

# Why Data Citation is a Computational Problem

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#### Outline

#### The power of abstraction

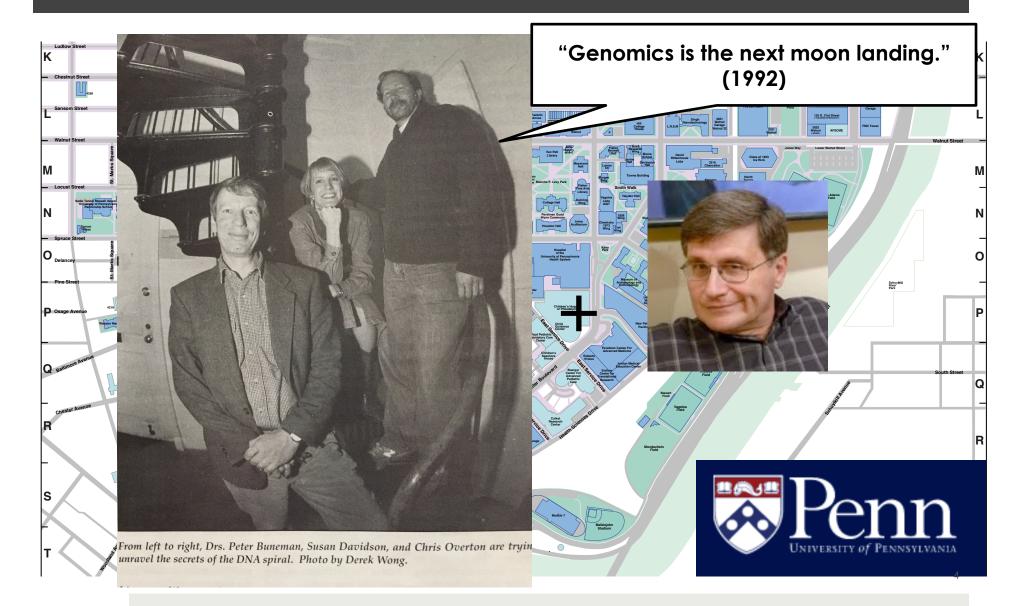
- And how it has helped with two of my favorite problems in bioinformatics
- New problem: data citation
- Bigger picture: Data Science

### The power of abstraction

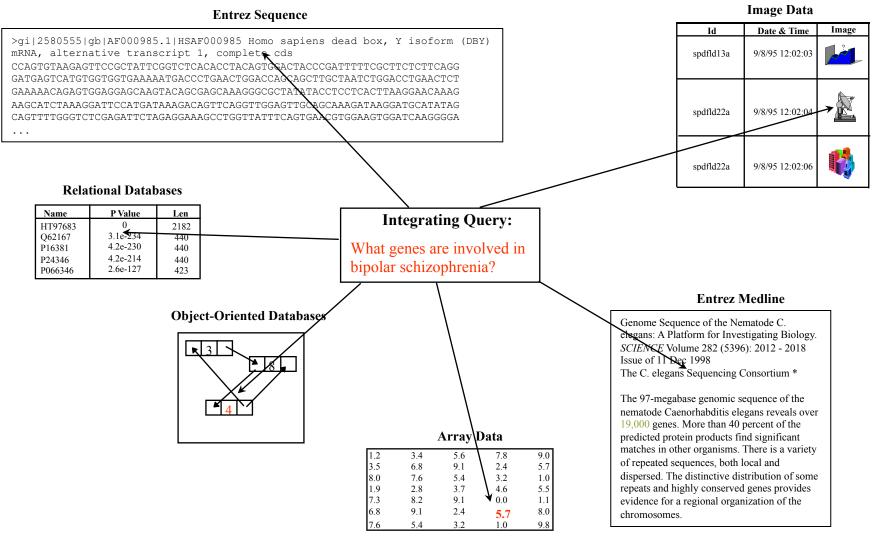
- The "right" abstraction is key to developing solutions to many practical problems.
  - Data Integration
  - Provenance
  - •
  - Data Citation
- Developing the right abstraction requires close collaboration between end-users, systems builders, and theoreticians.

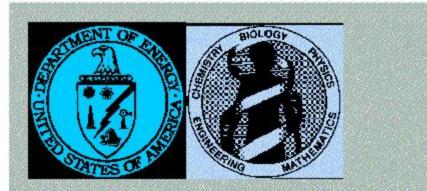


#### Databases meets bioinformatics



#### Example 1: Data Integration





#### Report of the Invitational DOE Workshop on

#### Genome Informatics, 26-27 April 1993

The Office of Health and Environmental Research of the Department of Energy (OHER/DOE) sponsored a meeting in Baltimore on 26–27 April of a group of experts to assess the state of current OHER-related bioinformatics efforts and to offer advice on planning and coordinating future activities. OHER has a considerable interest in bioinformatics, in large part, because of the DOE Human Genome and the Structural Biology programs.

TOPICS DISCUSSED IN DOE INFORMATICS SUMMIT

26-27 APRIL 1993, BALTIMORE, MD

"Until a fully relationalized sequence database is available, none of the queries in this appendix can be answered."

#### Why would they say that?

- Needed to pose set-oriented queries against multiple, heterogeneous databases, files, and software packages.
  - Most integration work at the time was based on the relational model
  - Embedded links in files: Clicking doesn't scale!
- Needed in-depth understanding of what data sources were available and what information they contained.

### Answering the "unanswerable"

- We were able to answer the "unanswerable queries" within about a month using our data integration system, Kleisli.
- Kleisli used a complex-object model of data, language based on comprehension syntax, and optimizations that went beyond relational systems.



Kyle Hart, Jonathan Crabtree,...

Leonid Libkin, Dan Suciu,...

