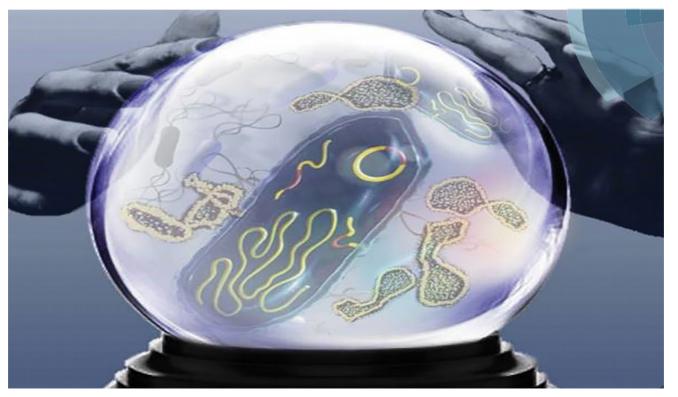




### **Multi-Omics Data Integration via Machine Learning**

Omics Integration and Systems Biology course Nikolay Oskolkov, Lund University, NBIS SciLifeLab, Sweden





@NikolayOskolkov



https://github.com/NikolayOskolkov

#### Image adapted from Molecular Omics, Issue 1, 2018

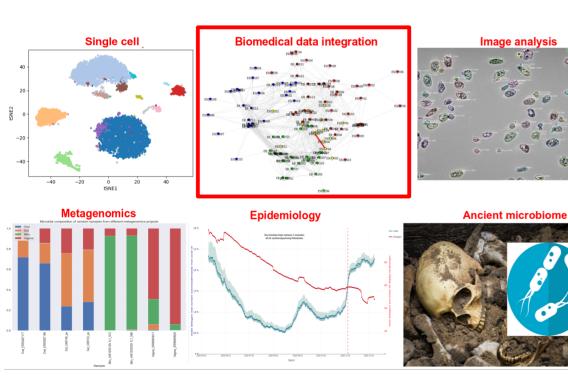


### Brief introduction: who am I



2007 PhD in theoretical physics

- 2011 medical genetics at Lund University
- 2016 working at NBIS SciLifeLab, Sweden

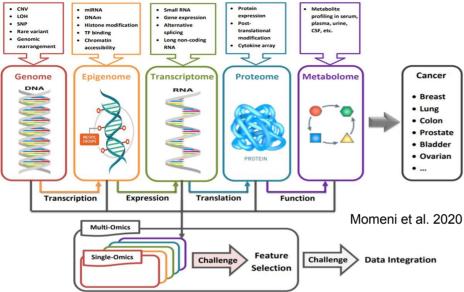








### Multi-Omics Begins: 2015 – until now



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Article Open access Published: 25 June 2024

#### Predicting type 2 diabetes via machine learning integration of multiple omics from human pancreatic islets

Tina Rönn, Alexander Perfilyev, Nikolay Oskolkov & Charlotte Ling 🖾

Scientific Reports 14, Article number: 14637 (2024) Cite this article

Rönn et al., Scientific Reports 2024



#### https://github.com/NBISweden/workshop\_omics\_integration

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### Introduction: High Dimensional Biological Data



### Various types of data around us

#### **Tabular**

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#### Text

#### Editing Wikipedia articles on

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#### Engage with editors

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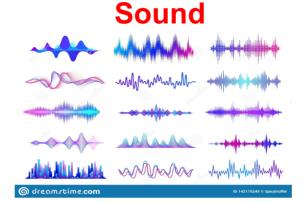
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## DATA

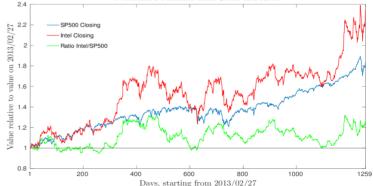
Video



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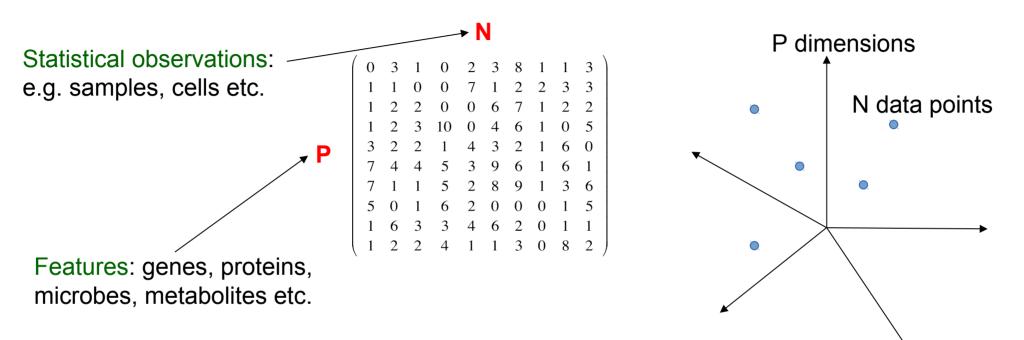
#### Time Series Normalized Financial Time Series and Ratio







