## Lecture 1: Medical Databases

#### CSCI6410/EPAH6410/CSCI4148

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## Learning Objectives

- Overview of the types of medical database
- Ways of maintaining data privacy with medical databases and some of their trade-offs
- How and why ontologies and survey weights are used in medical databases
- Key strategies/approaches for exploratory data analysis
- Different types of dimensionality reduction
- Basics of supervised learning
- Accessing feature importances
- Aggregating simple/weak models to improve performance: boosting and bagging

## What is a database?

Examples include:

Medical Charts

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Examples include:

- Medical Charts
- Phone Book
- Dictionaries
- Spreadsheet

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Ordering:

- Index
- Defined fields
- Standardisation

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Ordering:

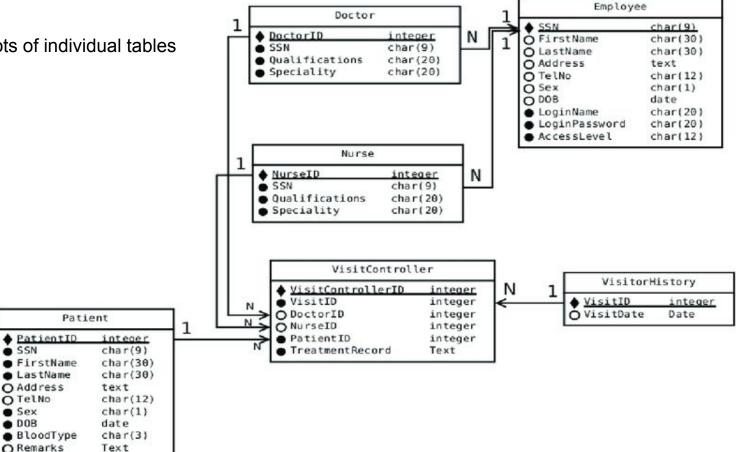
- Index
- Defined fields
- Standardisation

Organisation make some tasks easier/harder:

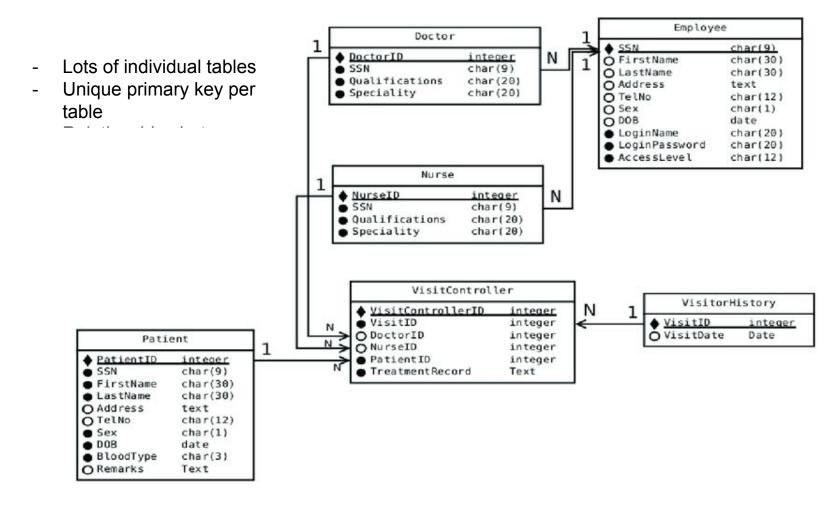
- Find all patients with the same condition
- Find the longest word in a dictionary
- Find an a number from an address in a phonebook

PART A - PRESENT HEALTH HISTORY (continued)				
GENERAL HEALTH, ATTITUDE AND HABITS (continued)				
ave you recently had any changes in your: If yes, please explain: arital status? No Yes				
th or work? No. Yes				
ssidence? No Yes				
re vou having any legal problems				
trouble with the law? No Yes				
PART B – PAST HISTORY	PART C - BODY SYSTEMS REVI	EW		
FAMILY HEALTH Have any blood relatives had any of the following illnesses?				
tease give the following information about your immediate If so, indicate relationship (mother, brother, etc.) amby: Illness Family Members	MEN Please answer questions 1 through 12, then skip to question 18, WOMEN: Please start on question 6,			
Age, If Age At State of Health Or Asthine	1 DHLY			
	4 ONLY Have you had or do you have			
Father Cancer	prostate trouble?			
Nother	Do you have any ancust proceents or with impatency? Have you even had soms or lesions on your penie?	No Yes		
and	Have you ever had sores or		C	
Sisters ) [ Rheumatoid Arthritis			0	
	from your panis? Do you ever have pain, tumps	No Yes	0	
Geut	Do you war have pair, lumps	No. Yes		
Nildren	or paeting in your testicles? . Ik here if you wish to discuss any special problems a	ith the doctor,	N	
Mercal Problems		New Occasionally Frequently		
Suicide	Is it apreetimes hard to start your urine flow?		F	
				-
	Chert No			
I. HOSPITALIZATIONS, SURGERIES ANDRUS/CLINI-REC* HEALTH HISTORY QUE	STIONNAIRE		D	
lease list all times you have been hospitals in identification information	Today's Data			4
Year Operation Name Date of Birth		Navar Occasionally Fragmently	E	
Occupation Marical Status				
Marsa Satur			N	
PART A - PRESENT HEALTH HISTO	RY			
IL ILLNESS AND MEDICAL PHOBLE			T	
Tease mark with an IX) any of the following				
f you are not certain when an illness started, Please list the medical problems for which you came to see the doctor. About when did they to	egin?			
Iness (X) Problems	Date Began			
ve or eve lid infection	C		A	
Recome		No Yes		457
bher eve problems	0	No Yes		
ar Trouble  What concerns you must about these problems?		the doctor		
	N	New Occasionally Prequently		
Imp threat				
Instructions	se describe the problems and write			
Iness or Medical Problem Physician or Medical Facility Strain and Str	ity <u>City</u>			
loerculasis		······		No.
Dher lung problems	D	No Yes		
Sph blood pressure II, MEDICATIONS		Yes		
	ecryption (such as aspirin, cold tablets or E	No Yes	Co	
vitemin supplements)		Yes		
Hardening of arteries)	N			
Seart murmur		and the second se		
Directed standition         III. ALLEGROUS AND SENSITIVITIES           Istmach-doublend ulcer	T	No Yes		
Itemachiduodenal ulcer	saps, household items, pollens, bee	No. Yes.		
Nerricultaria	Effect	Yes		
Charles Charle		No		
Separati s		No Yes, Traveled in		
Althadder trouble	— — A	Yes, Traveled in		
	Good Excellent	Mondes Strailpox		50
	Good Excellent	Petio Typhoid		
		No		
Has your appetite changed?	Increased Stayed same	Nep Pos		
Has your weight changed?	ieinedlbs.No change	197114 5/83		
Has your overall gep' changed?	IncreasedStayed same	IN THIS PAGE Page	1	
	Less than I need			
Bo you smokas' Smokes: No Yes How many each day? Digarettes	If yes, how many years? CopersPipesfull			
Have you ever smoked? Smoked No. Yes	If yes, how many years?			
Now many each day?	Cigars Pipesfull bink Beers Glasses of Wine			
Do you drink alsoholis beverages? Alsohol No	binkReersGlasses of Wine	and the second		A PARTY AND
Mave you ever had a problem with alcohol? Prior problem: No Yes	of hard liquor - per day			
How much coffee or tea do viou usually drink?	fee or tea a day.			
Do you regularly wear seathering?				
DO YOU Many business Presently DO YOU	Rear Institutivy Property			1200
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Lots of individual tables \_

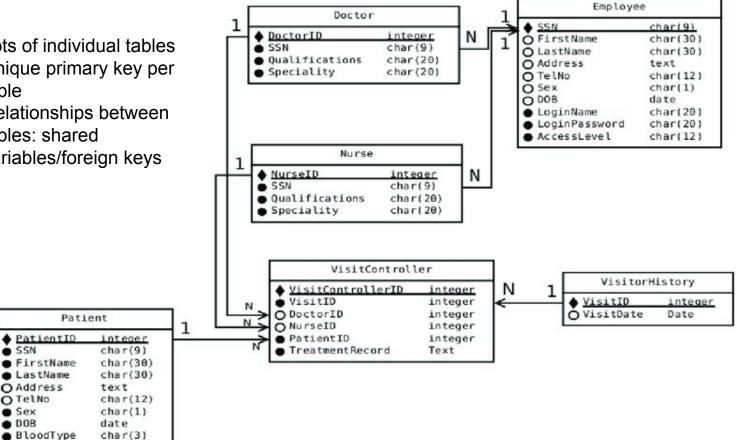


http://dx.doi.org/10.1016/j.procs.2015.08.441



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- Lots of individual tables
- Unique primary key per table
- Relationships between \_ tables: shared variables/foreign keys



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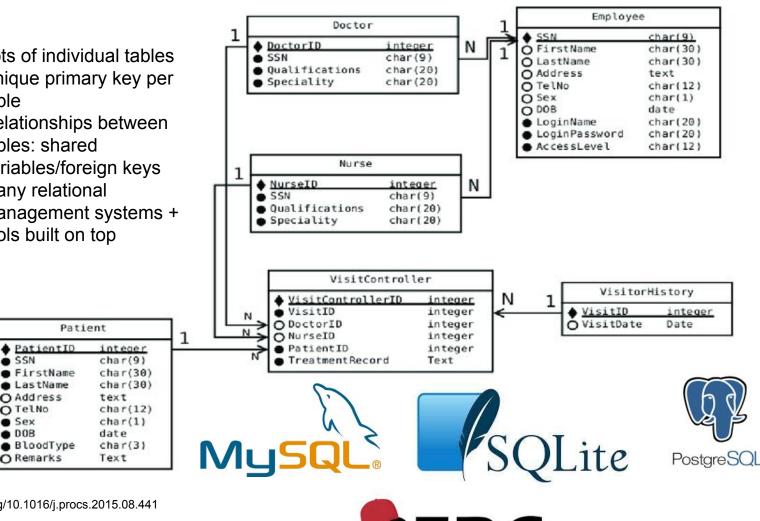
**O** Remarks

