## Lecture 1: Medical Databases

#### CSCI6410/EPAH6410/CSCI4148

Finlay Maguire (finlay.maguire@dal.ca)

## 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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Examples include:

- Medical Charts
- Phone Book
- Dictionaries
- Spreadsheet

Ordering:

- Index
- Defined fields
- Standardisation

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Examples include:

- Medical Charts
- Phone Book
- Dictionaries
- Spreadsheet

Ordering:

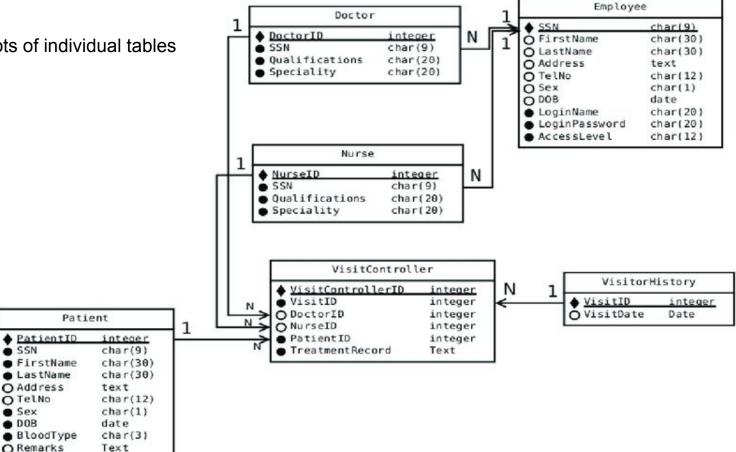
- Index
- Defined fields
- Standardisation

Organisation make some tasks easier/harder:

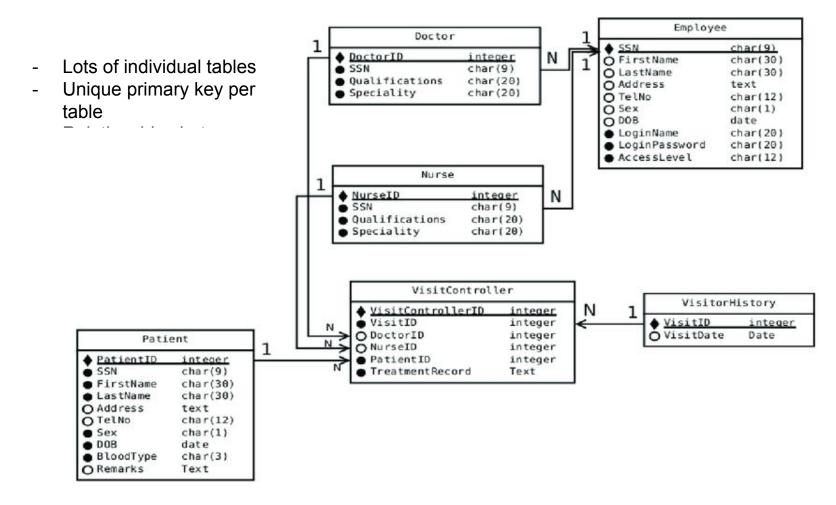
- Find all patients with the same condition
- Find the longest word in a dictionary
- Find an a number from an address in a phonebook

| PART A - PRESENT HEALTH HISTORY (continued)  |   |   |                       |   |
|--|---|---|-----------------------|---|
| GENERAL HEALTH, ATTITUDE AND HABITS (continued)  |   |   |                       |   |
| ave you recently had any changes in your: If yes, please explain:<br>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.)<br>amby: Illness Family Members   | MEN Please answer questions 1 through 12, then<br>skip to question 18,<br>WOMEN: Please start on question 6,  |   |                       |   |
| Age, If Age At State of Health Or Asthine  | 1 DHLY  |   |                       |   |
|  | 4 ONLY<br>Have you had or do you have   |   |                       |   |
| Father Cancer  | prostate trouble?   |   |                       |   |
| Nother   | Do you have any ancust proceents<br>or with impatency?<br>Have you even had soms or<br>lesions on your penie? | No Yes  |                       |   |
| and  | Have you ever had sores or  |   | C                     |   |
| Sisters ) [ Rheumatoid Arthritis   |   |   | 0                     |   |
|  | from your panis?<br>Do you ever have pain, tumps  | No Yes  | 0                     |   |
| Geut   | Do you war have pair, lumps   | No. Yes   |                       |   |
| Nildren  | or paeting in your testicles? .<br>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<br>How many each day? Digarettes   | If yes, how many years?<br>CopersPipesfull  |   |                       |   |
| Have you ever smoked? Smoked No. Yes   | If yes, how many years?   |   |                       |   |
| Now many each day?   | Cigars Pipesfull<br>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  |
| Feel nervous? Ever feel like com-  | 0.250 2002021 0.2020  |   |                       |   |
|  |   |   |                       |   |
| Find it hand to Feel bored with<br>make decisions?your life?   |   |   | A DE A DE A DE A DE A | CALL OF A REAL                                  |
| Loss your temper? Use marguane?  |   |   |                       |   |
|  |   |   |                       | Ar an and a los                                 |
| Werry a lot? Use "herd drugs"?   |   |   |                       |   |
| Tire easily? Do you asset to talk to the   |   |   |                       |   |
| Tire easily? Do you want to talk to the<br>Nave trouble relaxing? donor about a narroad  | natter? No Yes  | All March   |                       |   |
| Tire easily? Do you want to talk to the<br>Have stroy texual problems? doctor about a personal<br>Have tory texual problems?   | natter? No Yes  |   |                       |   |
| Tire easily? Do you want to talk to the<br>Nave trouble relaxing? donor about a narroad  | STOCK NO. 19-711-4 5/83   | 2 Day   |                       |   |

Lots of individual tables \_

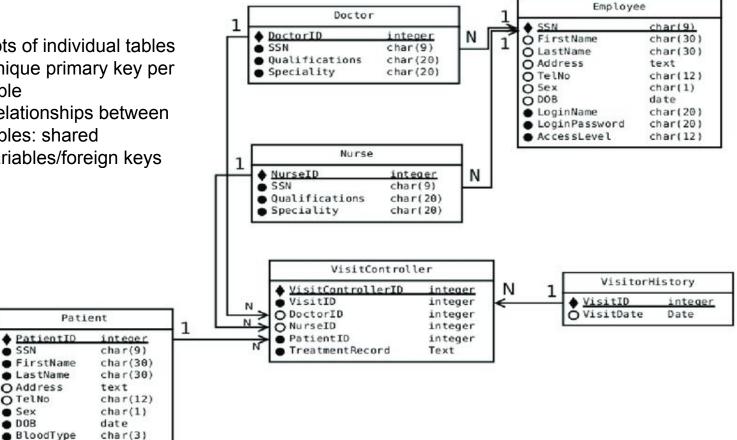


http://dx.doi.org/10.1016/j.procs.2015.08.441



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

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



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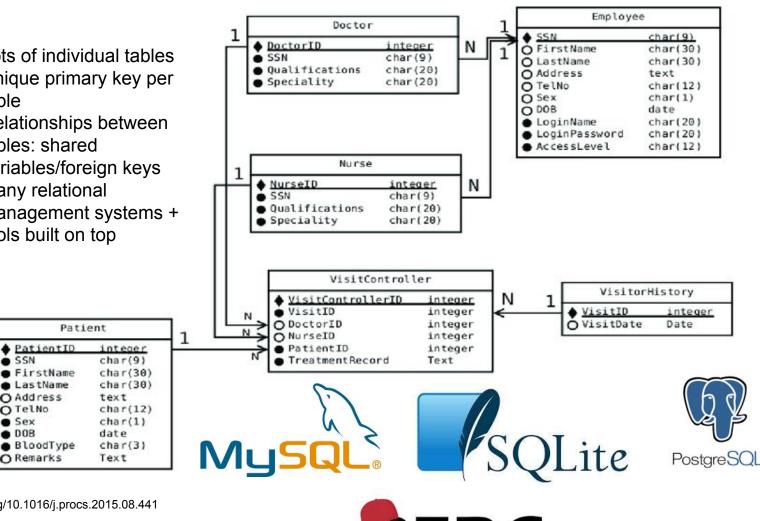
**O** Remarks