#### **Biological Data are High Dimensional**



### High Dimensional Data: P >> N

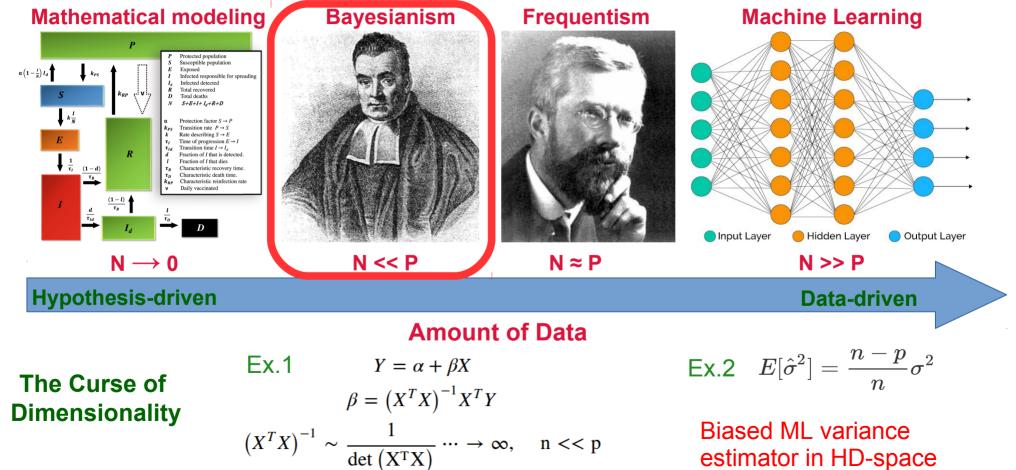
For a robust statistical analysis, one should properly "sample" the P-dimensional space, hence large sample size is required, N >> P

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### NRSS Some types of data analysis in Life Sciences J SciLifeLab

**P** is the number of features (genes, proteins, genetic variants etc.) **N** is the number of observations (samples, cells, nucleotides etc.)

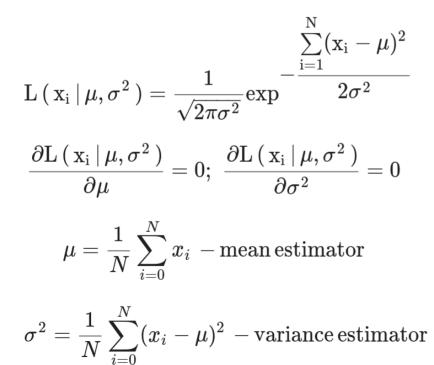
#### Biology / Biomedicine

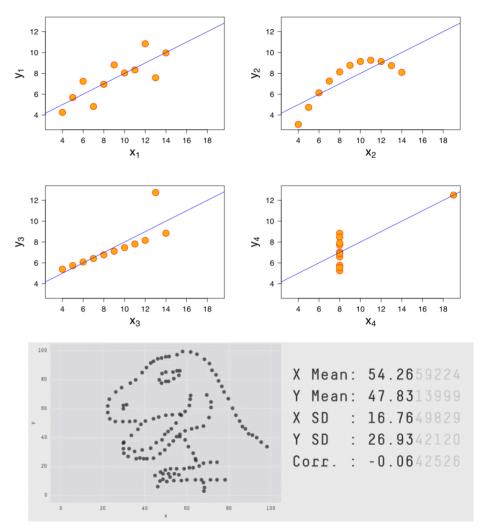


### Some peculiarities of Frequentist statistics

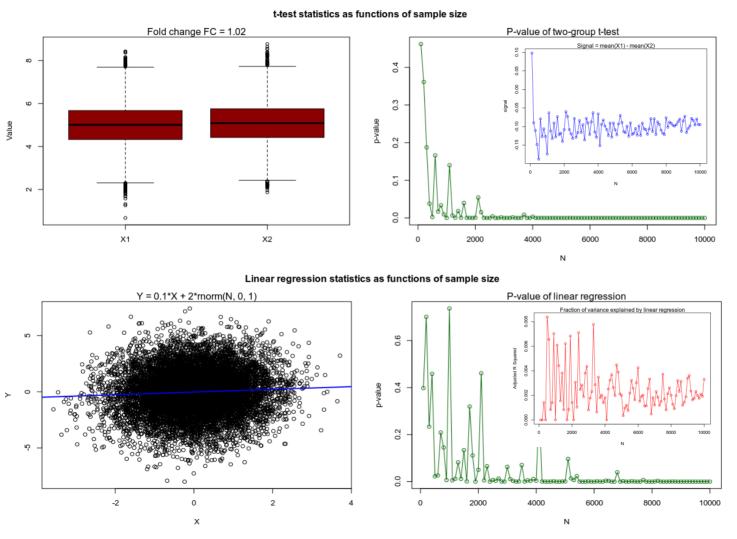


- Maximum likelihood based
- Focus on summary statistics
- Focus too much on p-values