Text

• Sex

D0B

- Lots of individual tables
- Unique primary key per table
- Relationships between \_ tables: shared variables/foreign keys
- Many relational management systems + tools built on top



Research Electronic Data Capture

http://dx.doi.org/10.1016/j.procs.2015.08.441

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O Address

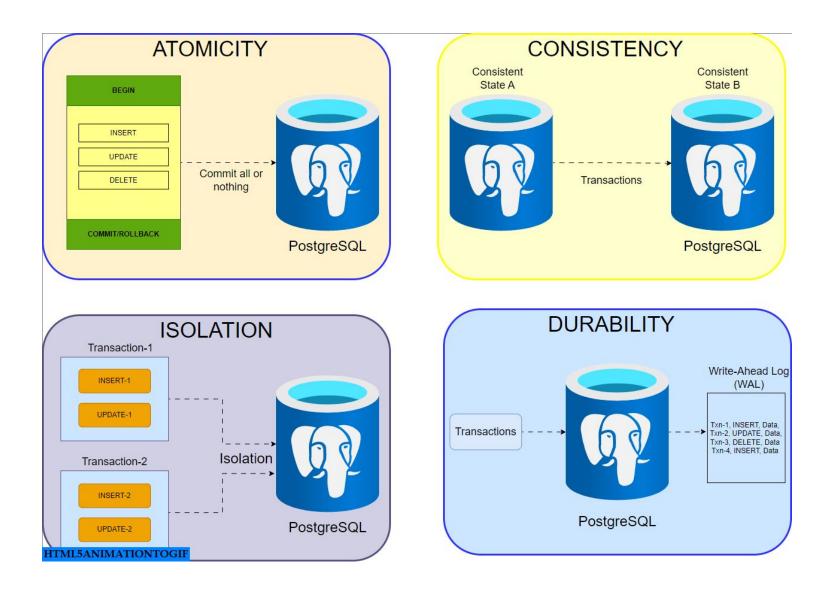
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#### Most relational databases support ACID properties



## Queried using Structured Query Language (SQL)

- Non-procedural Language
- Standardised/powerful/flexible

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```
flights %>%
```

```
select(contains("delay")) %>%
show_query()
```

```
#> <SQL>
```

```
#> SELECT `dep_delay`, `arr_delay`
```

```
#> FROM `nycflights13::flights`
```

```
flights %>%
```

```
group_by(month, day) %>%
summarise(delay = mean(dep_delay)) %>%
```

```
show_query()
```

```
#> Warning: Missing values are always removed in SQL.
```

```
#> Use `AVG(x, na.rm = TRUE)` to silence this warning
```

```
#> <SQL>
```

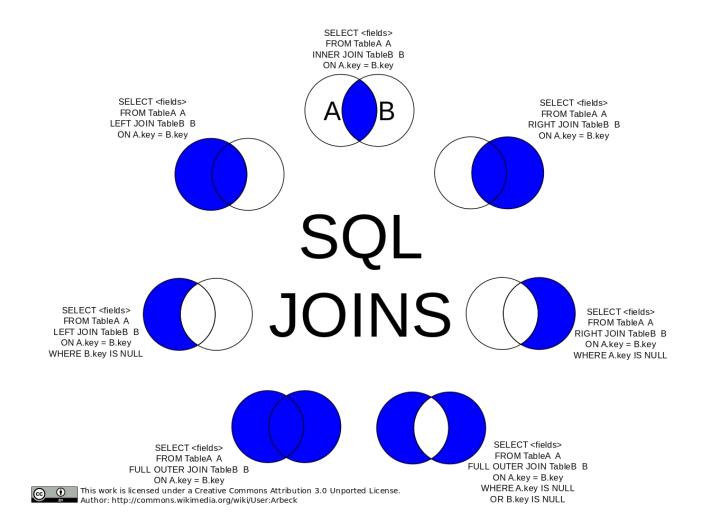
```
#> SELECT `month`, `day`, AVG(`dep_delay`) AS `delay`
```

