Aleksandra Perz Wren Lab Oklahoma Medical Research Foundation

### Overview

- MNEMONIC
  - Goals
  - Data acquisition and processing
  - Results and current state
- PubQC
  - Goals
  - Results so far

# There is knowledge out there: objectives

Bring in the already available knowledge to interpret a new finding

Find samples that are similar: learn something new about the finding based on the literature

Compare shifts observed between conditions: find samples that exhibit similar changes in taxonomic abundance

Predict characteristics of the finding: confirm the finding

Make and evaluate statements about global relationships between entities

A researcher's interface to database

### Data

- Batch-download count data from EBI
- Represent counts as a fraction of total count within a sample (compositional data)
- Set low-count observations to zero
- TF-IDF transform counts (term frequency - inverse document frequency)
- Calculate cosine distances

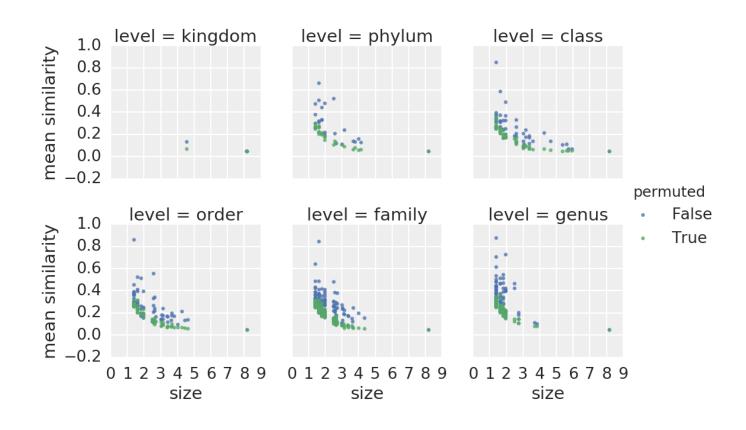
### Entities and entity hierarchy:

- Samples
  - Projects
  - Biomes
  - Keywords
  - Contrasts
- Taxa
  - Genera
  - Families
  - •
- Genes
  - Functions

### Validation?

Comparison of results for samplesample cosine distance between taxonomic data and functional data Comparison of mean similarity within taxonomic levels against permuted values

 Mantel test: 0.28 Permuted: ~0.00 (10439 samples)



### Where I stand

Metadata browsing

http://10.84.146.16:9000/home

 Sample-sample (also project-project, biome-biome)

http://10.84.146.16:9000/projects/ERP010458 http://10.84.146.16:9000/biomes/Fecal

Taxon-taxon

http://10.84.146.16:9000/taxa/k\_\_Bacteria;%20p\_\_Firmicutes;%20c\_\_Clostridia;%20o\_\_Clostridiales;%20f\_\_Peptostreptococcaceae;%20g\_[Clostridium];%20s\_\_difficile

• Contrasts (differential abundance)

http://10.84.146.16:9000/contrasts/soil-fecal

 Data management, optimization: getting results for > 300 samples and 3000 taxons is very slow!

# Sample, project, biome results

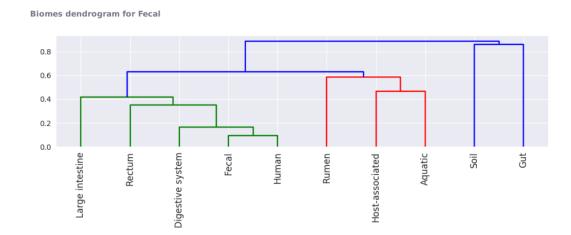
- Precalculated distance matrix for all sample-sample relationships
- Collapsing and averaging for a higher-level entity (e.g. project)

Biomes most similar to Fecal Samples most similar to ERS940246

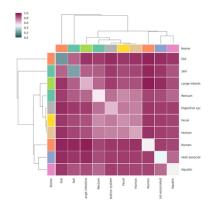
For agglomerative entities like project,