### **NB**S Frequentist stats: too much focus on p-values **SciLifeLab**



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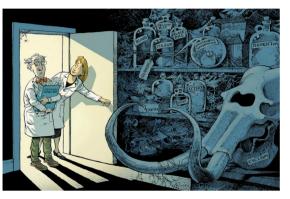
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nature



It is questionable whether p-value is the best metric for ranking features

### **B** Frequentist stats struggles with high-dimensional data **SciLifeLab**

1 n <- 20 # number of samples

- 2 p <- 2 # number of features / dimensions
- 3 Y <- rnorm(n)
- 4 X <- matrix(rnorm(n \* p), n, p)</pre>
- 5 summary(lm(Y ~ X))

Call: lm(formula = Y ~ X)

Residuals: Min 1Q Median 3Q Max -2.0522 -0.6380 0.1451 0.3911 1.8829

Coefficients: Estimate Std. Error t value Pr(>|t|)

(Intercept) 0.14950 0.22949 0.651 0.523 X1 -0.09405 0.28245 -0.333 0.743 X2 -0.11919 0.24486 -0.487 0.633

Residual standard error: 1.017 on 17 degrees of freedom Multiple R-squared: 0.02204, Adjusted R-squared: -0.09301 F-statistic: 0.1916 on 2 and 17 DF, p-value: 0.8274

#### Going to higher dimensions $\rightarrow$

1 n <- 20 # number of samples
2 p <- 10 # number of features / dimensions
3 Y <- rnorm(n)
4 X <- matrix(rnorm(n \* p), n, p)
5 summary(lm(Y ~ X))</pre>

Call: lm(formula = Y ~ X)

Residuals: Min 1Q Median 3Q Max -1.0255 -0.4320 0.1056 0.4493 1.0617

#### Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	0.54916	0.26472	2.075	0.0679	
X1	0.30013	0.21690	1.384	0.1998	
X2	0.68053	0.27693	2.457	0.0363	*
X3	-0.10675	0.26010	-0.410	0.6911	
X4	-0.21367	0.33690	-0.634	0.5417	
X5	-0.19123	0.31881	-0.600	0.5634	
X6	0.81074	0.25221	3.214	0.0106	*
X7	0.09634	0.24143	0.399	0.6992	
X8	-0.29864	0.19004	-1.571	0.1505	
X9	-0.78175	0.35408	-2.208	0.0546	
X10	0.83736	0.36936	2.267	0.0496	*

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.8692 on 9 degrees of freedom Multiple R-squared: 0.6592, Adjusted R-squared: 0.2805 F-statistic: 1.741 on 10 and 9 DF, p-value: 0.2089

Going to even higher dimensions  $\rightarrow$ 

1 n <- 20 # number of samples
2 p <- 20 # number of features / dimensions
3 Y <- rnorm(n)
4 X <- matrix(rnorm(n \* p), n, p)
5 summary(lm(Y ~ X))</pre>

Call: lm(formula = Y ~ X)

Residuals: ALL 20 residuals are 0: no residual degrees of freedom!

Coefficients: (1 not defined because of singularities)

	Estimate	Std.	Error	t	value	Pr(> t )
(Intercept)	1.34889		NaN		NaN	NaN
X1	0.66218		NaN		NaN	NaN
X2	0.76212		NaN		NaN	NaN
X3	-1.35033		NaN		NaN	NaN
X4	-0.57487		NaN		NaN	NaN
X5	0.02142		NaN		NaN	NaN
X6	0.40290		NaN		NaN	NaN
X7	0.03313		NaN		NaN	NaN
X8	-0.31983		NaN		NaN	NaN
X9	-0.92833		NaN		NaN	NaN
X10	0.18091		NaN		NaN	NaN
X11	-1.37618		NaN		NaN	NaN
X12	2.11438		NaN		NaN	NaN
X13	-1.75103		NaN		NaN	NaN
X14	-1.55073		NaN		NaN	NaN
X15	0.01112		NaN		NaN	NaN
X16	-0.50943		NaN		NaN	NaN
X17	-0.47576		NaN		NaN	NaN
X18	0.31793		NaN		NaN	NaN
X19	1.43615		NaN		NaN	NaN
X20	NA		NA		NA	NA

Residual standard error: NaN on θ degrees of freedom Multiple R-squared: 1, Adjusted R-squared: NaN F-statistic: NaN on 19 and θ DF, p-value: NA

