ICMAT
INSTITUTO DE CIENCIAS MATEMÁTICAS

Some ML applications in Online Marketing and Molecule Design

Roi Naveiro

From academia to industry

With **a bit** of creativity, **some** knowledge and **a lot** of effort; you can do incredible stuff...

From academia to industry

With **a bit** of creativity, **some** knowledge and **a lot** of effort; you can do incredible stuff…

…if you know some math/stats/programming!

What are we gonna see

- Online Marketing
- Demo 1
- Molecular Design
- Demo 2

Online Marketing - The problem

- Xeerpa collects data from social loggings
  - Likes on facebook
  - Posts in Twitter
  - Photos in IG…
- **Goal (at large):** process this information and analyse it to improve marketing decisions
- Many things to be done!
- We will see how to process information coming from:
  - Likes
  - Images

Online Marketing - Information coming from (Facebook) likes

- Facebook defines many categories such as: IPAs, Veggie Food, Soccer, Rock ‘n’ Roll
- Every category contains many Facebook pages (that users could like)

$$q = (q_1, \ldots, q_T) \text{ where } q_i = 1$$

$$\text{if page belongs to category and 0 otherwise}$$

- Similarly, users are represented as vector d.

- Goal: score every user in every category

Online Marketing - Scoring people based on Facebook likes

“A common problem in Information Retrieval (IR) is the following: given a corpus of documents, each of them represented by a sequences of words, how to find the more relevant documents to a given query. This problem reduces to assigning a score to a (query, document) pair.”

This is the same! Words are Facebook pages, Users are documents, Categories are queries

Online Marketing - Scoring people based on Facebook likes

- IR assigns a number for each word in each document, that weights the importance of a word in a document

- Assign a weight to each like

- Two thoughts:
  - If there is no like, what should be the weight?
  - Should a like to Real Madrid be as important as a like to Cultural y Deportiva Leonesa?

- TF-IDF (as in IR)

Online Marketing - Scoring people based on Facebook likes

- Term Frequency
  - 1 if like is present 0 otherwise
  - 1 / (Number of likes)

- Inverse document frequency (how much info a like provides?)

$$\log\left(\frac{N}{n_t+1}\right)+1$$

- tf-idf = tf * idf

Online Marketing - Scoring people based on Facebook likes

- Each user is a vector

$$v(d) \text{ where } v(d)_i \text{ tf-idf of the i-th like}$$

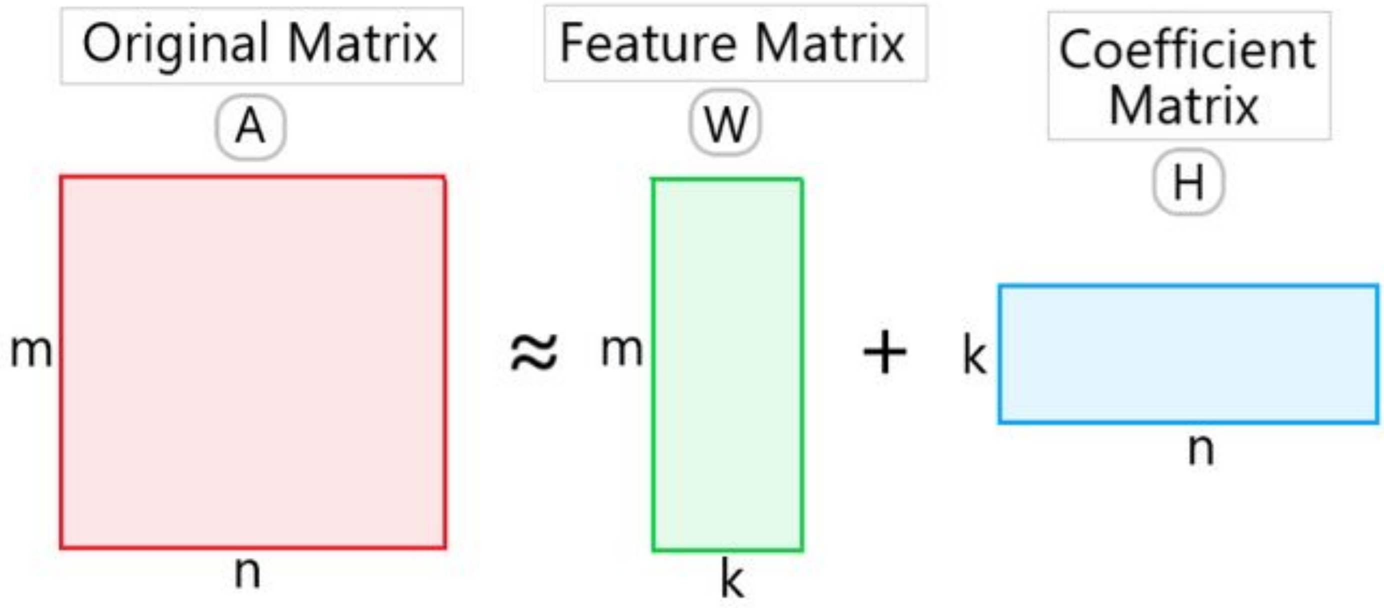
- Same for categories q!
- A common score

$$\text{score}(d, q) = \frac{v(d) \cdot v(q)}{|v(d)||v(q)|}$$

- Lives in [0,1]
- User with no likes in category will have 0
- User liking all pages in category (and with no other likes) will have 1

