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We don’t talk about Semantic Web Technologies

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https://www.psdi.ac.uk/

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About Me

- Senior Enterprise Fellow at University of Southampton
- Pathfinder Lead & Researcher for PSDI Project: Process Recording
- Coordinates AI4SD & Future Blood Testing Network
- Research Interests: Semantic Web Technologies, IoT, Research Data Management, Digitisation, Lab of the Future, Paperless Labs, Re-use of Technology
- @SamiKanza

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Lets talk about the Semantic Web

Conclusions

- **The Semantic Web is coming!**
  - Joint development between DARPA/EU/and W3C communities
  - Languages and tools are available to play with
    - Http://www.daml.org/
  - W3C interest group available for those wishing to join the discussion
    - Www-rdf-logic@w3c.org (live or archived)
  - Ongoing DoD and commercial projects
- **Come join us**
  - Submit ontologies/marked up pages
  - Develop tools or help test ours
- **Get in on the next big thing early!**

www.daml.org

https://www.wi-consortium.org/wicweb/pdf/wi-hendler.pdf

WI-2001: Maebashi, Japan

MiND

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Common Misconceptions

The concept of machine-understandable documents does not imply some magical artificial intelligence allowing machines to comprehend human mumblings. It relies solely on the machine's ability to solve well-defined problems by performing well-defined operations on well-defined data. So, instead of asking machines to understand people's language, the new technology, like the old, involves asking people to make some extra effort, in repayment for which they get major new functionality – just as the extra effort of producing HTML mark-up is outweighed by the benefit of having content searchable on the web.

Berners-Lee, T. and Hendler, J., 2001. Publishing on the semantic web. *Nature*, *410*(6832), pp.1023-1024.

Berners-Lee, T., Hendler, J. and Lassila, O., 2001. The semantic web. Scientific american, 284(5), pp.34-43.

The Semantic Web will enable machines to COMPREHEND semantic documents and data, not human speech and writings.

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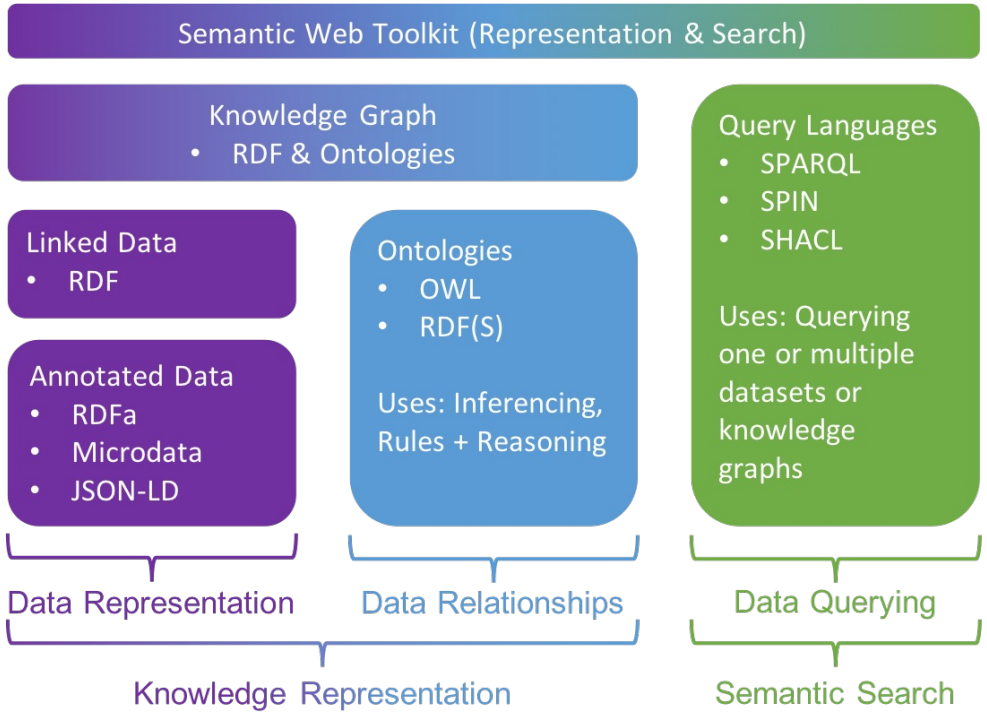
So what is the Semantic Web?