#### This is another way we face the Curse of Dimensionality in computational biology



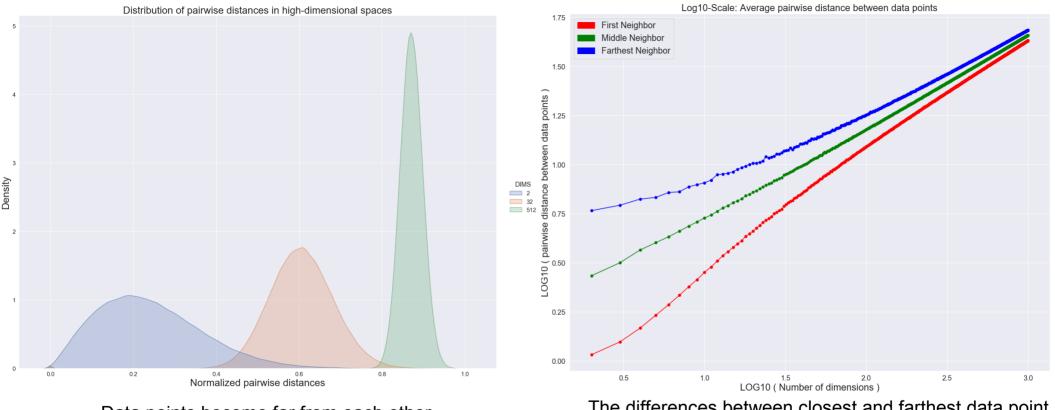


### More on the Curse of Dimensionality



### **Distances in High Dimensions**

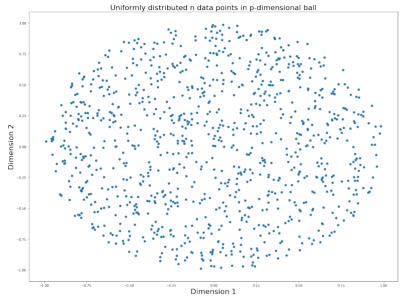


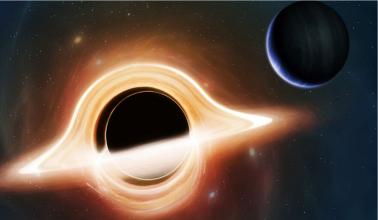


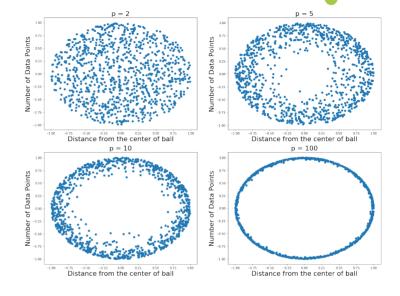
Data points become far from each other and equidistant in high dimensions The differences between closest and farthest data point neighbours disappears in high-dimensional spaces: can't run cluster analysis

#### In high-dimensional space we can not separate cases and controls any more

### **B**S High-dimensional data make black holes







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High-dimensional data can be viewed as having a **"hole in the middle"**, hence the concept of mean / centroid loses its validity, hence we can't use Gaussian distribution

### Literature on the Curse of Dimensionality

POINTS OF SIGNIFICANCE

### The curse(s) of dimensionality

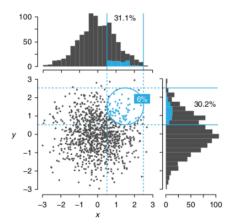
There is such a thing as too much of a good thing.

#### Naomi Altman and Martin Krzywinski

e generally think that more information is better than less. However, in the 'big data' era, the sheer number of variables that can be collected from a single sample can be problematic. This embarrassment of riches is called the 'curse of dimensionality'<sup>1</sup> (CoD) and manifests itself in a variety of ways. This month, we discuss four important problems of dimensionality as it applies to data sparsity<sup>1,2</sup>, multicollinearity<sup>3</sup>, multiple testing<sup>4</sup> and overfitting<sup>5</sup>. These effects are amplified by poor data quality, which may increase with the number of variables.

Throughout, we use *n* to indicate the sample size from the population of interest and *p* to indicate the number of observed variables, some of which may have missing values for some samples. For example, we may have n = 1,000 subjects and p = 200,000 single-nucleotide polymorphisms (SNPs).

First, as the dimensionality *p* increases, the 'volume' that the samples may occupy grows rapidly. We can think of each of the *p* 



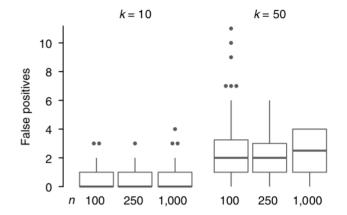
#### Fig. 1 | Data tend to be sparse in higher

**dimensions.** Among 1,000 (*x*, *y*) points in which both *x* and *y* are normally distributed with a mean of 0 and s.d.  $\sigma$  = 1, only 6% fall within  $\sigma$  of (*x*, *y*) = (1.5, 1.5) (blue circle). However, when the data are projected into a lower dimension—shown by histograms—about 30% of the points (all bins within blue called lines) are within a cf 1.5. Plue A and 100 to have the minor allele a. If we tabulate on two SNPs, A and B, we will expect only ten samples to exhibit both minor alleles with genotype ab. With SNPs A, B and C, we expect only one sample to have genotype abc, and with four or more SNPs, we expect empty cells in our table. We need a much larger sample size to observe samples with all the possible genotypes. As *p* increases, we may quickly find that there are no samples with similar values of a predictor.