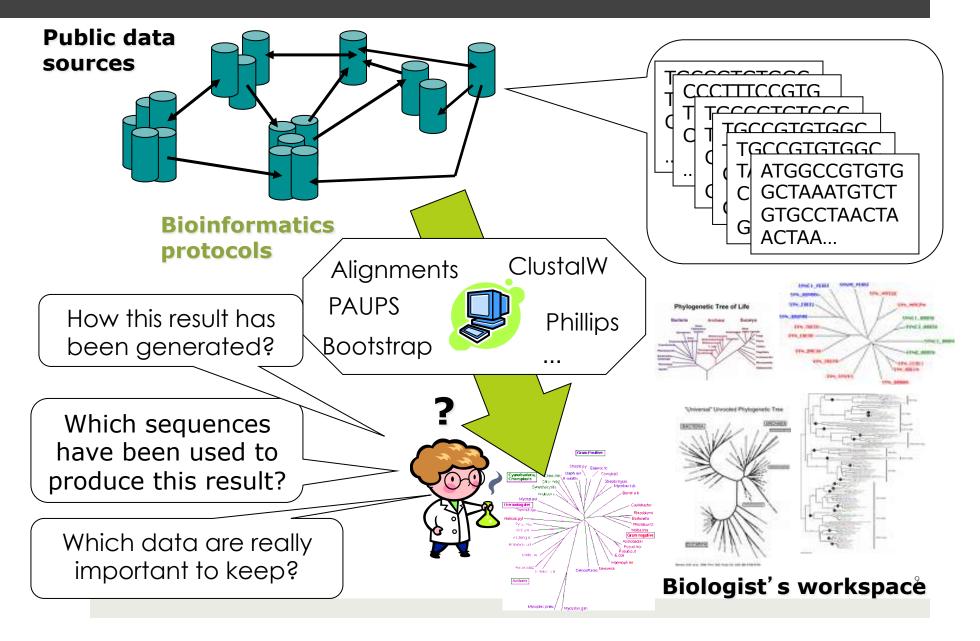
BioGuideSRS (Cohen-Boulakia)

...Ś

The Q Query System (Ives)



#### Example 2: Provenance



#### Different types of provenance

- "Coarse-grained" workflow provenance
  - Kepler (Ludaescher et al.), Pegasus (Deelman, Gil et al.), Taverna (Goble, Oinn et al.), Vistrails (Freire et al.),...
- "Fine-grained" database style provenance
  - Why and Where: Buneman, Khanna, Tan
  - Provenance Semirings: Tannen, Green, Karvouranakis
  - Trio: Widom, Cui, Weiner et al
- Event logs (ordering, timing, causality matters)
  - Provenance-Aware Storage Systems: Seltzer et al
  - Secure Network Provenance: Zhou, Loo, Haeberlen

#### The problem with provenance...



### Continuing challenges...

- Combining difference types of provenance
- Tools to query, explore, and understand provenance
- Summarizing provenance
- Approximating provenance
- ...

#### Outline

The power of abstraction

#### New problem: data citation

- State of the art
- Citations for general queries
- Building a citation system
- Bigger picture: Data Science



### Data Citation

# Publication is changing

- Information is increasing published on the web.
- Much of this information is in curated databases – crowd- or expert-sourced data
- These datasets are complex, structured, and evolving, and contributors need to be acknowledged

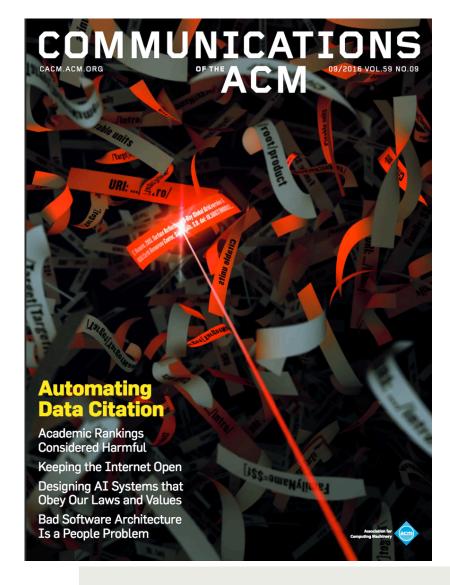


An expert-driven guide to pharmacological targets and the substances that act on them.

#### Citation: Principles and Standards

- Large number of organizations are involved, and standards are emerging: Datacite, DataONE, GEOSS, D-Lib Alliance, DCC, COPDES, Force-11, AGU, ESIP, DCMI, CODATA, ICSTI, IASSIST, ICSU...
  - Force 11: "Data citations should be accorded the same importance in the scholarly record as citations of other research objects, such as publications."
  - DataCite: "We believe that you should cite data in just the same way that you can cite other sources of information, such as articles and books."
  - Amsterdam Manifesto: "Data should be considered citable products of research."

### Our manifesto...



- Principles and standards for data citation are unlikely to be used unless the process of extracting information is coupled with that of providing a citation for it.
- We need to automatically generate citations as the data is extracted.
- Data citation is a computational problem.

Buneman, Davidson, Frew: Why data citation is a computational problem. <u>Commun. ACM 59(9)</u>: 50-57 (2016)

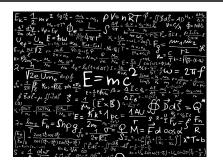
#### What is a (conventional) citation?

- A collection of "snippets" of information: authors, title, date, etc. and some kind of access mechanism
- Not exactly provenance
- Self contained, immutable (to within some choice of format)
- Needed for a variety of reasons: kudos, currency, authority, recognition, access...

Buneman, Davidson, Frew: Why data citation is a computational problem, Commun. ACM, 59(9): 50—57 (2016)

## Citation goes beyond DOIs

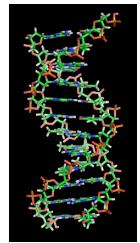
Ann. Phys., Lpz 18 639-641



#### Einstein:

Does the inertia of a body depend on its energy content?

Nature, 171,737-738



#### Watson and Crick:

Molecular Structure of Nucleic Acids; a structure for deoxyribose nucleic acid









An expert-driven guide to pharmacological targets and the substances that act on them.