- The Web of Linked Data
- Creating machine-readable/understandable data
- A way to bring context and meaning to data
- A set of common standards for data representation, integration, and search



https://www.sciencedirect.com/science/article/pii/B978012801238311520X?via%3Dihub

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So where did this all go wrong?

https://www.pinterest.co.uk/pin/539306124105554567/

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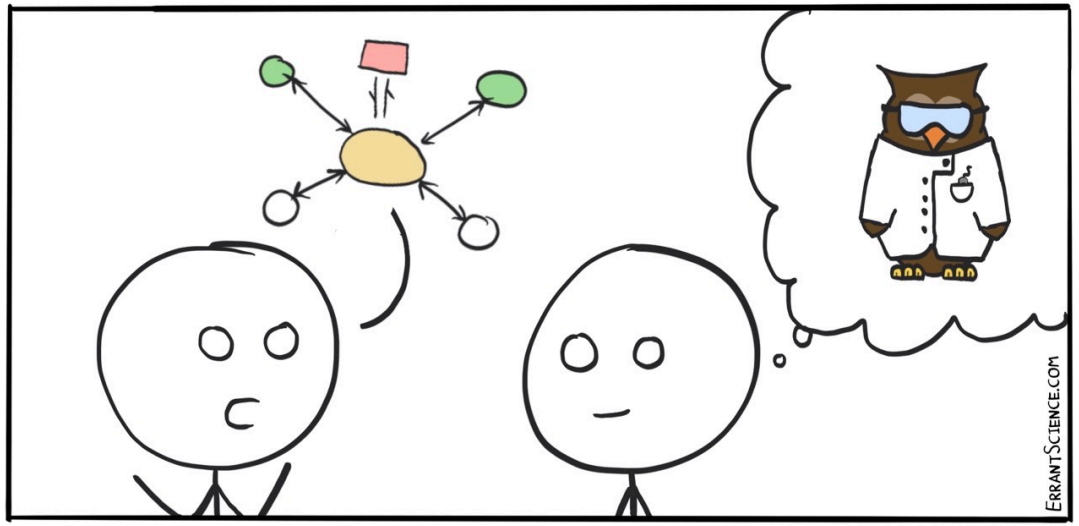
Ontologies

- Too many ontologies (and yet not enough?)
- “Lets just make a new one” mentality
- Lack of standards for Ontologies (aside from the biology sphere)
- Ontology projects frequently don’t consider the full data lifecycle
- Ontologies aren’t always well maintained
- Ontologies aren’t always FAIR
- Ontology tools are poor or expensive



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Linked Data Creation/Conversion

- Tools to convert structured data into linked data are still lacking
- R2RML even with additional libraries is repetitive
- Existing tools (OpenRefine or Karma) are very clunky and require a lot of human editing
- Writing custom scripts seems to be the best current method but isn't very user friendly

https://imgflip.com/memegenerator/

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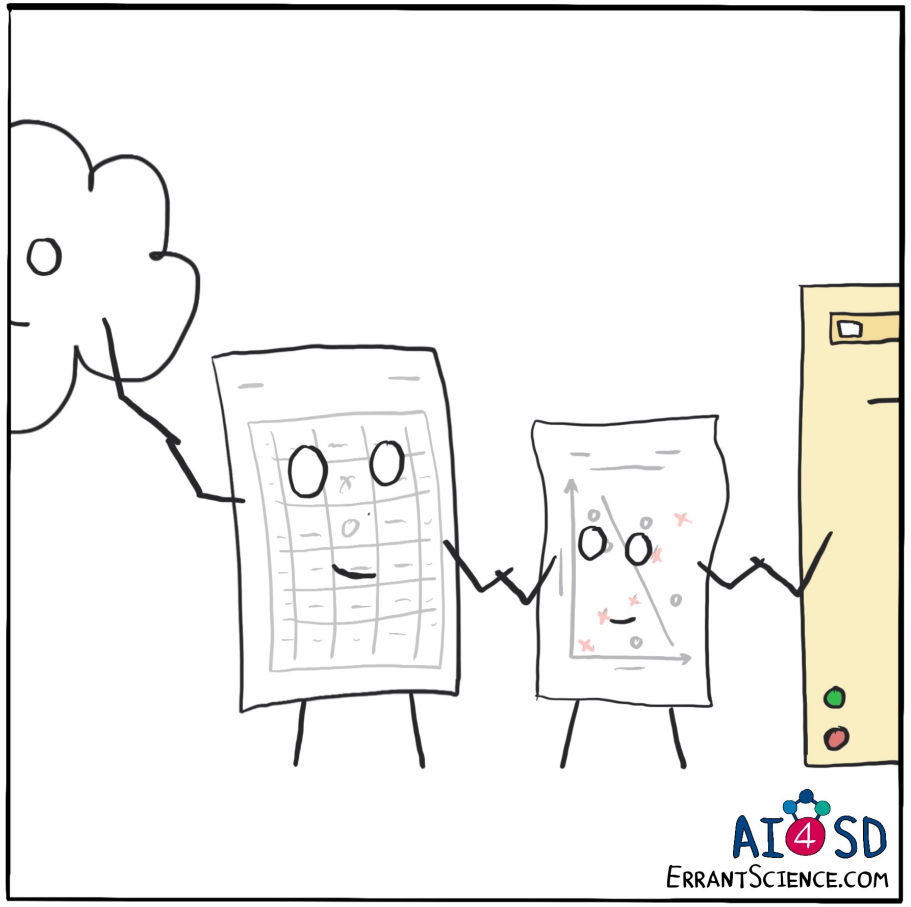
Data Storage & Data Types

- Some data doesn't lend itself well to being represented semantically (e.g. numerical classifications)
- Large datasets lead to even larger knowledge graphs
- Issues with reading, writing and deleting data with certain (free) versions of triple stores



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Given these issues, why should we care?