Even with just five SNPs, our ability to predict and classify the samples is impeded because of the small number of subjects that have similar genotypes. In situations where there are many gene variants, this effect is exacerbated, and it may be very difficult to find affected subjects with similar genotypes and hence to predict or classify on the basis of genetic similarity.

If we treat the distance between points (e.g., Euclidian distance) as a measure of similarity, then we interpret greater distance as greater discimilarity. As a increases, this

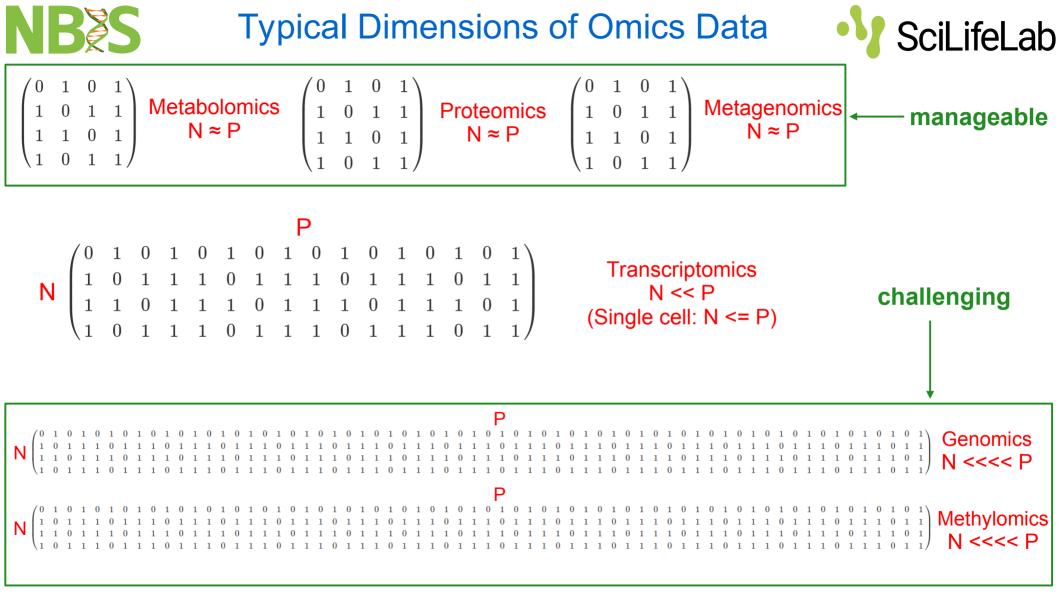
Altman N, Krzywinski M. The curse(s) of dimensionality. Nat Methods. 2018 Jun;15(6):399-400. doi: 10.1038/s41592-018-0019-x. PMID: 29855577.



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**Fig. 3** | The number of false positives increases with each additional predictor. The box plots show the number of false positive regression-fit *P* values (tested at  $\alpha = 0.05$ ) of 100 simulated multiple regression fits on various numbers of samples (n = 100, 250 and 1,000) in the presence of one true predictor and k = 10 and 50 extraneous uncorrelated predictors. Box plots show means (black center lines), 25th and 75th percentiles (box edges), and minimum and maximum values (whiskers). Outliers (dots) are jittered.