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

SSN

O Address

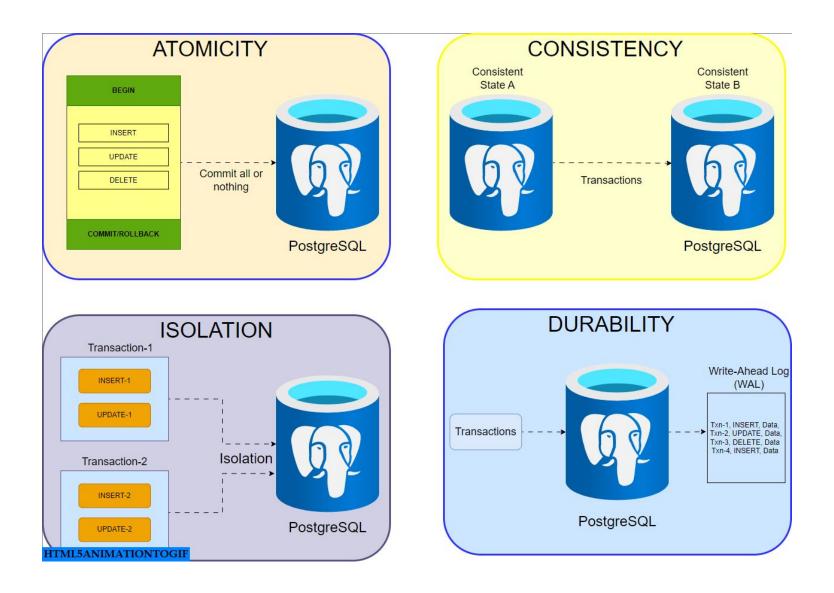
O Remarks

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Sex

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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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- Non-procedural Language
- Standardised/powerful/flexible
- Basis of many data tools
- Well-supported by dbplyr

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- Non-procedural Language
- Standardised/powerful/flexible
- Basis of many data tools
- Well-supported by dbplyr

```
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>
```