- Defining Common Shared Vocabularies
- Machine Readable Data
- Interoperable Metadata
- Linking Datasets
- Inferencing
- Semantic Search
- Unlocking the potential of AI/ML

https://imgflip.com/i/4x69cr

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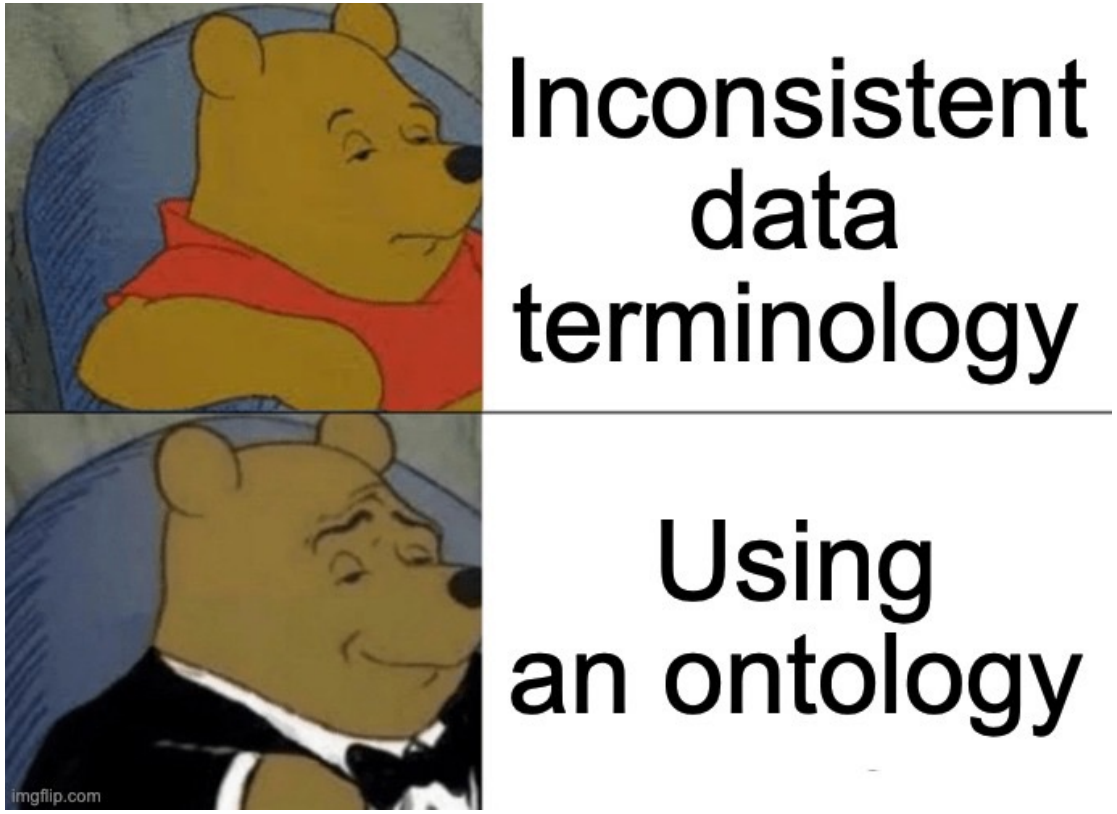
Common Shared Vocabularies

- Define a common set of terms to describe scientific data concepts consistently
- Markup your datasets to talk about the SAME concepts