```
#> FROM `nycflights13::flights`
```

```
#> GROUP BY `month`, `day`
```

```
flights %>%
  select(distance, air_time) %>%
  mutate(speed = distance / (air_time / 60)) %>%
  show_query()
#> <SQL>
#> SELECT `distance`, `air_time`, `distance` / (`air_time` / 60.0) AS `speed`
#> FROM (SELECT `distance`, `air_time`
#> FROM `nycflights13::flights`)
```

#### SQL enables complex joins/queries



#### Fun way to learn basic SQL

https://mystery.knightlab.com/



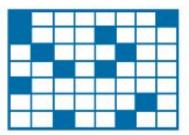
Can you find out whodunnit?



## Are all databases relational?

- Less common than relational in medicine
- General focus on flexibility & performance
- Mostly for very large/unusual datasets or high demand:
  - User data / security audit data
  - Medical image data
- Or unusual data structures:
  - Contact tracing
  - Ontologies
- Or both:
  - Social media data

https://phoenixnap.com/kb/database-types

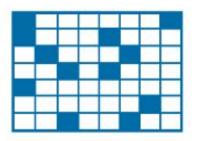


#### Column based



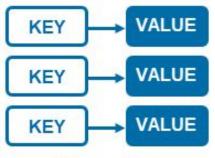
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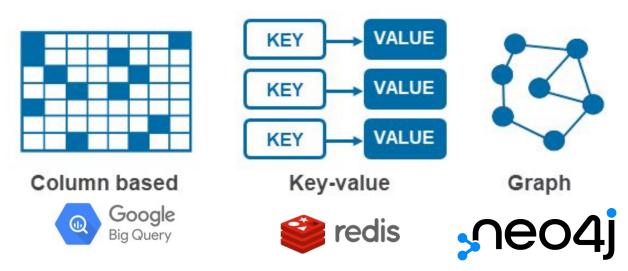


Key-value



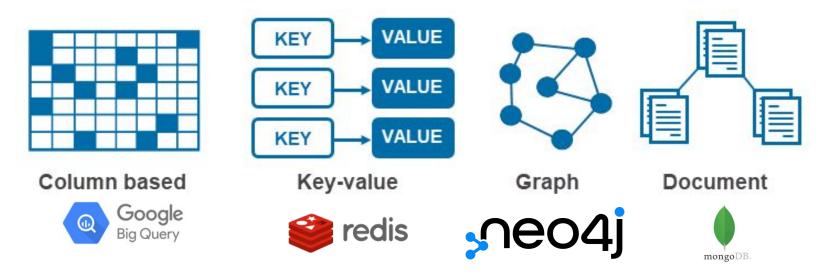
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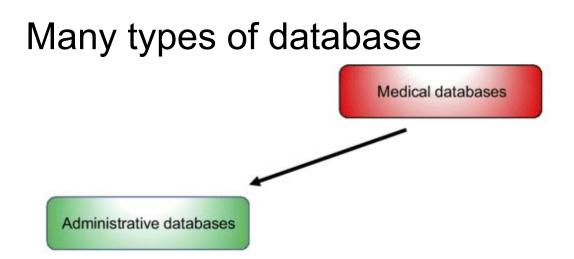


## What are medical databases?

#### Many types of database

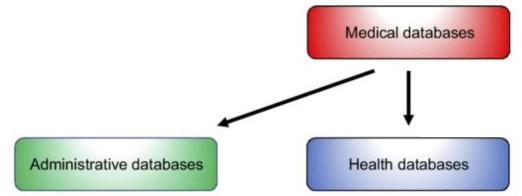
Medical databases

All types of registries and databases that contain health-related data



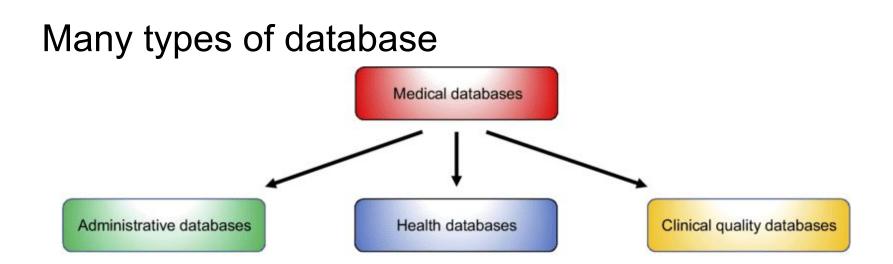
Register individuals according to geographic area, health insurance program, or attendance at a particular hospital or clinic

## Many types of database

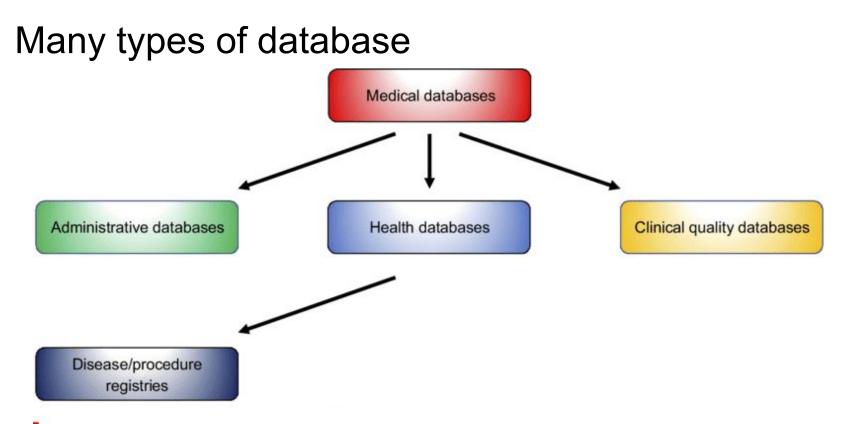


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Register health data for the purpose of surveillance and research



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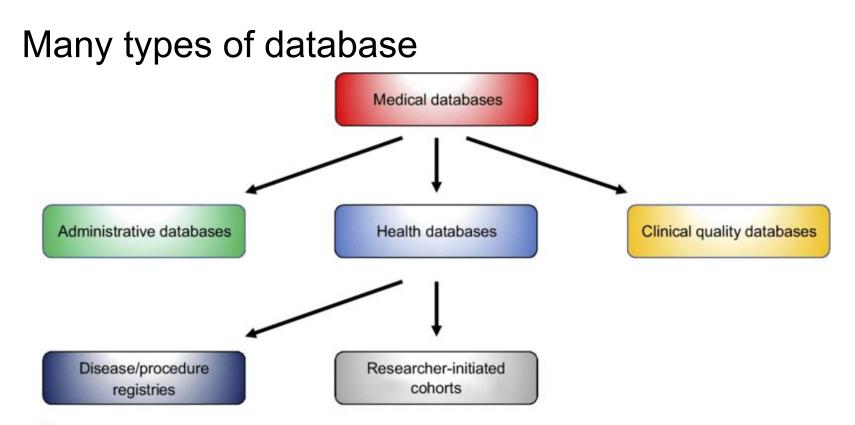


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Register detailed clinical data for clinical quality control

Register patients according to diagnosis or procedure



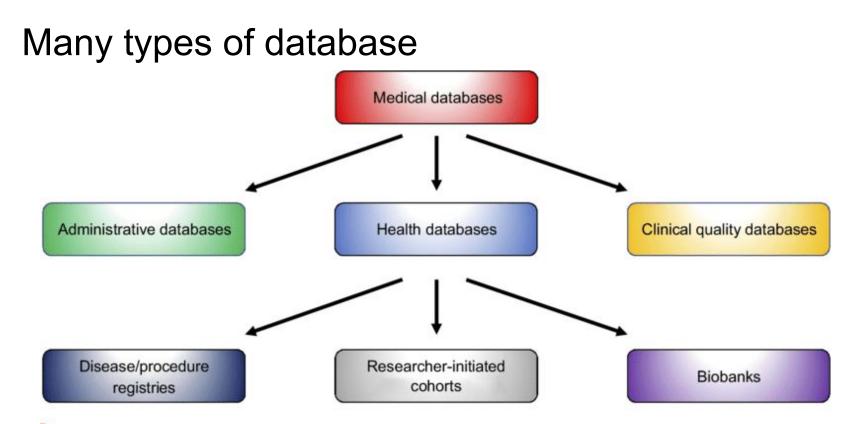
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Store biological samples (eg, blood and tissue)

## Consider primary record type

- Individual procedures e.g., arthroplasty
- Prescriptions e.g., colistin
- Disease/Illness e.g., ovarian cancer
- Hospital Admission/Discharge
- Individual health interactions
- Patient
- Person
- Population

## Sampling scope

- Single physician
- Group of physicians
- Hospital
- Health Authority
- Province
- National
- International

Generalisability

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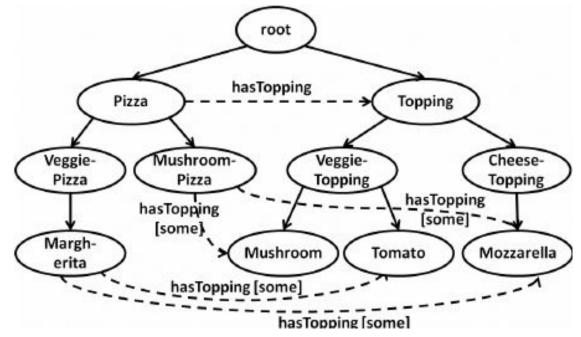
Challenge of standardisation

Generalisability

# How do medical databases try to handle standardisation?

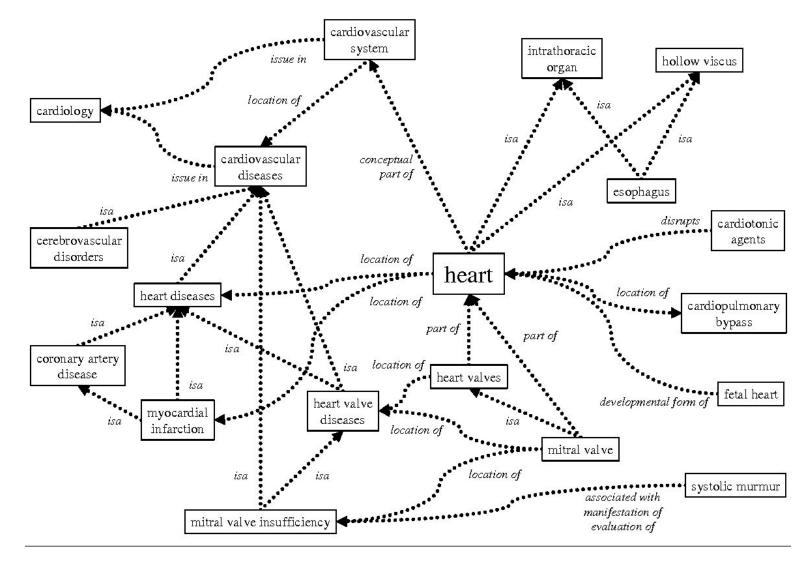
#### Ontologies for standardisation

- Standardised terms e.g., Pizza, Tomato, Mozzarella
- Standardised types of relationships between terms
- Acyclic links between terms
- Manual curation
- Automated curation

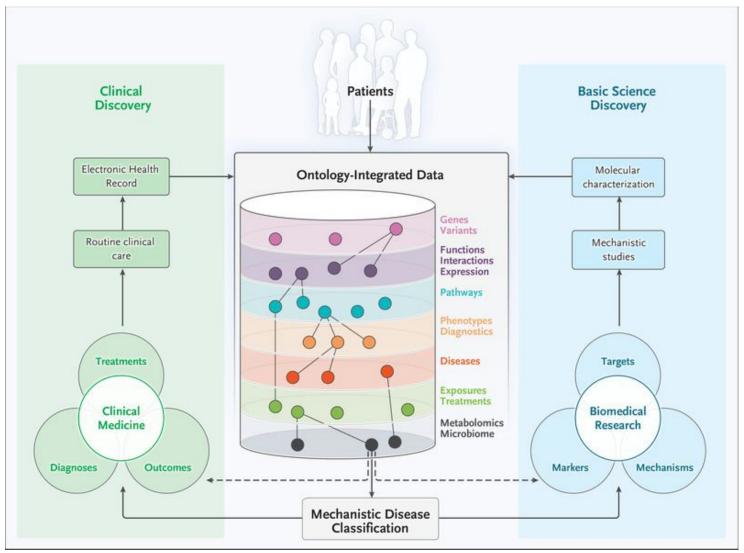


 $https://www.researchgate.net/figure/Example-pizza-ontology-represented-as-a-graph-G-a-and-a-changed-version-of-the-pizza_fig1_236842047$ 

## **Medical Ontologies**



### Ontologies for linking diverse types of data



International Statistical Classification of Diseases and Related Health Problems (ICD-9, ICD-10)

- 2 ontologies
