

Interdisciplinary collaboration

“the whole is greater than the sum of its parts”

~ Aristotele



Olga Dethlefsen
olga.dethlefsen@nbis.se

Introduction: talking from experience

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Can I ask you a question? I'm trying to understand the results of this copy number variations analysis and I'd thought I would ask you as you have been working with EVERYTHING (~ NBIS colleague)

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BEng/MSc in Technical Physics, PL



MSc internship, FR



PhD in Bioinformatics, UK

Medical Statistician, Oxford, UK



Post-docs experiences



KI, Sweden & RIKEN, Japan

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Medical Statistician, Oxford, UK



Post-docs experiences
KI, Sweden & RIKEN, Japan



- ❖ at NBIS since 2015
- ❖ “bioinformatics expert”
- ❖ 40+ projects
- ❖ across multiple omics
- ❖ medical focus

Introduction: session's aim



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- * to highlight and discuss some of the collaboration aspects worth thinking about**

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- * to introduce “reproducibility” concepts covered more in day 2

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- * to prepare a first draft of a “Good collaboration checklist”**

Introduction: session's aim

Show,
don't tell



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Introduction: theory

https://docs.google.com/document/d/1MpefgEuklXooeo86Q5bX_wjD4RQxMHT9OIY1jEQA2q4/edit?usp=sharing

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“the act of working together with other people or organisations to create or achieve something”

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- trust
- attachment
- clarity and alignment
- speed
- technology, geography and culture

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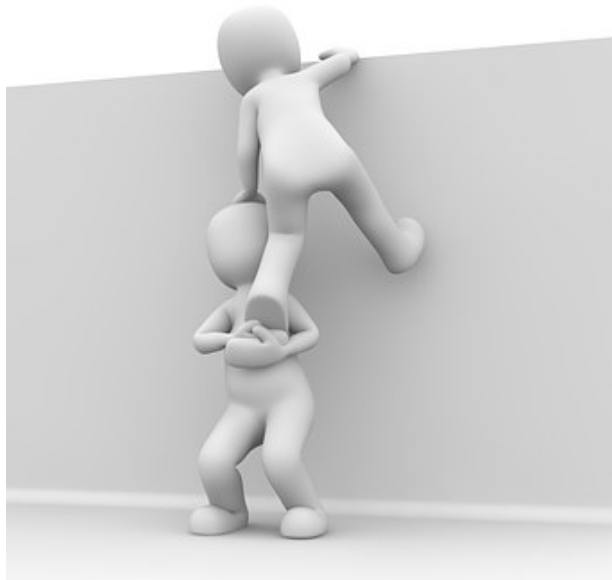
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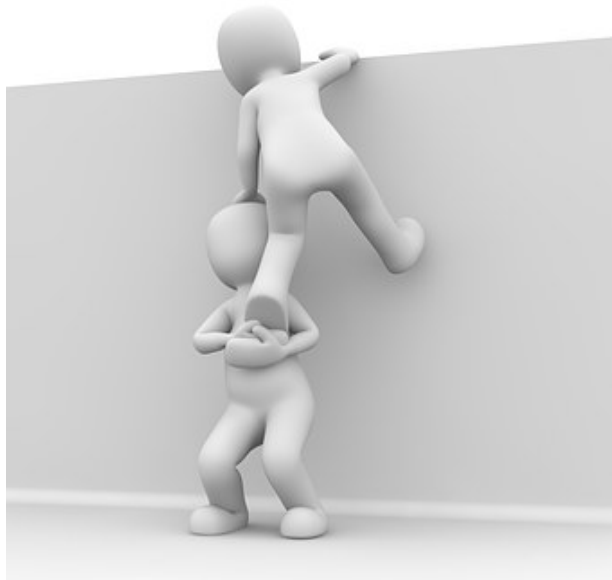
- trust
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- clarity and alignment
- speed
- technology, geography and culture

- diversity
- speed
- engagement
- productivity



Alignment on a collective goal

- **missing details**
- **conflicting incentives**
- **conflicting prioritisation**
- **conflict avoidance**



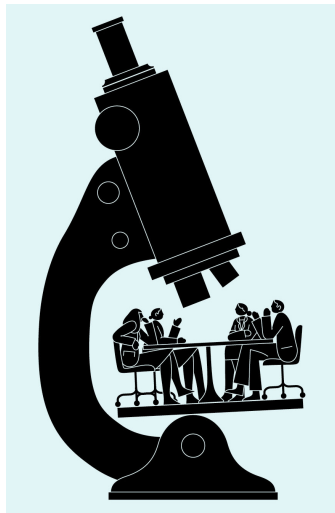
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Team players

- **core team**
- **others joining as needed**
- **roles and responsibilities**
 - e.g. facilitators, evaluators
 - e.g. coordinators, communicators
- **engage leadership support**
- **setting the team for success**



THE WORK ISSUE

What Google Learned From Its Quest to Build the Perfect Team

New research reveals surprising truths about why some work groups thrive and others falter.

- Equality of distribution of conversational turn-talking
- Highly average social sensitivity



<https://rework.withgoogle.com/print/guides/5721312655835136/>

<https://www.nytimes.com/2016/02/28/magazine/what-google-learned-from-its-quest-to-build-the-perfect-team.html?smid=pl-share>