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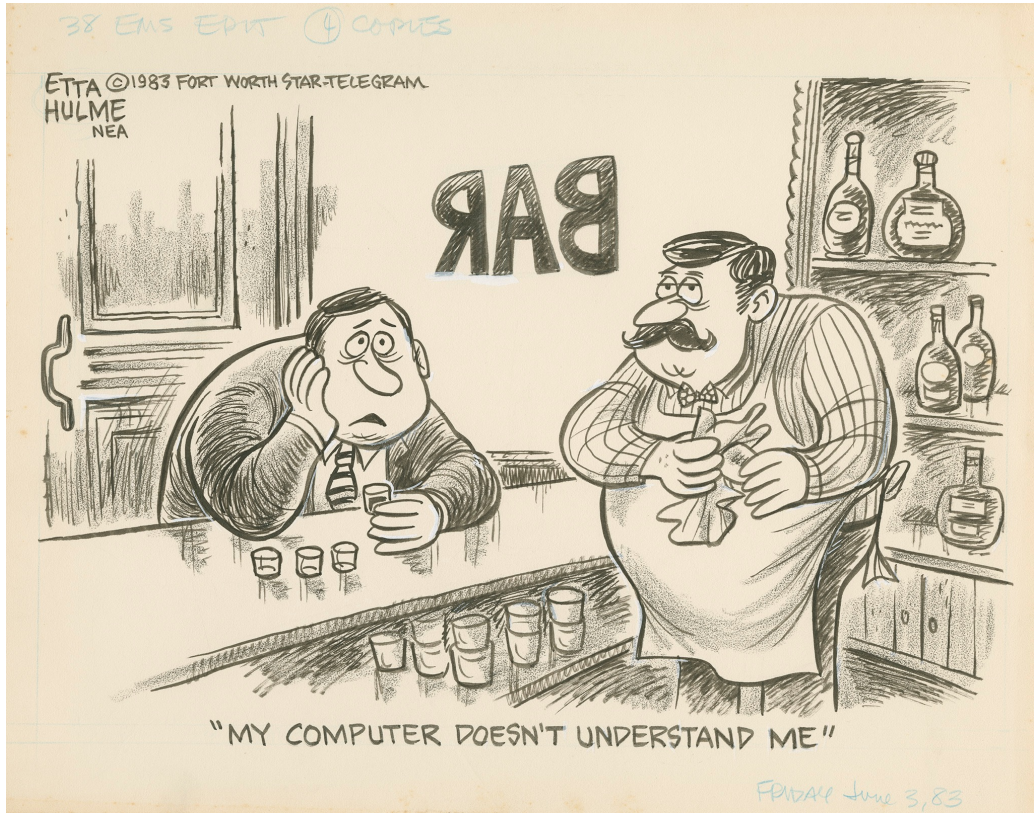
Machine Readable Data

- How can computers be expected to analyse and make decisions on scientific data they don't understand?



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Rich Interoperable Metadata

- Adding rich interoperable semantic metadata to your documents / webpages adds a whole new dimension to your data

https://www.pinterest.co.uk/jaci_mize/metadata/

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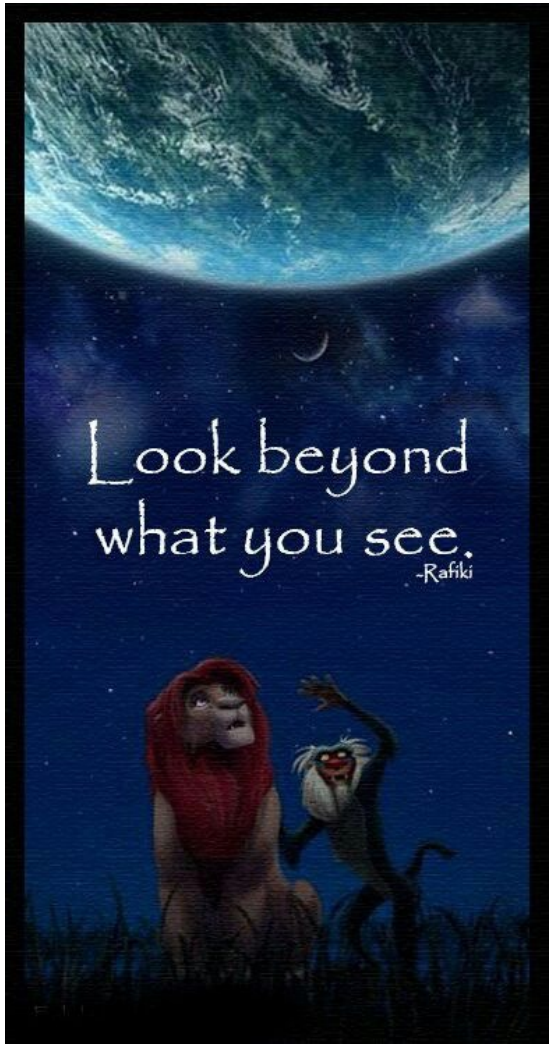
Semantic Knowledgebases

- Scientific Research can be significantly enhanced by linking datasets together to create knowledgebases:
  - Find undiscovered links
  - Answer questions that cannot be addressed with a single data source
  - Very useful for domains like drug discovery which require the integration of disparate datasets



https://www.pinterest.co.uk/pin/2674081014251214/

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Inferencing

- Description Logic can be embedded into Ontologies
- This enables machines to “infer” additional information that is not explicitly defined in the data

https://quoteswell.com/cheshire-cat-quotes/

Example: If we know that:

```
Sami isAllergicTo Juniper
Gin hasBotanical Junpier
```