Biome 2	Metric
Fecal	0.719689
Rectum	0.731858
<u>Human</u>	0.752949
Digestive system	0.766736
Large intestine	0.858444
Soil	0.876893
<u>Aquatic</u>	0.889793
<u>Host-associated</u>	0.905403
Gut	0.917661
Rumen	0.917746

Sample 2	Metric
ERS940246	0.000000
ERS939804	0.261820
ERS939485	0.324476
ERS941546	0.346890
ERS939653	0.348082
ERS920506	0.353270
ERS941537	0.355168
ERS915909	0.356859
ERS915910	0.358304
ERS918534	0.358816
ERS940404	0.360702
ERS918534	0.358816







### TODO:

• Include more metrics (already implemented in taxon comparison)

### Taxon results

HOME

HELP

**ABOUT** 

# K\_BACTERIA; P\_FIRMICUTES; C\_CLOSTRIDIA; O\_CLOSTRIDIALES; F\_PEPTOSTREPTOCOCCACEAE; G\_[CLOSTRIDIUM]; S\_DIFFICILE

#### DOWNLOAD TABLE

Tf-idf cosine; ascending=True

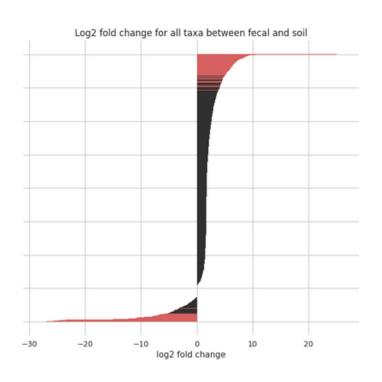
Taxon 2	Tf-idf cosine	N overlapping	Fisher exact p-value	Correlation	Chisquare kernel
k_Bacteria; p_Firmicutes; c_Clostridia; o_Clostridiales; f_Peptostreptococcaceae; g_[Clostridium]; s_difficile	0.000000	2596.0	0.000007	1.000000	1.0
k_Bacteria; p_Firmicutes; c_Clostridia; o_Clostridiales; f_Peptostreptococcaceae; g_; s_	0.283319	2452.0	0.000010	0.642032	0.0
k_Bacteria; p_Firmicutes; c_Clostridia; o_Clostridiales; f_Clostridiaceae; g_Clostridium; s_neonatale	0.297549	1176.0	0.000007	0.133426	0.0
k_Bacteria; p_Firmicutes; c_Clostridia; o_Clostridiales; f_Clostridiaceae; g_Clostridium; s_perfringens	0.329332	1937.0	0.000009	0.139407	0.0
k_Bacteria; p_Firmicutes; c_Clostridia; o_Clostridiales; f_Clostridiaceae; g_Clostridium; s_butyricum	0.387502	1207.0	0.000006	0.086361	0.0
k_Bacteria; p_Firmicutes; c_Clostridia; o_Clostridiales; f_Eubacteriaceae; g_Pseudoramibacter_Eubacterium; s_	0.439118	619.0	0.000006	0.158153	0.0
k_Bacteria; p_Firmicutes; c_Bacilli; o_Lactobacillales; f_Carnobacteriaceae; g_; s_	0.466686	771.0	0.000007	0.195472	0.0
k Bacteria; p Firmicutes; c Erysipelotrichi; o Erysipelotrichales; f Erysipelotrichaceae; g Coprobacillus; s cateniformis	0.467144	657.0	0.000005	0.121383	0.0
k Bacteria; p Firmicutes; c Bacilli; o Lactobacillales; f Enterococcaceae; g Enterococcus; s	0.475901	2300.0	0.000009	0.031046	0.0
k_Bacteria; p_Firmicutes; c_Bacilli; o_Lactobacillales; f_Enterococcaceae; g_Enterococcus; s_casseliflavus	0.484032	1258.0	0.000008	0.112064	0.0
k_Bacteria; p_Firmicutes; c_Erysipelotrichi; o_Erysipelotrichales; f_Erysipelotrichaceae; g_[Eubacterium]; s_dolichum	0.494058	1383.0	0.000010	0.141750	0.0
k_Bacteria; p_Firmicutes; c_Bacilli; o_Lactobacillales; f_; g_; s_	0.497414	1666.0	0.000010	0.032788	0.0
k Bacteria; p Firmicutes; c Bacilli; o Lactobacillales; f Enterococcaceae; g Vagococcus; s	0.500240	1556.0	0.000008	0.030739	0.0
k_Bacteria; p_Firmicutes; c_Bacilli; o_Lactobacillales; f_Leuconostocaceae; g_Weissella; s_	0.505225	1012.0	0.000008	0.105376	0.0
k_Bacteria; p_Firmicutes; c_Clostridia; o_Clostridiales; f_Clostridiaceae; g_; s_	0.523169	2566.0	0.000007	0.137969	0.0
k_Bacteria; p_Actinobacteria; c_Coriobacteriia; o_Coriobacteriales; f_Coriobacteriaceae; g_Eggerthella; s_lenta	0.529286	1162.0	0.000010	0.104832	0.0
k_Bacteria; p_Firmicutes; c_Bacilli; o_Lactobacillales; f_Leuconostocaceae; g_; s_	0.554177	897.0	0.000008	0.023938	0.0