Online Marketing - Community detection

Detect communities of similar users

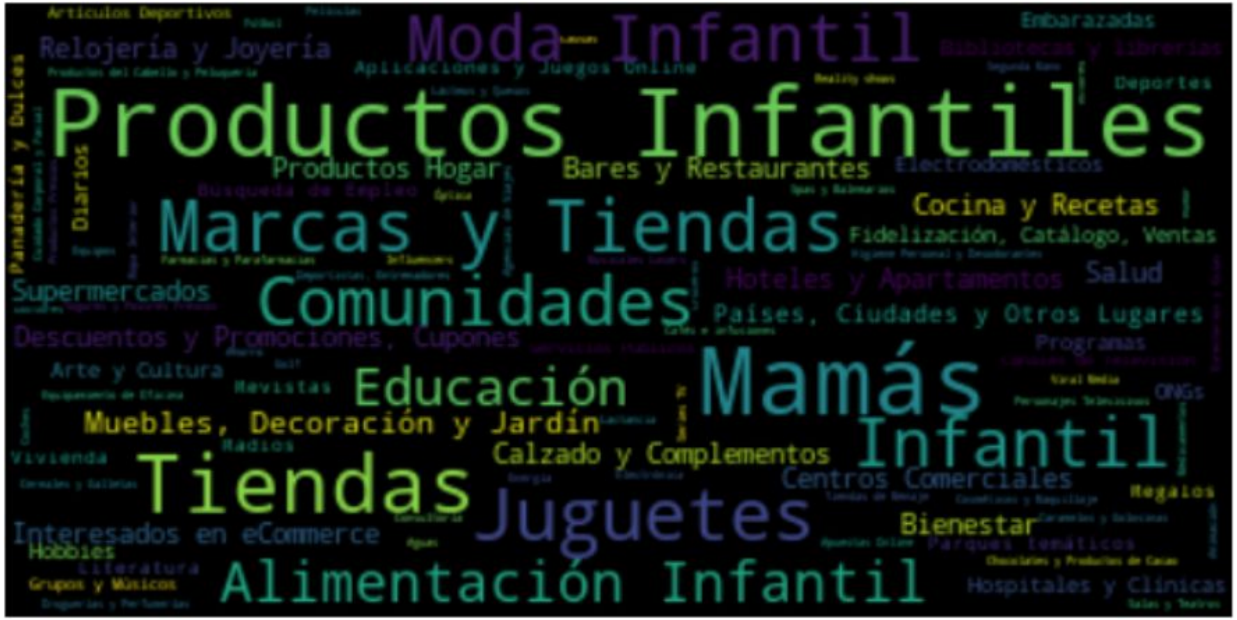


Minimize reconstruction error

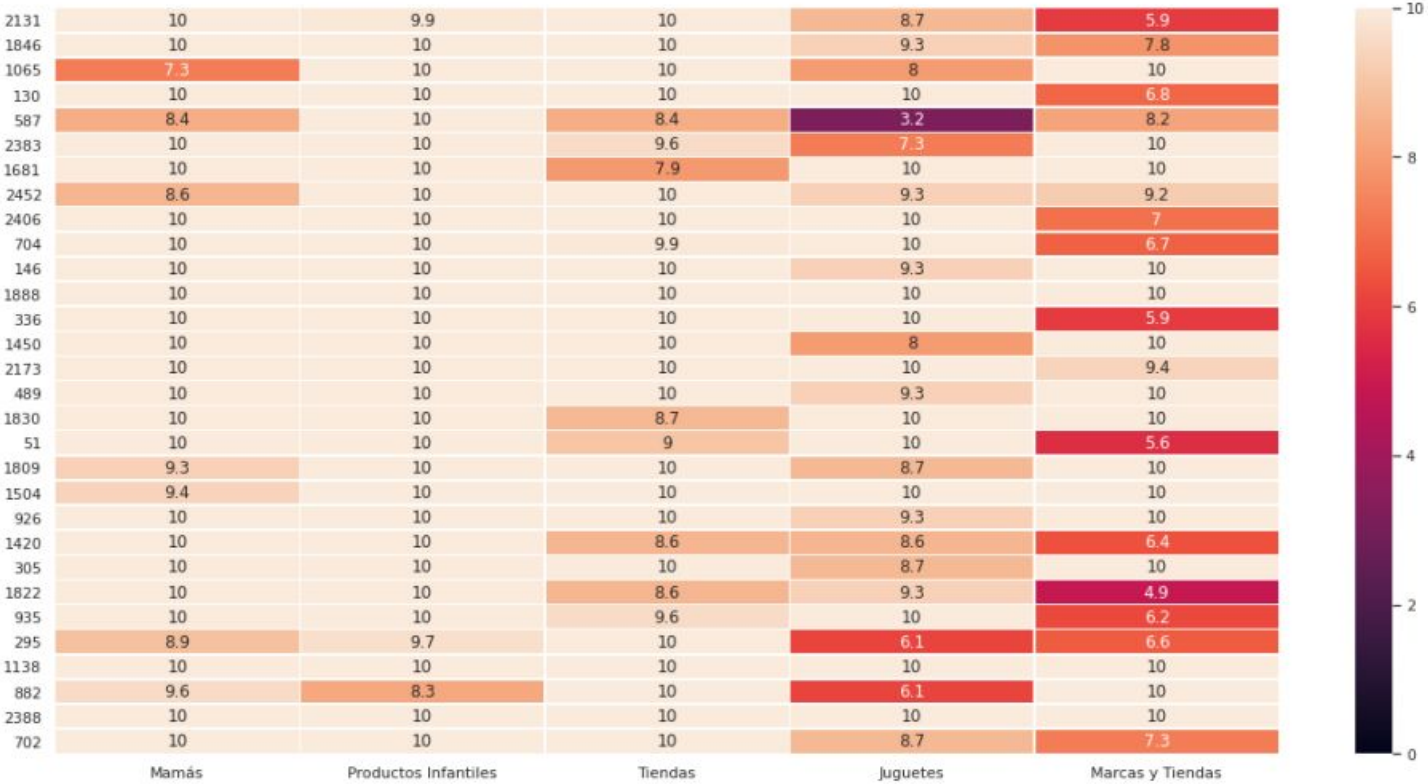
$$\|A - WH\|^2 \sum_{i=1}^{n} = \sum_{j=1}^{n} (X_{ij} - [WH]_{ij})^2$$

