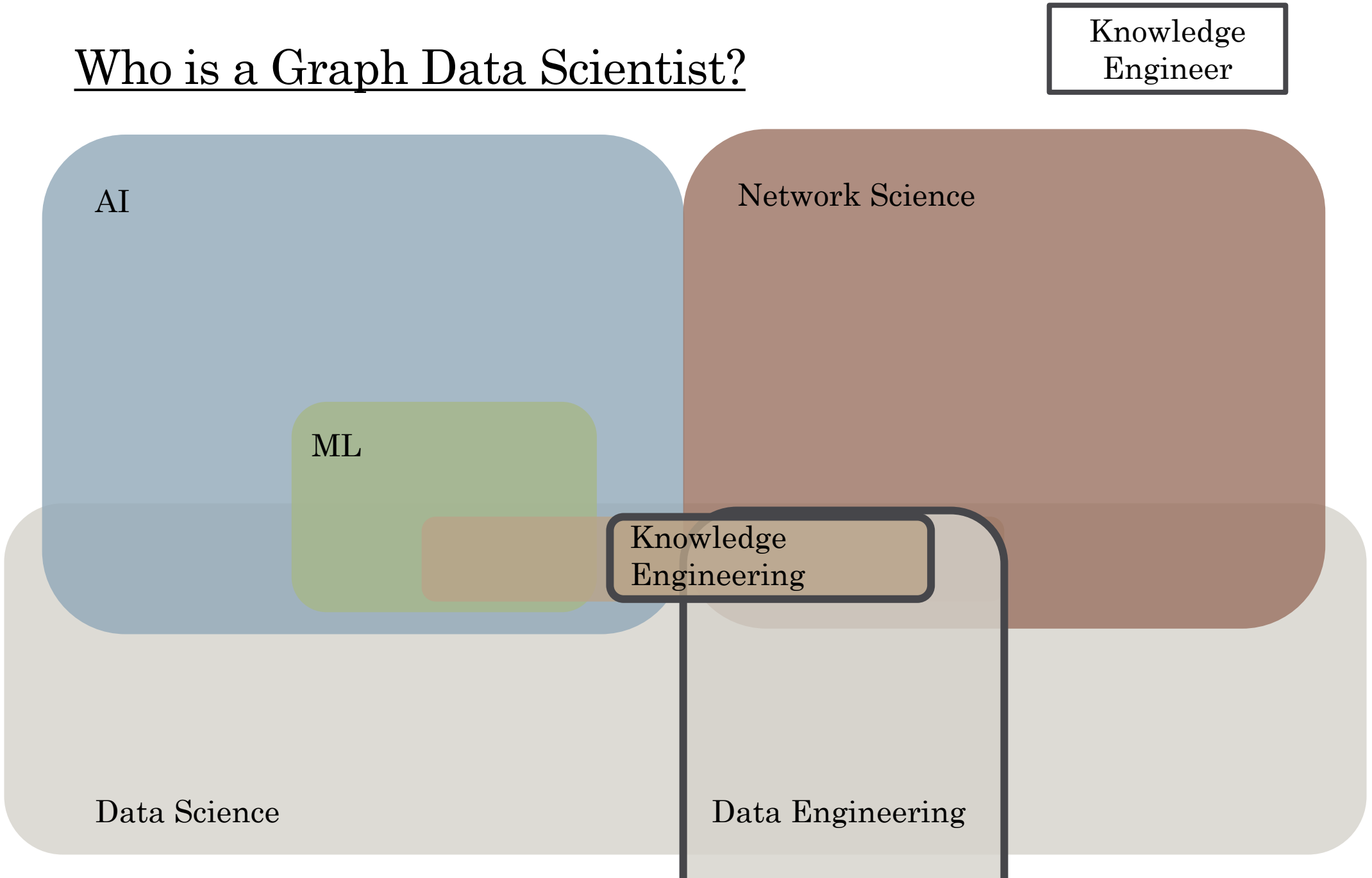