### TODO:

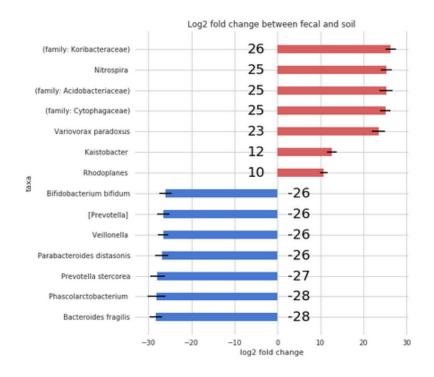
- Add genus, family, ... collapsing
- Draw plots for taxon results similar to sample results

### **Contrasts**

### **SOIL-FECAL**



Comparison of fecal to soil (reference).



Comparison of fecal to soil (reference).

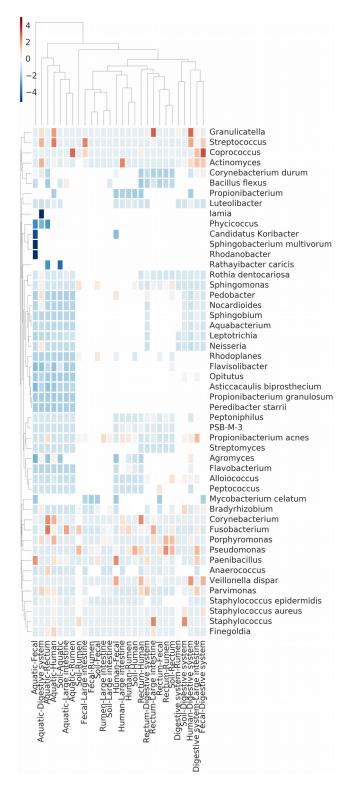
Showing 14 out of 282 taxa for which adjusted p-value < 0.01.

Standard errors are shown.

### TODO:

- Add a possibility to specify arbitrary groups of samples
- Log fold change plots for higher taxonomy levels

# One step higher: cluster contrasts



### PubQC

Correct errors in scientific publications submitted to journals ("Reviewer n+1" scheme)