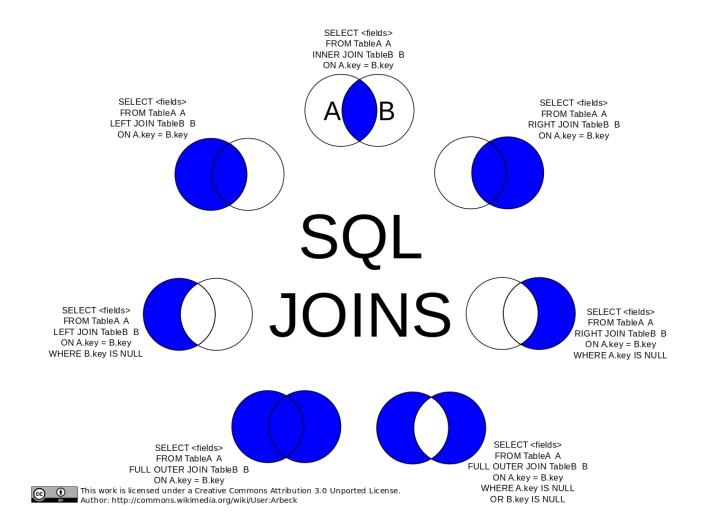
```
#> SELECT `month`, `day`, AVG(`dep_delay`) AS `delay`
```

```
#> 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/



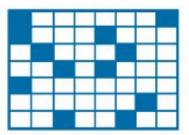
Can you find out whodunnit?



## 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

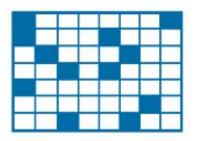


#### Column based



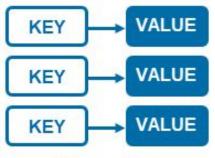
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Column based



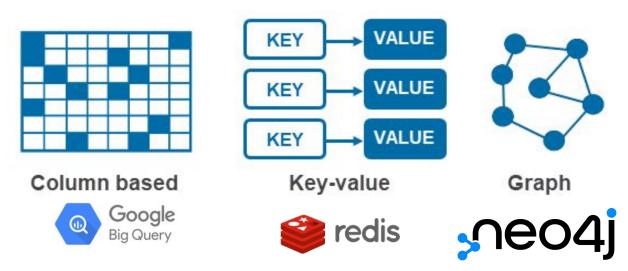


Key-value



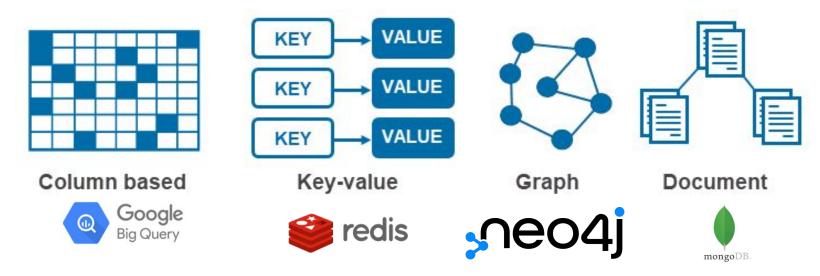
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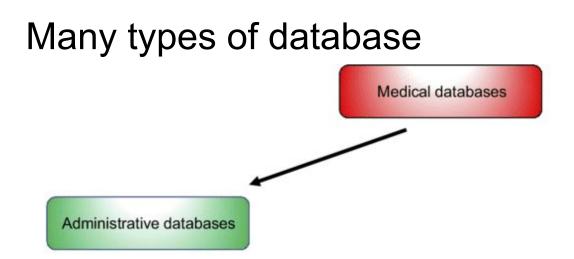


## What are medical databases?

#### Many types of database

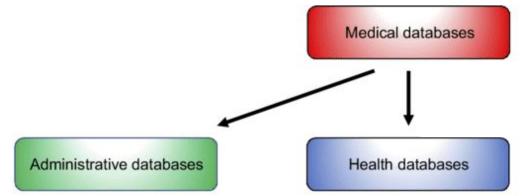
Medical databases

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



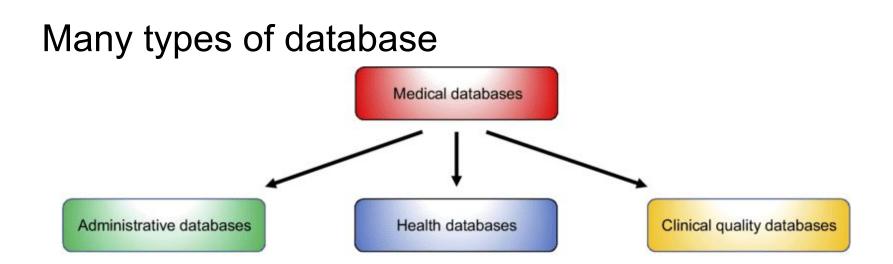
Register individuals according to geographic area, health insurance program, or attendance at a particular hospital or clinic

## Many types of database

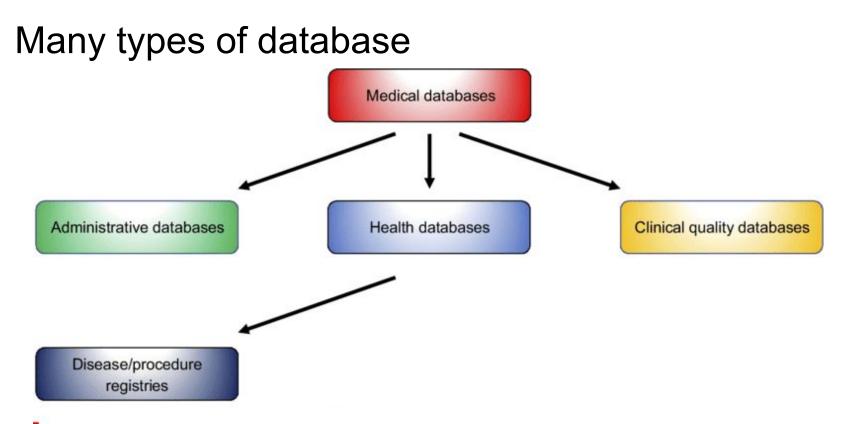


All types of registries and databases that contain health-related data Register individuals according to geographic area, health insurance program, or attendance at a particular hospital or clinic

Register health data for the purpose of surveillance and research



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 Register health data for the purpose of surveillance and research Register detailed clinical data for clinical quality control

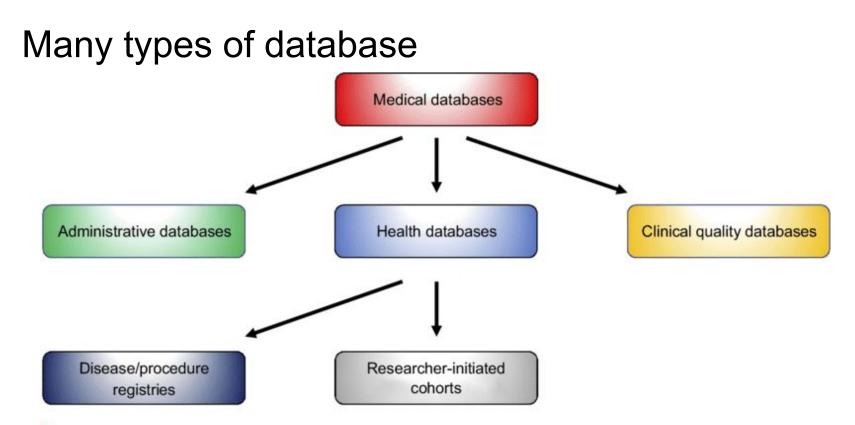


Register individuals according to geographic area, health insurance program, or attendance at a particular hospital or clinic

Register health data for the purpose of surveillance and research

Register detailed clinical data for clinical quality control

Register patients according to diagnosis or procedure



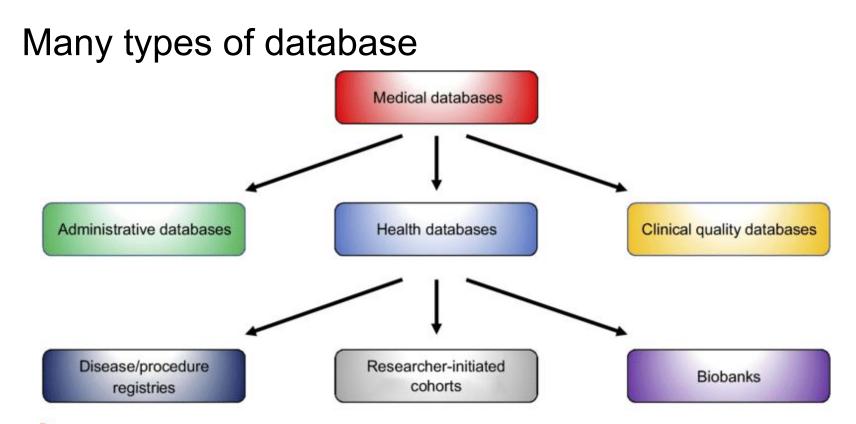
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Store biological samples (eg, blood and tissue)

## 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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- Single physician
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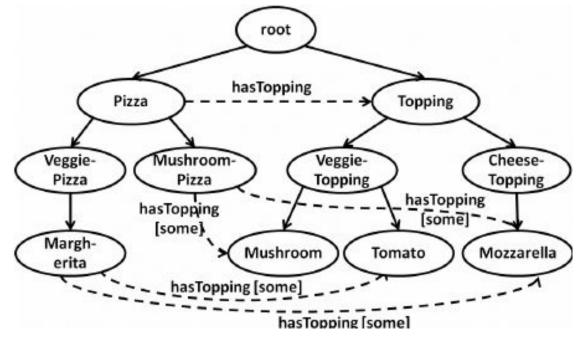
Challenge of standardisation

Generalisability