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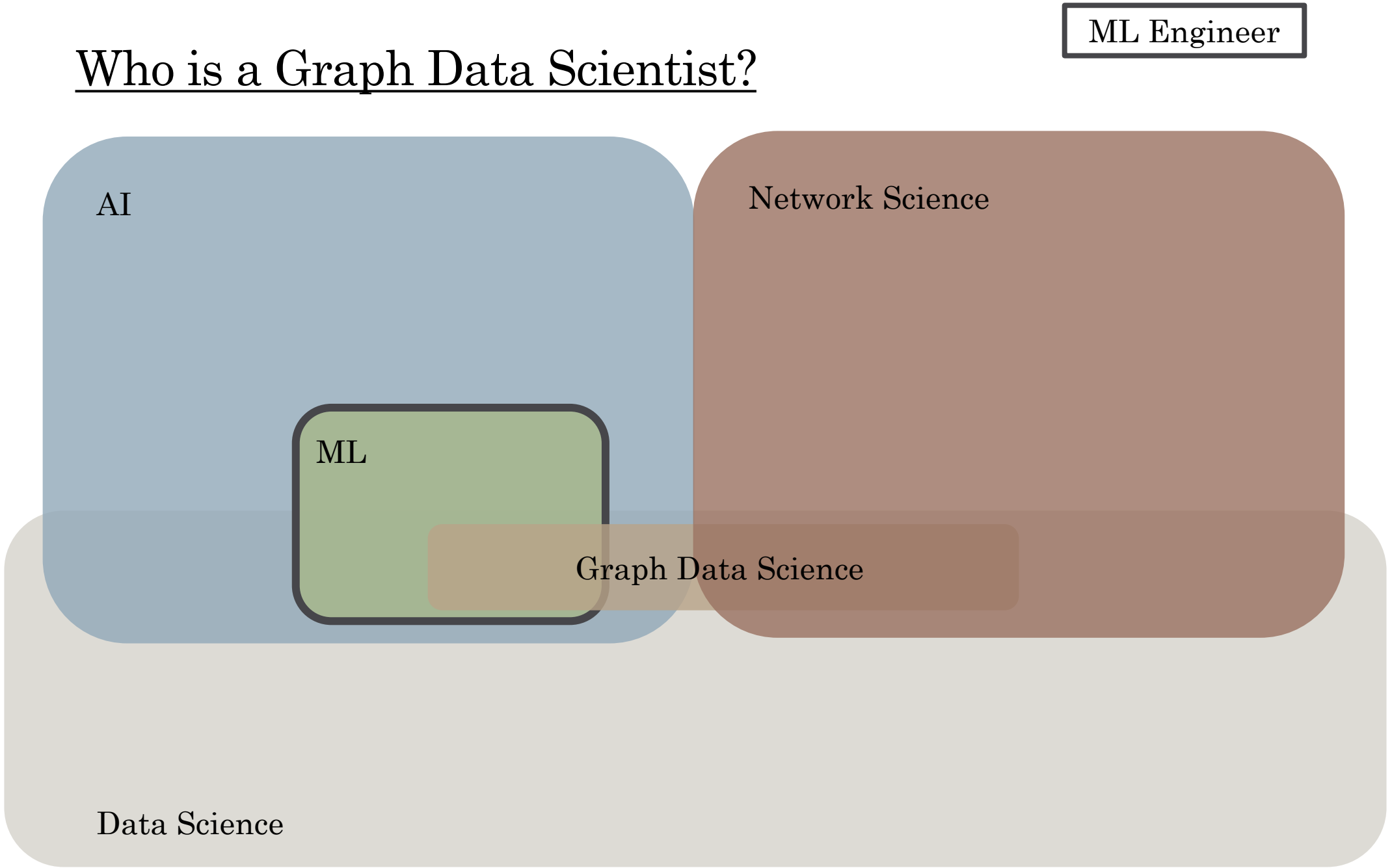