Online Marketing - Community detection

Women between 30 and 50



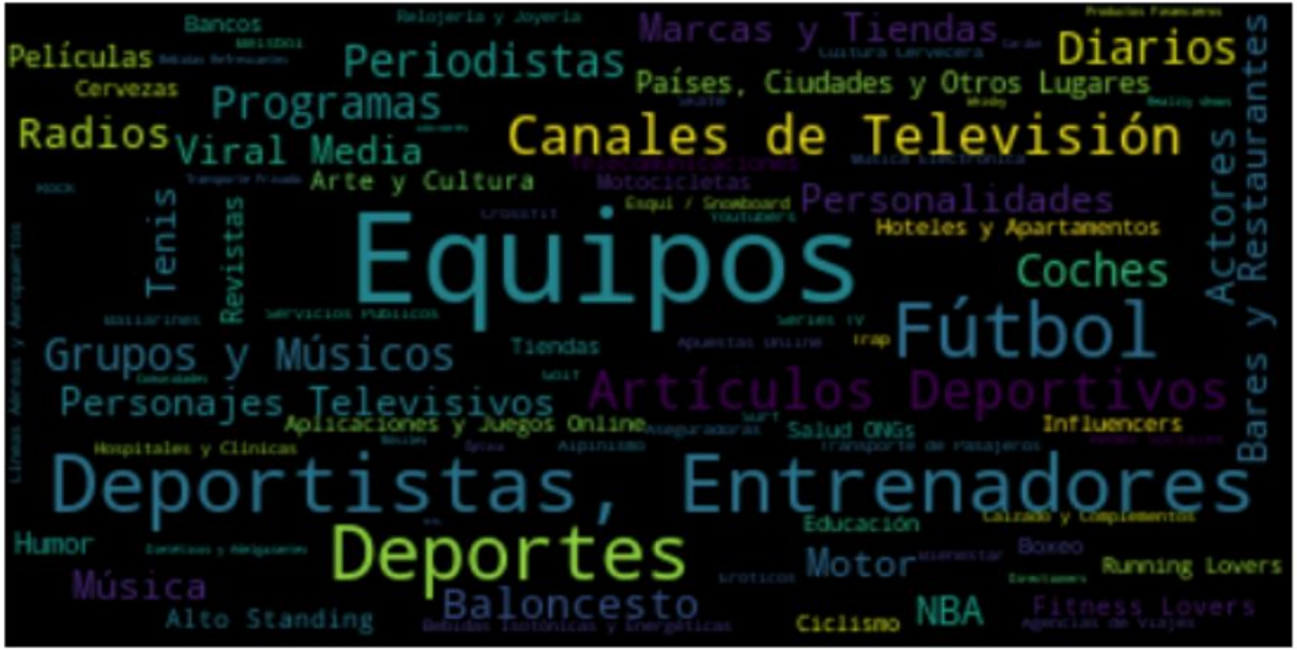
Online Marketing - Community detection



	Mamás	Productos Infantiles	Tiendas	Juguetes	Marcas y Tiendas
2131	10	9.9	10	8.7	5.9
1846	10	10	10	9.3	7.8
1065	7.3	10	10	8	10
130	10	10	10	10	6.8
587	8.4	10	8.4	3.2	8.2
2383	10	10	9.6	7.3	10
1681	10	10	7.9	10	10
2452	8.6	10	10	9.3	9.2
2406	10	10	10	10	7
704	10	10	9.9	10	6.7
146	10	10	10	9.3	10
1888	10	10	10	10	10
336	10	10	10	10	5.9
1450	10	10	10	8	10
2173	10	10	10	10	9.4
489	10	10	10	9.3	10
1830	10	10	8.7	10	10
51	10	10	9	10	5.6
1809	9.3	10	10	8.7	10
1504	9.4	10	10	10	10
926	10	10	10	9.3	10
1420	10	10	8.6	8.6	6.4
305	10	10	10	8.7	10
1822	10	10	8.6	9.3	4.9
935	10	10	9.6	10	6.2
295	8.9	9.7	10	6.1	6.6
1138	10	10	10	10	10
882	9.6	8.3	10	6.1	10
2388	10	10	10	10	10
702	10	10	10	8.7	7.3