# How do medical databases try to handle standardisation?

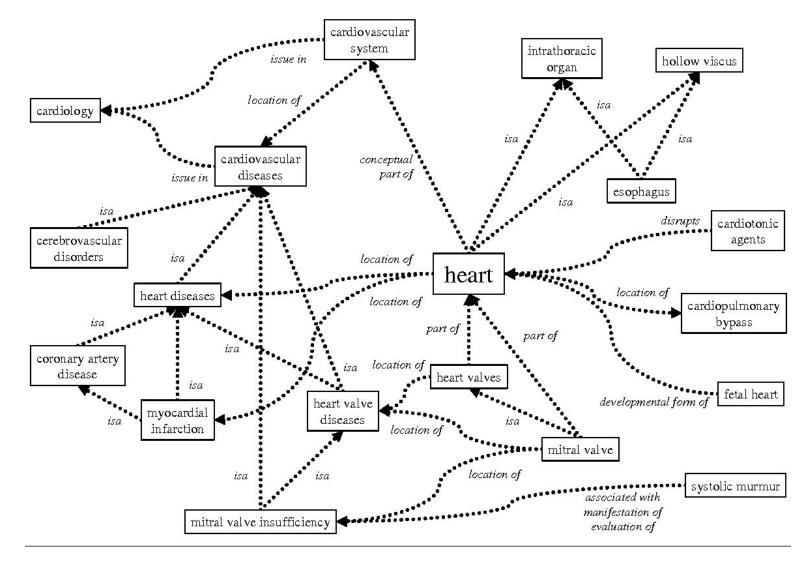
#### Ontologies for standardisation

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

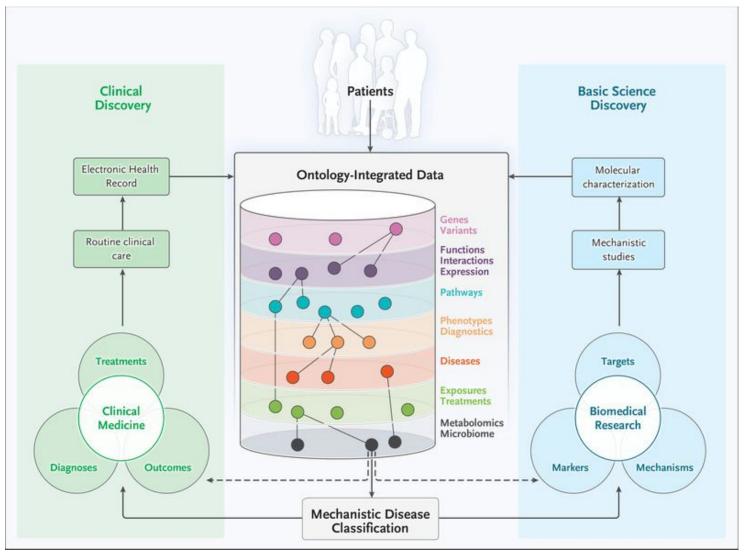


 $https://www.researchgate.net/figure/Example-pizza-ontology-represented-as-a-graph-G-a-and-a-changed-version-of-the-pizza_fig1_236842047$ 

## **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<br>Structure | Old  | New  |
|                        | <ul> <li>ICD-9-CM</li> <li>3 -5 characters</li> <li>First character is<br/>numeric or alpha</li> <li>Characters 2-5 are<br/>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<br/>be alpha or numeric</li> </ul> |
| Procedure<br>Structure | <ul> <li>ICD-9-CM</li> <li>3-4 characters</li> <li>All characters are numeric</li> <li>All codes have at least 3 characters</li> </ul>         | <ul> <li>ICD-10-PCS</li> <li>ICD-10-PCS has 7<br/>characters</li> <li>Each can be either<br/>alpha or numeric</li> <li>Numbers 0-9; letters<br/>A-H, J-N, P-Z</li> </ul>   |

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."

|                        | ICD-9-CM   | ICD-10 code sets   |
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| ICD-                   | 10 Code Structure Change   | es (selected details)  |
| Diagnosis<br>Structure | Old  | New  |
|                        | <ul> <li>ICD-9-CM</li> <li>3 -5 characters</li> <li>First character is<br/>numeric or alpha</li> <li>Characters 2-5 are<br/>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<br/>be alpha or numeric</li> </ul> |
| Procedure<br>Structure | <ul> <li>ICD-9-CM</li> <li>3-4 characters</li> <li>All characters are numeric</li> <li>All codes have at least 3 characters</li> </ul>         | <ul> <li>ICD-10-PCS</li> <li>ICD-10-PCS has 7<br/>characters</li> <li>Each can be either<br/>alpha or numeric</li> <li>Numbers 0-9; letters<br/>A-H, J-N, P-Z</li> </ul>   |

https://www.cdc.gov/nchs/icd/icd10cm\_pcs\_backg round.htm

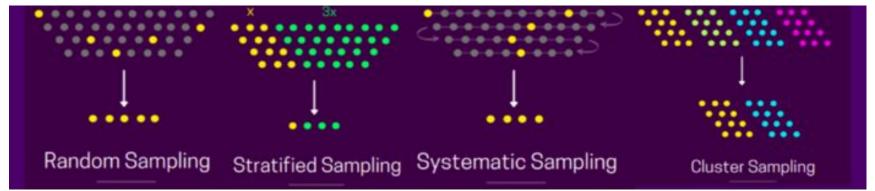
### How do we sample from medical databases?

### 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

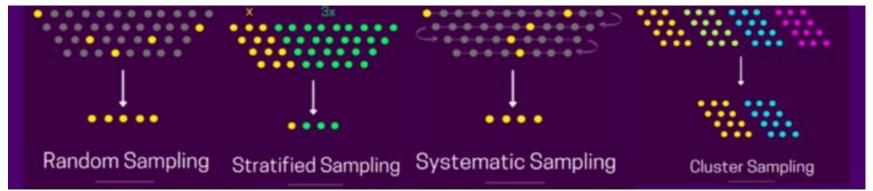
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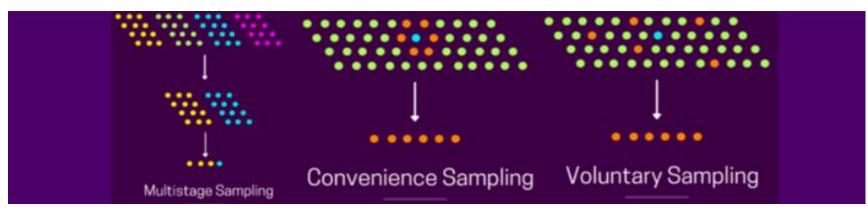


https://towardsdatascience.com/8-types-of-sampling-techniques-b21adcdd2124