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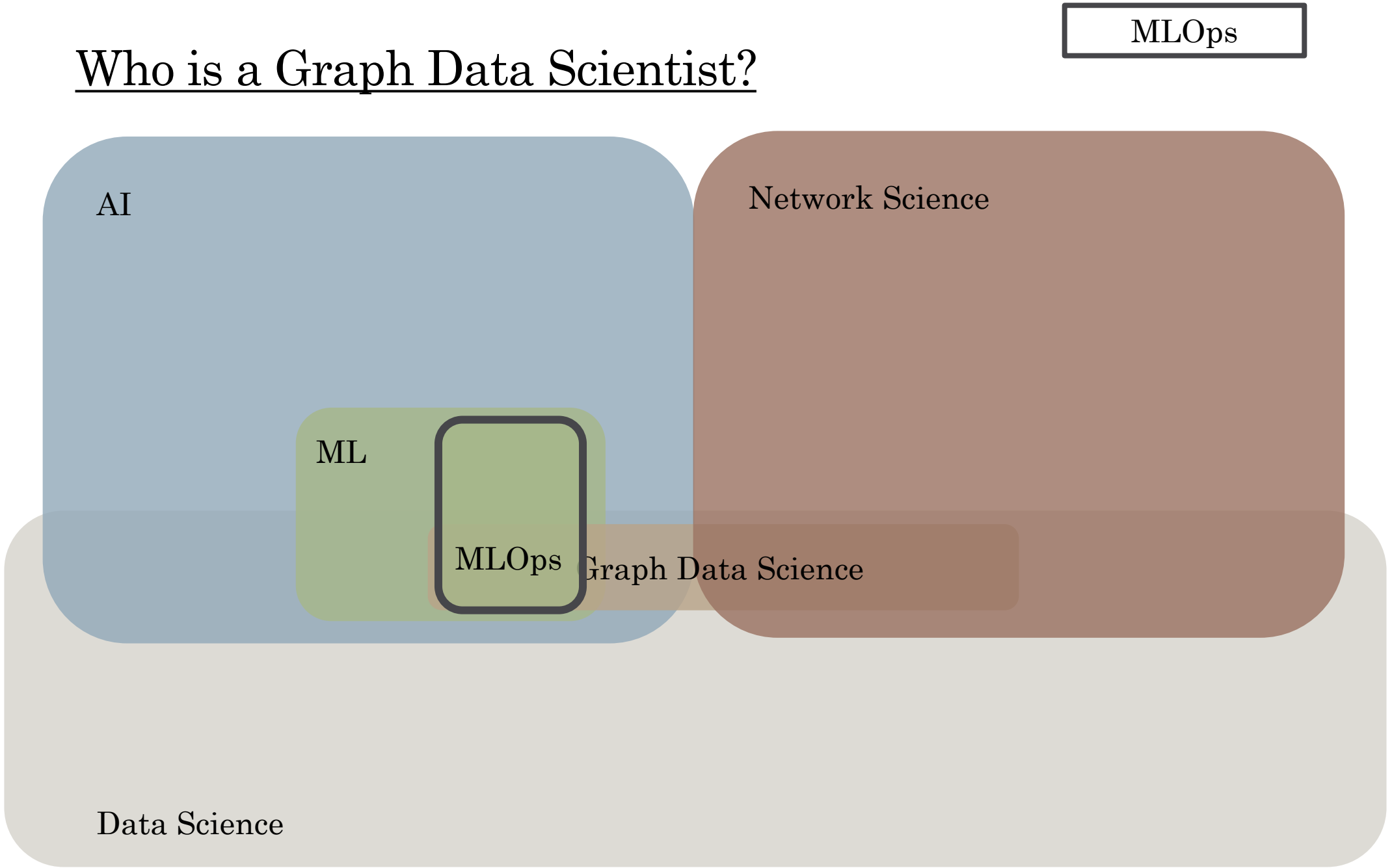