Then we can infer: `Sami isAllergicTo Gin`

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Semantic Search

- Search on CONCEPTS across LINKED DATASETS

https://garfield.com/comic?keywords=Jon&page=1113

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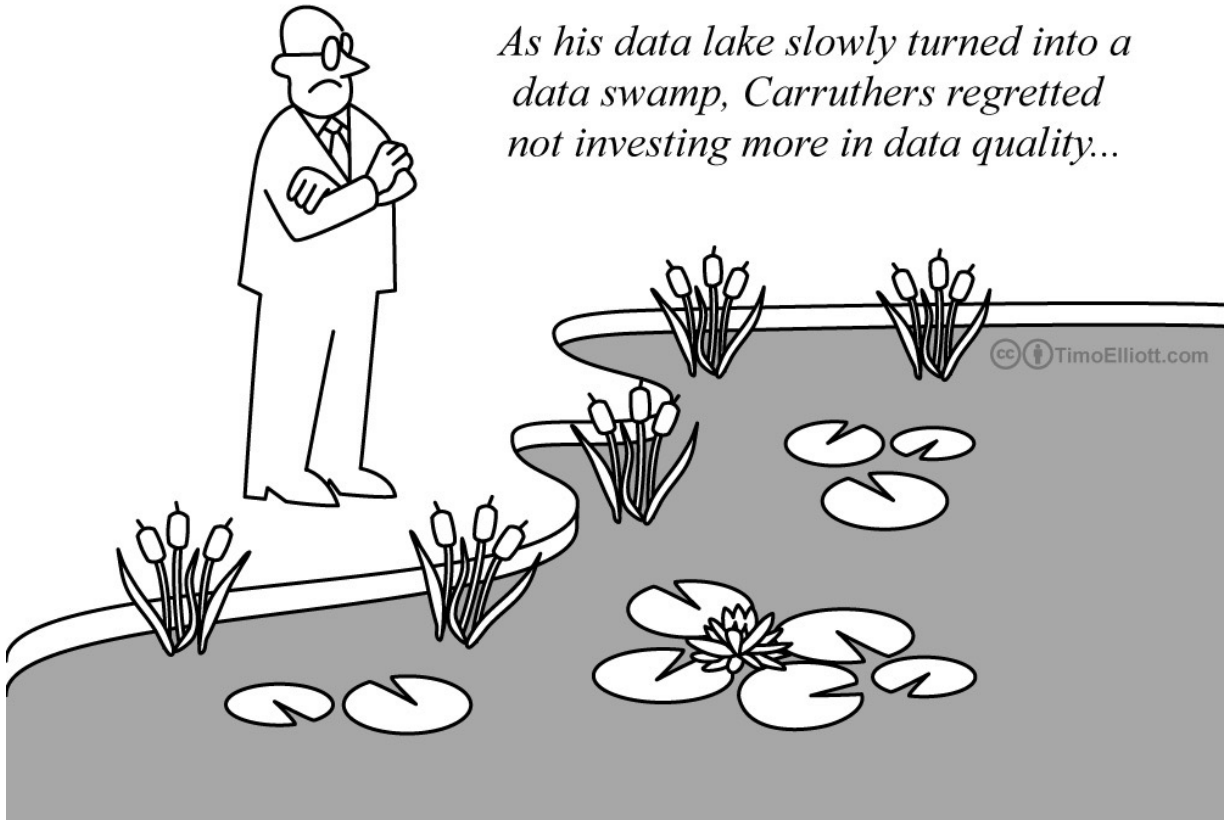
Unlock the Potential of AI & ML

- Don’t waste your algorithms time with poorly formed inconsistent data



https://timoelliott.com/blog/cartoons/more-analytics-cartoons

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So what can we do?

https://memegenerator.net/instance/68158697/hermione-leviosa-swish-flick

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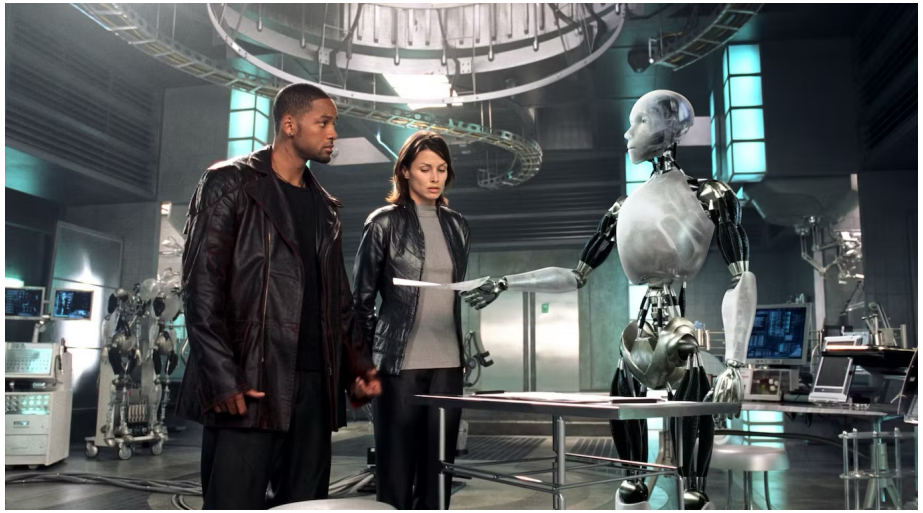
You need to ask the right questions