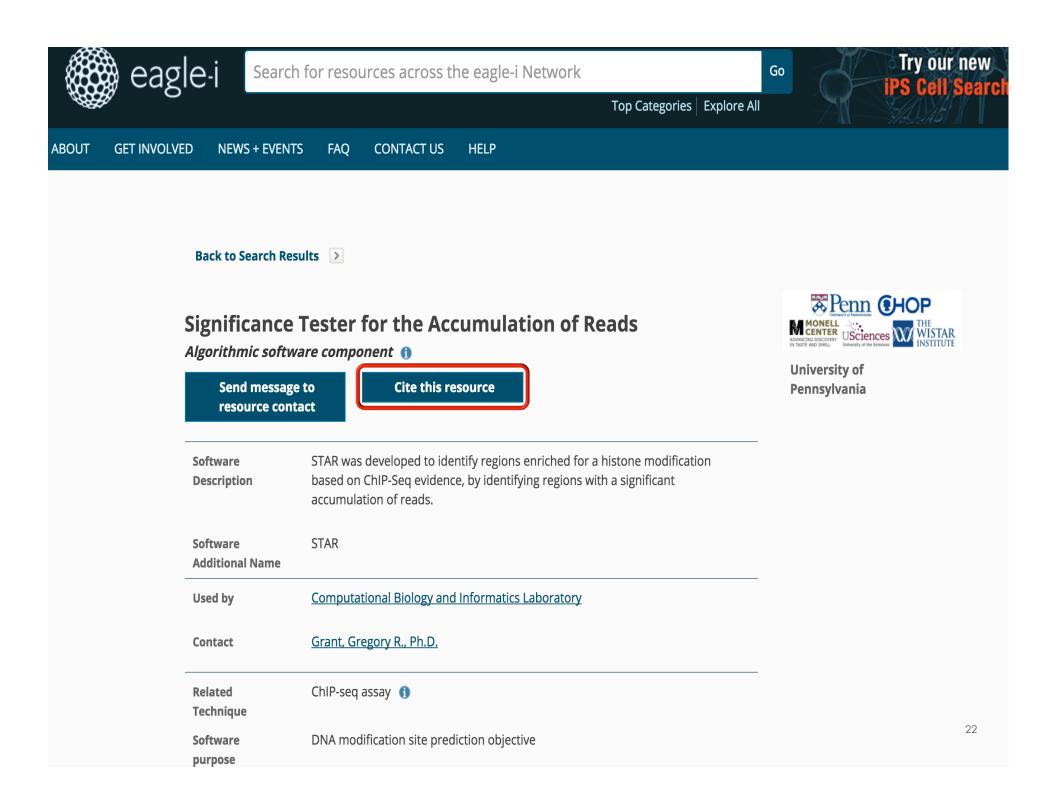
## State of the art in data citation ...

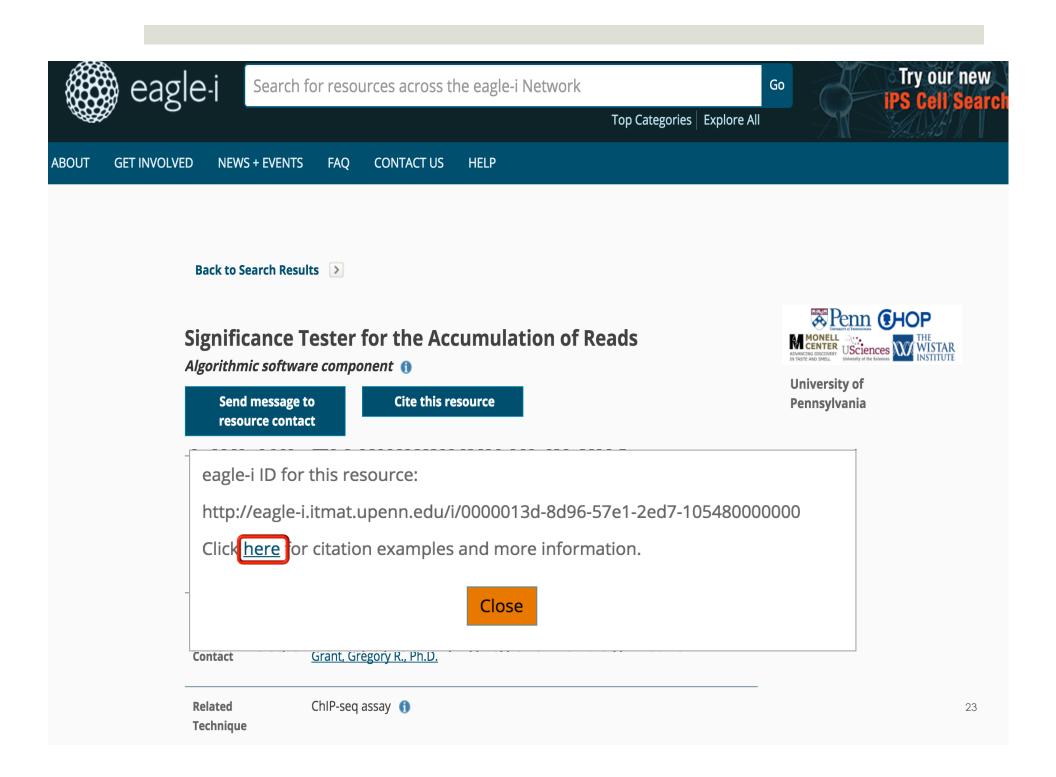
#### Example 1: eagle-i

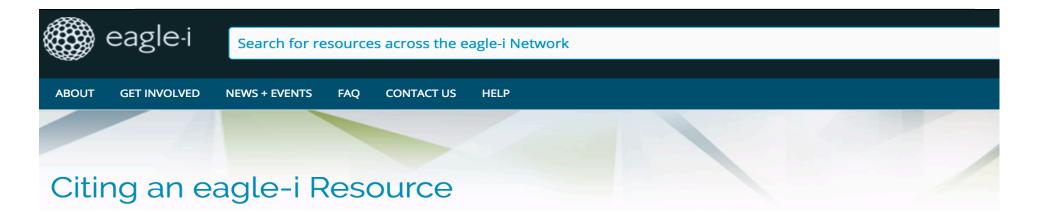
- A "resource discovery" tool built to facilitate translational science research.
- Developed by a consortium of universities under NIH funding, headed by Harvard.