Analyze the errors in scientific literature in the wild

# PubQC

Total accessible abstracts: 27,444,507

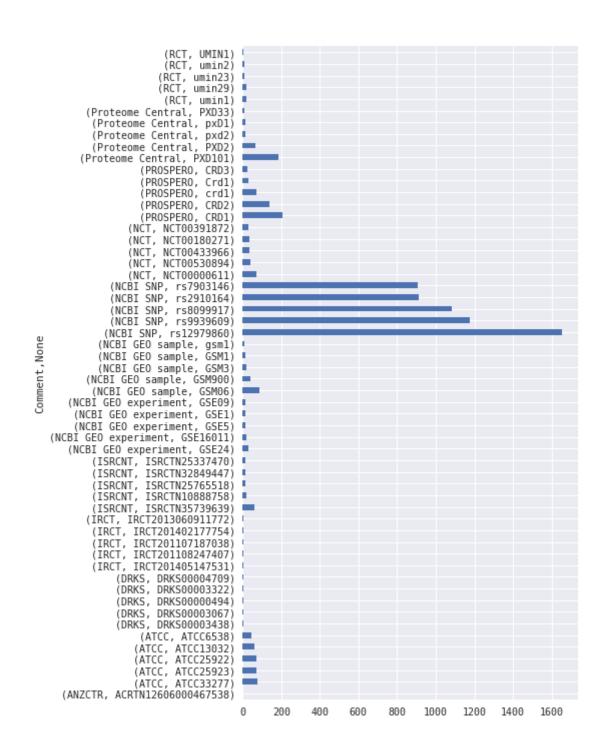
statistical term	(all abstracts)	10932987
CI, OR, p-value	(almost all abstracts)	7268408
concentrations	(script was interrupted)	1182067
ID	(all abstracts)	251868
chemical/gene	(subset abstracts)	128301
URL	(all abstracts)	65995
e-mail address	(subset abstracts)	0
θ	0 0.2 0.4 0.6	0.8 1.0 le7

http://10.84.146.16:9001/home

http://10.84.146.16:2460/notebooks/pubqc\_test\_results.ipynb

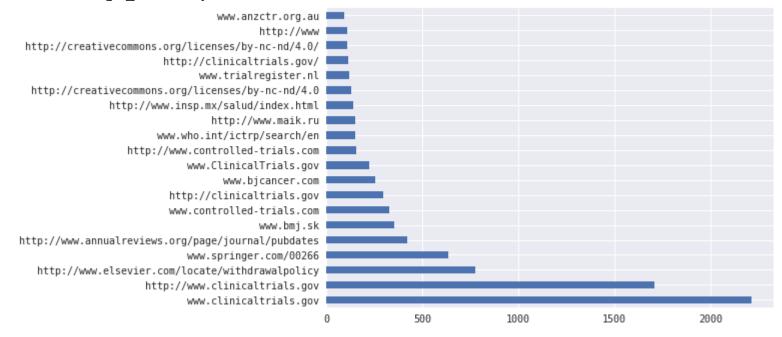
### PubQC – IDs (regex)

- 251,868 found
- Belinostat (PXD101) is a novel HDAC inhibitor with IC50 of 27 nM in a cellfree assay, with activity demonstrated in cisplatin-resistant tumors
- rs12979860 is a SNP near the IL28B gene, encoding interferon-lambda-3 (IFN-lambda-3)
- rs9939609 is a SNP in the fat mass and obesity associated FTO gene, aka the "Fat Gene"
- ATCC 33277 Porphyromonas gingivalis genome - human pathogen
- rs8099917 is related to hepatitis C treatment response
- GSE16011 is a glioma cohort
- (TODO) GSM1 is a protein, GSM06 is a cell line, CRD1 a protein domain, etc.



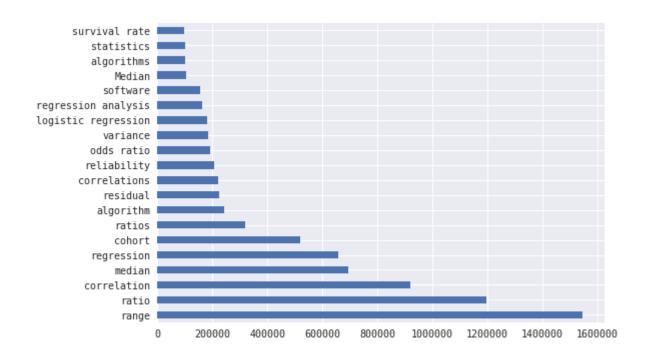
### PubQC – URLs (regex)

- 65,995 found
- www.springer.com/00266 aesthetic plastic surgery (??)
- (TODO) 'http://www' is almost always matched when there's a space after the 'www.'
- (TODO) spaCy results were rubbish why?
- (TODO) programatically get respone from the server