- What is your use case for semantics?
- Do you need an ontology?
- Do you need a knowledge graph?
- How much data do you need to represent semantically?
- What data would benefit from being in a semantic format?
- What do you want your data to look like and how are you going to use it?



https://www.inverse.com/culture/sci-fi-movies-january-2023-hbo-max-i-robot

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Consider your Conversion in Advance

- Converting data into linked data is non-trivial
- Conceptualising an Ontology vs using it in a dataset are two different things
- You need to consider the entire semantic data lifecycle of a project

https://www.woorank.com/en/blog/implement-semantic-web

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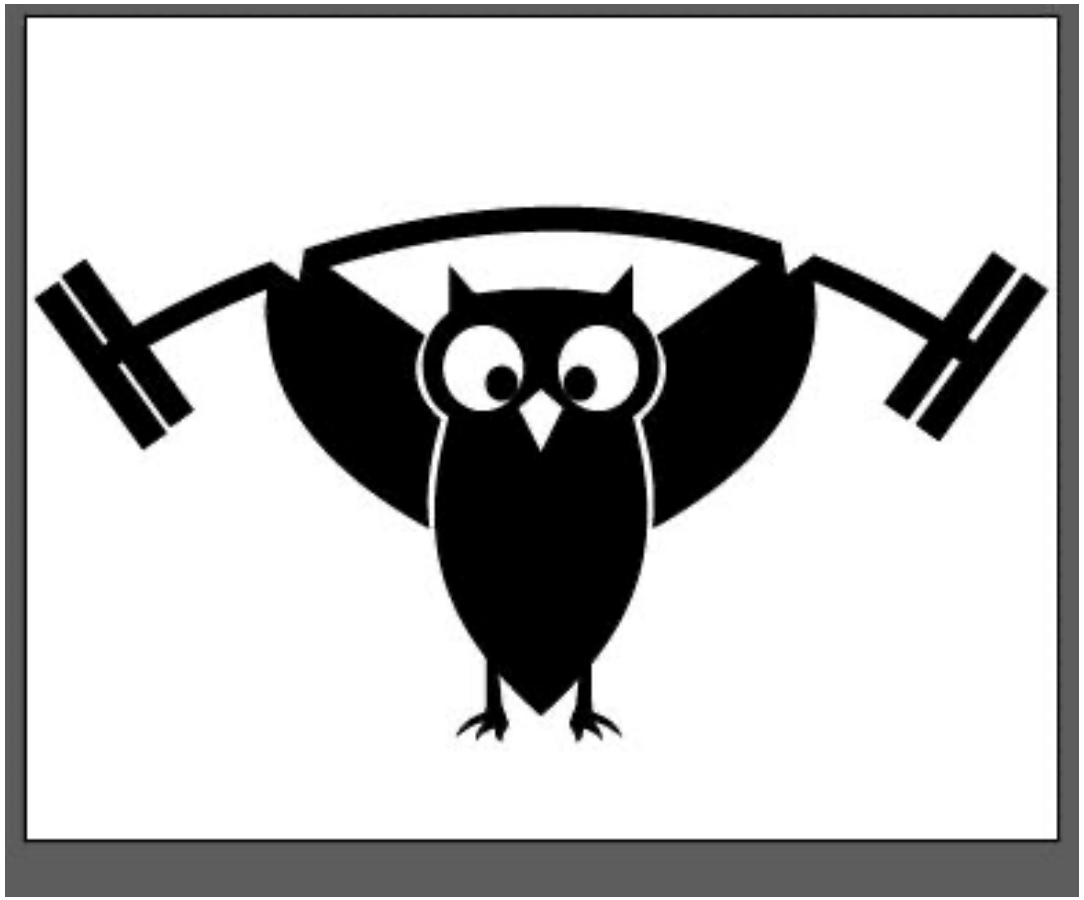
Think about the WHY and the WHAT



https://cuk00jan.wordpress.com/2014/02/14/who-is-alpha-owl/

- Think about WHY you are making Ontologies and WHAT they are for
- Play to OWLS Strengths

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Re-use and extend Ontologies where possible