Penn is a member.

- End users: researchers who wish to share information about research resources (Core Facilities, iPS cell lines, software resources).
- Data is stored and distributed as RDF files (graph database).
- Resources have a "Cite this resource" button!

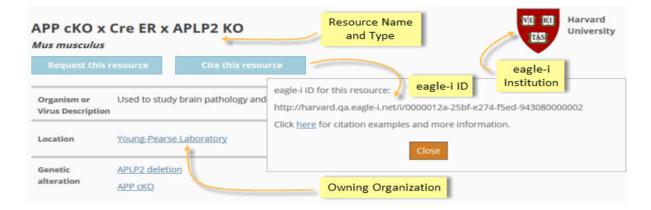






#### Citing eagle-i resources is an easy way to give credit.

The formats suggested below provide the minimum information necessary to identify and credit the resource provider, and are designed to provide a traceable, durable, and unambiguous reference for the resource being cited. These suggestions can and should be used along with those from other resource identifiers (i.e. Antibody Registry ID, Addgene, DSHB, RRID) or from the journal publishing your work.



Note that for all types, the names of Core Facilities or other ambiguously named organizations should be followed by the name of the affiliated eagle-i institution in order to disambiguate them (e.g. *Flow Cytometry Core. Montana State University vs. Flow Cytometry Core. Dartmouth College*).

#### **Citation Guidelines**

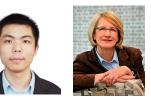
Although only the most commonly cited types are listed below, the same rules can be used to cite any eagle-i resource.

### Automating citation in eagle-i

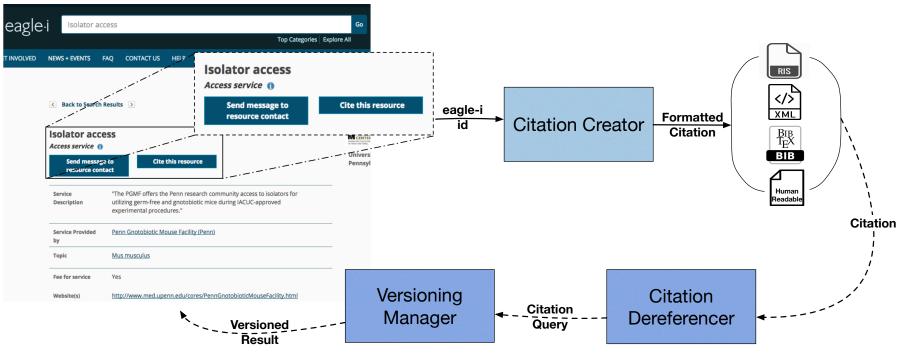








A. Alawini, L. Chen, S. B. Davidson, N. Da Silva, G. Silvello: "Automating data citation: the eagle-I experience." JCDL 2017.



#### Example 2: IUPHAR

- IUPHAR Guide to Pharmacology is a database of information about drug targets, and the prescription medicines and experimental drugs that act on them.
- Information is presented to users through a hierarchy of web views, with an underlying relational implementation.

Targets are arranged into groups called "families"

Contents of the database are generated by hundreds of experts who, in small groups, contribute to portions of the database. Thus the authorship depends on what part of the database is being cited.



## Citations in IUPHAR

- Citation to the IUPHAR database as a whole (the root) is a traditional paper written by the main curators (owners) of the database.
- Each IUPHAR Family and Family Introduction page has an independent citation.
  - Information about a Family is managed by a set of curators, which may be different for each family.
  - The detailed Family Introduction page is written by a set of contributors, which may be different from the curators of the Family.

## Citations in IUPHAR, cont.

#### Family page

Home	About Targets Ligands Resources	IUPHAR/BPS Guide to PHARMACOLOGY		
► Hom	e   Targets  G protein-coupled receptors  Glucagon rec	ceptor family		
Glucagon receptor family Unless otherwise stated all data on this page refer to the human proteins. Gene information is provided for human (Hs), mouse (Mm) and rat (Rn). Expand all sections Collapse all sections				
Overvie	W			
0	« Hide	More detailed introduction		
	The glucagon family of receptors (nomenciature as agreed by the <u>NC-UPHAR</u> Subcommittee on the Glucagon receptor family [18]) are activate the endogenous peptide (27-44 aa) hormones glucagon (GCG, P01275), glucagon-like peptide 1 (GCG, P01275), glucagon-like peptide 2 (GCG, P012 gluccee-dependent insulinotropic polypeptide (also known as gastric inhibitory polypeptide (GIP, P0381)), GHRH (GHRH, P01266) and secretin (SCT P00863), One commo precursor (GCG) generates glucagon (GCG, P01275), glucagon-like peptide 1 (GCG, P01275) and glucagon-like peptide 2 (GC P01275) peptides [12].			

#### Database page citation:

Miller, Drucker, Bataille, Chan, Delagrange, Göke, Mayo, Thorens, Hills. Glucagon receptor family. Accessed on 08/05/2017. IUPHAR/BPS Guide to PHARMACOLOGY, http://www.guidetopharmacology.org/ GRAC/FamilyDisplayForward?FamilyId=1.

#### Family Introduction page



agon receptor family: Introduction

Annotation status: 
Annotated and awaiting review. Please contact us if you can help with reviewing. » Email us

#### General

Glucagon, glucagon-like peptide 1 (GLP-1), and glucagon-like peptide 2 (GLP-2) are peptide hormones encoded by a single common prohormone precursor, proglucagon (5,62). The sequence of 29 amino acid (aa) pancreatic glucagon is highly conserved in mammals. Glucagon is synthesised mainly in islet A cells and the brain and has also been localised to specific cells in the stomach and intestine in some species [61]. Further processing of glucagon may also produce the C-terminal undecapeptide miniglucagon, a powerful inhibitor of insulin secretion [23].