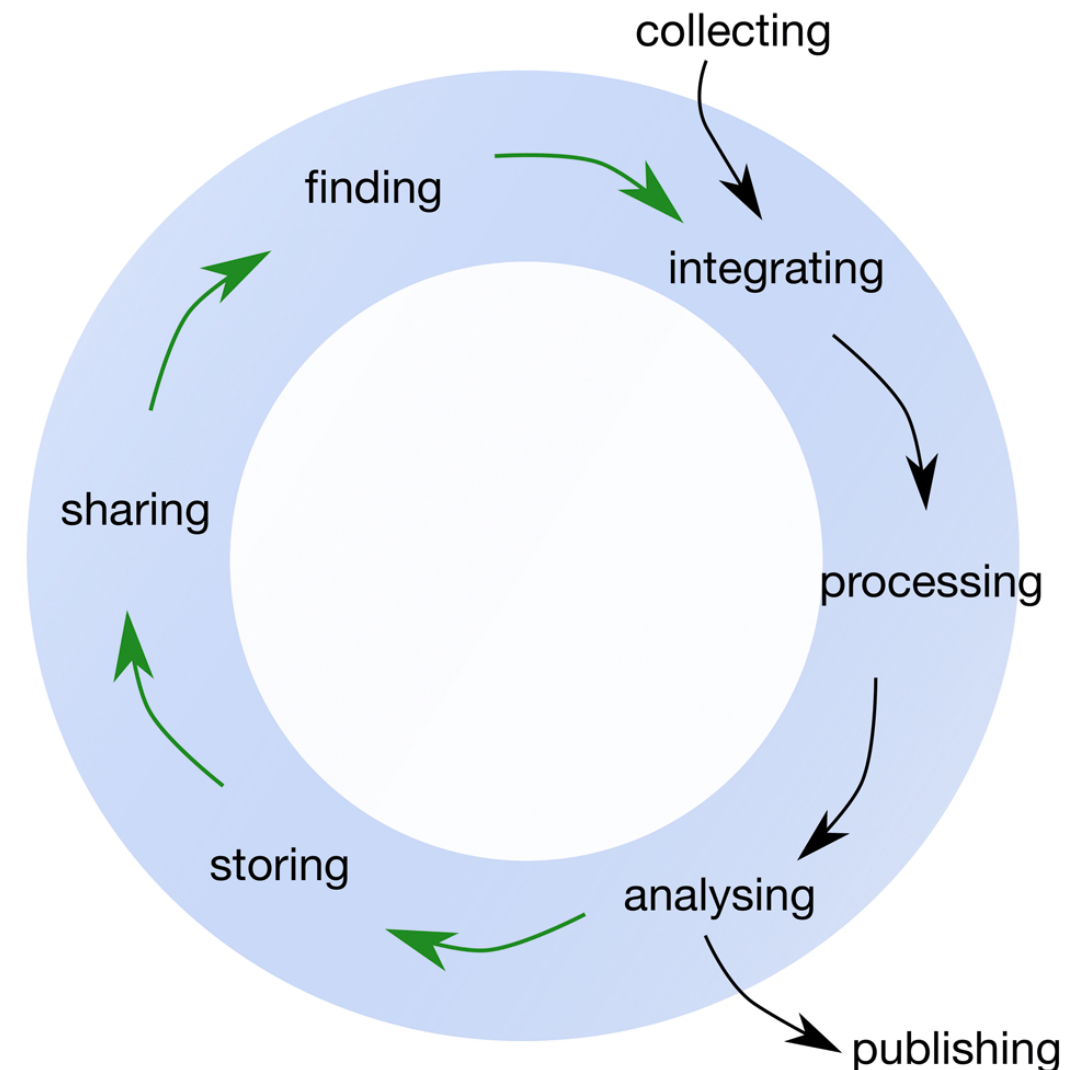
Project management main steps

- ☒ **defining project**
- ☒ **listing tasks**
- ☒ **estimate times and costs**
- ☒ **assess risk and prepare action plans**
- ☒ **monitor progress & costs**
- ☒ **review**

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Simplified Data Life Cycle framework for bioscience, biomedical and bioinformatics data

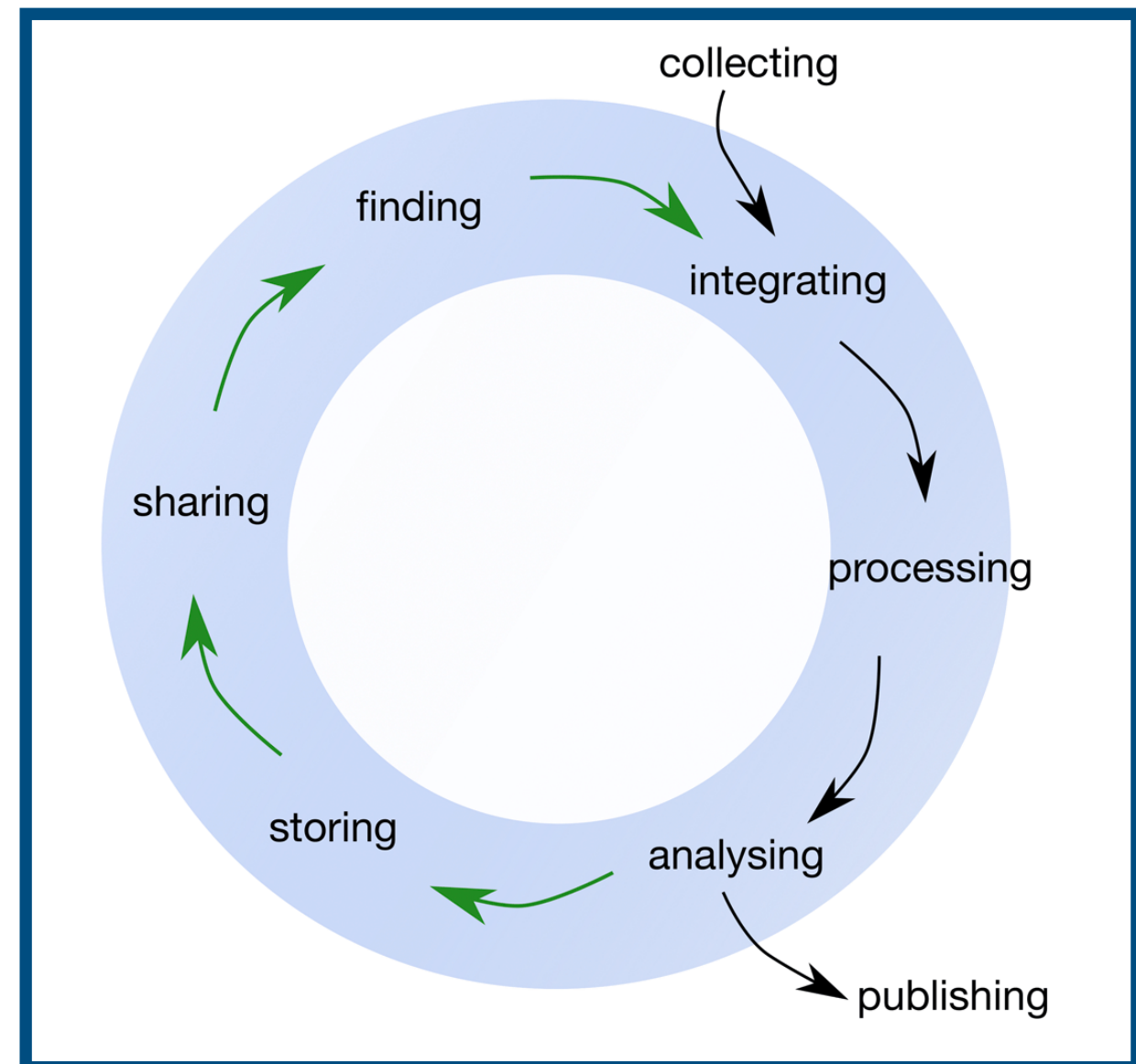


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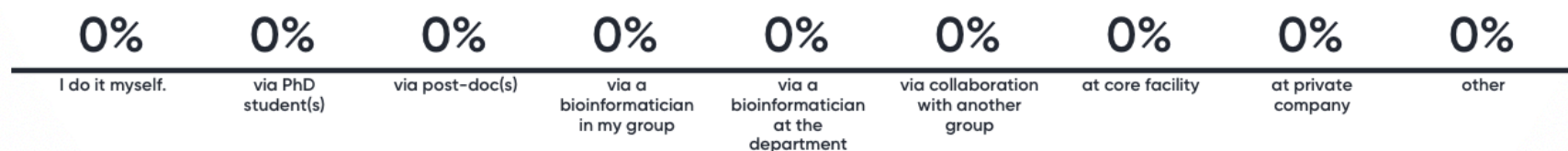
potential bioinformatics needs





Go to www.menti.com and use the code 50 54 91

How do you get bioinformatics done?





https://docs.google.com/document/d/1MpefgEuklXooeo86Q5bX_wjD4RQxMHT9OIY1jEQA2q4/edit?usp=sharing



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most likely unrealistic, admirable, lonely



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is there a second supervisor? asking for troubles, if not



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bioinformatician**

it may be a good set-up for the group, and hopefully for the bioinformatician; is anyone discussing with him / her career development?



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wait, have you double-checked that the default pipelines and workflows are applicable to your project, worth time and money?



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may be great, but what really motivates these bioinformaticians? And how does the core facility work?