#### Correcting for multiple testing does not solve the problem of too many false-positive hits

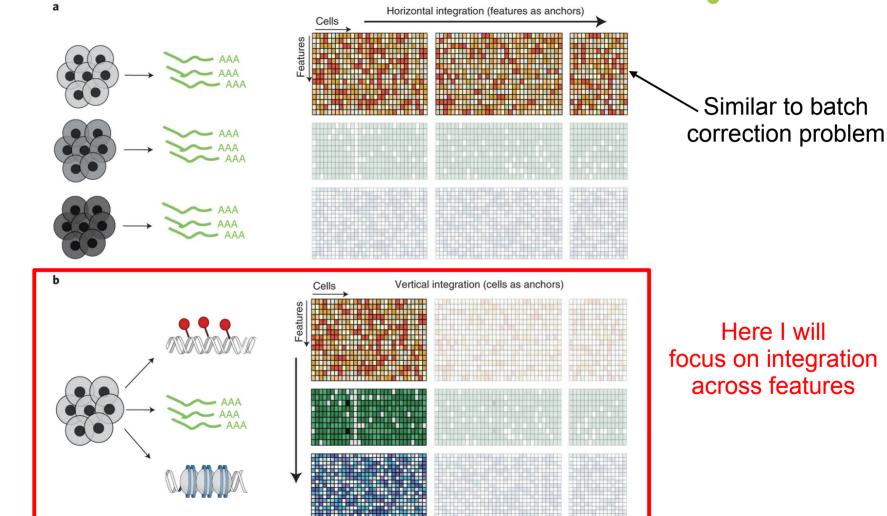






### **Multi-Omics Data Integration**

### **NB**S Integration Across Features vs. Samples SciLifeLab

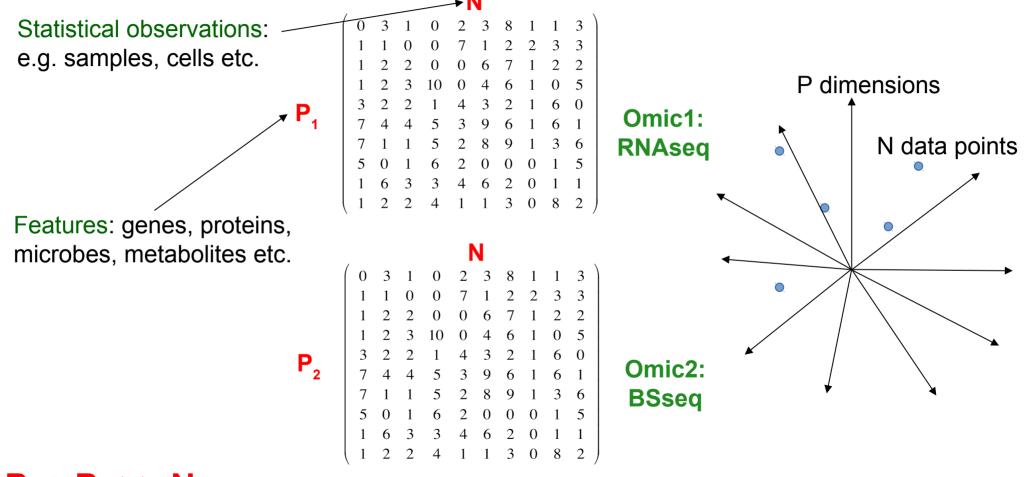


Argelaguet et al., 2021



### **Integrating Omics Across Features**



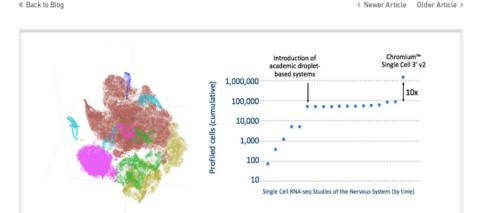


 $P_1 + P_2 >> N$  integration across features leads to even more high-dimensional data

### **Big Data in Single Cell Genomics**



# CAREERS BLOG 10X UNIVERSITY



### Our 1.3 million single cell dataset is ready 🙆 • \*\*\*\*\* 🍖 to download

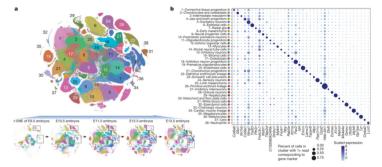


POSTED BY: grace-10x, on Feb 21, 2017 at 2:28 PM

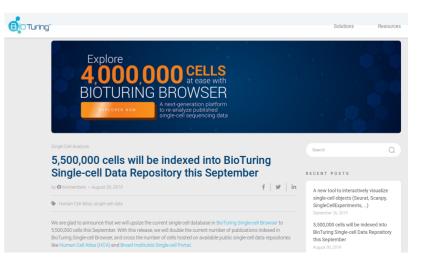
At ASHG last year, we announced our 1.3 Million Brain Cell Dataset, which is, to date, the largest dataset published in the single cell RNA-sequencing (scRNA-seq) field. Using the Chromium™ Single Cell 3' Solution (v2 Chemistry), we were able to sequence and profile 1,308,421 individual cells from embryonic mice brains. Read more in our application note Transcriptional Profiling of 1.3 Million Brain Cells with the Chromium™ Single Cell 3' Solution. MENU V nature

Fig. 2: Identifying the major cell types of mouse organogenesis.

From: The single-cell transcriptional landscape of mammalian organogenesis

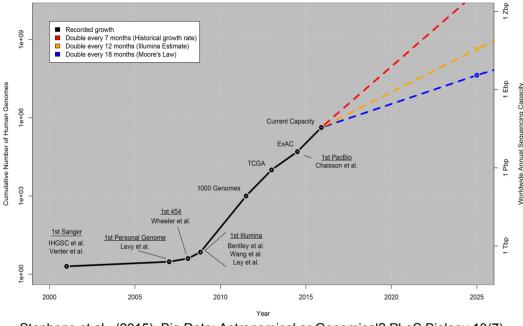


a, t-SNE visualization of 2,026,641 mouse embryo cells (after removing a putative doublet cluster), coloured by cluster identity (ID) from Louvain clustering (in b), and annotated on the basis of marker genes. The same t-SNE is plotted below, showing only cells from each stage (cell numbers from left to right: n = 151,000 for E9.5; 370,279 for E10.5; 602,784 for E11.5; 468,088 for E12.5; 434,490 for E13.5). Primitive erythroid (transient) and definitive erythroid (expanding) clusters are boxed. b, Dot plot showing expression of one selected marker gene per cell type. The size of the dot encodes the percentage of cells within a cell type in