### Sampling strategy

- Exhaustive in a database isn't always exhaustive in true population
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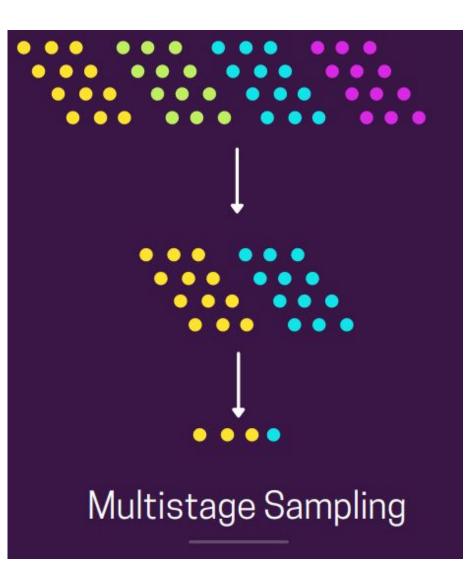
https://towardsdatascience.com/8-types-of-sampling-techniques-b21adcdd2124

### 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



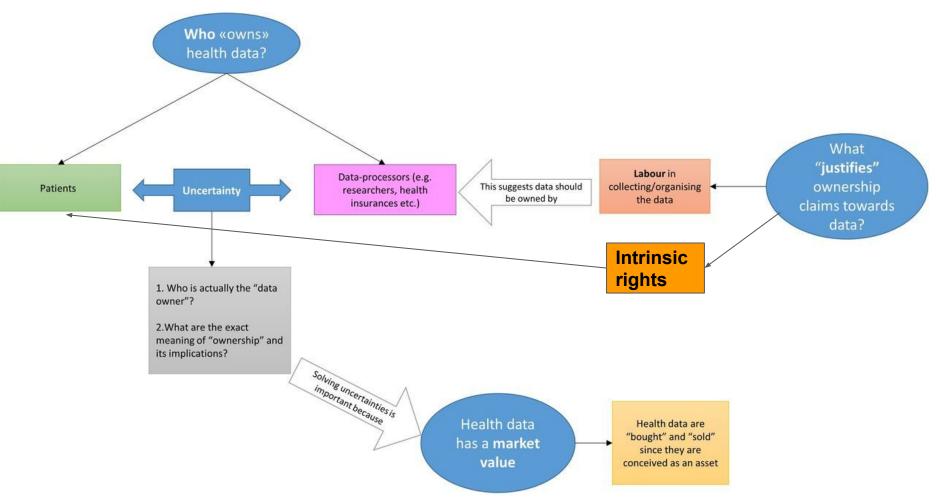
### Types of weights

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  - Based on collected data
  - Typically biases in whose data is collected
  - Over-represented groups need to be under-weighted
- Often many different weights are combined:



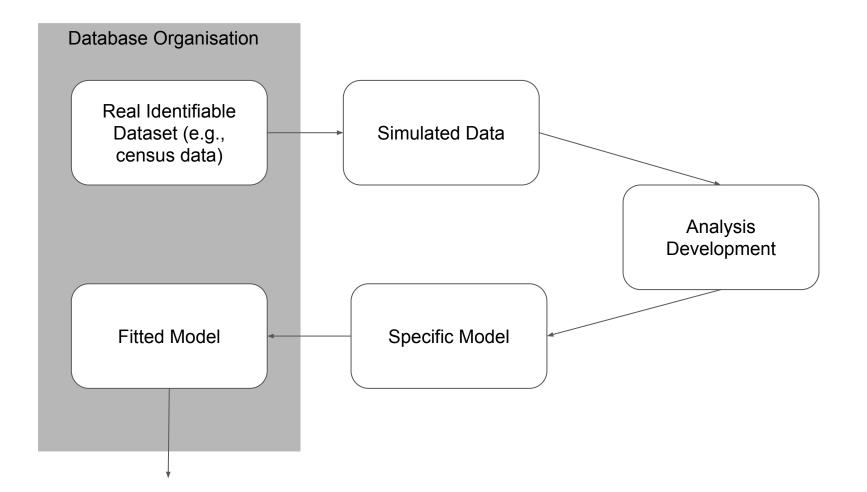
### Who actually owns this data?

### Data Ownership is Difficult



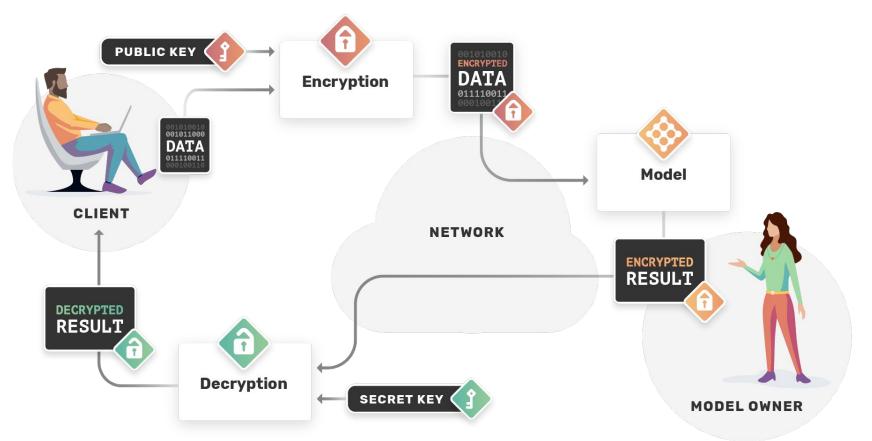
# How do you protect privacy in these databases?

### No direct data access



Shared data but encrypted: homomorphic encryption

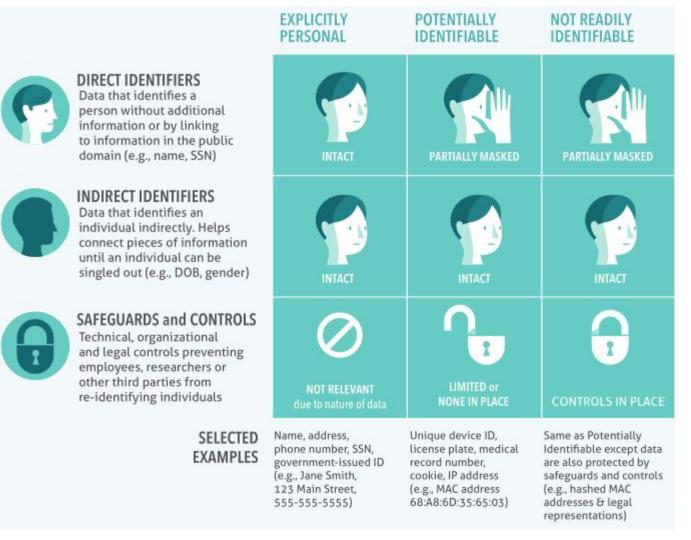
Partial to fully homomorphic encryption



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

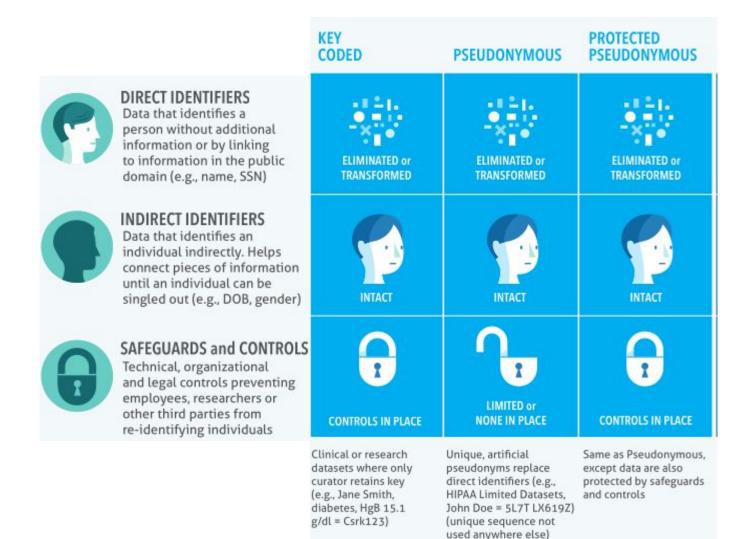
Both are difficult and limited... so how can we share data directly but safely?

### Data privacy is a continuum



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

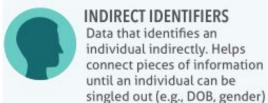
### Indirectly identifiable: Pseudonymous Data



### 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

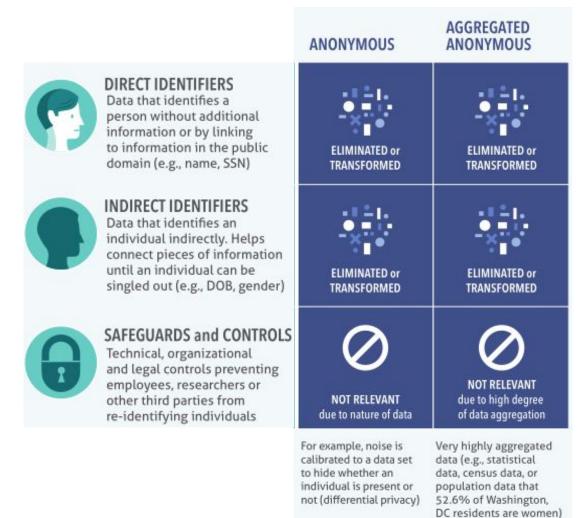
Technical, organizational and legal controls preventing employees, researchers or other third parties from re-identifying individuals



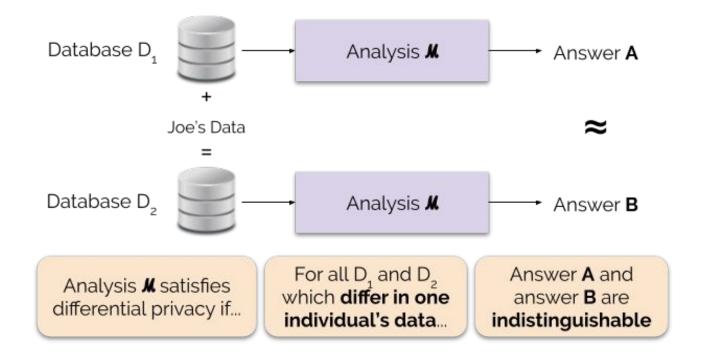
Data are suppressed, generalized, perturbed, swapped, etc. (e.g., GPA: 3.2 = 3.0-3.5, gender: female = gender: male)

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

### Non-identifiability Guarantee: Anonymous Data

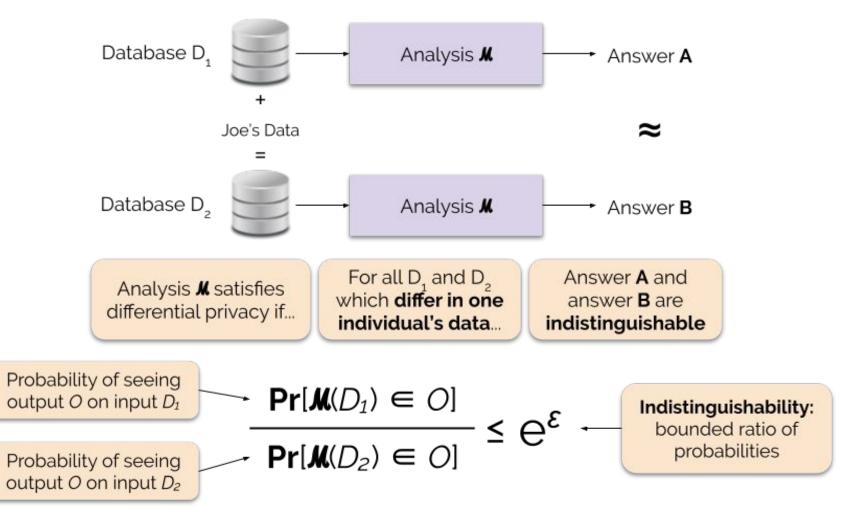


### Differential privacy: no singling out individuals



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

### Differential privacy: no singling out individuals

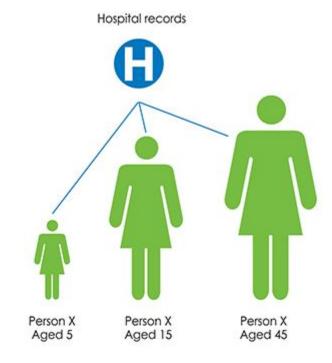


https://www.nist.gov/blogs/cybersecurity-insights/differential-privacy-privacy-preserving-data-analysis-introduction-our

### 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

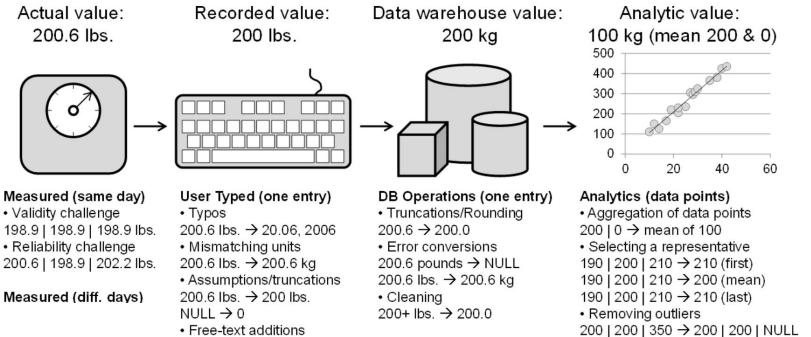
### Let's take a short break!

# 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

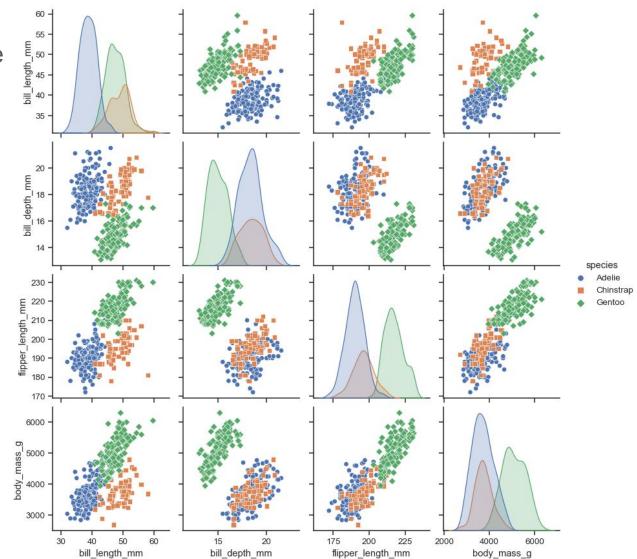