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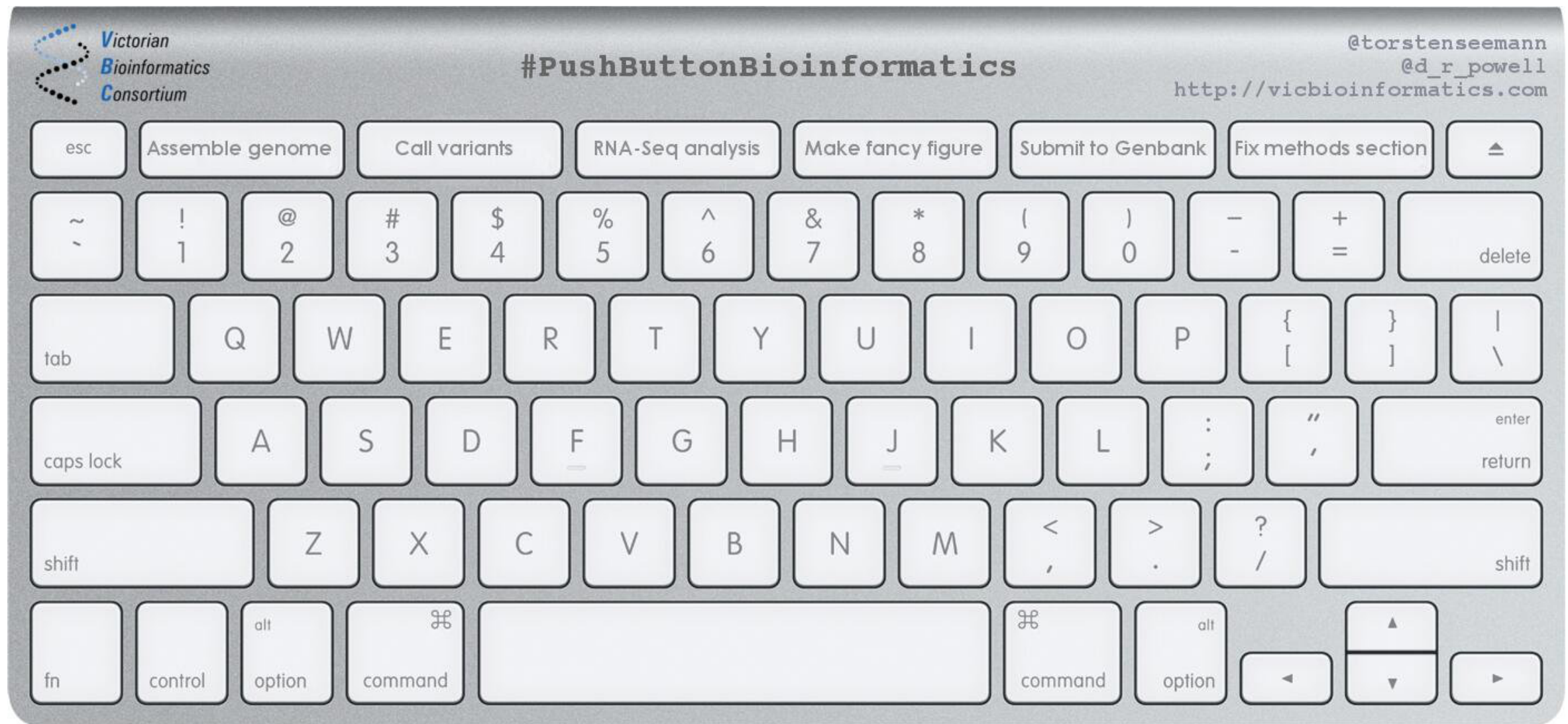
**at an external
company**

will you ever see the code and be able to explain M&M?

NO



#PushButtonBioinformatics





“Biological data will continue to pile up unless those who analyse it are recognised as creative collaborators in need of career paths”

– Jeffrey Chang, 2015



Over 18 months, 46 data-analysis projects undertaken at the bioinformatics core of the University of Texas Health Science Center at Houston required 34 different types of analysis — most were used infrequently. Each project demanded unique combinations of analyses, demonstrating how bioinformaticians must be versatile, creative and collaborative.



Core services: Reward bioinformaticians; *Nature* **520**, 151–152 (09 April 2015) doi:10.1038/520151a

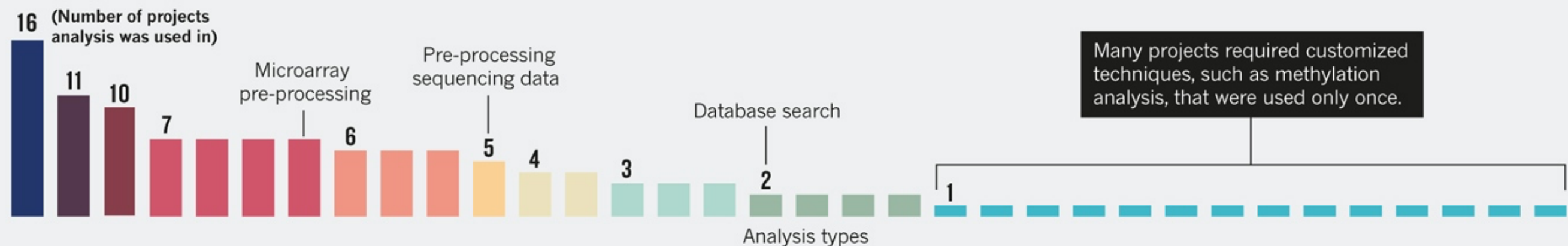


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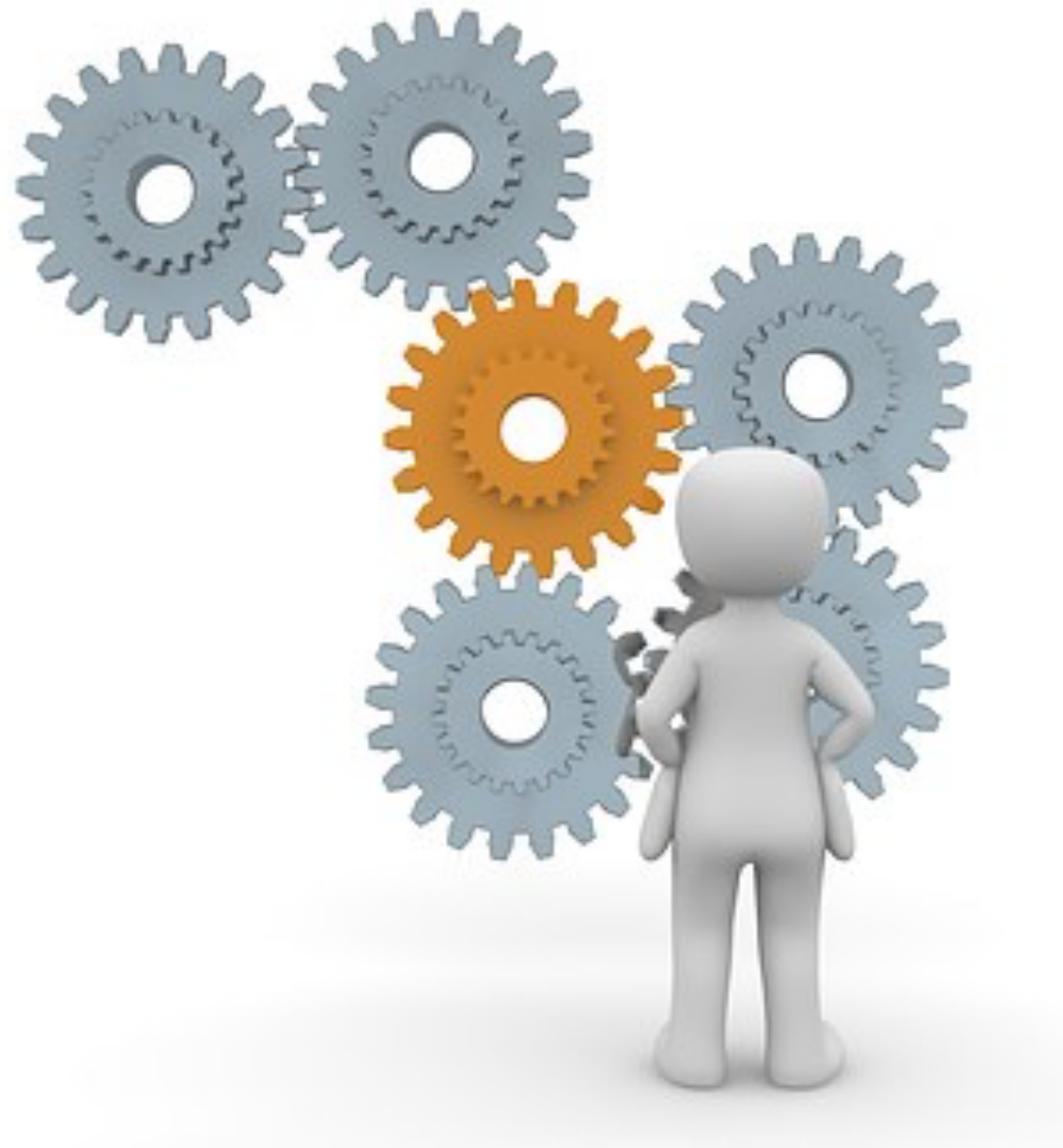