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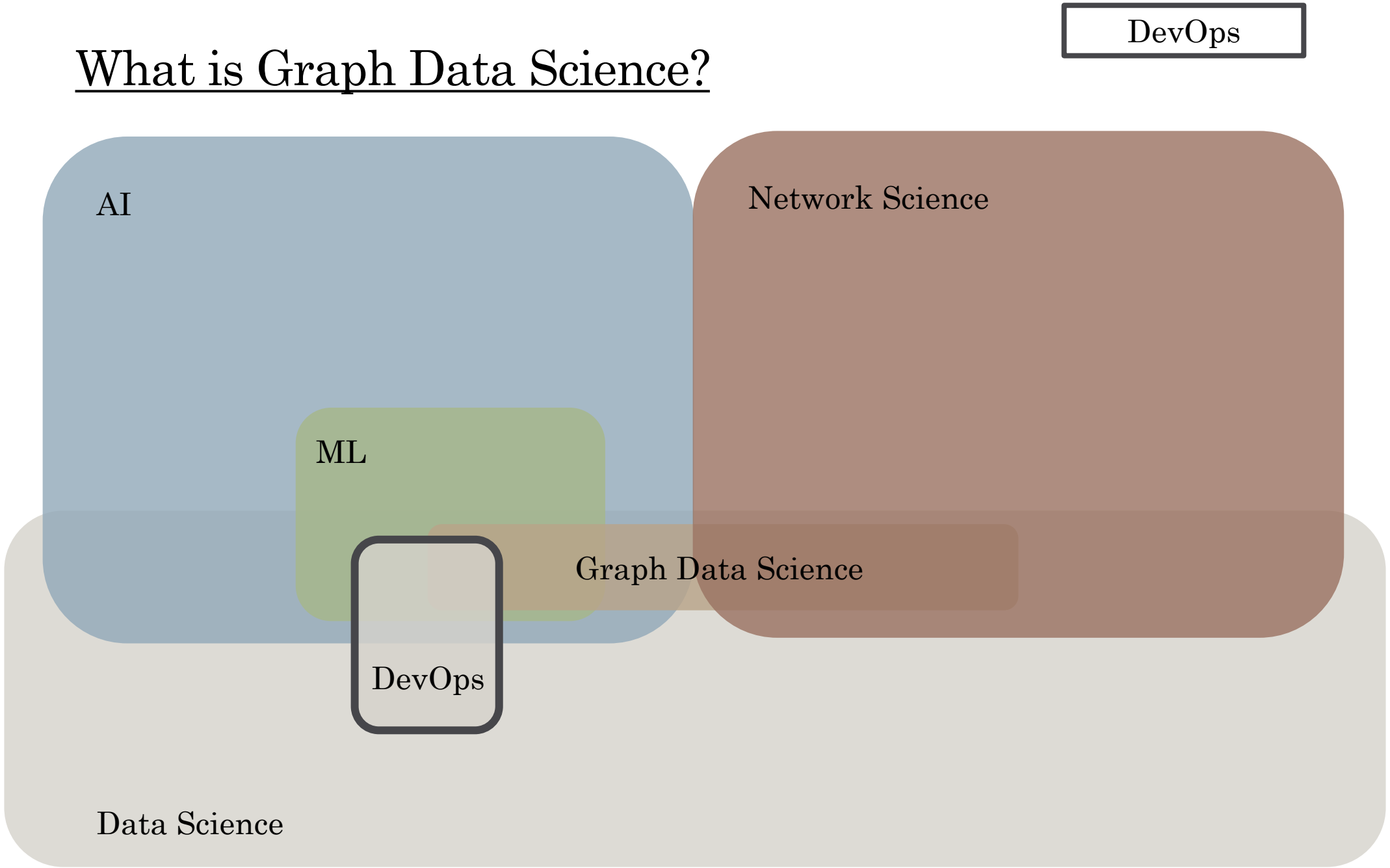

A work week in the life of a GDS

Monday	Tuesday	Wednesday	Thursday	Friday
Emails / chat	Emails / chat	Emails / chat	Emails / chat	Emails / chat
• Data analysis • AIML dev • Other software dev • Debugging	Team call Other call/email	Project support activities (e.g. documentation, maintenance, git, venvs, gpu)	• Data analysis • AIML dev • Software dev • Debugging • R&D	Continuous learning Other call/email
Lunch/office chat	Lunch/office chat	Lunch/office chat	Lunch/office chat	Lunch/office chat
Calls / meetings • Manager • Stakeholders • Business • Peers • Knowledge sharing	• Data analysis • AIML dev • Other software dev • Debugging • R&D	Alignment calls Data-related work (engineering, DevOps)	Other call/email Documentation Preparing slides Dashboard dev	• Data analysis • AIML dev • Other software dev • Debugging • R&D