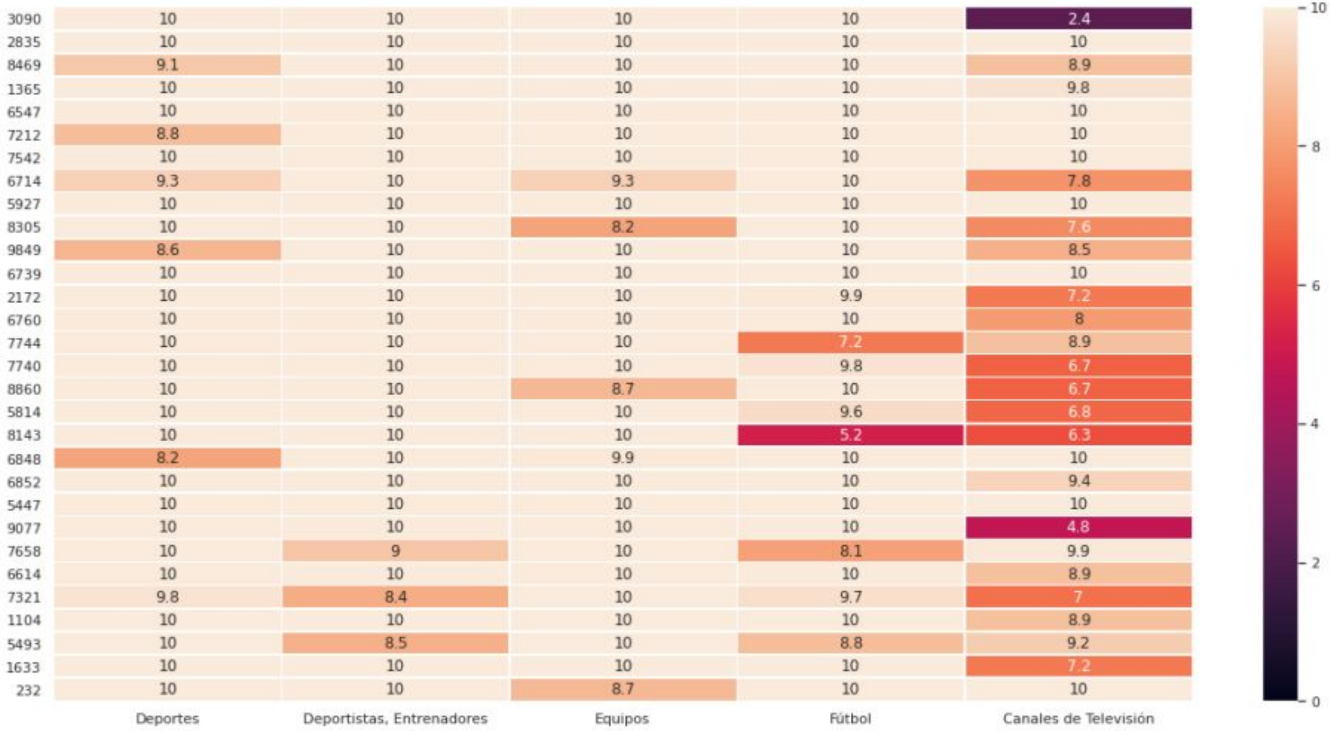
Online Marketing - Community detection

Men between 30 and 50



Online Marketing - Community detection

Men between 30 and 50



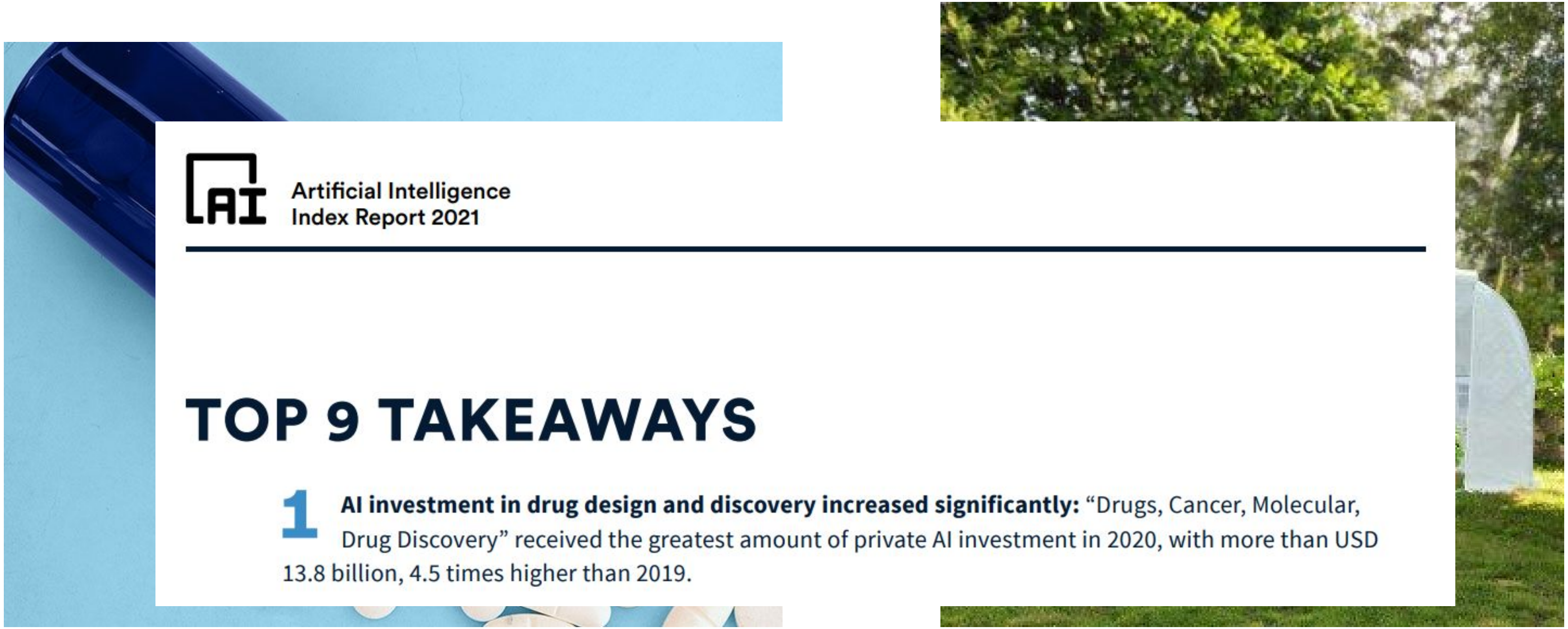
	Deportes	Deportistas, Entrenadores	Equipos	Fútbol	Canales de Televisión
3090	10	10	10	10	2.4
2835	10	10	10	10	10
8469	9.1	10	10	10	8.9
1365	10	10	10	10	9.8
6547	10	10	10	10	10
7212	8.8	10	10	10	10
7542	10	10	10	10	10
6714	9.3	10	9.3	10	7.8
5927	10	10	10	10	10
8305	10	10	8.2	10	7.6
9849	8.6	10	10	10	8.5
6739	10	10	10	10	10
2172	10	10	10	9.9	7.2
6760	10	10	10	10	8
7744	10	10	10	7.2	8.9
7740	10	10	10	9.8	6.7
8860	10	10	8.7	10	6.7