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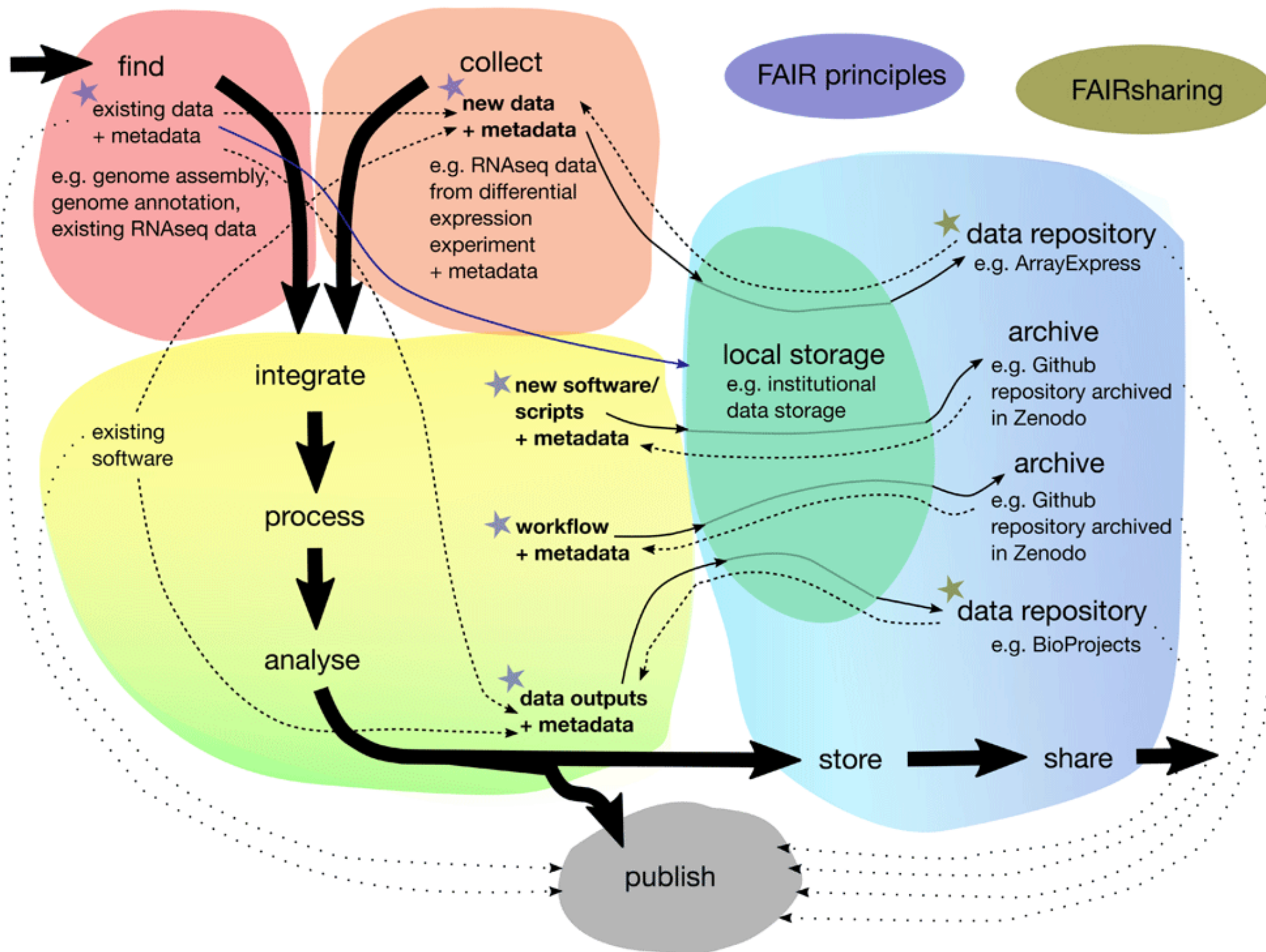
“87% of analysis time was spent on projects that had the characteristics of research...These findings suggest that to foster team-based multidisciplinary research, institutions must adopt policies that recognise contributions to research by applied bioinformatics scientists.”

– Jeffrey Chang, 2019

Practicalities: key aspects



A short intro to how we work & reproducibility



Griffin PC, Khadake J, LeMay KS et al. Best practice data life cycle approaches for the life sciences [version 2; peer review: 2 approved]. F1000Research 2018, 6:1618 (<https://doi.org/10.12688/f1000research.12344.2>)

* DATA



Sharing data with a statistician / bioinformatician

- ❖ The raw data
- ❖ The tidy / clean dataset
- ❖ A code book describing each variable and its values in the tidy data set
- ❖ An explicit and exact recipe to go from 1 to 2 and 3

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Expecting back

- ❖ An analysis script that performs each of the analyses
- ❖ The exact computer code
- ❖ All output files and figures generated