Under review

Slide from Dr. Hadi Kharrazi

9 months & >25 rules to clean weight

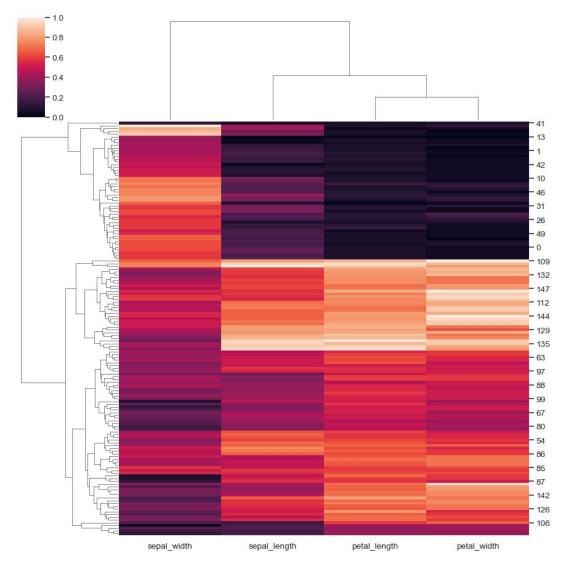
### **Exploratory Data Analysis**

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



### **Exploratory Data Analysis**

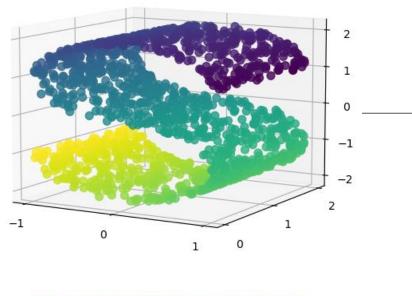
- Individual variable distributions
- Pairwise variable distributions
- Distributions
   relative to
   variable(s) of
   interest
- Hierarchical clustering of variables
- Point analysis of extreme values

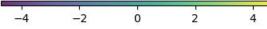


### How do I look at all the data together?

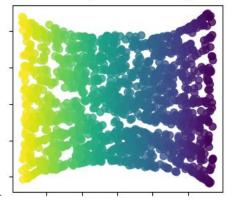
# Many dimensions to few: Manifold learning, Ordination, Decomposition, Dimensionality reduction

Original S-curve samples

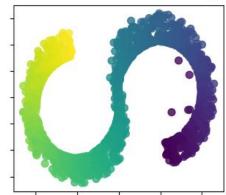




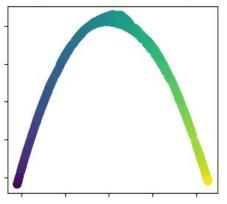
Isomap Embedding



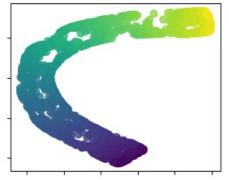
Multidimensional scaling



Spectral Embedding

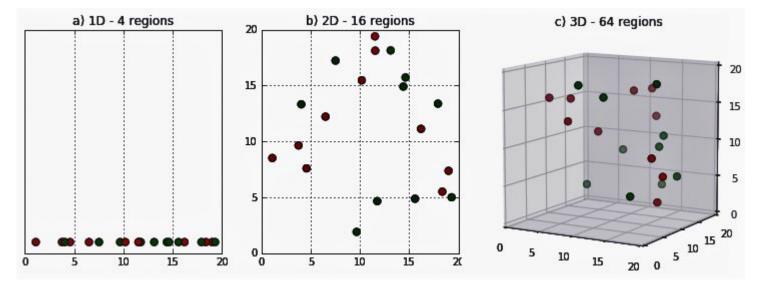


T-distributed Stochastic Neighbor Embedding



### Why is this hard?

### High dimensional data is sparse

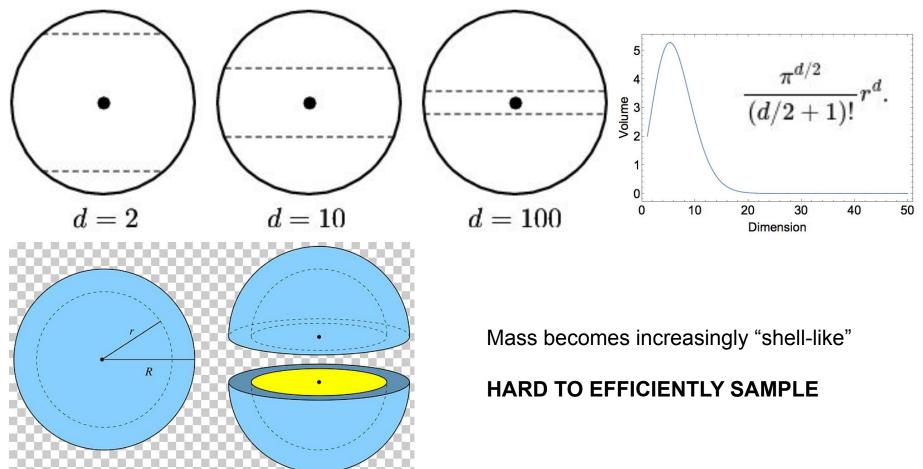


https://medium.com/analytics-vidhya/the-curse-of-dimensionality-and-its-cure-f9891ab72e5c

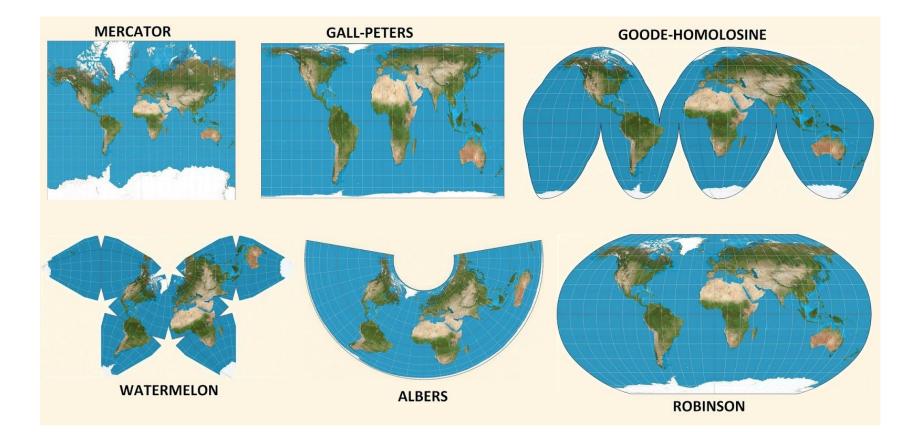
#### High dimensional space is counterintuitive

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

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



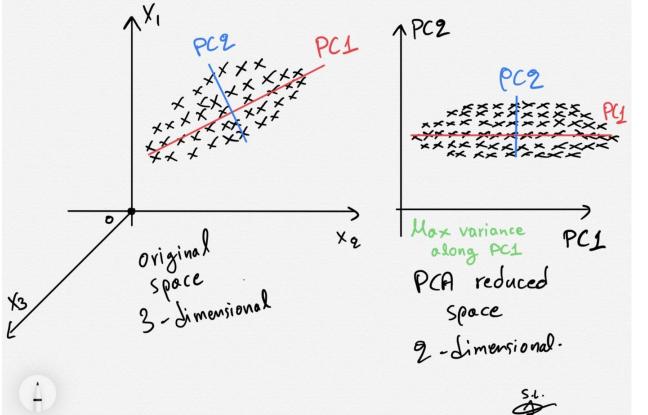
#### No representation is perfect



## 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

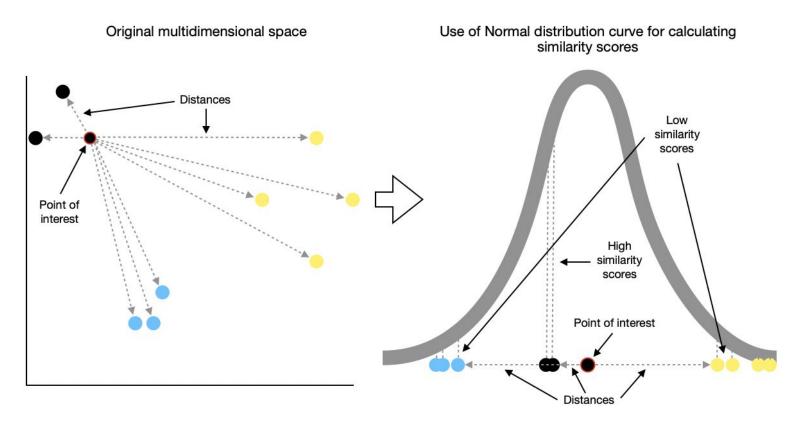
https://towardsdatascience.com/pca-clearly-explained-how-when-why-to-use-it-and-feature-importance-a-guide-in-python-7c274582c37e

#### MultiDimensional Scaling (MDS): Distances

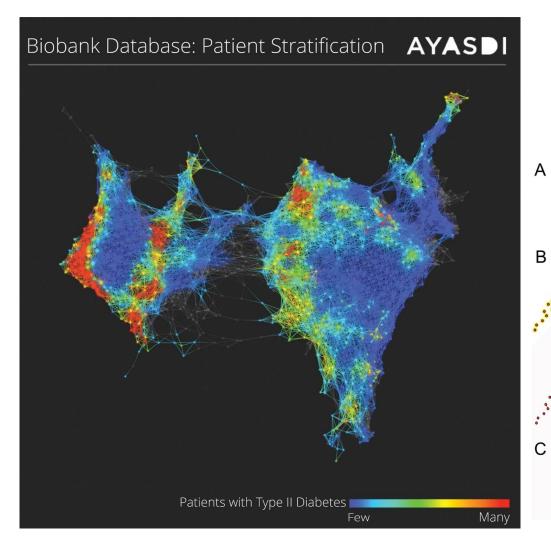
 $||x_i - x_j||)^2$  $(d_{ij} - d_{ij})$  $Stress_D(x_1, x_2, \ldots, x_N)$  $||x_i - x_i||$  is the  $d_{ii}$  is the actual distance Where  $x_1, \ldots, x_N$  are The goal of the we have calculated distance between data points with their algorithm is to between the two the two new set of minimize the 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

 $H_1$ 

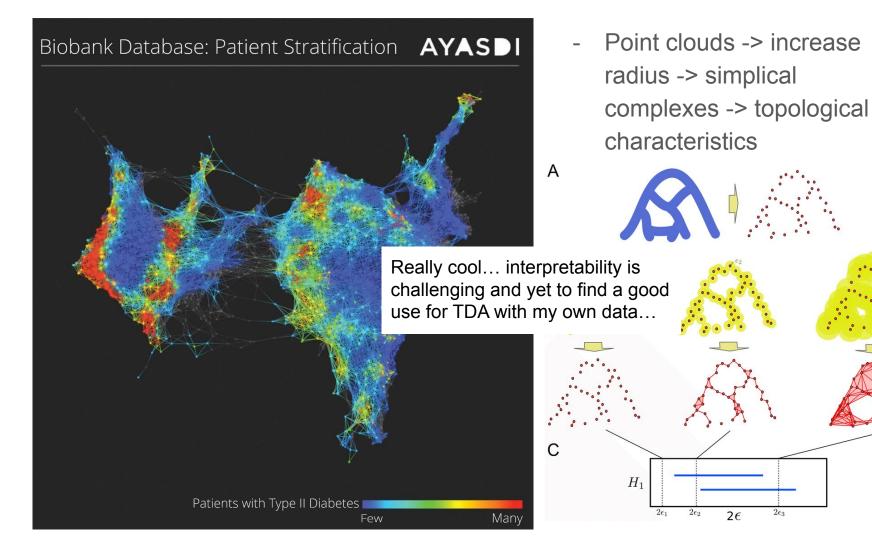
 $2\epsilon_1$ 

 $2\epsilon_2$ 

 $2\epsilon$ 