To cite this family introduction, please use: Miller, Drucker, Bataille, Chan, Delagrange, Göke, Mayo, Thorens, Hills. Glucagon receptor family, introduction. Accessed on 08/05/2017. IUPHAR/BPS Guide to PHARMACOLOGY, http://www.guidetopharmacology.org/ GRAC/FamilyIntroductionForward?FamilyId=1.

## Why not just hard code citations?

- Citations vary with what part of of the database is being cited.
  - There are a very large number of "parts" of a database.
- In the future, IUPHAR would like to enable general queries
  - Queries may combine "parts" in different ways.
- We cannot expect to create a citation for each possible query result.
- Citations should be lifted up to schema-level specifications so they can be reasoned about.



# Citations for general queries

### The citation generation problem

- It is common for database owners to supply citations for some parts (views) of the database, V<sub>1</sub> ... V<sub>n.</sub>.
- So the problem becomes: Given a query Q, can it be rewritten using the views? That is, is there a Q<sub>i</sub> such that

#### $\forall D \in S. Q(D) = Q_i(V_{i1}(D), \dots, V_{ik}(D))$

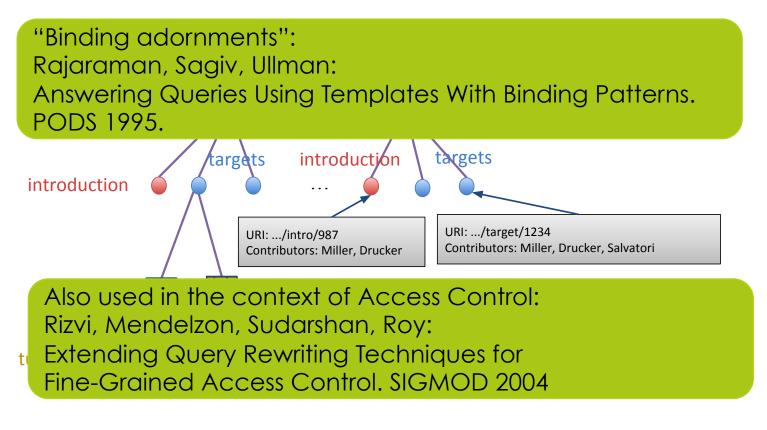
If so, the citations for V<sub>i1</sub>..., V<sub>ik</sub> could be used to create a citation for Q.

## Answering queries using views

- The problem of answering queries using views has been well studied and is generally hard – but in our context may be tractable.
  - A. Halevy. Answering queries using views: A survey. VLDB J., 10(4):270–294, 2001.
  - Lenzerini. Data Integration: A Theoretical Perspective: PODS, 2002.
  - A. Deutsch, L. Popa, and V. Tannen. Query reformulation with constraints. SIGMOD Record, 35(1): 65–73, 2006.
  - F. Afrati, C. Li and J. Ullman. Using views to generate efficient evaluation plans for queries. JCSS 73(5): 703 -724, 2007.

### "Parameterized" views

In IUPHAR there are views for Family and Family Introduction pages, parameterized by FID, and views for Target pages, parameterized by FID, TID



### Effect of parameters

Parameterized views define a family of views, one for each value of the parameter.

FID	FName	Туре
1	Glucagen receptor	GPCR
2	CLR (calcitonin receptor-like receptor)	GPCR
3	Peptidases and proteinases	Kinase
4	A multifunctional molecule, adenosine	Kinase
5	Chromatin modifying enzymes	Kinase

 $\lambda$  F. V1(F, N,Ty) :- Family(F, N, Ty)

V4(F, N,Ty) :- Family(F, N, Ty)

"Instantiated views": V1(F, N, Ty)(1), V1(F, N, Ty)(2),..., V1(F, N, Ty)(5)

## Citation views

#### To specify a citation, there are three components:

□ View definition: spe "Universal" across different

Citation query: spec information to includ types of databases (e.g. relational, XML, RDF...)

pecifi Simplifies reasoning hippets over queries and views

w to construct the formation

We call this trip. a citation

ew.

For now, we will focus on the view definition, which is expressed in Datalog.

#### **IUPHAR:** Citation views

Schema: Family(<u>FID</u>, FName, Type) FamilyIntro(<u>FID</u>, Text) Person(<u>PID</u>, PName, Affiliation) FC(<u>FID</u>, <u>PID</u>) FIC (<u>FID</u>, <u>PID</u>)

**View definitions:** 

 $\lambda$  F. V1(F, N,Ty) :- Family(F, N, Ty)  $\lambda$  F. V2(F, Tx) :- FamilyIntro(F, Tx)

Citation queries:

 $\lambda$  F. C<sub>V1</sub>(F, PN) :- Family(F, N, Ty), FC(F, P), Person(P, PN)  $\lambda$  F. C<sub>V2</sub>(F, PN) :- FamilyIntro(F, Tx), FIC(F, P), Person(P, PN)

# Generating citations

- If the query matches a view definition, we can use the associated citation query and function.
- But what if it doesn't?
  - Nothing matches the query
  - A set of view definitions are used to rewrite the query
  - More than one set of view definitions can be used to rewrite the query

# What is a "good" citation?

- Contains appropriate snippets of information
   E.g. as suggested by DataCite Schema
- Allows the data as it appeared at time of citation to be retrieved
  - Query and timestamp
  - Proll and Rauber: Scalable data citation in dynamic, large databases: Model and reference implementation (IEEE Big Data 2013).
- Concise
- Specific
- Our approach enables the DBA to specify the tradeoff between conciseness and specificity.