Bioinformatics File Formats

* Bioinformatics File Formats

FASTA

*.fa, *.fasta, *.sa

A simple way to represent nucleotide or amino acid sequences of nucleic acids and proteins; 2 lines per entry

```
>XR_002086427.1 Candida albicans SC5314 uncharacterized ncRNA (SCR1), ncRNA
```

```
TGGCTGTGATGGCTTTTAGCGGAAGCGCGCTGTTTCGCGTACCTGCTGTTTGTTGAAAATTTAAGAGCAAAGTGTCCGGCTCGATCCCTGCGAATTGAATTCTGAACGCTAGAGT  
AATCAGTGTCTTTCAAGTTCTGGTAATGTTTAGCATAACCACTGGAGGGAAGCAATTCAGCACAGTAATGCTAATCGTGGTGGAGGCGAATCCGGATGGCACCTTGTTTGTTGA  
TAAATAGTGCGGTATCTAGTGTTGCAACTCTATTTTT
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AATCAGTGTCTTTCAAGTTCTGGTAATGTTTAGCATAACCACTGGAGGGAAGCAATTCAGCACAGTAATGCTAATCGTGGTGGAGGCGAATCCGGATGGCACCTTGTTTGTTGA
TAAATAGTGCGGTATCTAGTGTTGCAACTCTATTTTT

FASTQ

***.fastq, *.fq, *.sanfastq**

Puts together sequence and its quality score Q; 4 lines per entry

@K00188:208:HFLNGBBXX:3:1101:1428:1508 2:N:0:CTTGTA
ATAATAGGATCCCTTTTCCTGGAGCTGCCTTTAGGTAATGTAGTATCTNATNGACTGNCNCCANANGGCTAAAGT
+
AAAFFJJJJJJJJJJJJJJJJJJJJFJJFJJJJJFJJJJJJJJJJJJJJJJJJ#FJ#JJJJF#F#FJJ#F#JJJFJJJJ

Sequence Alignment Map, generated following mapping of the reads to reference sequence; BAM a binary equivalent; header lines (@) followed by 1 line per entry

1:497:R:-272+13M17D24M	113	1	497	37	37M	15	100338662	0	CGGGTCTGACCTGAGGAG
AACTGTGCTCCGCCTTCAG	0;==--=9;	>>>>=>>>>>>>>>=>>>>>>>>>	XT:A:U	NM:i:0	SM:i:37	AM:i:0	X0:i:1	X1:i:0	XM
:i:0	X0:i:0	XG:i:0	MD:Z:37						
19:20389:F:275+18M2D19M	99	1	17644	0	37M	=	17919	314	TATGACTGCTAATAATACCTACACAT
GTTAGAACCAT	>>>>>>>>>>>>>>>>><<>>><<>>4::>>:<9	RG:Z:UM0098:1	XT:A:R	NM:i:0	SM:i:0	AM:i:0	X0:i:4	X1	
:i:0	XM:i:0	X0:i:0	XG:i:0	MD:Z:37					
19:20389:F:275+18M2D19M	147	1	17919	0	18M2D19M	=	17644	-314	GTAGTACCAACTGTAAGT

QNAME	FLAG	RNAME	POS	MAPQ	CIGAR	RNEXT	PNEXT	TLEN	SEQ
272+13M17D24M	113	1	497	37	37M	15	100338662	0	CGGGTCTGACCTGAGGAG
CCGCCTTCAG	0;==--==9;>>>>=>>>>>>>>=>>>>>>>>					XT:A:U	NM:i:0 SM:i:37 AM:i:0		X0:i:1 X1:i:0 XM
O:i:0 XG:i:0 MD:Z:37									
F:275+18M2D19M	99	1	17644	0	37M	=	17919	314	TATGACTGCTAATAATACCTACACAT
AT	>>>>>>>>>>>>>>>>>>>><<>><<>>4::>>:<9					RG:Z:UM0098:1	XT:A:R NM:i:0 SM:i:0 AM:i:0		X0:i:4 X1
M:i:0 X0:i:0 XG:i:0 MD:Z:37									
F:275+18M2D19M	147	1	17919	0	18M2D19M	=	17644	-314	GTAGTACCAACTGTAAGT

Example :

<https://samtools.github.io/hts-specs/VCFv4.2.pdf>

VCF *.vcf

Variant Calling Format/File, used to store gene sequence variations, header lines (##) followed by 1 liner per entry

```
##FORMAT=<ID=GT,Number=1,Type=String,Description="Genotype">
##FORMAT=<ID=GQ,Number=1,Type=Integer,Description="Genotype Quality">
##FORMAT=<ID=DP,Number=1,Type=Integer,Description="Read Depth">
##FORMAT=<ID=HQ,Number=2,Type=Integer,Description="Haplotype Quality">
#CHROM POS ID REF ALT QUAL FILTER INFO FORMAT NA000001 NA000002 NA000003
20 14370 rs6054257 G A 29 PASS NS=3;DP=14;AF=0.5;DB;H2 GT:GQ:DP:HQ 0|0:48:1:51,51 1|0:48:8:51,51 1/1:43:5:.,.
20 17330 . T A 3 q10 NS=3;DP=11;AF=0.017 GT:GQ:DP:HQ 0|0:49:3:58,50 0|1:3:5:65,3 0/0:41:3
20 1110696 rs6040355 A G,T 67 PASS NS=2;DP=10;AF=0.333,0.667;AA=T;DB GT:GQ:DP:HQ 1|2:21:6:23,27 2|1:2:0:18,2 2/2:3
5:4
20 1230237 . T . 47 PASS NS=3;DP=13;AA=T GT:GQ:DP:HQ 0|0:54:7:56,60 0|0:48:4:51,51 0/0:61:2
20 1234567 microsat1 GTC G,GTCT 50 PASS NS=3;DP=9;AA=G GT:GQ:DP 0/1:35:4 0/2:17:2 1/1:40:3
```

GFF/GTF

*.gff, *.gff2, *.gff3, *.gtf

General Feature Format / Gene Transfer Format, used for describing genes and other features of DNA, RNA and protein sequences

GTF

```
1 transcribed_unprocessed_pseudogene gene 11869 14409 . + . gene_id "ENSG00000223972"; gene_name "DDX11L1"; gene_source "havana"; gene_biotype "transcribed_unprocessed_pseudogene";
1 processed_transcript transcript 11869 14409 . + . gene_id "ENSG00000223972"; transcript_id "ENST00000456328"; gene_name "DDX11L1"; gene_source "havana"; transcript_biotype "processed_transcript";
```

GFF

```
X Ensembl Repeat 2419108 2419128 42 . . hid=trf; hstart=1; hend=21
X Ensembl Repeat 2419108 2419410 2502 - . hid=AluSx; hstart=1; hend=303
X Ensembl Repeat 2419108 2419128 0 . . hid=dust; hstart=2419108; hend=2419128
X Ensembl Pred.trans. 2416676 2418760 450.19 - 2 genscan=GENSCAN00000019335
X Ensembl Variation 2413425 2413425 . + .
X Ensembl Variation 2413805 2413805 . + .
```

Fields

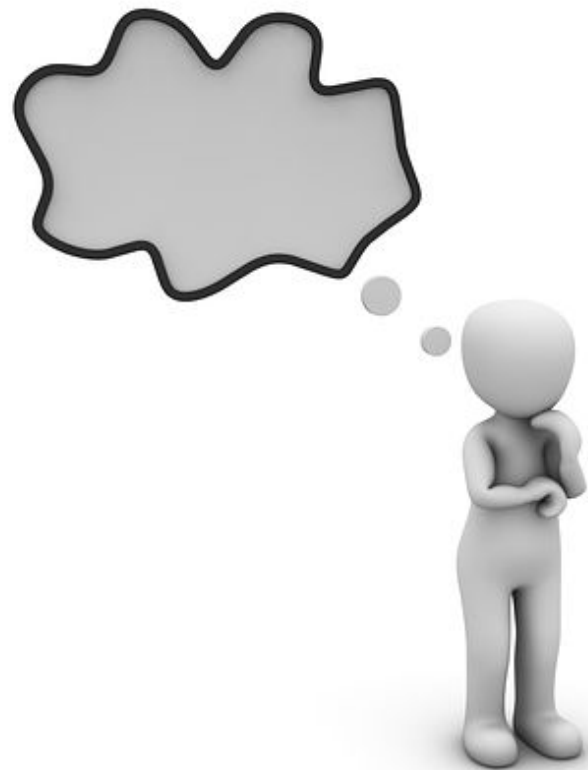
Fields **must** be tab-separated. Also, all but the final field in each feature line must contain a value; "empty" columns should be denoted with a '.'

1. **seqname** - name of the chromosome or scaffold; chromosome names can be given with or without the 'chr' prefix. **Important note:** the seqname must be one used within Ensembl, i.e. a standard chromosome name or an Ensembl identifier such as a scaffold ID, without any additional content such as species or assembly. See the example GFF output below.
2. **source** - name of the program that generated this feature, or the data source (database or project name)
3. **feature** - feature type name, e.g. Gene, Variation, Similarity
4. **start** - Start position of the feature, with sequence numbering starting at 1.
5. **end** - End position of the feature, with sequence numbering starting at 1.
6. **score** - A floating point value.
7. **strand** - defined as + (forward) or - (reverse).
8. **frame** - One of '0', '1' or '2'. '0' indicates that the first base of the feature is the first base of a codon, '1' that the second base is the first base of a codon, and so on..
9. **attribute** - A semicolon-separated list of tag-value pairs, providing additional information about each feature.

source: <https://www.ensembl.org/info/website/upload/gff.html>

Let's discuss: share your experiences in any of the following

- ❖ locating data
- ❖ describing data (metadata)
- ❖ coding data (continuous, ordinal, categorical, missing, censored)
- ❖ sharing data



* Unix-like operating systems

Unix, 1960s, Bell Labs

“Unix philosophy” of creating small, modular utilities that do one thing and do them well.

Commonly used for: working with files and directories; checking file sizes, previewing data, summary statistics