- There are lots of ontologies out there! See if there's any you can re-use before making a new one (Search Papers/OLS/Google)
- Re-use doesn't just mean ontologies! You can re-use design patterns as well!
- Consider trying to create an extension to an existing ontology if appropriate

https://www.fosteropenscience.eu/content/cartoonreusable-data

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Modularize your Ontologies

- Break your ontologies into smaller related modules

Relation to time / Granularity	Continuant				Occurrent
	Independent			Dependent	
Complex of organisms	Family, community, deme, population		Environment	Population phenotype	Population process
Organ and organism	Organism (NCBI Taxonomy)	(FMA, CARO)		Organ function (FMP, CPRO)	Phenotypic Quality (PaTO)	Biological process (GO)
Cell and cellular component	Cell (CL)	Cell component (FMA, GO)		Cellular function (GO)		
Molecule	Molecule (ChEBI, SO, RnaO, PrO)			Molecular function (GO)		Molecular process (GO)

https://www.researchgate.net/publication/268412593_Ontology-Based_Knowledge_Representation_of_Experiment_Metadata_in_Biological_Data_Mining/figures?lo=1

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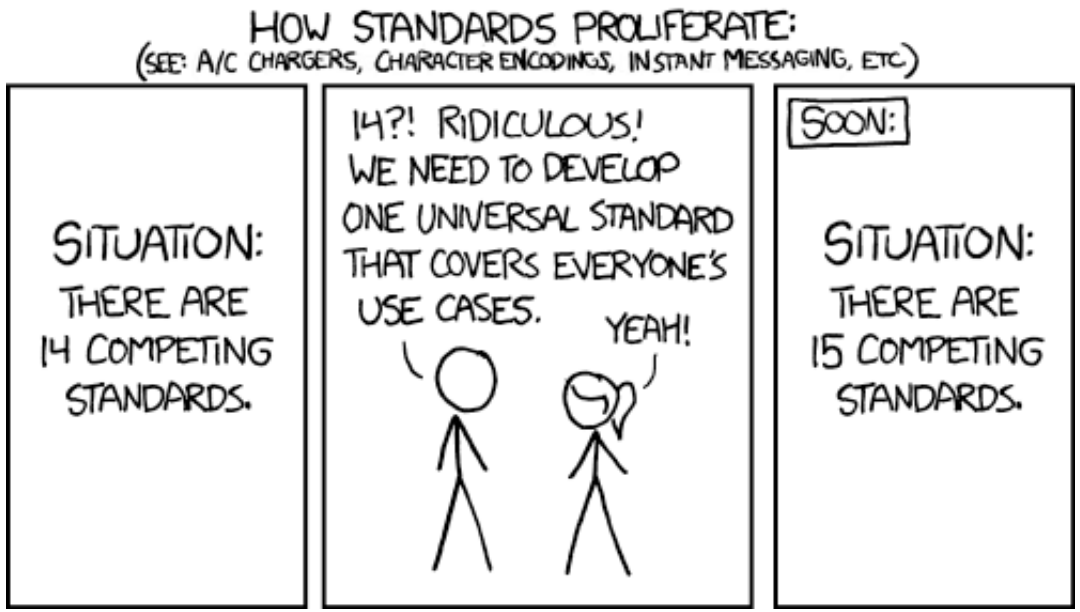
Don’t forget your standards

- Even your standards should have standards
- Consider:
  - Design patterns
  - Upper Level Ontologies
  - Consistency