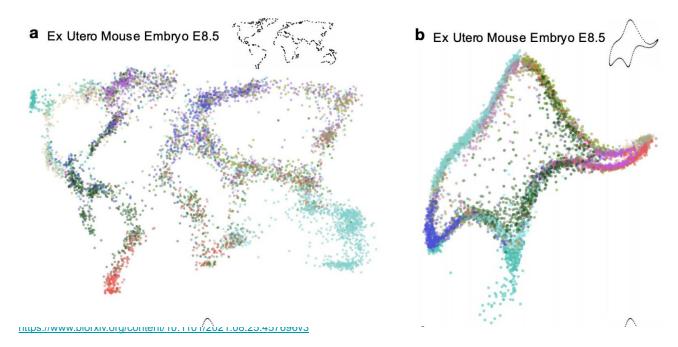
 $2\epsilon_3$ 

### **Topological Data Analysis**



#### Avoid over-interpreting single plots

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

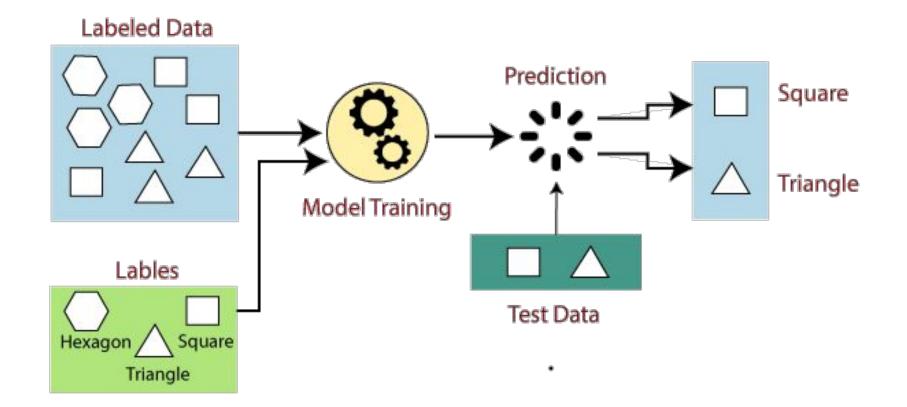


"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk." - Von Neumann

# Predicting using tabular data

# Predicting using tabular data

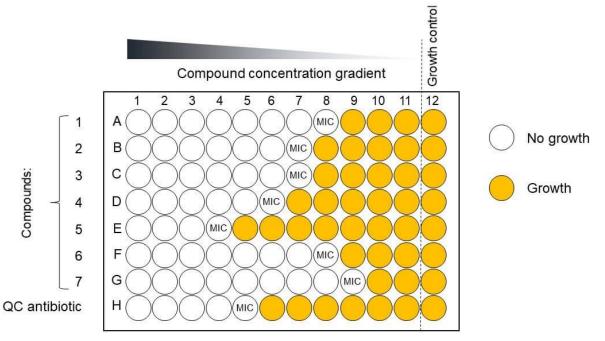
#### **Predicting Labels or Values**



#### Values can be complex: interval prediction

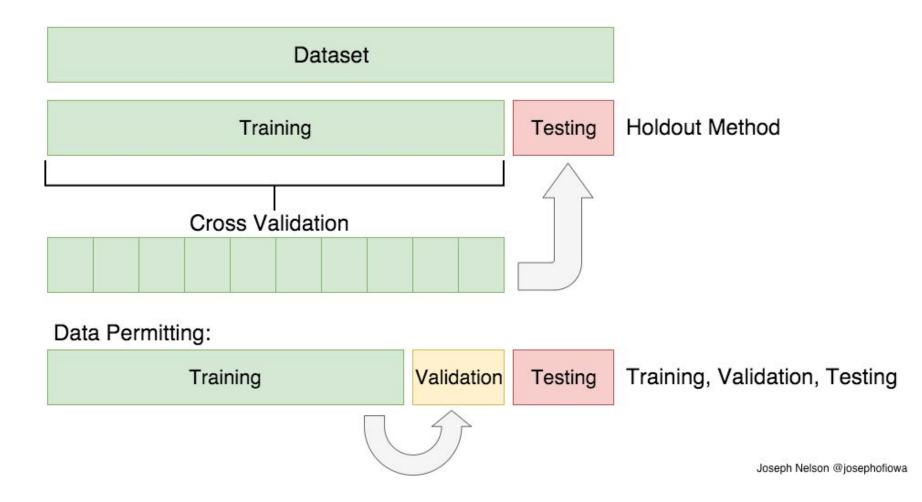
- MIC > highest concentration = <u>right-censored</u>
- MIC < lowest concentration = <u>left-censored</u>
- Serial Dilutions: MIC of x actually [x/2, 2x] = <u>unequal error</u>

#### Interpretation of microdilution MIC results



©Emery Pharma

#### Overfitting 101: Test-Train Split

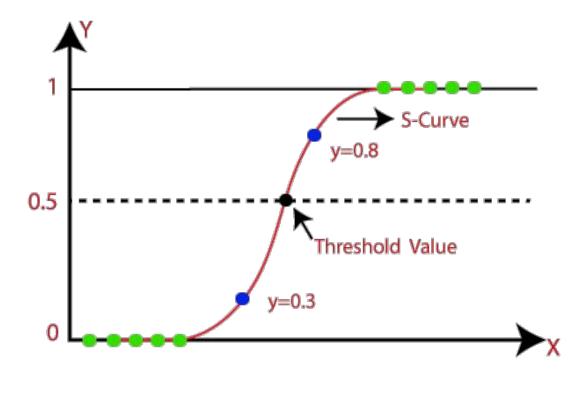


#### Start simple: linear regression

|   | 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><br>P: One-sample t-test<br>N: Wilcoxon signed-rank         | t.test(y)<br>wilcox.test(y)  | lm(y ~ 1)<br>lm(signed_rank(y) ~ 1)   | ✓<br>for N >14         | One number (intercept, i.e., the mean) predicts <b>y</b> .<br>- (Same, but it predicts the <i>signed rank</i> of <b>y</b> .)   |                             |
|   | P: Paired-sample t-test<br>N: Wilcoxon matched pairs                                    | t.test(y1, y2, paired=TRUE)<br>wilcox.test(y1, y2, paired=TRUE)  | $lm(y_2 - y_1 \sim 1)$<br>$lm(signed_rank(y_2 - y_1) \sim 1)$   | √<br>f <u>or N ≥14</u> | One intercept predicts the pairwise y <sub>2</sub> -y <sub>1</sub> differences.<br>- (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><br>P: Pearson correlation<br>N: Spearman correlation            | cor.test(x, y, method='Pearson')<br>cor.test(x, y, method='Spearman')  | lm(y ~ 1 + x)<br>lm(rank(y) ~ 1 + rank(x))  | ✓<br>for N >10         | One intercept plus <b>x</b> multiplied by a number (slope) predicts <b>y</b> .<br>- (Same, but with <i>ranked</i> <b>x</b> and <b>y</b> )  | مىلېرىپ                     |