## IUPHAR: Generating the citation (1)

Schema: Family(<u>FID</u>, FName, Type) FamilyIntro(<u>FID</u>, Text) View definitions:  $\lambda$  F. V1(F, N,Ty) :- Family(F, N, Ty)  $\lambda$  F. V2(F, Tx) :- FamilyIntro(F, Tx)

A query is another Datalog expression (unparameterized).

Q<sub>1</sub>(F, N, Ty):- Family(F, N, Ty), F= 1

□ This can be rewritten using V1

Q<sub>1</sub>'(F, N, Ty):- V1(F, N, Ty)(1)

We can then construct a citation to Q in terms of the citation for V1(F, N, Ty)("1").

## IUPHAR: Generating the citation (2)

Schema: Family(<u>FID</u>, FName, Type) FamilyIntro(<u>FID</u>, Text) View definitions:  $\lambda$  F. V1(F, N,Ty) :- Family(F, N, Ty)  $\lambda$  F. V2(F, Tx) :- FamilyIntro(F, Tx)

Consider another input query

Q<sub>2</sub>(F, N, Y):- Family(F, N, Ty)

This can be rewritten using V1

Q<sub>2</sub>'(F, N, Y):- V1(F, N, Ty)

Now we must use all instantiations of V1 to construct a citation to Q

V1(F, N, Ty)(1), V1(F, N, Ty)(2),..., V1(F, N, Ty)(5)

#### IUPHAR: Generating the citation (3)

Schema: Family(<u>FID</u>, FName, Type) FamilyIntro(<u>FID</u>, Text) **View definitions:** λ F. V1(F, N, Ty) :- Family(F, N, Ty) ... V4(F, N, Ty) :- Family(F, N, Ty)

Consider the following query, with another view V4

 $Q_2(F, N, Y)$ :- Family(F, N, Ty), Ty="GPCR"

This can be rewritten using V1or V4 (alternate use)

Q<sub>2</sub>' (F, N, Ty):- V1(F, N, Ty) , Ty="GPCR" Q<sub>2</sub>''(F, N, Ty):- V4(F, N, Ty), Ty="GPCR"

We can then construct a citation to Q in terms of the citations V1(F, N, Ty)(1), V1(F, N, Ty)(2) or V4(F,N,Ty)

## IUPHAR: Generating the citation (4)

Schema: Family(<u>FID</u>, FName, Type) FamilyIntro(<u>FID</u>, Text) View definitions:  $\lambda$  F. V1(F, N,Ty) :- Family(F, N, Ty)  $\lambda$  F. V2(F, Tx) :- FamilyIntro(F, Tx)

Another query:

Q<sub>1</sub>(F, N, Ty, Tx):- Family(F, N, Ty), FamilyIntro(F, Tx), F= 1

□ This can be rewritten using V1 and V2 (**joint** use)

Q<sub>1</sub>'(F, N, Ty, Tx):- V1(F, N, Ty)(1), V2(F, Tx)(1)

We can then construct a citation to Q in terms of the citations for V1(F, N, Ty)(1) and V2(F, Tx)(1).

## Citation views as annotation

- Citation views are a type of annotation on tuples.
- Provenance is a form of annotation on tuples, which is well understood while being a veried through queries.
  2017 PODS Test
  - Green, Karvounarakis, Tannen: Provenance Semirings, POBs 2007;
- 2017 PODS Test of Time

- Joint use: joins of tuples
- Alternate use: unions and projections of tuples
- Can we use these ideas to understand how citation "annotations" on tuples are combined in general queries?

# Citation "semiring"?

Given a (conjunctive) query, we rewrite it to a set of minimal equivalent queries that contain at least one citation view.

• Let the set of queries obtained in this way be  $\{Q_1, ..., Q_n\}$ 

- Each Q<sub>i</sub> contains a set of citation views {V<sub>i1</sub>, ..., V<sub>imi</sub>}. The **joint** use (\*) of their citations constructs a citation for Q<sub>i</sub>, C(Q<sub>i</sub>).
   C(Q<sub>i</sub>) = C(V<sub>i1</sub>)\*...\*C(V<sub>imi</sub>)
- The alternate use (+) of each C(Q<sub>i</sub>) constructs a citation for Q, C(Q).

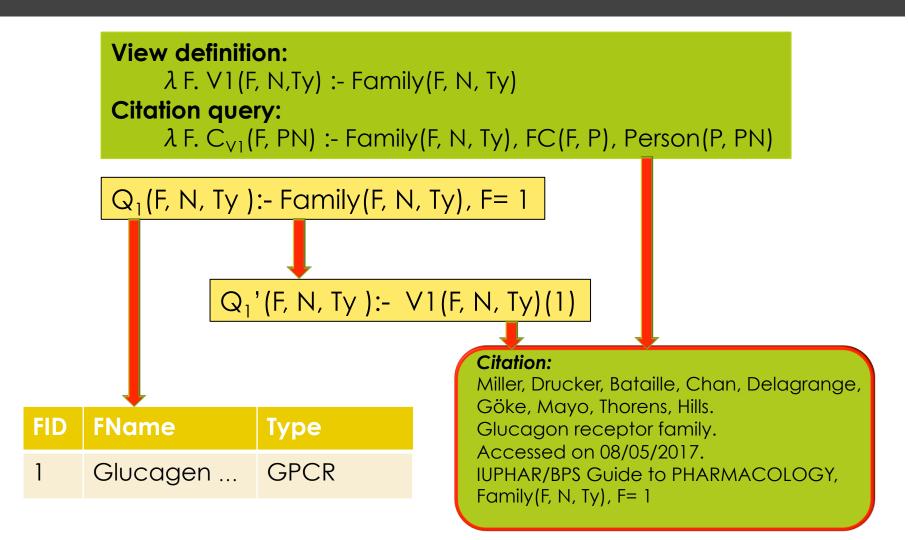
 $\square C(Q) = C(Q_1) + \dots + C(Q_n)$ 