```
# List directory content
[olga@rackham3 Fastq]$ ls -lh
total 23G
-rw-rw---- 1 5.8G Sep 10 09:18 P12516_101_R1.fastq
-rw-rw---- 1 5.8G Sep 10 09:18 P12516_101_R2.fastq
-rw-rw---- 1 5.4G Sep 10 09:18 P12516_102_R1.fastq
-rw-rw---- 1 5.4G Sep 10 09:18 P12516_102_R2.fastq

# Output the first part of files
head P12516_101_R1.fastq
@A00187:119:H72F7DRXX:2:1101:1072:1000 1:N:0:ATTACTCG
CAATGTTCTGCATGGTTATCGATCCGGAGGCTGCTAGCTTTCCAGCCAGAC
+
FFFFFFFFFFFFFFFFFFFFFFFF:FFFFFFFFFFFFFFFFFFFFFFFF
```

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```

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CAATGTTCTGCATGGTTATCGATCCGGAGGCTGCTAGCTTTCCAGCCAGAC
+
FFFFFFFFFFFFFFFFFFFF::FFFFFFFFFFFFFFFFFFFFFFFFFFFF
```

* High-performance computers & large-scale storage



Tetralith, NSC, Linköping University

e.g. <https://www.uppmax.uu.se>

UPPMAX (Uppsala Multidisciplinary Center for Advanced Computational Science) is Uppsala University's resource of high-performance computers, large-scale storage and know-how of high-performance computing (HPC)

Commonly used as: computational infrastructure and project/temporary data storage

* Bioinformatics tools

e.g. FastQC, SAMtools, BEDTools

```
# Use samtools to generate stats  
samtools stats example.sam
```

```
# Sort bed file  
bedutils sort example.bed
```

```
# Mapping reads to a reference  
star --genomeDir /proj/uppstore2019092/NBIS/Index/Star --readFilesIn /proj/snic2019-8-218/private/NBIS/Cutad  
apt/v03/Out/FC5_9.trim8.fastq.gz --readFilesCommand zcat --outFileNamePrefix /proj/uppstore2019092/NBIS/Star  
/Out/v03/FC5_9/FC5_9_ --runThreadN 4 --outFilterMultimapNmax 999 --outFilterMismatchNmax 3 --outSAMtype SAM  
--outSAMunmapped Within --outFilterMultimapScoreRange 1 --seedSearchStartLmax 15
```