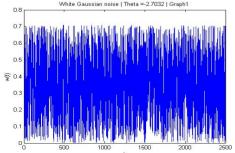


### Big in Size or Sample Size?

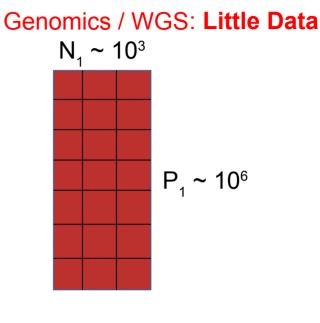
Growth of DNA Sequencing



Stephens et al., (2015). Big Data: Astronomical or Genomical? PLoS Biology 13(7)



A file with **White Noise** can also take a lot of disk space





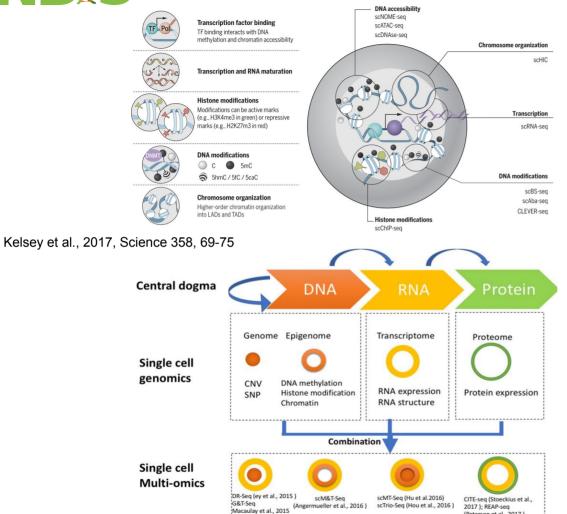
ScRNAseq: Big Data  $N_2 \sim 10^6$   $P_2 \sim 10^3$ 



### **Multi-Omics in Single Cell Genomics**

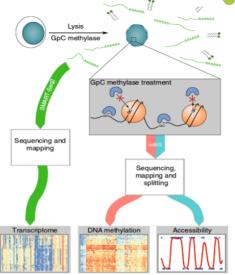
(Peterson et al., 2017)





Hu et al., 2018, Frontier in Cell and Developmental Biology 6, 1-13

NRX



Clark et al., 2018, Nature Communications 9, 781







# How to define and evaluate multi-Omics data integration?



### What I mean by Omics Integration



JIVE DISCO

**OnPLS** 

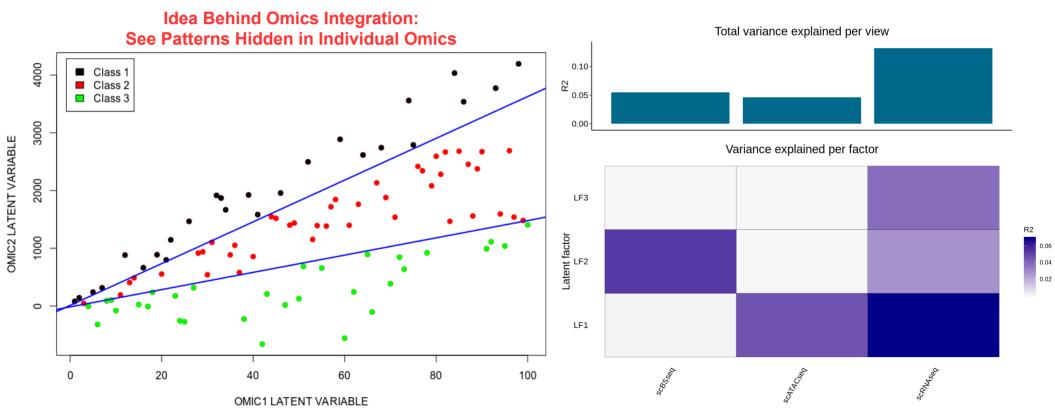








#### **Clustering of Clusters**





### How I Evaluate Omics Integration

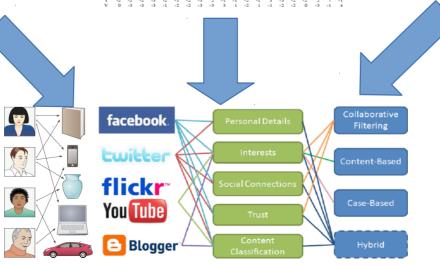
#### IMAGE (83%)