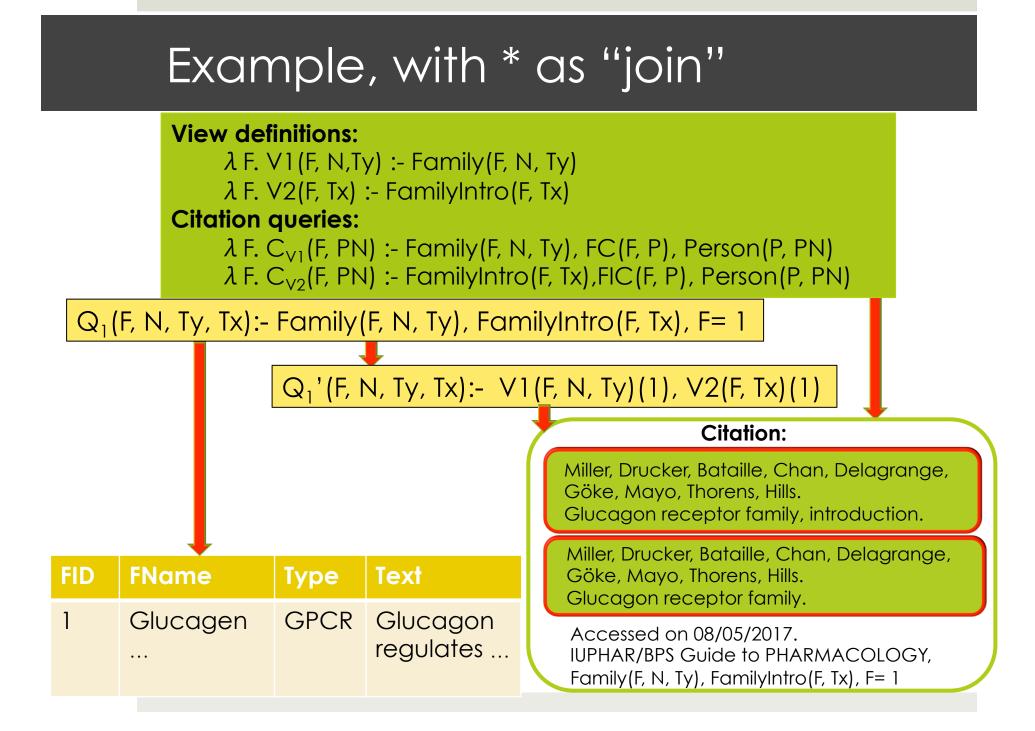
"Model for Fine-Grained Data Citation", CIDR 2017 S. Davidson, D. Deutch, T. Milo, and G. Silvello.

# Interpreting \* and +

- **Joint** use of citations:  $C(V_{i1})^*...^*C(V_{imi})$ 
  - \* could be union or some sort of join
  - E.g. in example 4, VI and V2 were jointly used: V1(F,N, Ty)("F123")\*V2(F, Tx)("F123")
- □ Alternate use of citations:  $C(Q_1) + ... + C(Q_n)$ 
  - + could be union or min (wrt some ordering on views)
  - E.g. in example 3, both the parameterized and unparameterized views on Family matched (V1(F, N, Ty)(1), V1(F, N, Ty)(2))+ V4
- Joint and alternate use are "policies" specified by the DBA

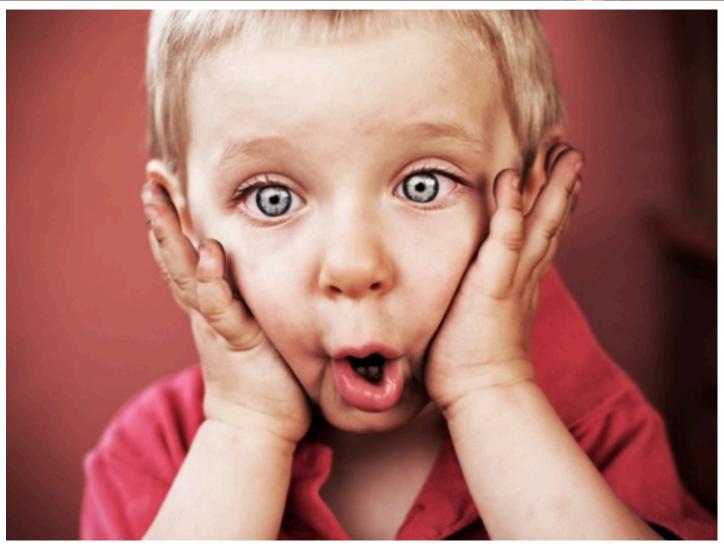
## Example of output citation





# Reaction of the DBA...





# "Partitioning" views

- In current practice, citation views are simple
   Project-select views of a single relation
- It is easily shown that if the views "partition" a relation then there is a single maximal rewriting using the views.
- And the implementation is much simpler...



# Building a citation system

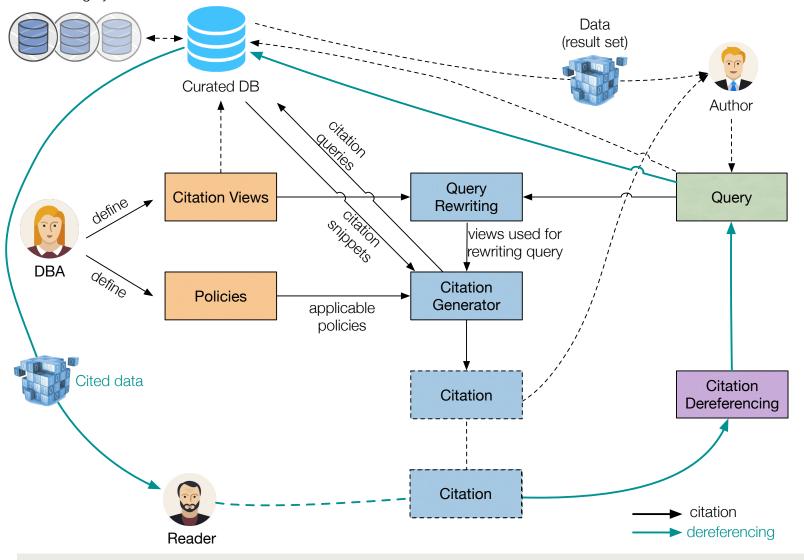
# The big picture

- Database owners need to be able to specify citation views for the database – schema level information.
- Database users ("authors") need to have citations "served up" as they extract data through queries.
- Dereferencing the citation should bring back the data to "readers" as of the time it was cited.