Installed Software

<https://www.uppmax.uu.se/resources/software/installed-software/>

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apt/v03/Out/FC5_9.trim8.fastq.gz --readFilesCommand zcat --outFileNamePrefix /proj/uppstore2019092/NBIS/Star
/Out/v03/FC5_9/FC5_9_ --runThreadN 4 --outFilterMultimapNmax 999 --outFilterMismatchNmax 3 --outSAMtype SAM
--outSAMunmapped Within --outFilterMultimapScoreRange 1 --seedSearchStartLmax 15
```



bio.tools

Database (Oxford). 2014; 2014: bau069.

PMCID: PMC4095679

Published online 2014 Jul 14. doi: [10.1093/database/bau069](https://doi.org/10.1093/database/bau069)PMID: [25024350](https://pubmed.ncbi.nlm.nih.gov/25024350/)

OMICtools: an informative directory for multi-omic data analysis

Vincent J. Henry,¹ Anita E. Bandrowski,² Anne-Sophie Pepin,³ Bruno J. Gonzalez,¹ and Arnaud Desfeux^{3,*}

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Abstract

Go to:

Recent advances in 'omic' technologies have created unprecedented opportunities for biological research, but current software and database resources are extremely fragmented. OMICtools is a manually curated metadatabase that provides an overview of more than 4400 web-accessible tools related to genomics, transcriptomics, proteomics and metabolomics. All tools have been classified by omic technologies (next-generation sequencing, microarray, mass spectrometry and nuclear magnetic resonance) associated with published evaluations of tool performance. Information about each tool is derived either from a diverse set of developers, the scientific literature or from spontaneous submissions. OMICtools is expected to serve as a useful didactic resource not only for bioinformaticians but also for experimental researchers and clinicians.

Database URL: <http://omictools.com/><https://omictools.com>

Sci Data. 2018; 5: 180023.

PMCID: PMC5827688

Published online 2018 Feb 27. doi: [10.1038/sdata.2018.23](https://doi.org/10.1038/sdata.2018.23)PMID: [29485625](https://pubmed.ncbi.nlm.nih.gov/29485625/)

Article

Datasets2Tools, repository and search engine for bioinformatics datasets, tools and canned analyses

Denis Torre,¹ Patrycja Krawczuk,¹ Kathleen M. Jagodnik,¹ Alexander Lachmann,¹ Zichen Wang,¹ Lily Wang,¹ Maxim V. Kuleshov,¹ and Avi Ma'ayan^{a,1}

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Abstract

Go to:

Biomedical data repositories such as the Gene Expression Omnibus (GEO) enable the search and discovery of relevant biomedical digital data objects. Similarly, resources such as OMICtools, index bioinformatics tools that can extract knowledge from these digital data objects. However, systematic access to pre-generated 'canned' analyses applied by bioinformatics tools to biomedical digital data objects is currently not available. Datasets2Tools is a repository indexing 31,473 canned bioinformatics analyses applied to 6,431 datasets. The Datasets2Tools repository also contains the indexing of 4,901 published bioinformatics software tools, and all the analyzed datasets. Datasets2Tools enables users to rapidly find datasets, tools, and canned analyses through an intuitive web interface, a Google Chrome extension, and an API. Furthermore, Datasets2Tools provides a platform for contributing canned analyses, datasets, and tools, as well as evaluating these digital objects according to their compliance with the findable, accessible, interoperable, and reusable (FAIR) principles. By incorporating community engagement, Datasets2Tools promotes sharing of digital resources to stimulate the extraction of knowledge from biomedical research data. Datasets2Tools is freely available from: <http://amp.pharm.mssm.edu/datasets2tools>.

<http://amp.pharm.mssm.edu/datasets2tools/>

*** Scripts and programs**
putting commands together



C++



THE
C
PROGRAMMING
LANGUAGE



*** Scripts and programs**
putting commands together



Main three (interpreted)



C++



THE
C
PROGRAMMING
LANGUAGE



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Main three (interpreted)



C++



THE
C
PROGRAMMING
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Compiled languages

*** Scripts and programs**
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Main three (interpreted)



C++



THE
C
PROGRAMMING
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Website development

Compiled languages

*** Scripts and programs**
putting commands together



Main three (interpreted)



C++



THE
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Website development

Compiled languages



open-source initiatives

*** Scripts and programs**
putting commands together



Main three (interpreted)



Website development



Compiled languages



open-source initiatives

- ❖ **Interpreted vs. compiled languages**
- ❖ **Script vs. program vs. tool vs. software**

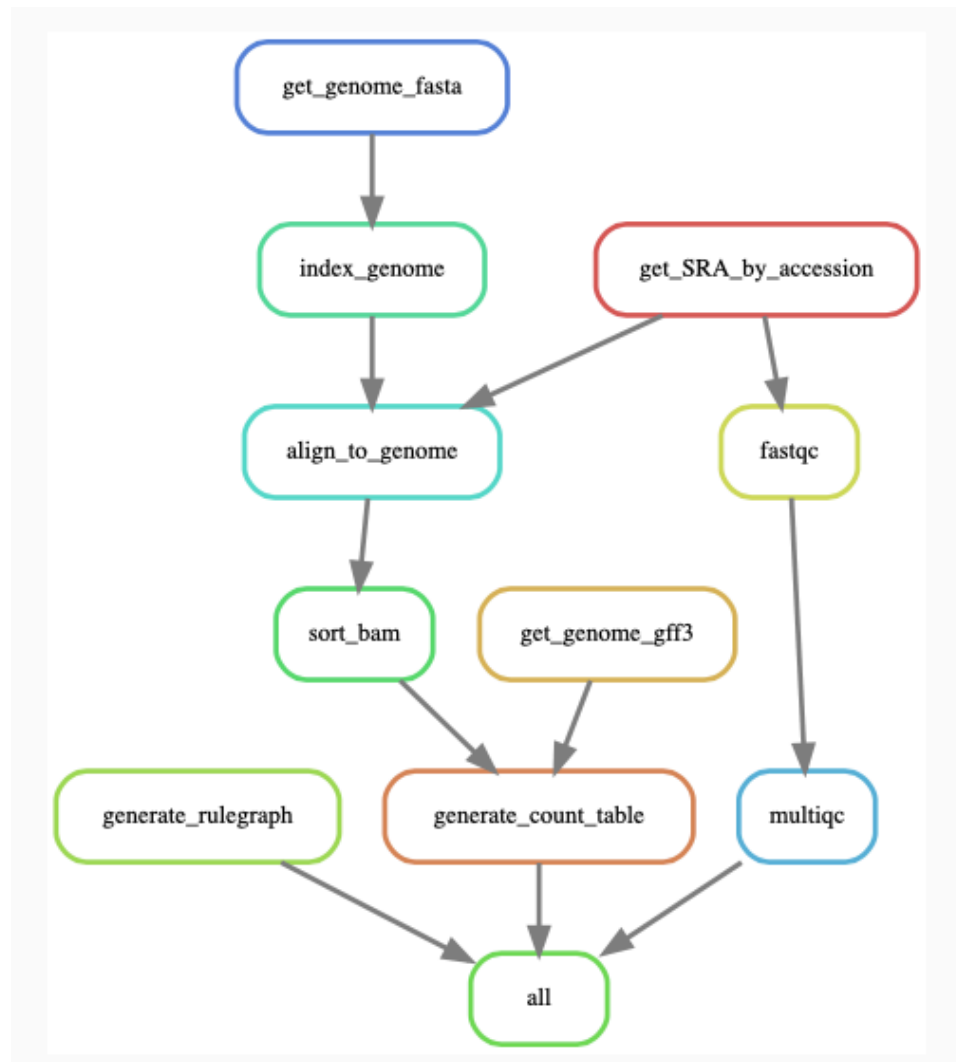
Read more:

<http://omgenomics.com/programming-languages/>