  - ICD-X-CM (medical diagnoses)
  - ICD-X-PCS (procedure coding)

## International Statistical Classification of Diseases and Related Health Problems (ICD-9, ICD-10)

- 2 ontologies
  - ICD-X-CM (medical diagnoses)
  - ICD-X-PCS (procedure coding)
- ICD-9 -> ICD-10 (2015)

	ICD-9-CM	ICD-10 code sets
Procedure	3,824 codes	71,924 codes
Diagnosis	14,025 codes	69, 823 codes
ICD-	10 Code Structure Change	es (selected details)
Diagnosis Structure	Old	New
	<ul> <li>ICD-9-CM</li> <li>3 -5 characters</li> <li>First character is numeric or alpha</li> <li>Characters 2-5 are numeric</li> </ul>	<ul> <li>ICD-10-CM</li> <li>3 -7 characters</li> <li>Character 1 is alpha</li> <li>Character 2 is numeric</li> <li>Characters 3 – 7 can be alpha or numeric</li> </ul>
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https://www.cdc.gov/nchs/icd/icd10cm\_pcs\_backg round.htm

## International Statistical Classification of Diseases and Related Health Problems (ICD-9, ICD-10)

- 2 ontologies
  - ICD-X-CM (medical diagnoses)
  - ICD-X-PCS (procedure coding)
- ICD-9 -> ICD-10 (2015)
- "V97.33XD: Sucked into jet engine, subsequent encounter."
- "Y93.D: V91.07XD: Burn due to water-skis on fire, subsequent encounter."
- "Z63.1: Problems in relationship with in-laws."
- "W22.02XD: V95.43XS:
   Spacecraft collision injuring occupant, sequela."

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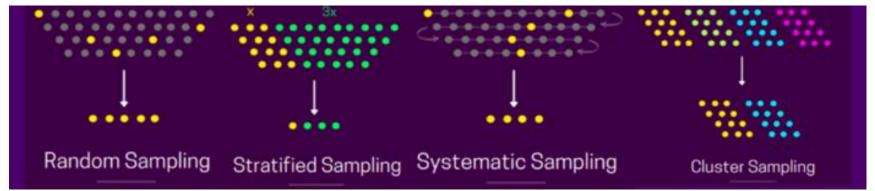
### How do we sample from medical databases?

### Sampling strategy

- Exhaustive in a database isn't always exhaustive in true population
- Numerous and often quite complex!
- Major source of bias so always carefully explore

### Sampling strategy

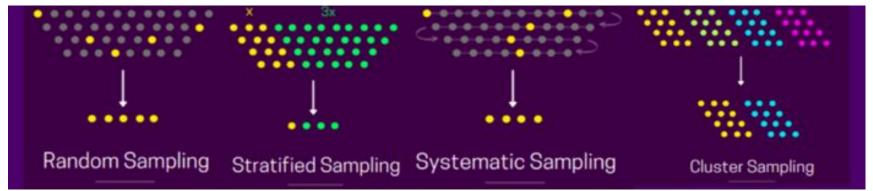
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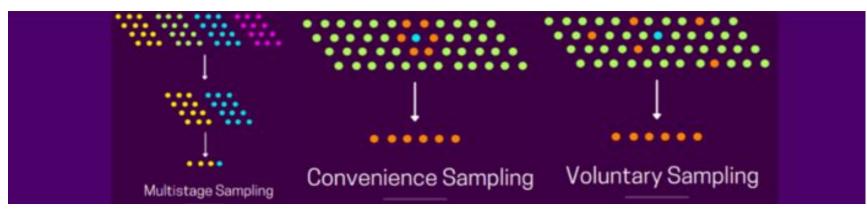


https://towardsdatascience.com/8-types-of-sampling-techniques-b21adcdd2124

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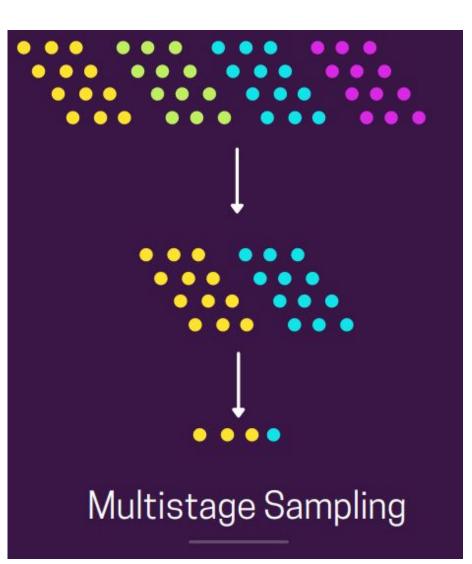
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### Survey/Sample weights

- Value/weight assigned to each record
- Make statistics calculated from database more representative of population
  - Weight=0.5 underweight this case
  - Weight=1
  - Weight=2 overweight the contribution of this case

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- Value/weight assigned to each record
- Make statistics calculated from database more representative of population
  - Weight=0.5 underweight this case
  - Weight=1
  - Weight=2 overweight the contribution of this case
- Complex sampling strategies (e.g., deliberate oversampling of some populations, biasing recruitment) mean weights **MUST** be used.
- Not directly supported in all machine learning libraries (sample\_weights implemented for some models)



### Types of weights

- Design Weights
  - Based on sampling strategy i.e., "design" of survey/database/data collection
  - Common to over-sample under-represented or rare groups
  - Need to correct for this or will overestimate statistics e.g., lower weight of over-sampled groups

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- Post-stratification / Non-response weights
  - Based on collected data
  - Typically biases in whose data is collected
  - Over-represented groups need to be under-weighted



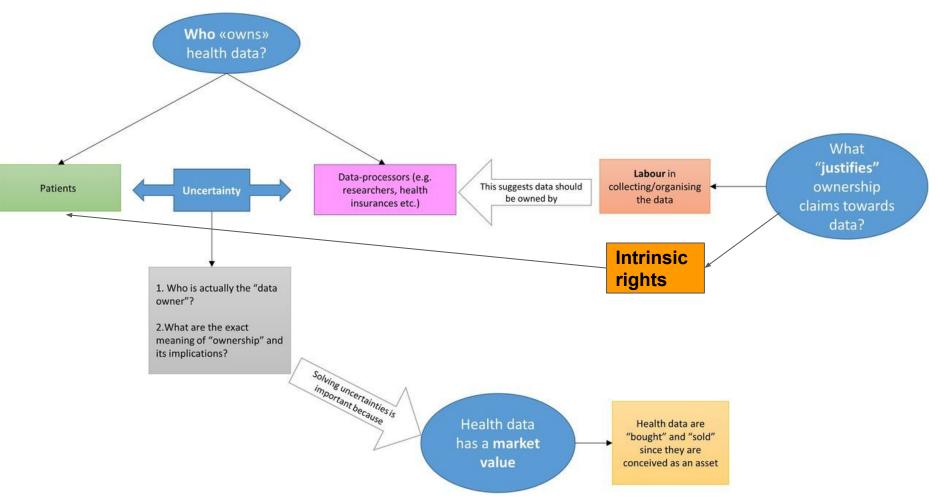
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- Often many different weights are combined:



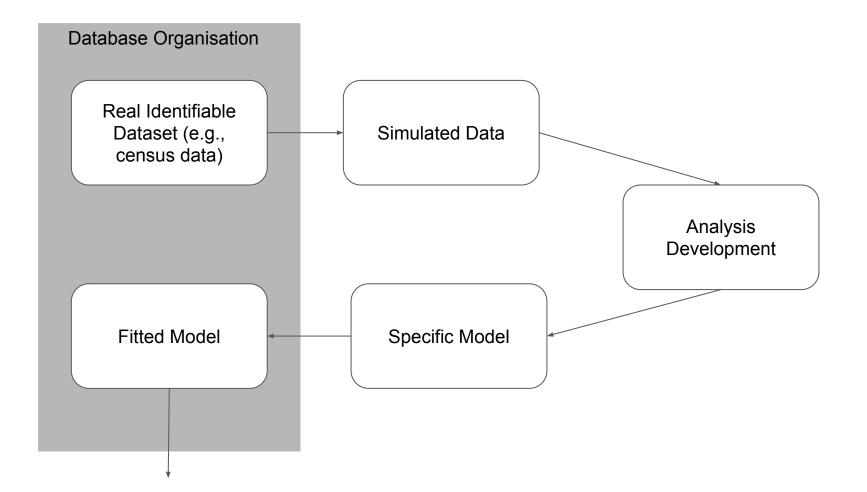
### Who actually owns this data?

### Data Ownership is Difficult



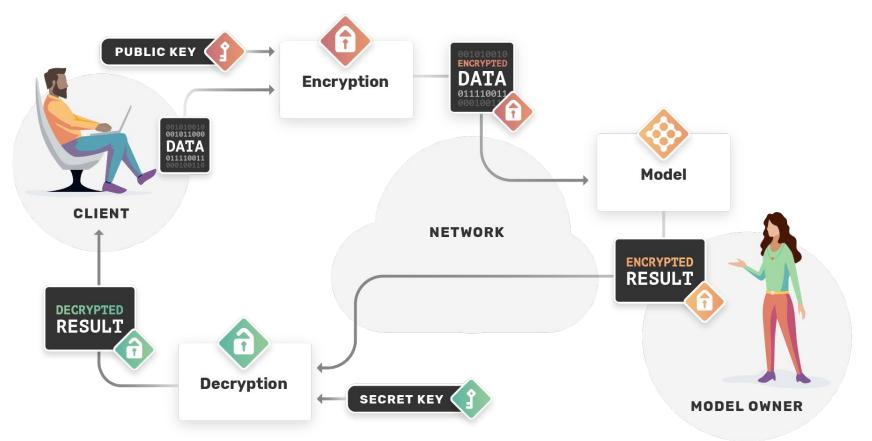
# How do you protect privacy in these databases?

### No direct data access



Shared data but encrypted: homomorphic encryption

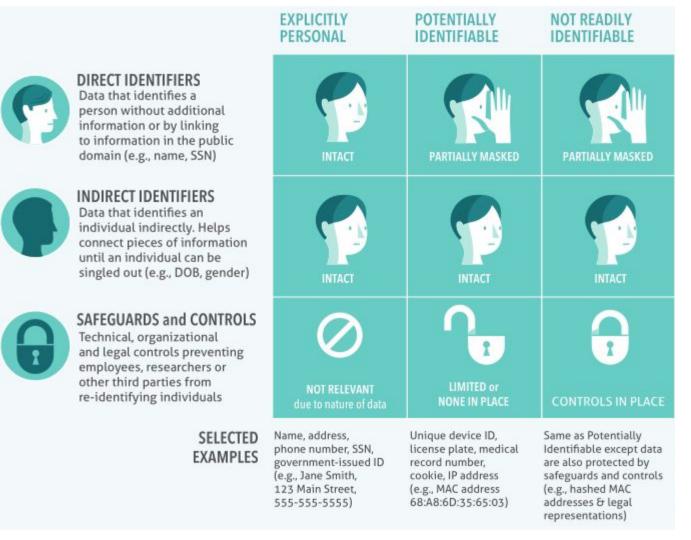
Partial to fully homomorphic encryption



https://research.aimultiple.com/homomorphic-encryption/

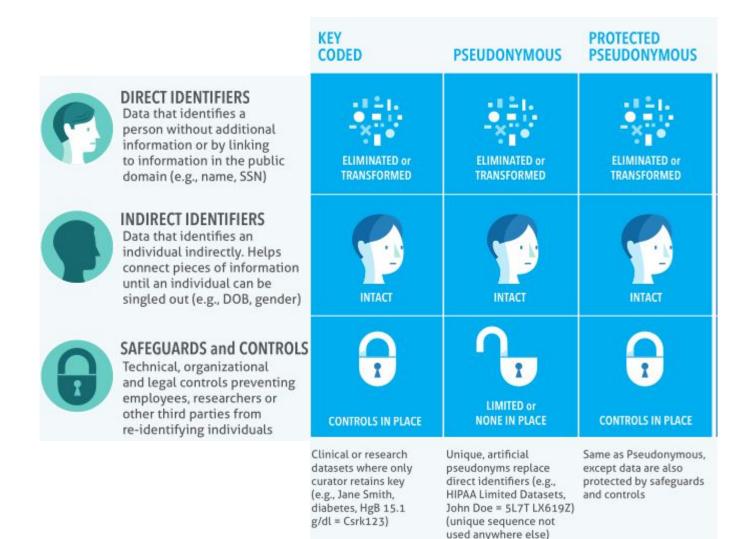
Both are difficult and limited... so how can we share data directly but safely?

### Data privacy is a continuum



https://fpf.org/wp-content/uploads/2016/04/FPF\_Visual-Guide-to-Practical-Data-DeID.pdf

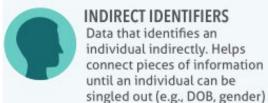
### Indirectly identifiable: Pseudonymous Data



### Identifiers removed/broken: De-Identified Data



DIRECT IDENTIFIERS Data that identifies a person without additional information or by linking to information in the public domain (e.g., name, SSN)



#### INDIRECT IDENTIFIERS Data that identifies an individual indirectly. Helps connect pieces of information until an individual can be

#### SAFEGUARDS and CONTROLS

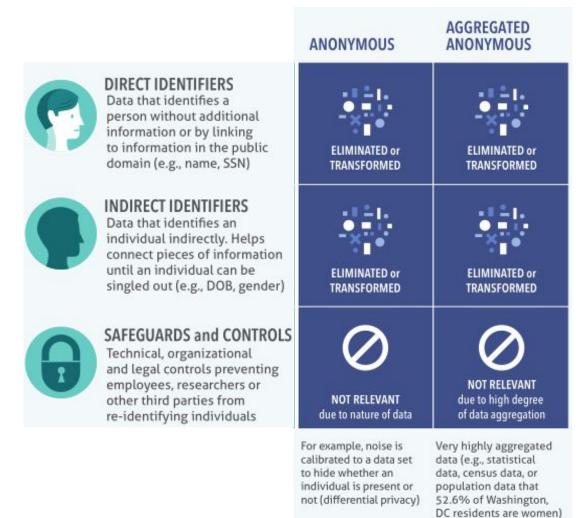
Technical, organizational and legal controls preventing employees, researchers or other third parties from re-identifying individuals



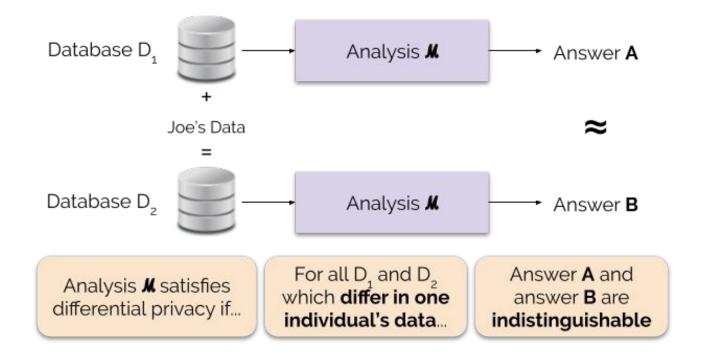
Data are suppressed, generalized, perturbed, swapped, etc. (e.g., GPA: 3.2 = 3.0-3.5, gender: female = gender: male)

Same as De-Identified. except data are also protected by safeguards and controls

### Non-identifiability Guarantee: Anonymous Data

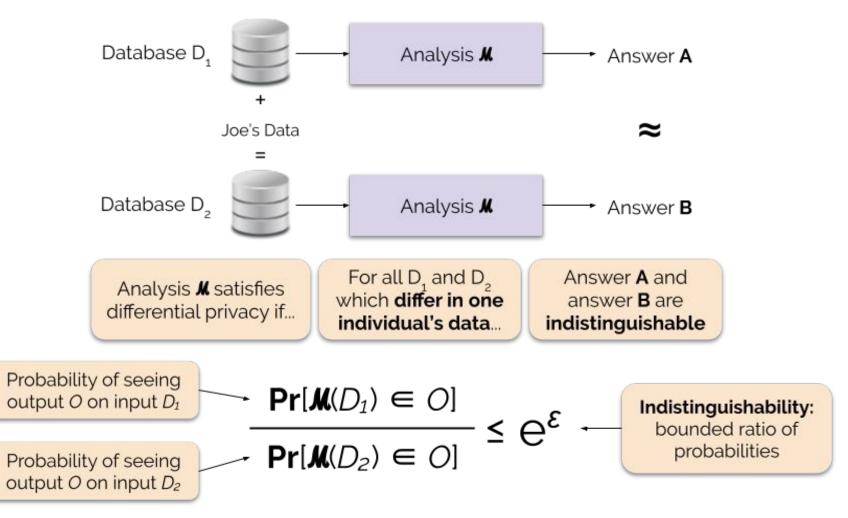


### Differential privacy: no singling out individuals



https://www.nist.gov/blogs/cybersecurity-insights/differential-privacy-privacy-preserving-data-analysis-introduction-our

### Differential privacy: no singling out individuals

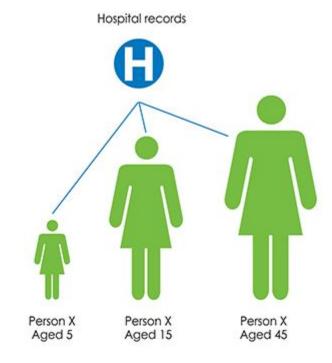


https://www.nist.gov/blogs/cybersecurity-insights/differential-privacy-privacy-preserving-data-analysis-introduction-our

### Data linkage is powerful but dangerous

- Linking between databases and resources -> identifiability
- Can be done probabilistically
- Often needs additional ethics/applications
- Can break a lot of data privacy operations





### Many different data access processes

- Buy access and get processed data
- Apply for individual fields and justify why
- Full pre-registration of analysis

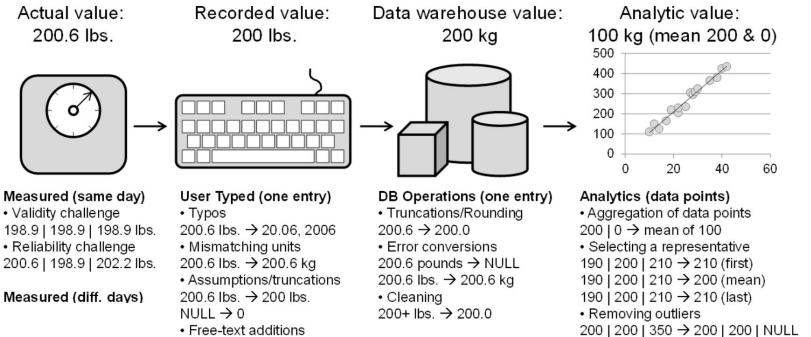
### Let's take a short break!

# So, you've got access to a database, what now?

### Data Cleaning: even "simple" fields can be a nightmare

### Data Quality





200.6 lbs. → 200.6 pounds

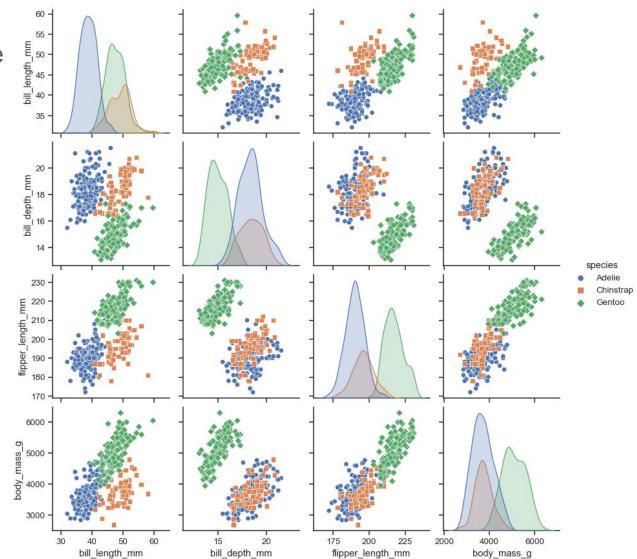
Under review

Slide from Dr. Hadi Kharrazi

9 months & >25 rules to clean weight

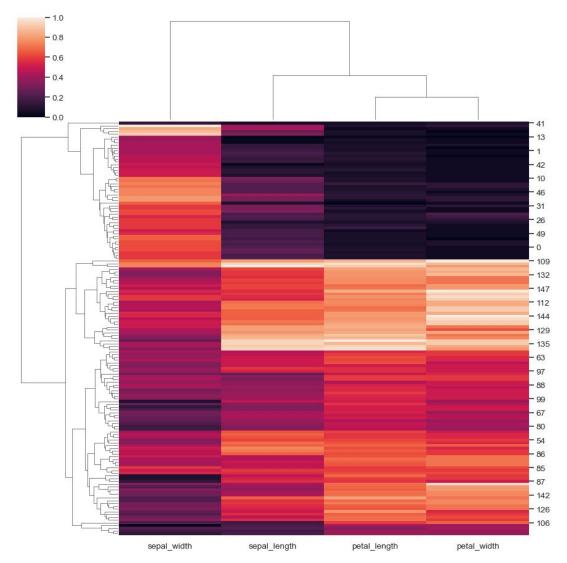
### **Exploratory Data Analysis**

- Individual variable distributions
- Pairwise variable distributions
- Distributions relative to variable(s) of interest
- Point analysis of extreme values



### **Exploratory Data Analysis**

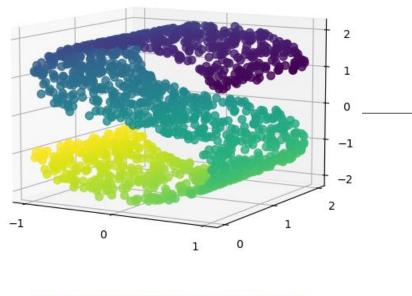
- Individual variable distributions
- Pairwise variable distributions
- Distributions
   relative to
   variable(s) of
   interest
- Hierarchical clustering of variables
- Point analysis of extreme values



### How do I look at all the data together?

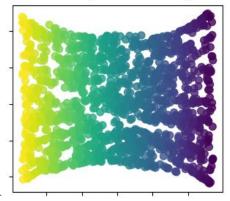
# Many dimensions to few: Manifold learning, Ordination, Decomposition, Dimensionality reduction

Original S-curve samples