5814	10	10	10	9.6	6.8
8143	10	10	10	5.2	6.3
6848	8.2	10	9.9	10	10
6852	10	10	10	10	9.4
5447	10	10	10	10	10
9077	10	10	10	10	4.8
7658	10	9	10	8.1	9.9
6614	10	10	10	10	8.9
7321	9.8	8.4	10	9.7	7
1104	10	10	10	10	8.9
5493	10	8.5	10	8.8	9.2
1633	10	10	10	10	7.2
232	10	10	8.7	10	10

Online Marketing - Scoring based on images!

- How to do score users in categories based on their IG images?
- We need to associate each image to a category or group of categories
- This has to be done automatically!
- **Demo**

Molecular design - Why?

Molecular design. Why?



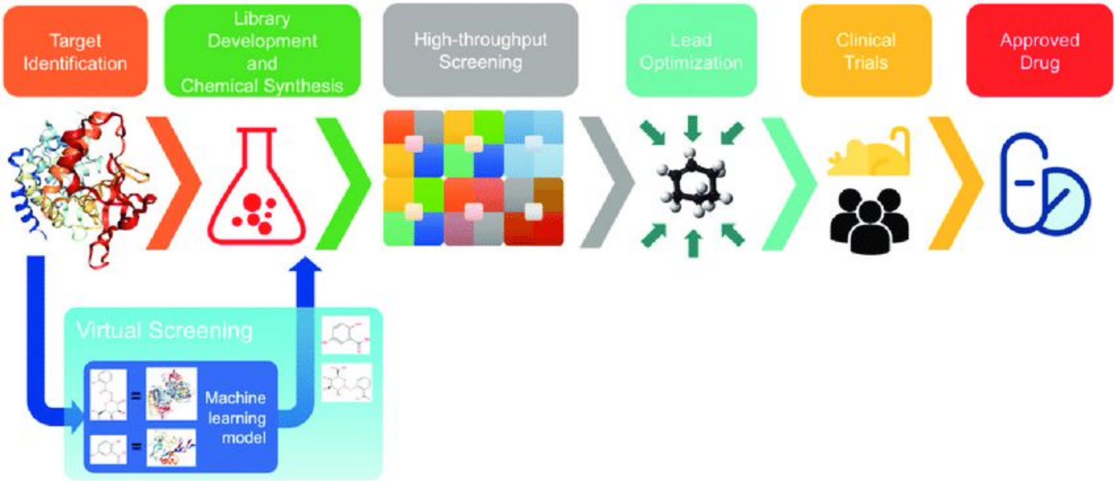
Artificial Intelligence
Index Report 2021