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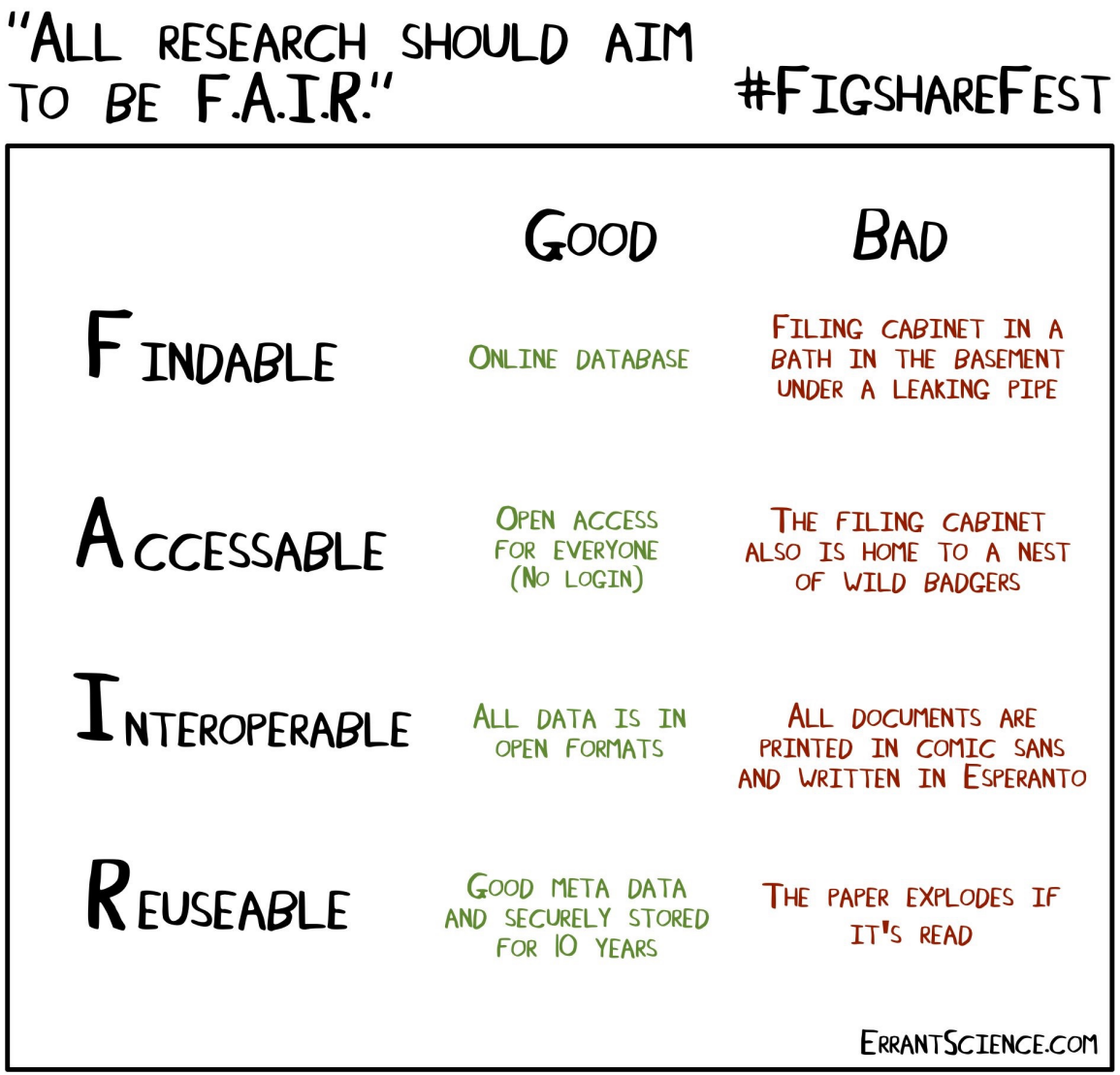
FAIR is a Four Letter Word



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Garbage In = Garbage Out

- GIGO can still apply even in the world of semantics

https://ffineis.github.io/blog/2017/09/13/case_for_big_govt.html

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Conclusions

- We're all in this together and we need to work together!
- A lot of the technology is there, we just need to use it properly!
- This is as much a human endeavor as a technical one!

https://www.thedesigngym.com/skip-collaboration-collaborations-sake/

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Relevant Publications & Talks

- Kanza, S., Willoughby, C., Gibbins, N., Whitby, R., Frey, J.G., Erjavec, J., Zupančič, K., Hren, M. and Kovač, K., 2017. Electronic lab notebooks: can they replace paper?. Journal of cheminformatics, 9(1), pp.1-15. https://doi.org/10.1186/s13321-017-0221-3
- Kanza, S., Stolz, A., Hepp, M. and Simperl, E., 2018. What does an ontology engineering community look like? A systematic analysis of the schema. org community. In The Semantic Web: 15th International Conference, ESWC 2018, Heraklion, Crete, Greece, June 3–7, 2018, Proceedings 15 (pp. 335-350). Springer International Publishing. https://doi.org/10.1007/978-3-319-93417-4_22
- Kanza, S., 2018. What influence would a cloud based semantic laboratory notebook have on the digitisation and management of scientific research? (Doctoral dissertation, University of Southampton). https://eprints.soton.ac.uk/421045/
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- Kanza, S. and Frey, J.G., 2019. A new wave of innovation in Semantic web tools for drug discovery. Expert Opinion on Drug Discovery, 14(5), pp.433-444. https://doi.org/10.1186/s13321-019-0345-8
- Kanza, S. and Frey, J.G., 2020. Semantic technologies in drug discovery—potential, practical, possibilities. http://dx.doi.org/10.1016/B978-0-12-801238-3.11520-X
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- Kanza, S., Willoughby, C., Bird, C.L. and Frey, J.G., 2022. eScience Infrastructures in Physical Chemistry. Annual Review of Physical Chemistry, 73, pp.97-116. https://doi.org/10.1146/annurev-physchem-082120-041521
- Kanza, S., Willoughby, C., Knight, N.J., Bird, C.L., Frey, J.G. and Coles, S.J., 2023. Digital research environments: a requirements analysis. *Digital Discovery*. https://doi.org/10.1039/D2DD00121G

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