**TEXT (78%)** 



#### Predict Facebook user interests



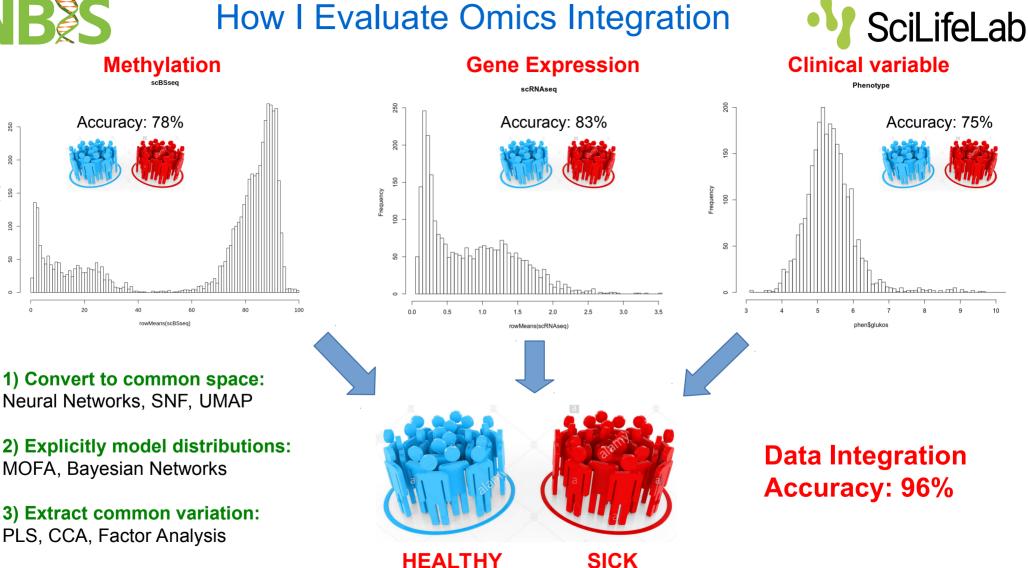
#### Data Integration Accuracy: 96%

**SciLifeLab** 

**SOUND (75%)** 

MANA

NR

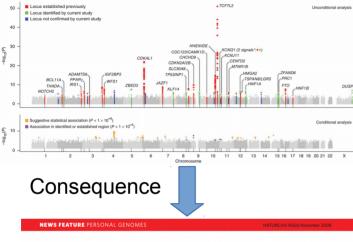




### **Prediction as a Criterion of Success**



#### Statistics searches for candidates





#### **The case of the missing heritability** B. Maher, Nature 456, 18-21 (2008)

#### Machine Learning optimizes prediction



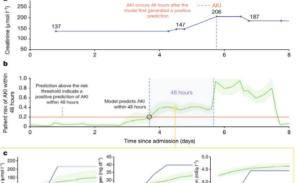
Nenad Tomašev , Xavier Glorot, [...] Shakir Mohamed

Nature 572, 116-119 (2019) Download Citation

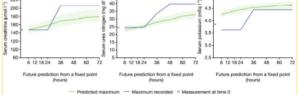
nature > letters > article

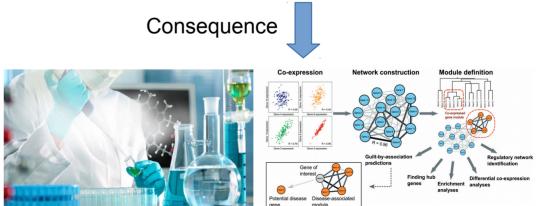
#### Abstract

The early prediction of deterioration could have an important role in supporting healthcare professionals, as an estimated 11% of deaths in hospital follow a failure to promptly recognize and treat deteriorating pattents<sup>1</sup>. To achieve this goal requires predictions of patient risk that are continuously updated and accurate, and delivered at an individual level with sufficient context and enough time to act. Here we develop a deep learning approach for the continuous risk prediction of future deterioration in patients, building on recent work that models adverse events from electronic health records<sup>23,44,56,18,9,00,12,13,14,55,67</sup> and using acute kidney injury—a common and potentially life-threatening condition<sup>31</sup>—as an exemplar. Our model was developed on a large, longitudinal dataset of electronic health records that cover diverse



From: A clinically applicable approach to continuous prediction of future acute kidney inkny







### Take Home Messages



- 1) Biological data are high-dimensional and notoriously difficult to analyze
- 2) Integration across Omics is often sensitive to the Curse of Dimensionality
- 3) Integrating across Omics we expect to discover novel patterns in the data
- 4) Increased prediction accuracy is an indication of successful data integration
- 5) Single cell Omics are promising for integration in terms of statistical power



### National Bioinformatics Infrastructure Sweden (NBIS)





Knut och Alice Wallenbergs Stiftelse



Vetenskapsrådet



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