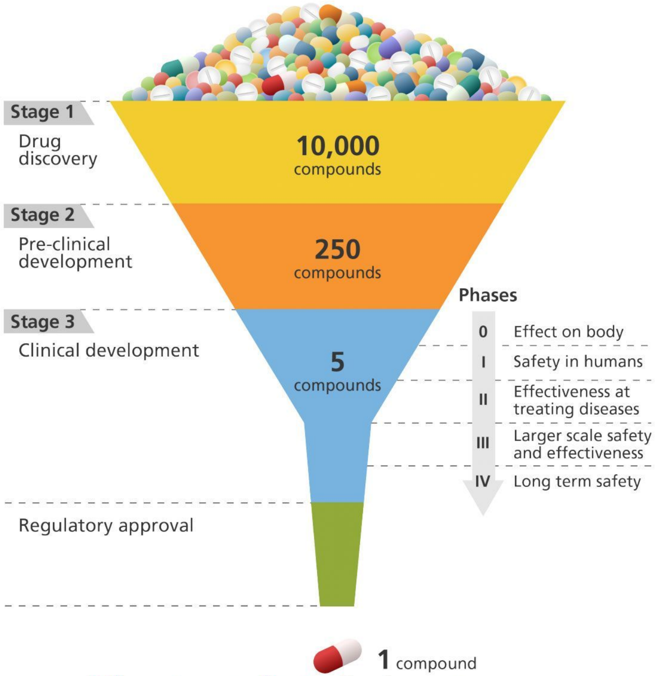
TOP 9 TAKEAWAYS

1 **AI investment in drug design and discovery increased significantly:** “Drugs, Cancer, Molecular, Drug Discovery” received the greatest amount of private AI investment in 2020, with more than USD 13.8 billion, 4.5 times higher than 2019.

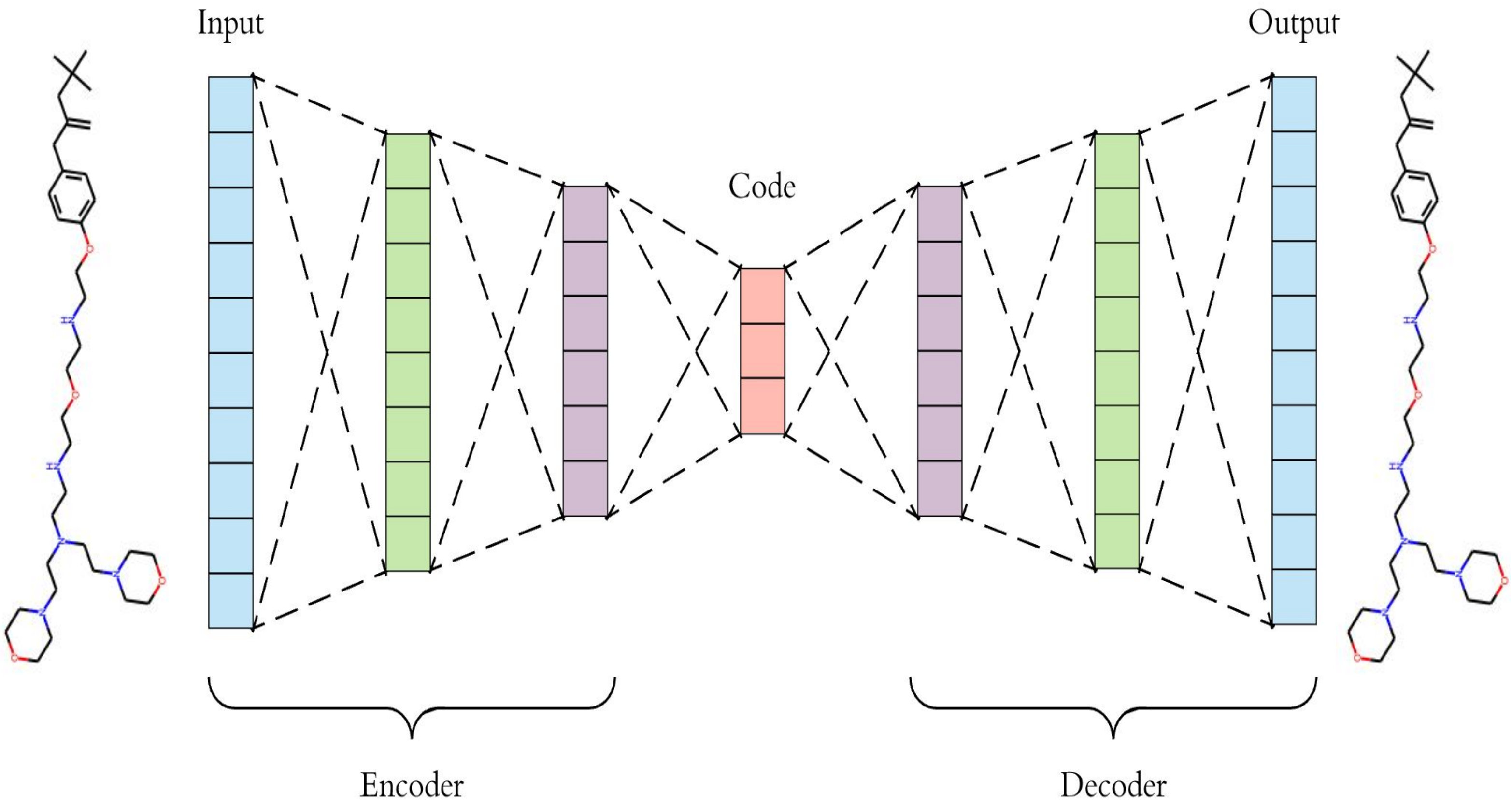
The process of discovering new molecules