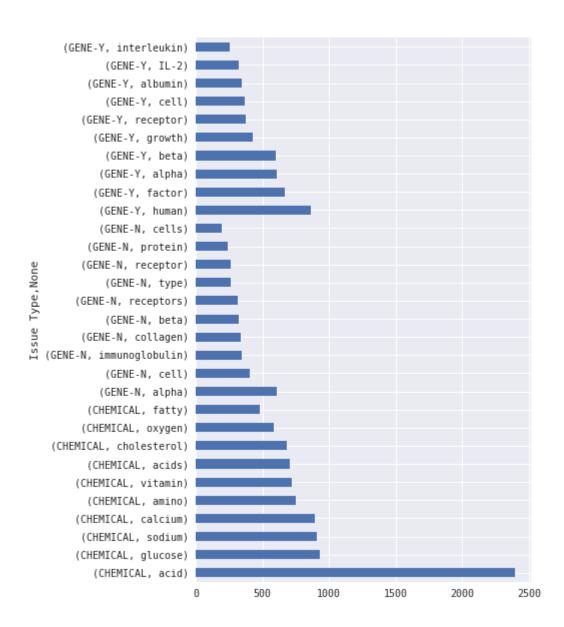
# PubQC – terms (simple pattern match)

- 10,932,987 found
- (TODO) ignore case

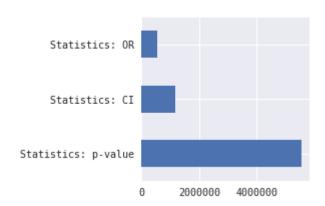


# PubQC – chemicals, genes (spaCy)

• 128,301 found, but...



## PubQC – CI, OR, p-value



- (TODO) scientific notation
- (TODO) recalculate statistics

• Number of values associated with each

Statistics:	CI	3	12043
		4	545
		2	12
		5	5
		6	4
Statistics:	0R	1	6208
		2	1
Statistics:	p-value	1	63403