<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2267699/>

* Workflows

automating tasks

tracking provenance



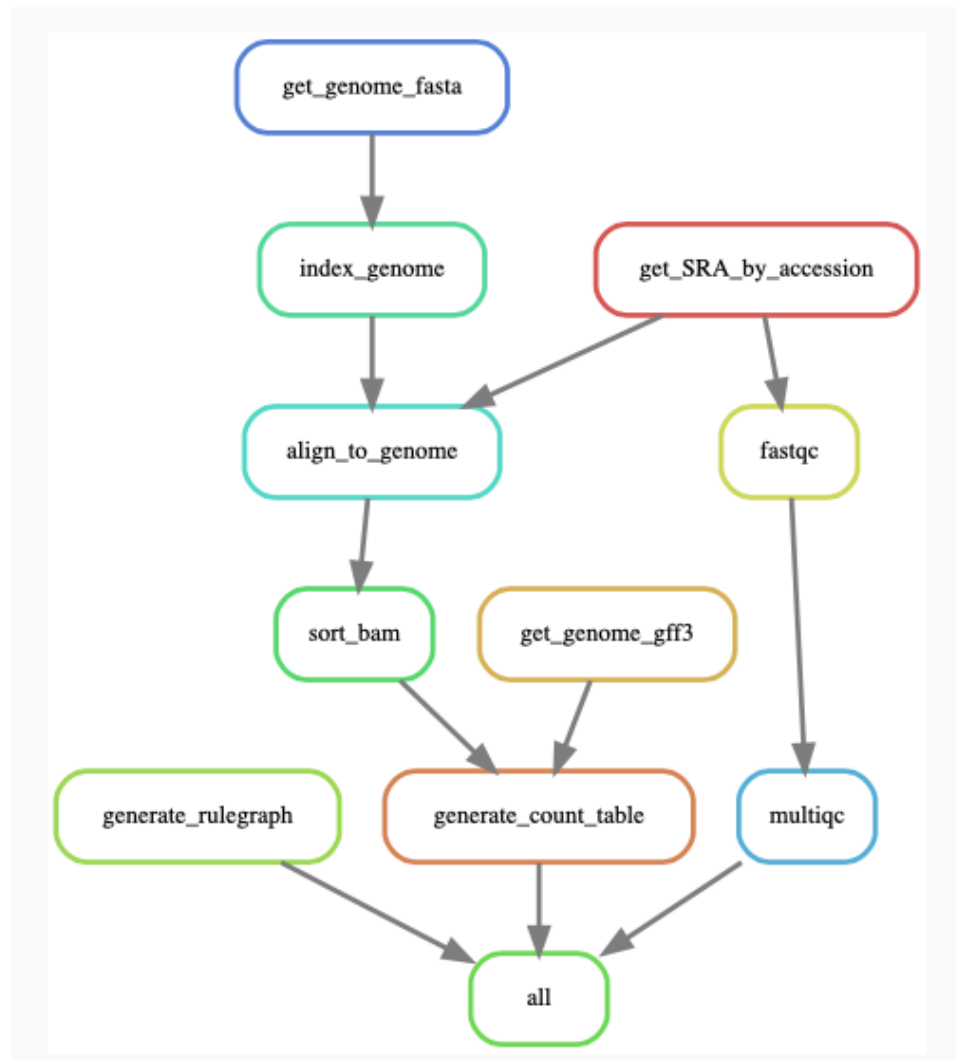
* Workflows

automating tasks
tracking provenance

TOOLBOX • 02 SEPTEMBER 2019

Workflow systems turn raw data into scientific knowledge

How workflow tools can make your computational methods portable, maintainable, producible and shareable.



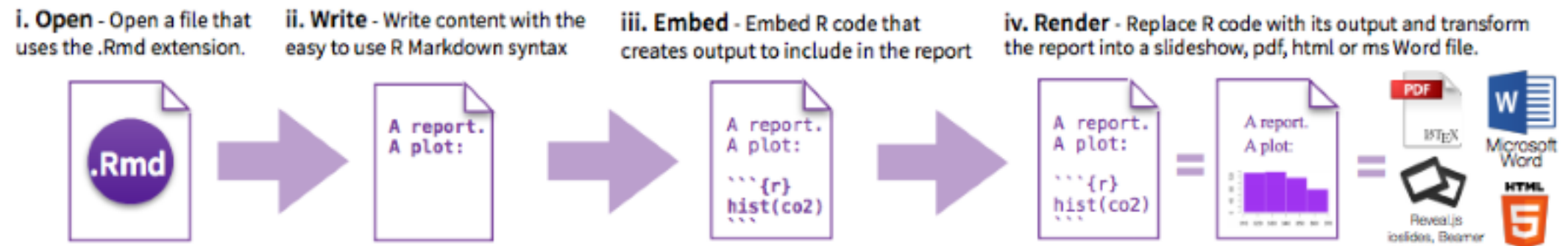
Snakemake

nextflow

Galaxy

* Literate computing & authoring

writing self-contained documents that include narrative and code used to generate both text and graphical results



* Literate computing & authoring

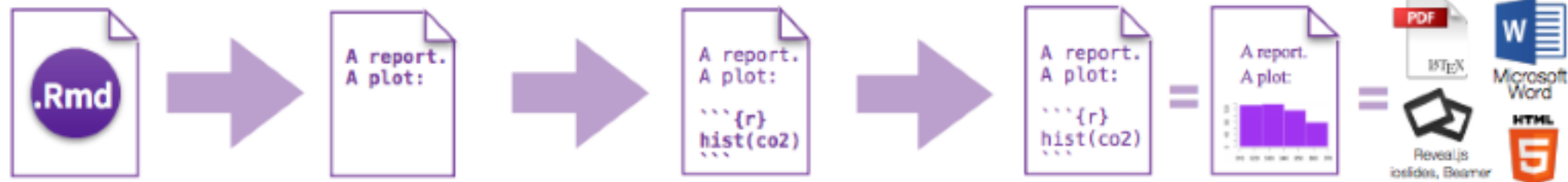
writing self-contained documents that include narrative and code used to generate both text and graphical results

i. **Open** - Open a file that uses the .Rmd extension.

ii. **Write** - Write content with the easy to use R Markdown syntax

iii. **Embed** - Embed R code that creates output to include in the report

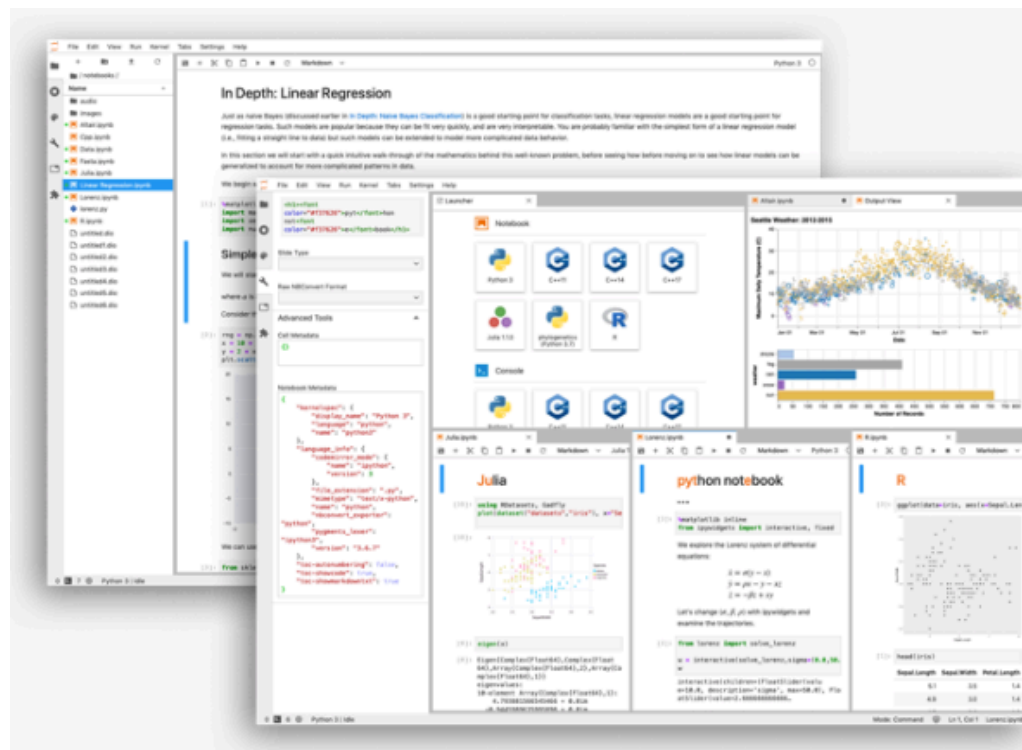
iv. **Render** - Replace R code with its output and transform the report into a slideshow, pdf, html or ms Word file.



The LATEX Project



Project Jupyter exists to develop open-source software, open-standards, and services for interactive computing across dozens of programming languages.



JupyterLab 1.0: Jupyter's Next-Generation Notebook Interface


JupyterLab is a web-based interactive development environment for Jupyter notebooks, code, and data. JupyterLab is flexible: configure and arrange the user interface to support a wide range of workflows in data science, scientific computing, and machine learning. JupyterLab is extensible and modular: write plugins that add new components and integrate with existing ones.

Try it in your browser

Install JupyterLab

* Version control

keeping a record of file changes over time
collaborating on a code development

The image is a screenshot of the Git website's header and main content area. At the top left is the Git logo (an orange diamond with a white branching diagram) followed by the word "git" in a bold, lowercase font. To the right of the logo is the tagline "--distributed-even-if-your-workflow-isnt". Further right is a search bar with the placeholder text "Search entire site...". Below the header, the main content area has a light gray background with a subtle diamond pattern. On the left, there are two paragraphs of text. The first paragraph describes Git as a "free and open source" distributed version control system. The second paragraph describes it as "easy to learn" and having a "tiny footprint with lightning fast performance". On the right side of the main content area is a diagram showing several stacks of white papers, each with a small colored bar at the top. These stacks are connected by thick, colored lines (red, blue, yellow) that represent different branches or workflows in a distributed version control system.

git --distributed-even-if-your-workflow-isnt

Search entire site...

Git is a **free and open source** distributed version control system designed to handle everything from small to very large projects with speed and efficiency.

Git is **easy to learn** and has a **tiny footprint with lightning fast performance**. It outclasses SCM tools like Subversion, CVS, Perforce, and ClearCase with features like **cheap local branching**, convenient **staging areas**, and **multiple workflows**.

<https://git-scm.com>

Git repository hosting services



* Capturing the computational environment



Package and environment manager

- ❖ As a package it enables installing a wide range of tools using one command `conda install`
- ❖ As an environment manager it allows creating and managing multiple different environments, e.g. different versions of the same package

* Capturing the computational environment



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Containers

- ❖ Full control of environment. Can be used to package entire scientific workflows, software, libraries and data, by isolating everything in a “container”

Summary



Team work and project planning

- ❖ **align on a common goal**
- ❖ **value team members**
- ❖ **communicate**

Summary



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Data sharing & bioinformatics

- ❖ **planning ahead when collecting and describing data**
- ❖ **a min. knowledge of unix skills and bioinformatics terms**

Summary



Team work and project planning

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Data sharing & bioinformatics

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Planning ahead:

- ❖ **reproducible research**
- ❖ **reproducible publications**
- ❖ **sustainability and long-term growth**

“Good collaboration checklist”

https://docs.google.com/document/d/1MpefgEuklXooeo86Q5bX_wjD4RQxMHT9OIY1jEQA2q4/edit?usp=sharing

Thank you!