A typical Data Science project workflow

1. Identify the problem / a business need

Icons from Flaticon (retrieved 2023-05-13)

A typical Data Science project workflow

1. Identify the problem / a business need
2. Formulate an idea in analytical ways, think of a solution
3. Implement a small prototype for the solution

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A typical Data Science project workflow

MONTHS

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5. Promote, validate with business, get feedback, evaluate
6. Improve and test again

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A YEAR

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A YEAR

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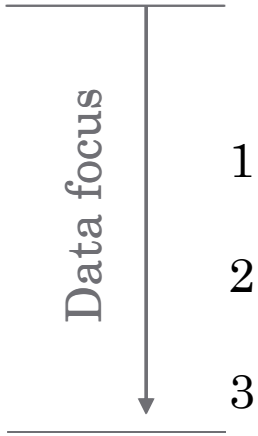
YEARS

8. Test and improve
9. Monitor and maintain

Icons from Flaticon (retrieved 2023-05-13)

A typical data modelling pipeline



1. Data collection
2. Data understanding
3. Data cleaning and processing

A typical data modelling pipeline

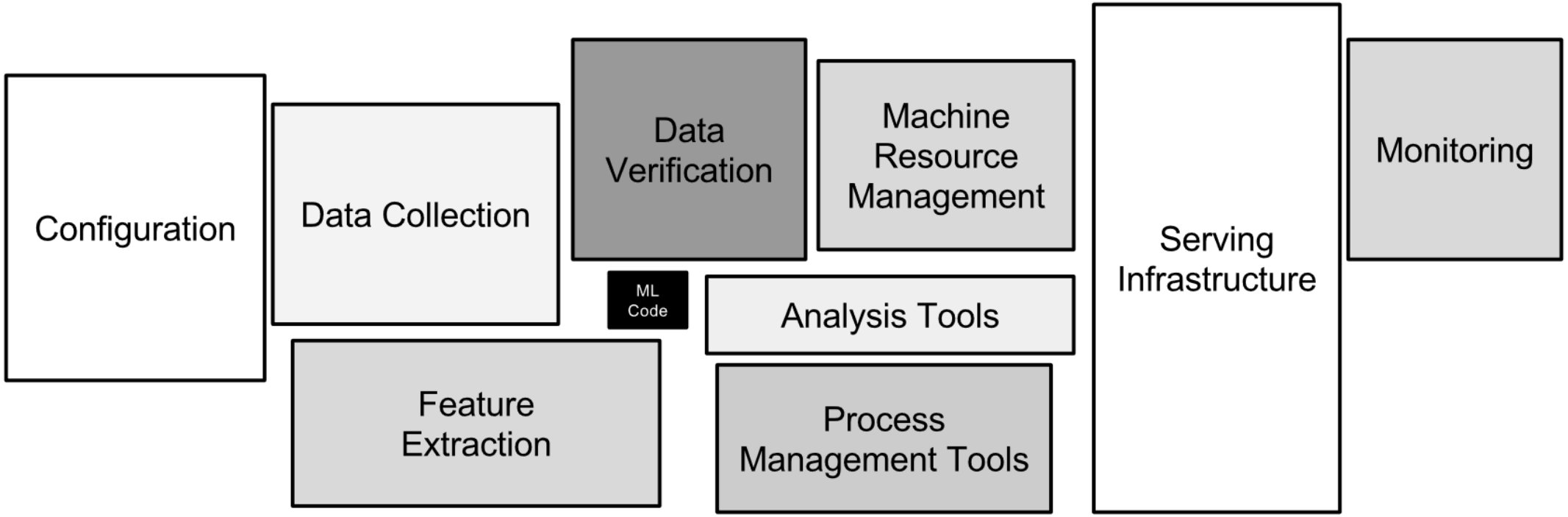
Data focus

1. Data collection
2. Data understanding
3. Data cleaning and processing

Data **and** model focus

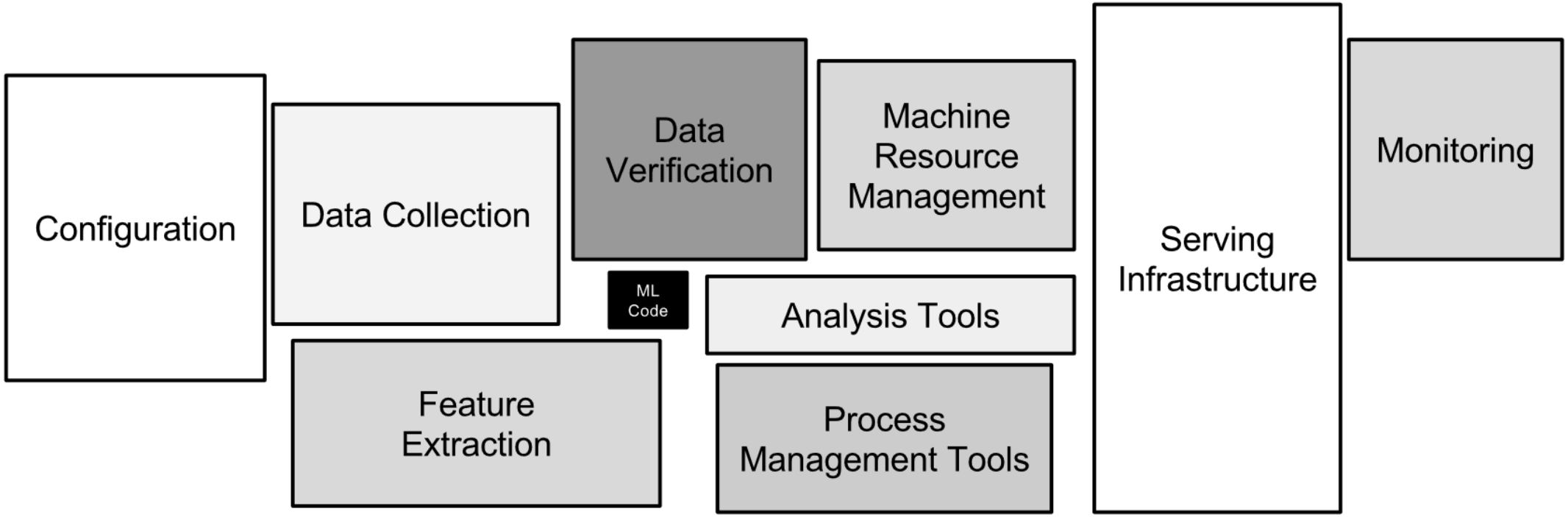
4. Model development and training
5. Model testing and business validation
6. Model deployment (and/or dashboard deployment)
7. Model maintenance (incl. retraining + retesting)

(Hidden) complexity of a data science project



Sculley *et al.*, NeurIPS **28** (2015)

(Hidden) complexity of a data science project



Sculley *et al.*, NeurIPS **28** (2015)

Additional conditions for success:

- IT support (infrastructure, model consumption, platforms)