- Pharma: average time discovery – market, 13 years
- Outside pharma: 25 years
- Crucial 1st step: **generate pool of candidates**
- Daunting task (e.g. 10^{23} – 10^{60} drug-like molecules)



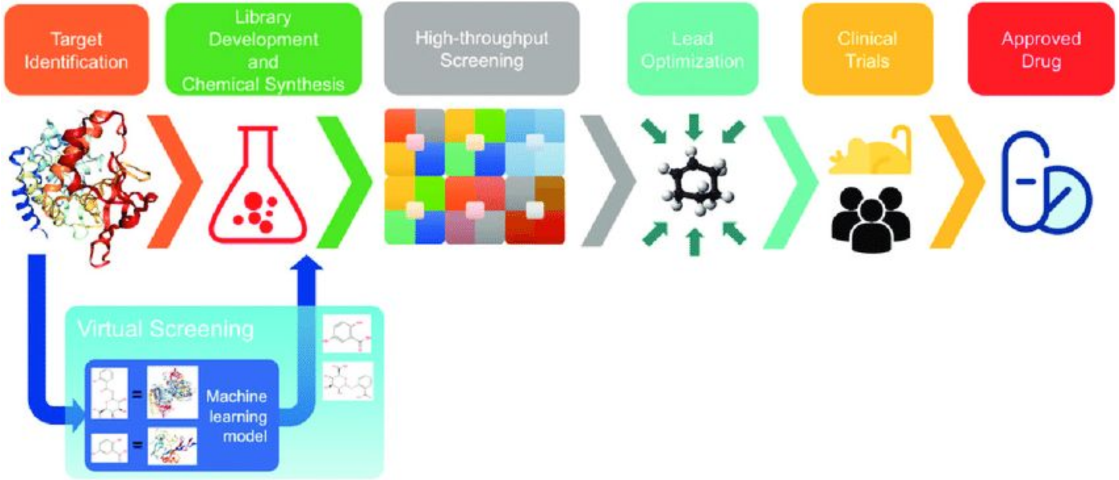


(Variational) Autoencoders



The old way and the soon-to-be-old way

- Old way
  - Human experts propose, synthesize and test (*in vitro*)
- Soon-to-be-old way: high throughput virtual screening (HTVS)
  - Predict properties through computational chemistry…
  - …leverage rapid **ML-based property predictions**



De novo molecular design

- Just existing molecules are explored
- Much time lost evaluating bad leads
- Traverse chemical space more “effectively”: reach **optimal molecules** with **less evaluations** than brute-force screening

> *“De novo molecular design is the process of* ***automatically proposing novel chemical structures*** *that* ***optimally satisfy desired properties****”*

Combinatorial, black-box, stochastic, multi-objective optimization with black-box constraints

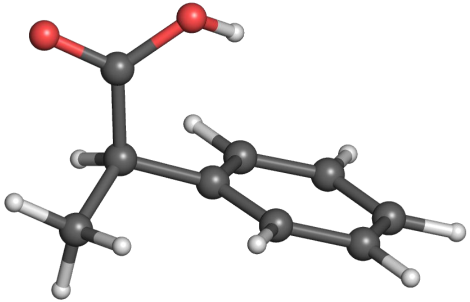
Automatically proposing novel chemical structures