Alawini, Davidson, Hu, Wu: Automating Data Citation in CiteDB. VLDB 2017 (Demo paper).

## Citation architecture

Versioning system

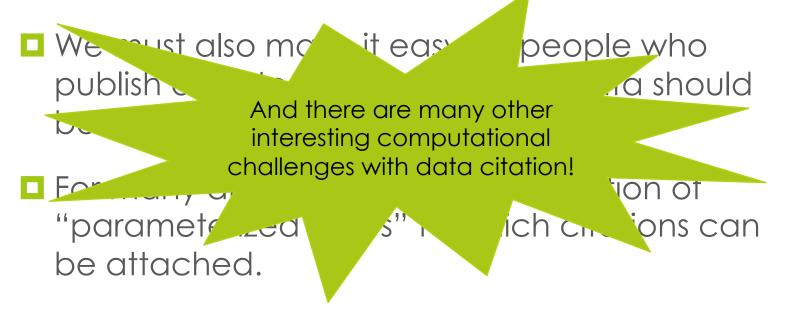


# Computational challenges

- Schema-level versus instance level?
  - Should we store the citations as annotations on tuples, or should we reason at the schema level and then calculate the citation?
- Given an expected query workload, what are the "best" citation views?
  - And are the necessary snippets of citation information in the schema?
- The number of alternative uses of citation views can be large.
  - Are there efficient algorithms to find the "best" according to some metric of quality (e.g. involving the number of views, the specificity of views, or related to a view hierarchy)?

#### Take home message

If we want people to cite the data they use, we need to make it easy for them to do so.



Joint and alternate use semantics are "policies" to be specified by the DBA

## Outline

- The power of abstraction
- New problem: data citation
- **Bigger picture: Data Science**



# The Tsunami of Data Science...

# Role of computing research in DS





- Report by CRA's Committee on Data Science
  - Lise Getoor (Chair), David Culler, Eric de Sturler, David Ebert, Mike Franklin, and H. V. Jagadish
- Topics:
  - Models for data representation, acquisition, storage and access.
  - Large scale system and algorithms.
  - Learning with biased, incomplete and heterogeneous data.
  - User interaction: with data and models.
  - Ethical use: privacy, fairness, transparency

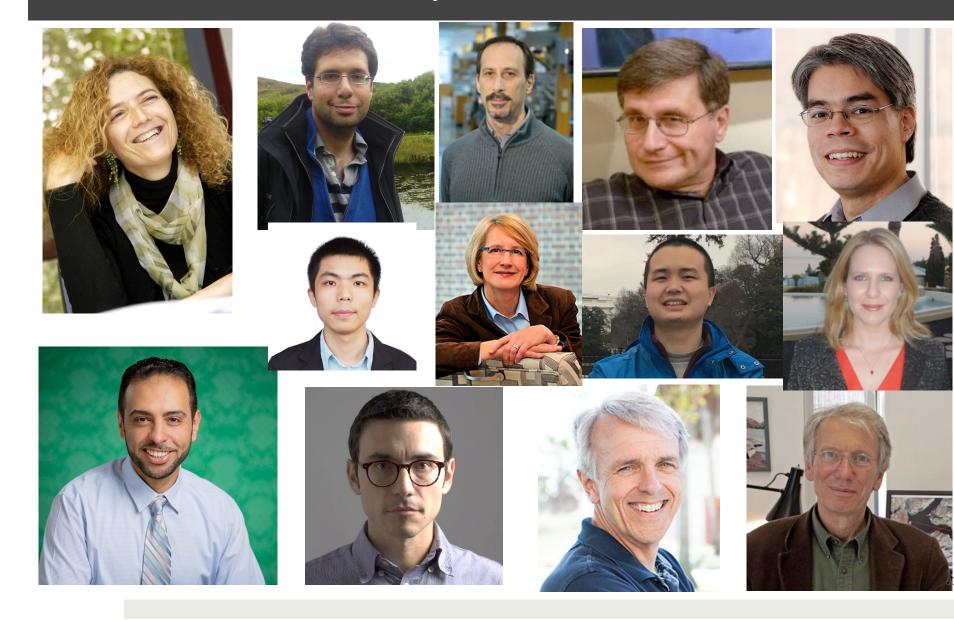
# My personal perspective...

Data Science= (CS+Stat+Math) ∩ (Science | Economics | Sociology | Business | Law |...)



- □ (Data Management) ∩ (Machine Learning)
- "Data Engineering" akin to "Software Engineering"
  - Collecting, cleaning and organizing data sets is reported to take nearly 80% of a data scientist's time yet is the least enjoyable part of their job
- "Why Analysis" of Algorithms
- Ethical data management

# Thanks to my collaborators



# And to our funders...



National Science Foundation WHERE DISCOVERIES BEGIN NSF IIS 1302212, NSF ACI 1547360,

. . .

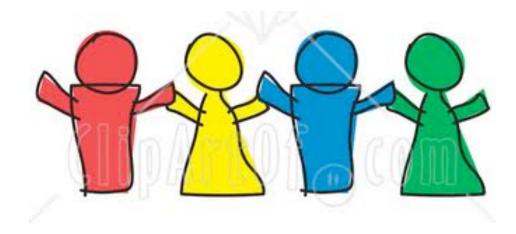


National Institutes of Health Turning Discovery Into Health

NIH 3-U01-EB-020954-02S1







# Questions?