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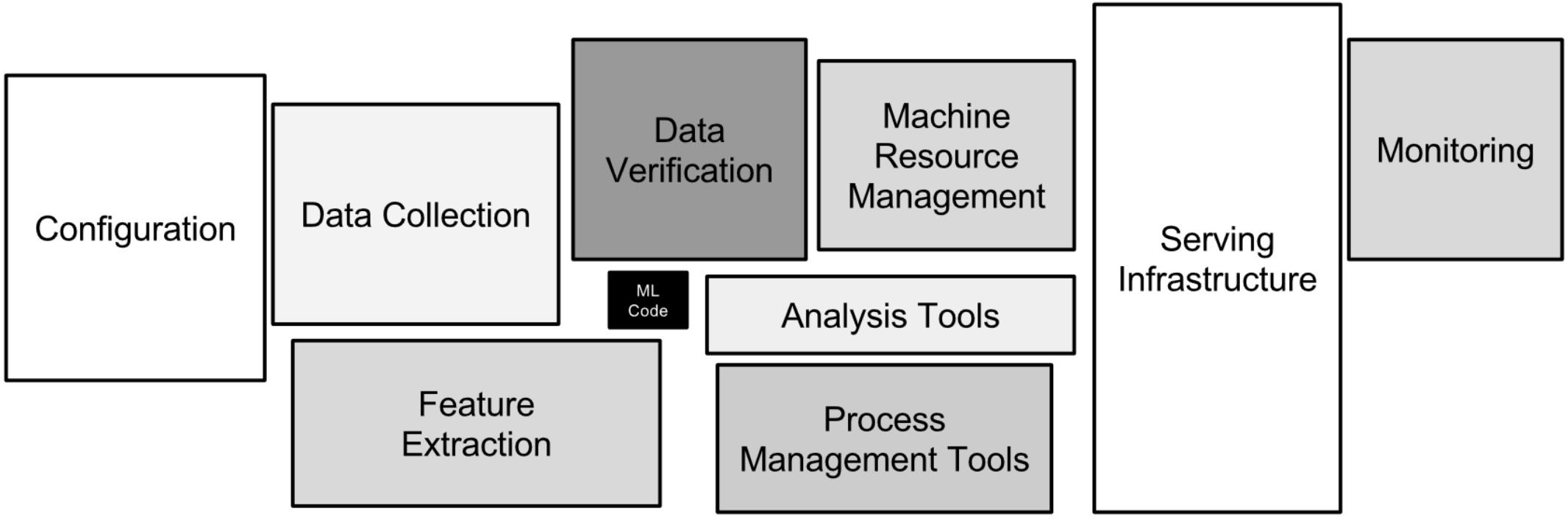

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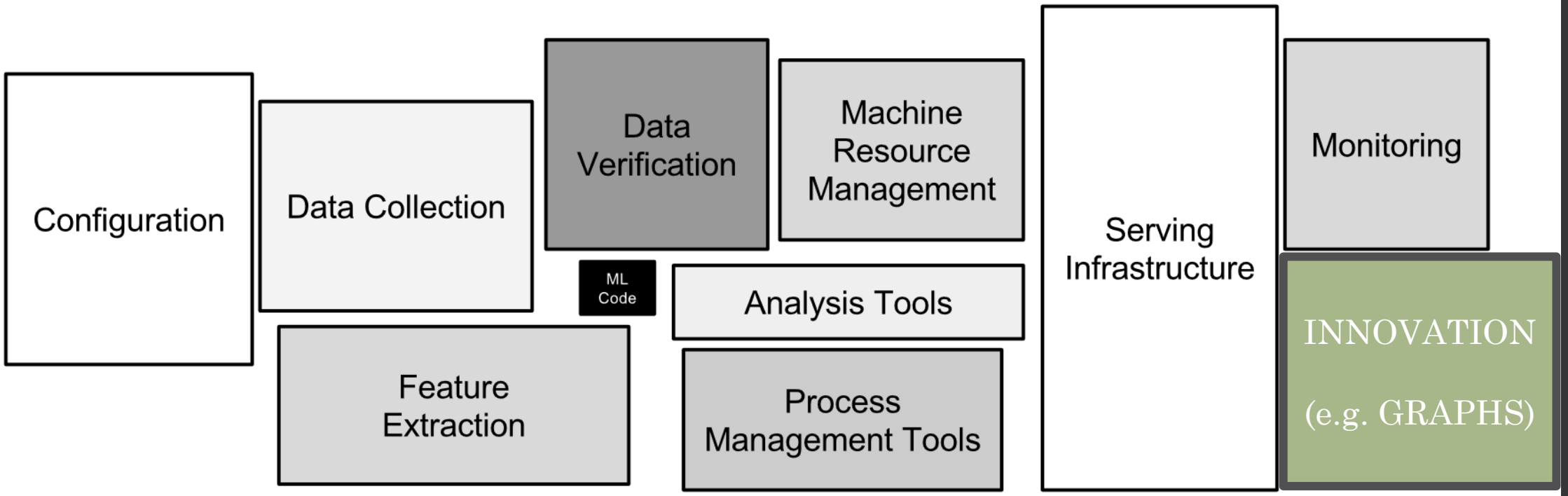

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