Extracted p-values

13836
11933
8188
3201
1857
1543
184
1
1

PMI D	Pattern	Location	value	Lower	Upper	Rec alcu late d OR	Pattern	Location	Context
3384 186	95% CI (CI)=(0.93, 3.17	(762, 785)	[95.0, 0.93, 3.17]	0.93	3.17		OR)=1.7 1	(752, 760)	ve to the NHWs [odds ratio (OR)=1.71; 95% CI (CI)=(0.93, 3.17)]. The risk of severe retinopathy (pr
3387 899	95% CI, 1.5-3.5	(943, 958)	[95.0, 1.5, 3.5]	1.5	3.5		OR=2.3	(935, 941)	eir place of residence indicated (OR=2.3; 95% CI, 1.5-3.5). There was a trend for patients to repor
3387 899	95% CI, 0.9-6.7	(1032, 1047)	[95.0, 0.9, 6.7]	0.9	6.7		OR=2.4	(1024, 1030)	s to report an unhappy childhood (OR=2.4; 95% CI, 0.9-6.7). Being unmarried, undergoing parental se
3389 360	3.94, CI=1.52- 10.20	(849, 868)	[3.94, 1.52, 10.2]	1.52	10.2		OR=3.94	(846, 853)	d an elevated risk for brain cancer (OR=3.94, CI=1.52-10.20). In addition, there was a linear relat
3389 361	1.72, CI 1.09-2.97	(750, 768)	[1.72, 1.09, 2.97]	1.09	2.97		OR 1.72	(747, 754)	the reduction division of the plant (OR 1.72, CI 1.09-2.97) including, in particular, Soderberg (OR
3389 361	1.71, CI 1.07-2.72	(810, 828)	[1.71, 1.07, 2.72]	1.07	2.72		OR 1.71	(807, 814)	including, in particular, Soderberg (OR 1.71, CI 1.07-2.72) and prebake (OR 2.26, CI. 1.27-4.02) po
3389 361	2.26, Cl. 1.27-4.02	(846, 865)	[2.26, 1.27, 4.02]	1.27	4.02		OR 2.26	(843, 850)	(OR 1.71, CI 1.07-2.72) and prebake (OR 2.26, CI. 1.27-4.02) potroom workers. The risk of IHD did n
3394 698	95% CI=1.6-4.9	(877, 891)	[95.0, 1.6, 4.9]	1.6	4.9		OR)=2.8	(868, 875)	eral cancer (adjusted odds ratio (OR)=2.8, 95% CI=1.6-4.9). Further, this relation was modified by t
3394 698	95% CI=1.2-3.0	(1003, 1017)	[95.0, 1.2, 3.0]	1.2	3		OR=1.9	(995, 1001)	initial cancer diagnosis (ratio of OR=1.9, 95% CI=1.2-3.0 for a five-year differential in time since
3394 698	95% CI=0.3-1.2	(1191, 1205)	[95.0, 0.3, 1.2]	0.3	1.2		OR=0.6	(1183, 1189)	h a 36% decrease in risk (adjusted OR=0.6, 95% CI=0.3-1.2); this estimate excluded the magnitude of
3394 707	95% CI=1.1-2.2	(520, 534)	[95.0, 1.1, 2.2]	1.1	2.2		OR)=1.6	(511, 518)	showed that male sex (odds ratio (OR)=1.6, 95% CI=1.1-2.2), maternal five-year age increase (OR=1.3,
3394 707	95% CI=1.1-1.5	(578, 592)	[95.0, 1.1, 1.5]	1.1	1.5		OR=1.3	(570, 576)	, maternal five-year age increase (OR=1.3, 95% CI=1.1-1.5), plural birth (OR=3.0, 95% CI=1.2-7.1) an
3394 707	95% CI=1.2-7.1	(617, 631)	[95.0, 1.2, 7.1]	1.2	7.1		OR=3.0	(609, 615)	.3, 95% CI=1.1-1.5), plural birth (OR=3.0, 95% CI=1.2-7.1) and black maternal race (OR=0.0, 95 perce
3395 581	95% CI=1.0-2.6	(634, 648)	[95.0, 1.0, 2.6]	1	2.6		OR)=1.6	(625, 632)	icultural production (odds ratio (OR)=1.6, 95% CI=1.0-2.6). A concomitant increase was detected for
3395	95%	(708 722)	[95 0 1 0 2 5]	1	25		OR=1.6	(700 706)	increase was detected for farmers (OR=1.6, 95% CI=1.0-

### PubQC – concentrations, percentages

 (TODO) Get chemicals in the proximity (extract noun?)

1:1 2:1 18:2 18:1 16:0	385 178 143 121 106	
100mg/kg) 50mg/kg) 12:0 200mg/kg) 5mg/kg) 19:00	8 8 8 7 7 7	
95% 50% 10% 20% 100% 5% 30% 90% 40% 25% 60%	10130 3683 2510 2378 2207 2033 1892 1857 1794 1744 1550	
70%	1465	

1369

1%

```
2.2%
Percent
(838, 842)
xed meat or chicken or pork or beef contributes 2.2%), the GI
emission is estimated to be 0.28 or 0
meat (CHEMICAL); chicken (CHEMICAL); pork (CHEMICAL)
```

0.5%
Percent (178, 182)
sound biomicroscopy. To determine the effect of 0.5% tropicamide and the resultant mydriasis on the tropicamide (CHEMICAL)

84% percent (635, 638) c SBR became fully granulated and finished with 84% and 99 of nitrogen and phosphorus removal, res nitrogen (CHEMICAL)

19.73ng/ml concentration (556, 567)

. Cutoff value for detecting stage B HF was 19.73ng/ml for catestatin with 90% sensitivity and 50.9 catestatin (CHEMICAL)

#### cat0

### **Column information**

Column name: cat0

Column type: object

Table: Summary by cat0

cat0	logistic							lognormal						normal					
	count	mean	std	min	25%	50%	75%	max	count	mean	std	min	25%	50%	75%	max	count	mean	std
а	189.0	0.253651	1.711486	-4.02	-0.880	0.10	1.2000	6.53	189.0	1.778730	2.267438	0.07	0.600	1.05	2.1100	18.72	189.0	-0.030159	1.032
b	160.0	-0.015062	1.716513	-5.16	-0.910	-0.21	0.9675	6.50	160.0	1.607500	1.690542	0.07	0.580	1.05	1.9625	10.46	160.0	0.009625	0.968
С	151.0	0.419073	2.052203	-8.76	-0.815	0.37	1.5350	5.83	151.0	1.766556	2.838467	0.09	0.515	1.09	1.9750	30.58	151.0	-0.012517	1.002