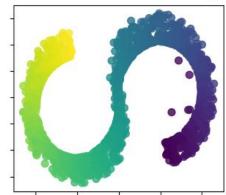




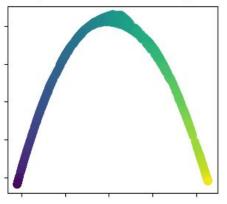
Isomap Embedding



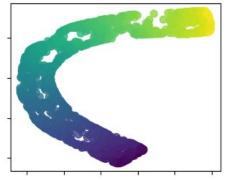
Multidimensional scaling



Spectral Embedding

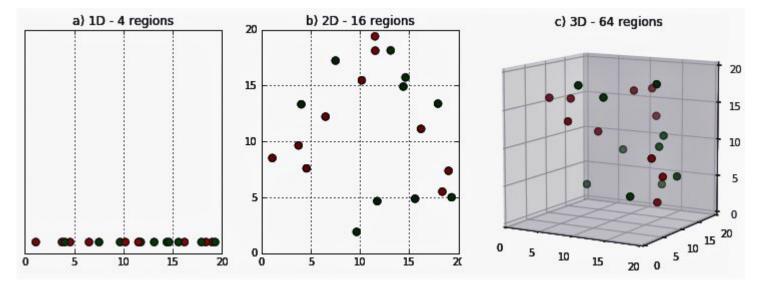


T-distributed Stochastic Neighbor Embedding



### Why is this hard?

### High dimensional data is sparse

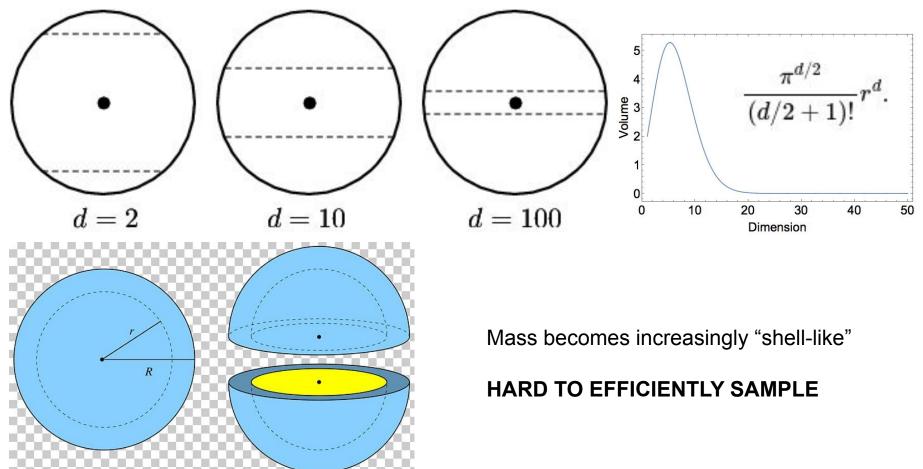


https://medium.com/analytics-vidhya/the-curse-of-dimensionality-and-its-cure-f9891ab72e5c

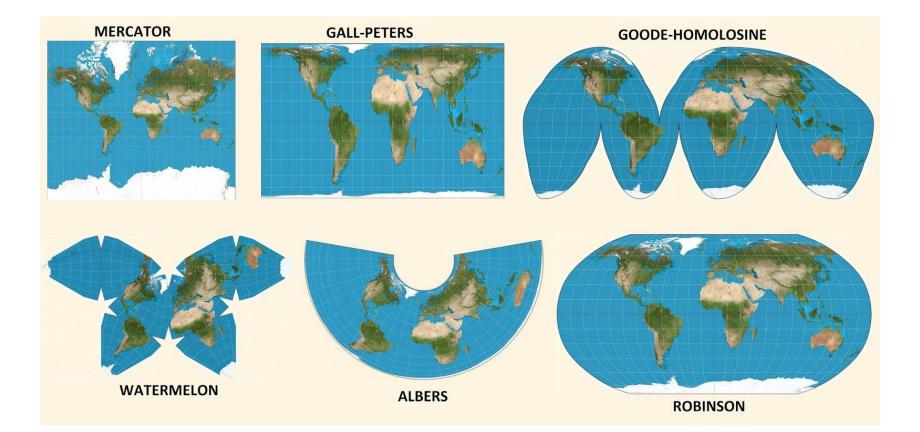
#### High dimensional space is counterintuitive

As dimensions increase volume enclosed by a d-sphere decreases  $\sim 0$ 

Band-size to capture 99% of the volume of a sphere:



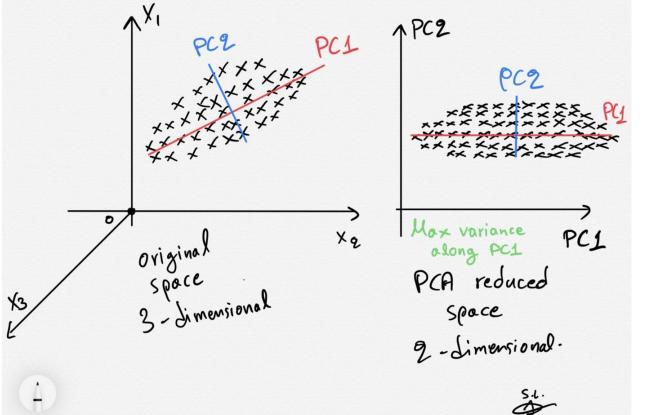
#### No representation is perfect



## So, how can we do it?

#### Principal Component Analysis (PCA): Variance

Mean center data -> Generate Covariance Matrix -> Eigendecomposition -> Sort Eigenvalues



How many components? Scree/elbow plot Scree plot Percentage of explained variances 50 -41.2% 40 30-8.49 20 -10 -0-Dimensions What variables contribute most to PCs? BiPlot

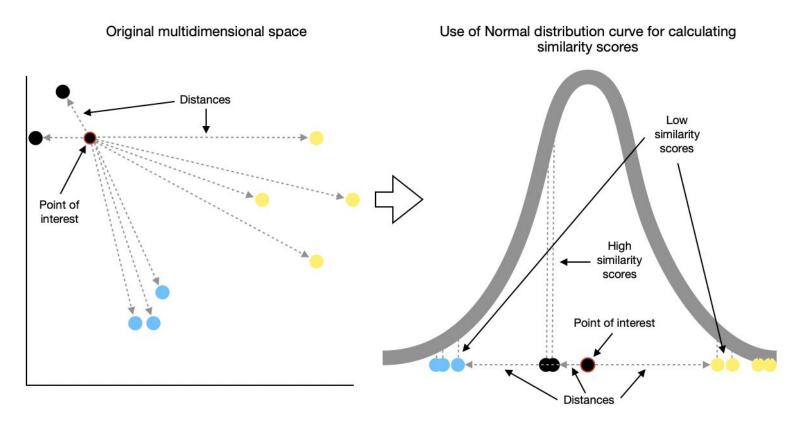
https://towardsdatascience.com/pca-clearly-explained-how-when-why-to-use-it-and-feature-importance-a-guide-in-python-7c274582c37e

#### MultiDimensional Scaling (MDS): Distances

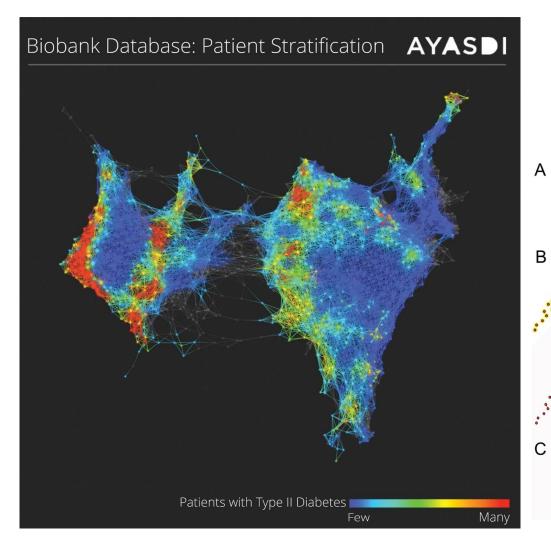
 $||x_i - x_j||)^2$  $(d_{ij} - d_{ij})$  $Stress_D(x_1, x_2, \ldots, x_N)$  $||x_i - x_i||$  is the  $d_{ii}$  is the actual distance Where  $x_1, \ldots, x_N$  are The goal of the we have calculated distance between data points with their algorithm is to between the two the two new set of minimize the value of corresponding data points corresponding data coordinates in lower stress. in their original points in their lower dimensional space. dimensional space. dimensional space. The closer the value of  $||x_i - x_j||$  is to  $d_{ij}$  the a b Non-Metric: Ranks 5 1.0 **Ordination distances** 9.0 Stress 3 0.2 0 0 2 5 3 5 3 Original dissimilarities Number of dimensions

#### t-SNE/UMAP: Probabilities

- Pairwise probability distribution in all dimensions
- Pairwise probability distribution in few dimensions
- Stochastic minimisation of KL divergence between distributions



### **Topological Data Analysis**



 Point clouds -> increase radius -> simplical complexes -> topological characteristics

 $H_1$ 

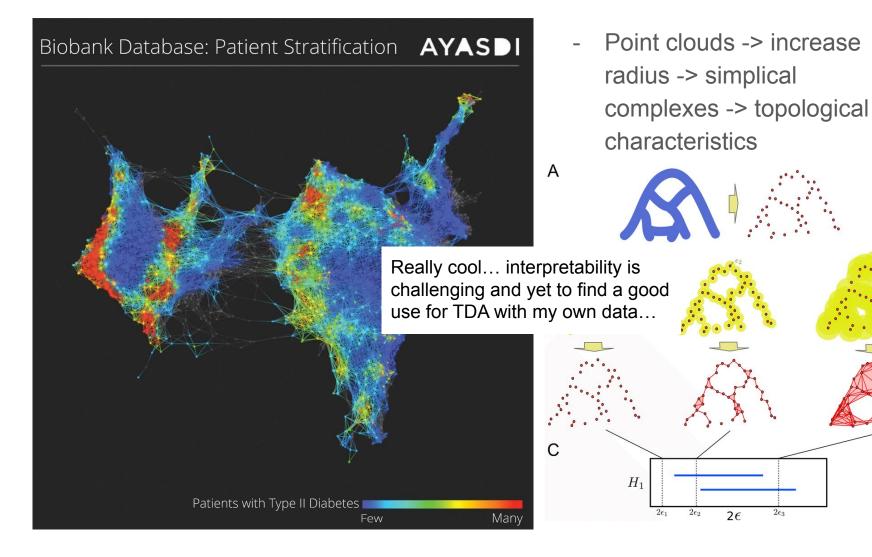
 $2\epsilon_1$ 

 $2\epsilon_2$ 

 $2\epsilon$ 

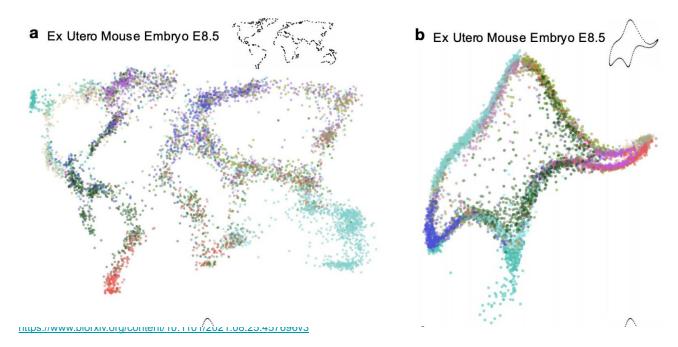
 $2\epsilon_3$ 

### **Topological Data Analysis**



#### Avoid over-interpreting single plots

- Sensitive to hyperparameters
- Beware analysing these non-linear projections
- Can contribute to confirmation bias

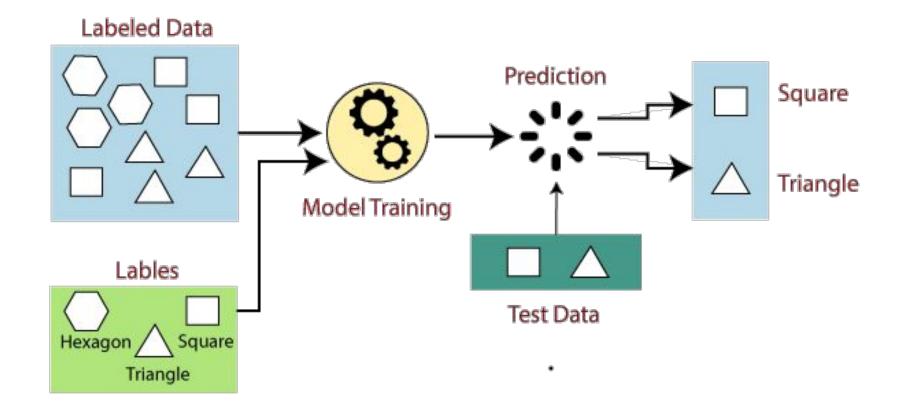


"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk." - Von Neumann

# Predicting using tabular data

# Predicting using tabular data

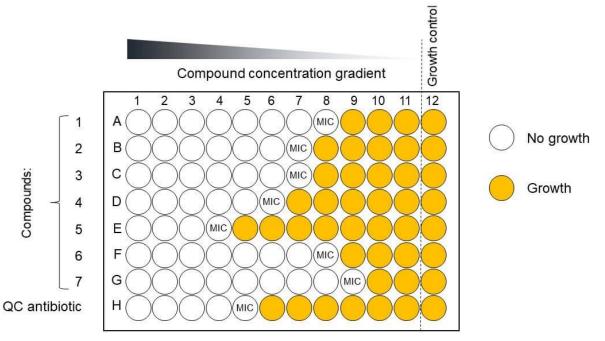
#### **Predicting Labels or Values**



#### Values can be complex: interval prediction

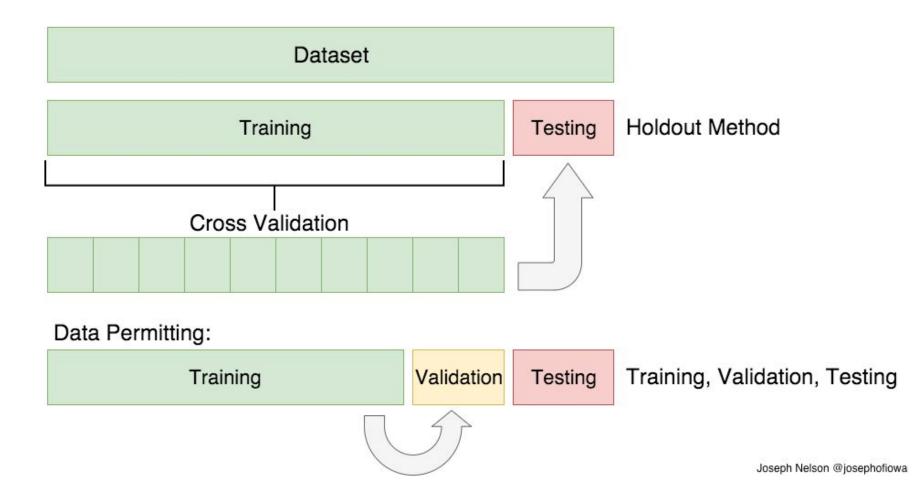
- MIC > highest concentration = <u>right-censored</u>
- MIC < lowest concentration = <u>left-censored</u>
- Serial Dilutions: MIC of x actually [x/2, 2x] = <u>unequal error</u>

#### Interpretation of microdilution MIC results



©Emery Pharma

#### Overfitting 101: Test-Train Split

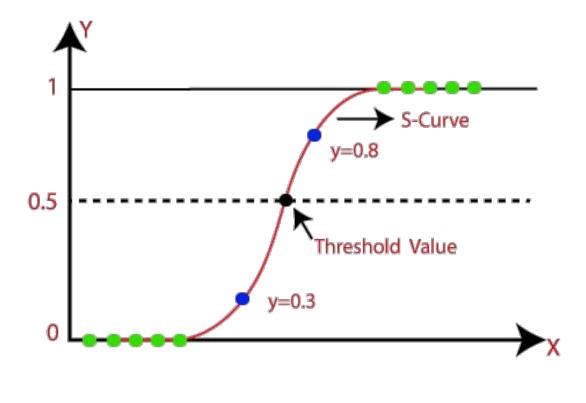