Two main ingredients

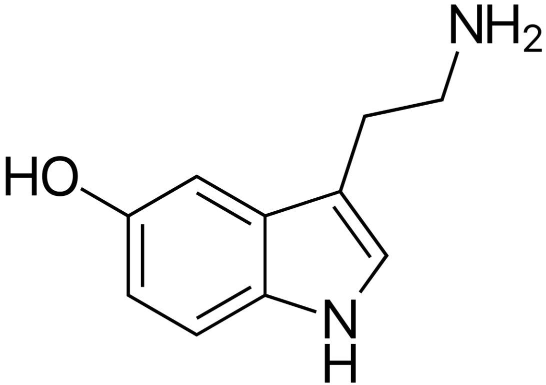
- Molecule representation
- Generative model

Representing molecules

Molecules are **3D QM objects** with: nuclei with defined positions surrounded by electrons described by complex wave-functions



- Digital encoding that serves as input to model
- **Uniqueness and invertibility**
- Trade-off: information lost vs complexity
  - 3D coord. representation (symmetries?)
  - More compact 2D (graph) representation
- 1D, 2D and 3D



1D representations - SMILEs

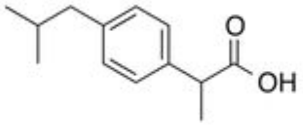
Simplified Molecular Input Line Entry System

Molecule as graph (bond length and conformational info is lost)

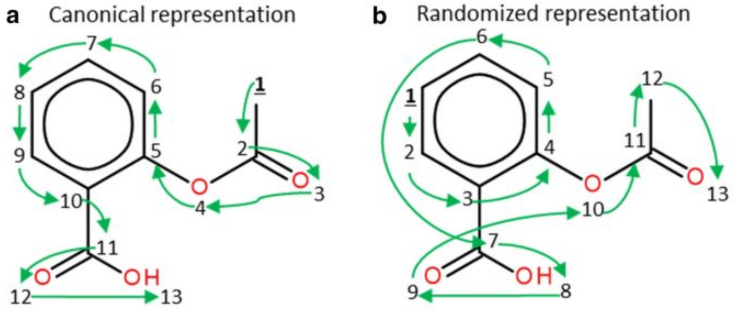
- Graph traversal
- Sequence of ASCII characters
- Non-unique → Canonical SMILES
- One-Hot-Encoding

- Leverage NLP techniques

- SMILE-based methods struggle to generate **valid** molecules
- Valid = valency rules
- Learn spurious grammar rules



Ibuprofen
CC(C)Cc1ccc(cc1)C(C)C(O)=O



CC(=O)Oc1ccccc1C(=O)O

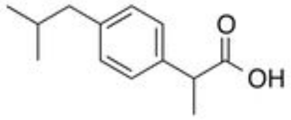
c1cc(c(cc1)C(O)=O)OC(C)=O

How to generate molecules?

Myriad of different ways. A useful distinction:

- Gradient-free methods
- Gradient-based methods

Recurrent Neural Networks



Ibuprofen
CC(C)Cc1ccc(cc1)C(C)C(O)=O

- Work on sequences (SMILES)
- Goal: given training sequences → learn to generate new sequences that resemble those of training.
- Sequence: $S_{1:T} = (S_1, \ldots, S_T)$ where $S_i \in \mathcal{V}$
- Training: maximum likelihood, equiv to minimize loss function:

$$L^{MLE} = -\sum_{s \in \mathcal{T}} \sum_{t=2}^{T} \log \pi_\theta(s_t | S_{1:T-1})$$

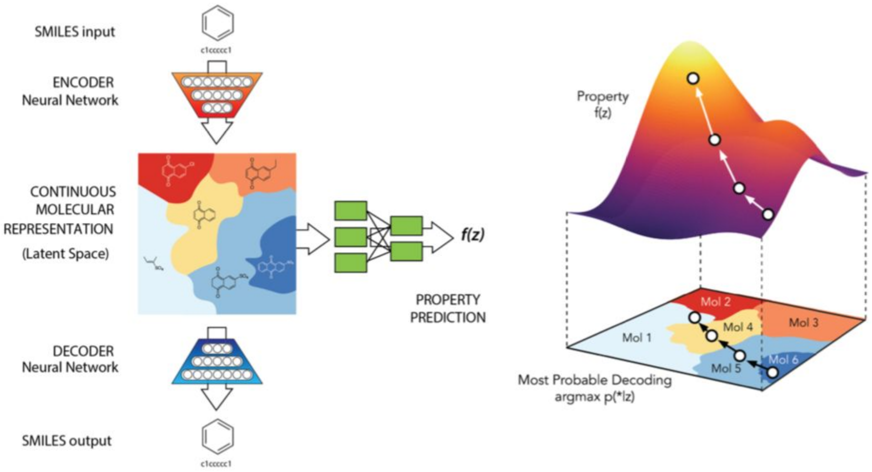
- Generation: sequentially sample from multinomial dist.
- Thermal rescaling

$$\hat{p}_i \propto \exp(\frac{p_i}{T})$$

Using properties to guide generation

2. Optimization with VAE

- Learn map from latent space to property (e.g. through GP)
- Optimize that map (gradient ascent, bayesian optimization, etc.)



Let’s generate some molecules!

Demo 2

Thanks!

CULTURAL 1923 1923 LEONESA

roi.naveiro@icmat.es

https://roinaveiro.github.io/

https://github.com/roinaveiro