#### Titles: MANOVA results for all variables

-	Df	Pillai	approx F	num_Df	den Df	Pr(>F)
cat0	2	0.014649	0.91312	8	990	0.5046
Residuals	497	-	-	-	-	-

### Titles: MANOVA results for response lognormal

-	Df	Sum Sq	Mean Sq	F value	Pr(>F)
cat0	2	3.0	1.5021	0.2839	0.753
Residuals	497	2629.5	5.2908	-	-

### Titles: MANOVA results for response logistic

-	Df	Sum Sq	Mean Sq	F value	Pr(>F)
cat0	2	15.04	7.5180	2.2633	0.1051
Residuals	497	1650.90	3.3217	-	-

### lognormal

### **Column information**

Column name: lognormal

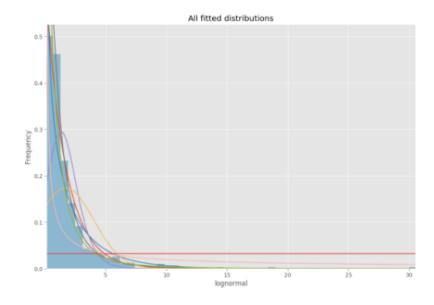
Column type: float64

Table: Column summary

count	mean	std	min	25%	50%	75%	max
500.0	1.72026	2.296861	0.07	0.58	1.065	2.0025	30.58

Table: Fitted distributions with best parameters and residual sum of squares

distribution	parameters	SSE
<u>beta</u>	a=0.98, $b=113.42$ , $loc=0.07$ , $scale=192.26$	0.185949
chi2	df=1.32, loc=0.07, scale=1.54	0.471846
<u>logistic</u>	loc=1.34, scale=0.85	0.626428
lognorm	s=0.97, loc=0.01, scale=1.06	0.0629841
norm	loc=1.72, scale=2.29	1.05756
<u>pareto</u>	b=2.02, loc=-1.83, scale=1.90	0.510913
<u>powerlaw</u>	a=0.27, loc=0.07, scale=33.09	1.124
uniform	loc=0.07, scale=30.51	2.09939



### Who Cares?

#### Maria K. E. Lahman<sup>1</sup>

#### Keywords

methodology, poetry, research poetry

I fantasize saying,
"Who CARES if
YOU think poetry
can be research?",
with a negligent
shrug of
shoulders.

Research IS poetry.

We are having a methodological ARGUMENT.

Tug of War,

Over our DEAD fetuses' bodies,<sup>1</sup> a girl's ANOREXIA,<sup>2</sup> my postpartum DEPRESSION<sup>3</sup> their HIV,<sup>4</sup> her MURDER,<sup>5</sup> his SUICIDE,<sup>6</sup> a daughter's racial IDENTITY,<sup>7</sup> their COMING OUT.<sup>8</sup>

Experience, story, research, poetry, inquiry, explorations, should fluster, perplex, unsettle method... METHODOLATRY.9

But I'd be lying.

Qualitative Inquiry
1-2
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journals.sagepub.com/home/qix

(\$)SAGE

```
I
know
I
care...
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#### Notes

- Lahman (2013).
- Chan (2003).
- Lahman (2008).
- Poindexter (2002).
- Lahman (2011).
- Teman (2010).
- Davis (2007).
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- Janesick (1994).

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Davis, A. M. (2007). SIP (School Induced Psychosis) poem for my daughter. Qualitative Inquiry, 13, 919-924.

Janesick ,V. J.(1994). The dance of qualitative research design – metaphor, methodolatry and meaning. In N. K. Denzin & Y. S. Lincoln (Eds.), Handbook of qualitative research. pp.209-219.Thousand Oaks, CA: Sage.

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