#### Start simple: linear regression

	Common name	Built-in function in R	Equivalent linear model in R	Exact?	The linear model in words	lcon
Simple regression: Im(y ~ 1 + x)	<b>y is independent of x</b> P: One-sample t-test N: Wilcoxon signed-rank	t.test(y) wilcox.test(y)	lm(y ~ 1) lm(signed_rank(y) ~ 1)	✓ for N >14	One number (intercept, i.e., the mean) predicts <b>y</b> . - (Same, but it predicts the <i>signed rank</i> of <b>y</b> .)	
	P: Paired-sample t-test N: Wilcoxon matched pairs	t.test(y1, y2, paired=TRUE) wilcox.test(y1, y2, paired=TRUE)	$lm(y_2 - y_1 \sim 1)$ $lm(signed_rank(y_2 - y_1) \sim 1)$	√ f <u>or N ≥14</u>	One intercept predicts the pairwise y <sub>2</sub> -y <sub>1</sub> differences. - (Same, but it predicts the <i>signed rank</i> of y <sub>2</sub> -y <sub>1</sub> .)	<b>*</b>
	<b>y ~ continuous x</b> P: Pearson correlation N: Spearman correlation	cor.test(x, y, method='Pearson') cor.test(x, y, method='Spearman')	lm(y ~ 1 + x) lm(rank(y) ~ 1 + rank(x))	✓ for N >10	One intercept plus <b>x</b> multiplied by a number (slope) predicts <b>y</b> . - (Same, but with <i>ranked</i> <b>x</b> and <b>y</b> )	مىلېرىپ
	<b>y ~ discrete x</b> P: Two-sample t-test P: Welch's t-test N: Mann-Whitney U	t.test(y <sub>1</sub> , y <sub>2</sub> , var.equal=TRUE) t.test(y <sub>1</sub> , y <sub>2</sub> , var.equal=FALSE) wilcox.test(y <sub>1</sub> , y <sub>2</sub> )	$\begin{array}{l} Im(y\sim1+G_2)^{A}\\ gls(y\sim1+G_2,\ weights=^{B})^{A}\\ Im(signed_rank(y)\sim1+G_2)^{A} \end{array}$	✓ ✓ for N >11	An intercept for <b>group 1</b> (plus a difference if <b>group 2</b> ) predicts <b>y</b> . - (Same, but with one variance <i>per group</i> instead of one common.) - (Same, but it predicts the <i>signed rank</i> of <b>y</b> .)	Y
Multiple regression: $Im(y \sim 1 + x_1 + x_2 +)$	P: One-way ANOVA N: Kruskal-Wallis	aov(y ~ group) kruskal.test(y ~ group)	$\begin{split} ℑ(y\sim 1+G_2+G_3++G_N)^4 \\ ℑ(rank(y)\sim 1+G_2+G_3++G_N)^4 \end{split}$	√ for N >11	An intercept for <b>group 1</b> (plus a difference if group $\neq$ 1) predicts <b>y</b> . - (Same, but it predicts the <i>rank</i> of <b>y</b> .)	ixt+
	P: One-way ANCOVA	aov(y ~ group + x)	$Im(y \sim 1 + G_2 + G_3 + + G_N + x)^4$	~	- (Same, but plus a slope on x.) Note: this is discrete AND continuous. ANCOVAs are ANOVAs with a continuous x.	-
	P: Two-way ANOVA	aov(y ~ group * sex)	$\begin{array}{l} Im(y\sim 1+G_{2}+G_{3}++G_{N}+\\ S_{2}+S_{3}++S_{K}+\\ G_{2}^{*}S_{2}+G_{3}^{*}S_{3}++G_{N}^{*}S_{K}) \end{array}$	*	Interaction term: changing sex changes the $y \sim group$ parameters. Note: $G_{2:WN}$ is an indicator (0 or 1) for each non-intercept levels of the group variable. Similarly for $S_{2:WN}$ for sex. The first line (with G) is main effect of group, the second (with S <sub>2</sub> ) for sex and the third is the group × sex interaction. For two levels (e.g. male/female), line 2 would just be "S <sub>2</sub> " and line 3 would be S <sub>2</sub> multiplied with each G <sub>0</sub> .	   [Coming] 
	Counts ~ discrete x N: Chi-square test	chisq.test(groupXsex_table)	$\begin{array}{l} \mbox{Equivalent log-linear model} \\ glm(y \sim 1 + G_2 + G_3 + + G_N + \\ S_2 + S_3 + + S_K + \\ G_2^*S_2 + G_3^*S_3 + + G_N^*S_{K_1} \mbox{ family=})^A \end{array}$	*	Interaction term: (Same as Two-way ANOVA.) Note: Run glm using the following arguments: gim(model, family=poisson()) As linear-model, the Chi-square test is $log(y) = log(N) + log(a) + log(b) + log(a\beta)$ where $a_i$ and $\beta_i$ are proportions. See more info in the accompanying notebook.	Same as Two-way ANOVA