|   | <b>y ~ discrete x</b><br>P: Two-sample t-test<br>P: Welch's t-test<br>N: Mann-Whitney U | t.test(y <sub>1</sub> , y <sub>2</sub> , var.equal=TRUE)<br>t.test(y <sub>1</sub> , y <sub>2</sub> , var.equal=FALSE)<br>wilcox.test(y <sub>1</sub> , y <sub>2</sub> ) | $\begin{array}{l} Im(y\sim1+G_2)^{A}\\ gls(y\sim1+G_2,\ weights=^{B})^{A}\\ Im(signed_rank(y)\sim1+G_2)^{A} \end{array}$  | ✓<br>✓<br>for N >11    | An intercept for <b>group 1</b> (plus a difference if <b>group 2</b> ) predicts <b>y</b> .<br>- (Same, but with one variance <i>per group</i> instead of one common.)<br>- (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<br>N: Kruskal-Wallis   | aov(y ~ group)<br>kruskal.test(y ~ group)  | $\begin{split} ℑ(y\sim 1+G_2+G_3++G_N)^4 \\ ℑ(rank(y)\sim 1+G_2+G_3++G_N)^4 \end{split}$  | √<br>for N >11         | An intercept for <b>group 1</b> (plus a difference if group $\neq$ 1) predicts <b>y</b> .<br>- (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.)<br>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.<br>Note: $G_{2:WN}$ is an indicator (0 or 1) for each non-intercept levels of the group variable.<br>Similarly for $S_{2:WN}$ for sex. The first line (with G) is main effect of group, the second (with<br>S <sub>2</sub> ) for sex and the third is the group × sex interaction. For two levels (e.g. male/female),<br>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> . | <br>  [Coming]<br>          |
|   | Counts ~ discrete x<br>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.)<br>Note: Run glm using the following arguments: gim(model, family=poisson())<br>As linear-model, the Chi-square test is $log(y) = log(N) + log(a) + log(b) + log(a\beta)$ where $a_i$<br>and $\beta_i$ are proportions. See more info in the accompanying notebook.   | Same as<br>Two-way<br>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/

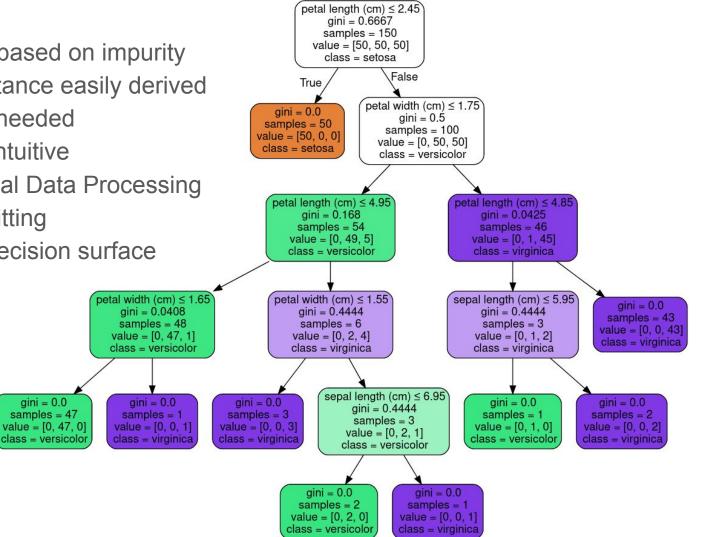
#### Add a sigmoid for classification



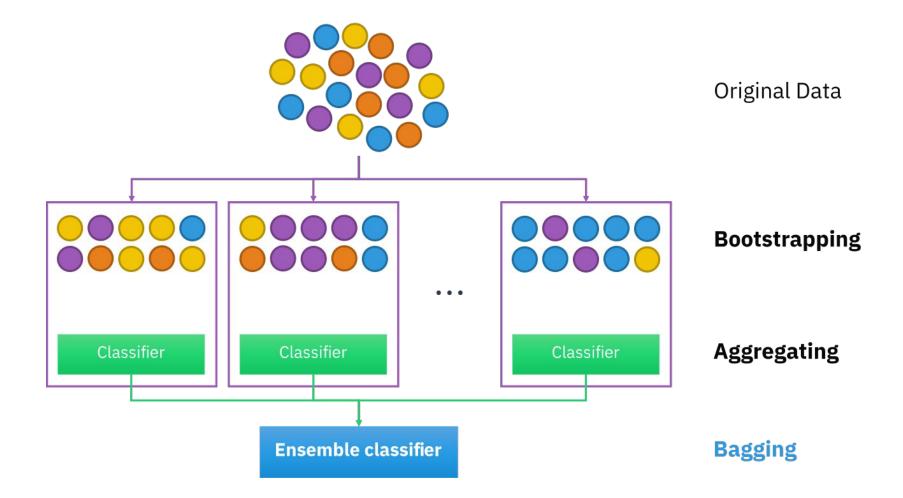
- Crude measure of feature importance (model coefficients)
- Specific feature selection can be a good idea
- Support for regularisation (Lasso/L1 -> sparsity vs Ridge/L2 -> minimal vs ElasticNet -> balance)
- Statistics has developed
  much better practices for
  treatment/interpretation
  of logistic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

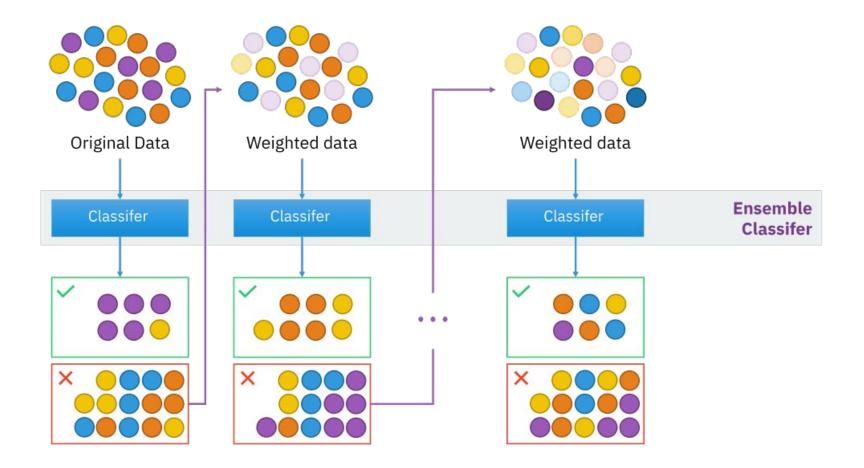


#### Many Decision Trees: Bagging



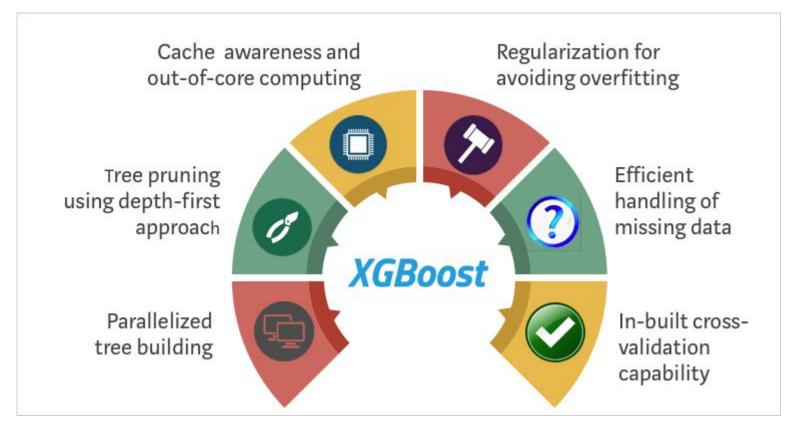
Random Forest: Bagging + Random Subset Per Split Feature Importance: Average impurity decrease

#### 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