Mu	N: Goodness of fit	chisq.test(y)	$gIm(y \sim 1 + G_2 + G_3 + + G_{N_1} family=)^{A}$	~	(Same as One-way ANOVA and see Chi-Square note.)	1W-ANOVA

https://lindeloev.github.io/tests-as-linear/

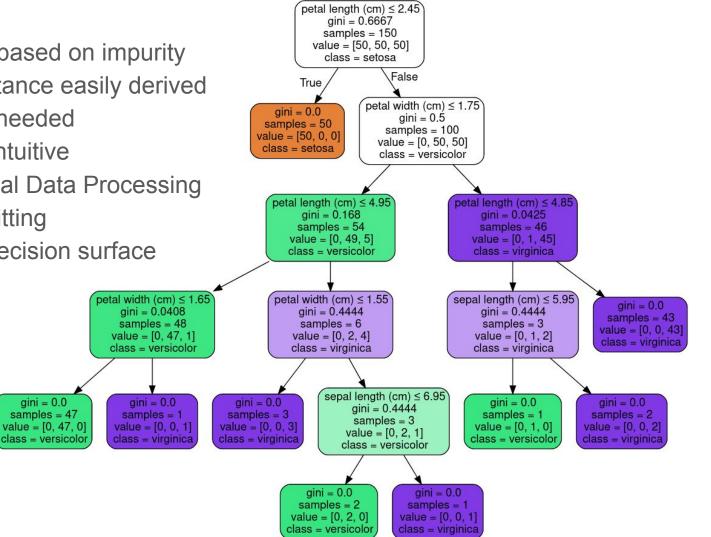
#### Add a sigmoid for classification



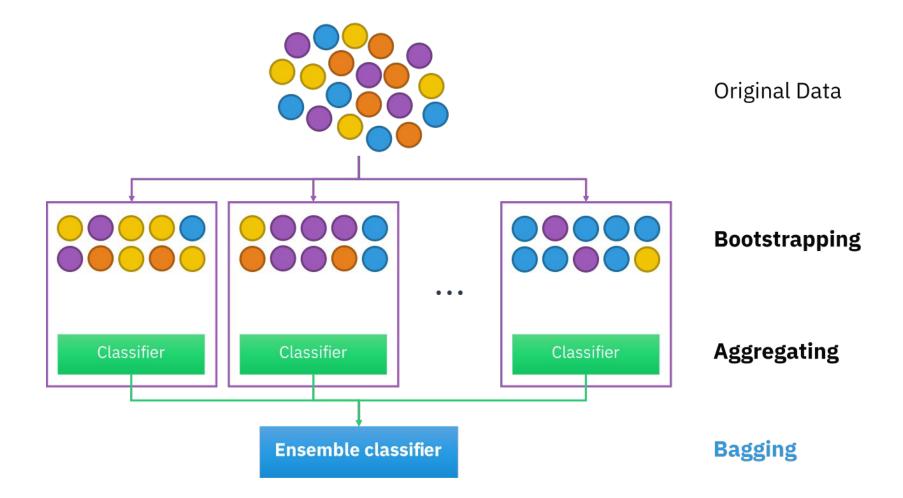
- Crude measure of feature importance (model coefficients)
- Specific feature selection can be a good idea
- Support for regularisation (Lasso/L1 -> sparsity vs Ridge/L2 -> minimal vs ElasticNet -> balance)
- Statistics has developed
  much better practices for
  treatment/interpretation
  of logistic regression

#### **Decision Trees**

- Dataset splits based on impurity \_
- Feature importance easily derived \_
- Pruning often needed
- Interpretable/Intuitive
- Require Minimal Data Processing
- Prone to overfitting
- Non-smooth decision surface

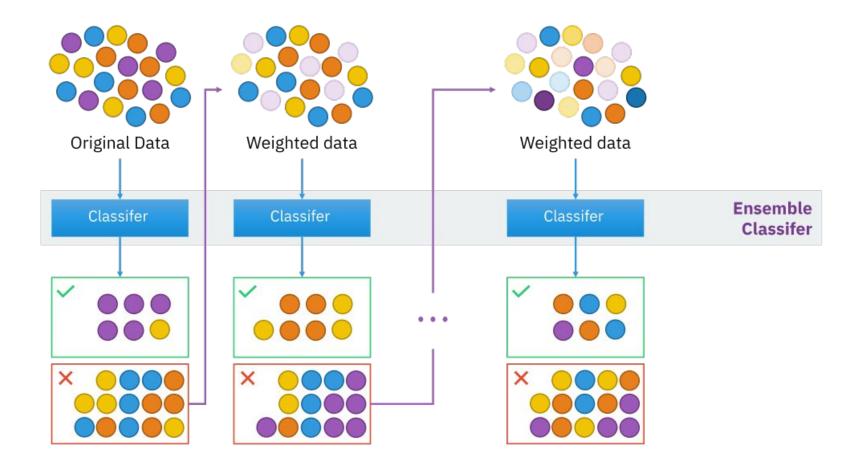


#### Many Decision Trees: Bagging



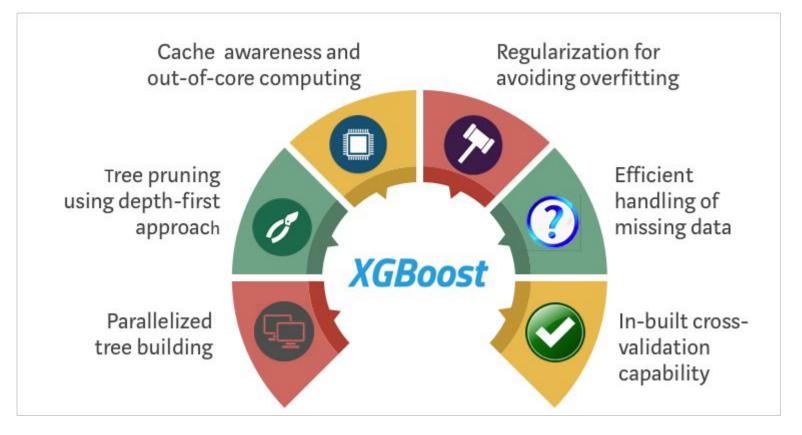
Random Forest: Bagging + Random Subset Per Split Feature Importance: Average impurity decrease

#### Boosting: AdaBoost, Gradient Boosting, XGBoost



#### Gradient Boosting: XGBoost

- Normal boosting is easy to overfit => regularisation
- Use stochastic gradient descent (technically Newton-Raphson variant)
- Many efficiency improvement



# Decision Trees methods regularly outperform deep learning on tabular data

Tree-based methods deal well with common features of tabular data (even compared to well-tuned neural networks):

- Heterogeneous data
- Ignoring uninformative data
- Non-smooth decision boundaries
- Moderate size & dimensionality
- Skewed or heavy-tailed feature distributions and other forms of dataset
- Rotational invariance (column/row order is not informative)

But: difference is often negligible (except in computational efficiency!)

Why do tree-based models still outperform deep learning on typical tabular data?

Léo Grinsztajn Soda, Inria Saclay leo.grinsztajn@inria.fr Edouard Oyallon MLIA, Sorbonne University Gaël Varoquaux Soda, Inria Saclay When Do Neural Nets Outperform Boosted Trees on Tabular Data?

Duncan McElfresh\*<sup>1,2</sup>, Sujay Khandagale<sup>3</sup>, Jonathan Valverde<sup>4</sup>, Vishak Prasad C<sup>5</sup>, Ganesh Ramakrishnan<sup>5</sup>, Micah Goldblum<sup>6</sup>, Colin White<sup>1,7</sup>

> <sup>1</sup> Abacus.AI, <sup>2</sup> Stanford, <sup>3</sup> Pinterest, <sup>4</sup> University of Maryland, <sup>5</sup> IIT Bombay, <sup>6</sup> New York University, <sup>7</sup> Caltech

#### Overview

- Medical databases are usually relational and are defined by their origin, primary record type, scope, and sampling strategy
- Standardisation is important and ontologies support that in medical databases
- Survey weights are key to compensate for complex sampling
- There is a continuum of approaches to retain data privacy (and data ownership is a complex issue)
- Individual and joint distributions are key EDA tools
- Dimensionality reduction (PCA, MDS, t-SNE) is very useful but can be challenging/misleading
- Start with simple classifiers e.g., logistic regression/decision tree
- Combine weak classifiers via bagging (bootstrapping data: Random Forest special form) or boosting (sequential training model on errors: AdaBoost/XGBoost) to improve performance.
- XGBoost gold-standard but requires more tuning than AdaBoost