





#### Where do we come from?

Université Paris 7 Denis Diderot UFR de Physique

Thèse en vue de l'obtention du diplôme de docteur de l'université de Paris 7 en physique Ecole doctorale 517, Particules-Noyaux-Cosmos

Etude théorique et expérimentale des corrections électrofaibles au processus de production inclusive de jets

Développement de méthodes de détection de topologies extrèmes

Nicolas MERIC

Thèse réalisée au CEA, LPNHE, LPTHE Sous la direction de : Gavin Salam et Philippe Schwemling

Thèse soutenue le jeudi 19 septembre 2013.

Deep learning @ATLAS

DreamQuark established 2014

## **Empower your action thanks to science**

 My background: computational plasma physics, turbulence modeling

=> originally applied ML to analyze experimental data & simulation data







Fraud & Compliance



Fraud detection AML Compliance supervision

# BANKS & INSURANCE



Marketing

Product upsell/cross-sell
Propensity
Customer segmentation
Satisfaction & anti-churn
Product recommendation



Risk

Risk model Credit scoring Fragile clients Recovery







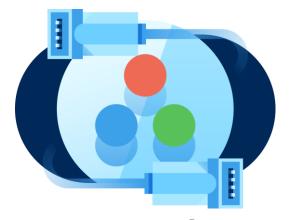
Transparency of decisions



Ability to do more business



Ease of use



Ease of deployment



## DreamQuark software is market-proven

THEY TRUST US





## **BNP PARIBAS**

















**AG2R LA MONDIALE** 

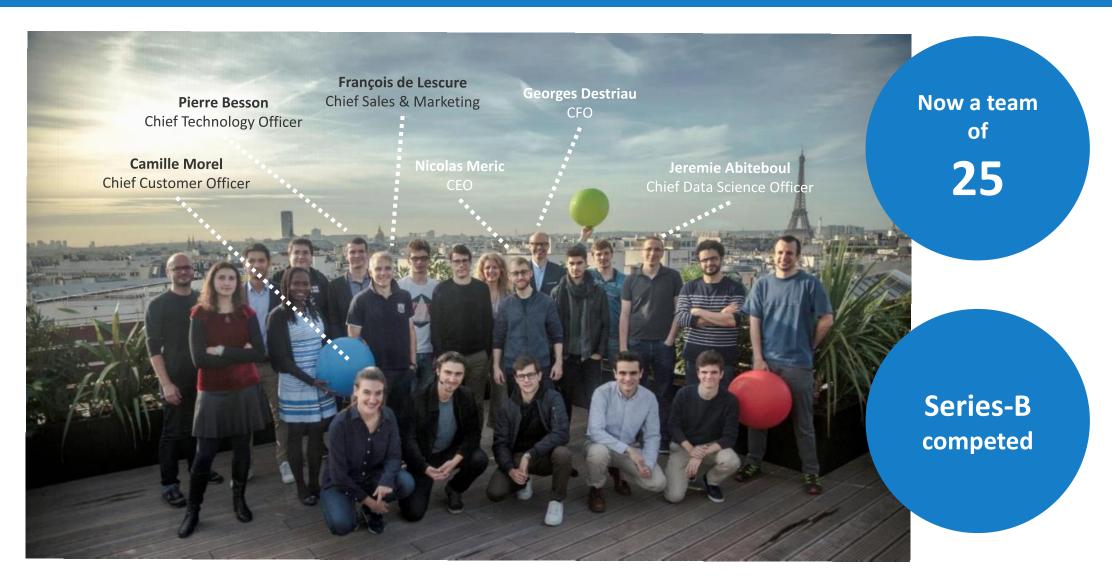




RECENT AWARDS



# The success of a team





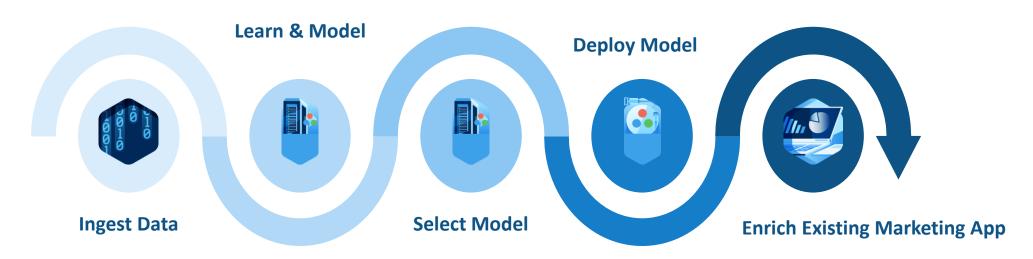


## Leverage data to reinvent the customer experience

To make it a reality in large scale production, DreamQuark created an AI platform for business experts:

Simple & zero-code Enterprise grade IT Top data-driven decisions

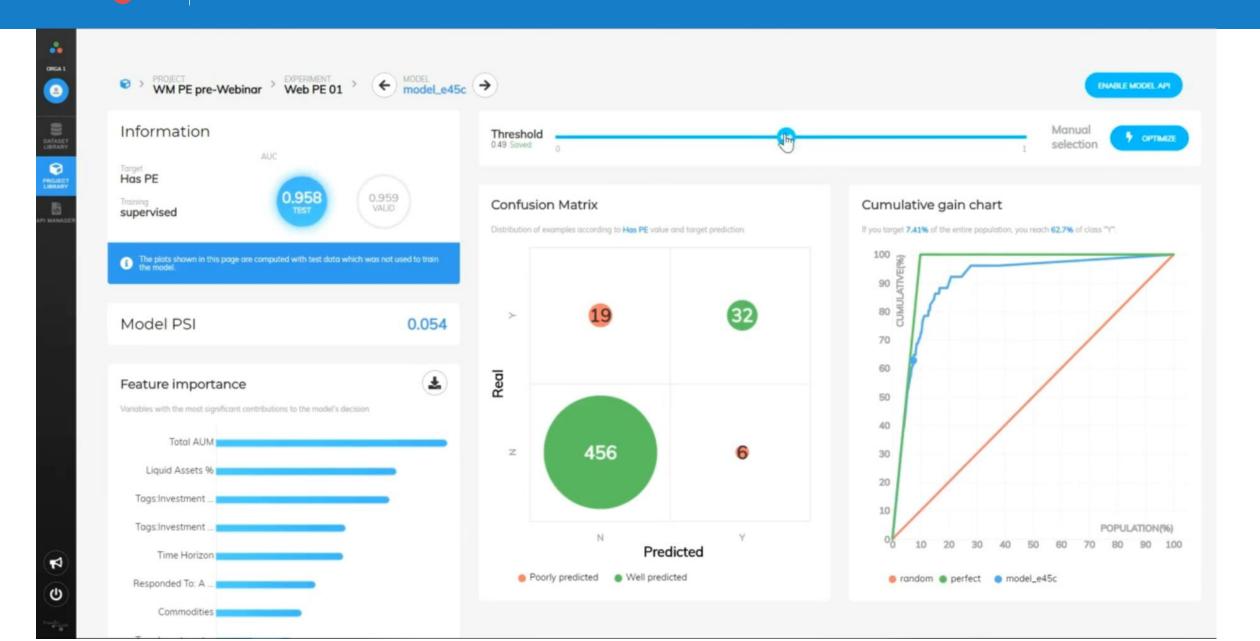
On-prem or SaaS Multi-tenant Transparent & trustworthy



Empower business analysts with predictive analytics => Citizen Data Scientist

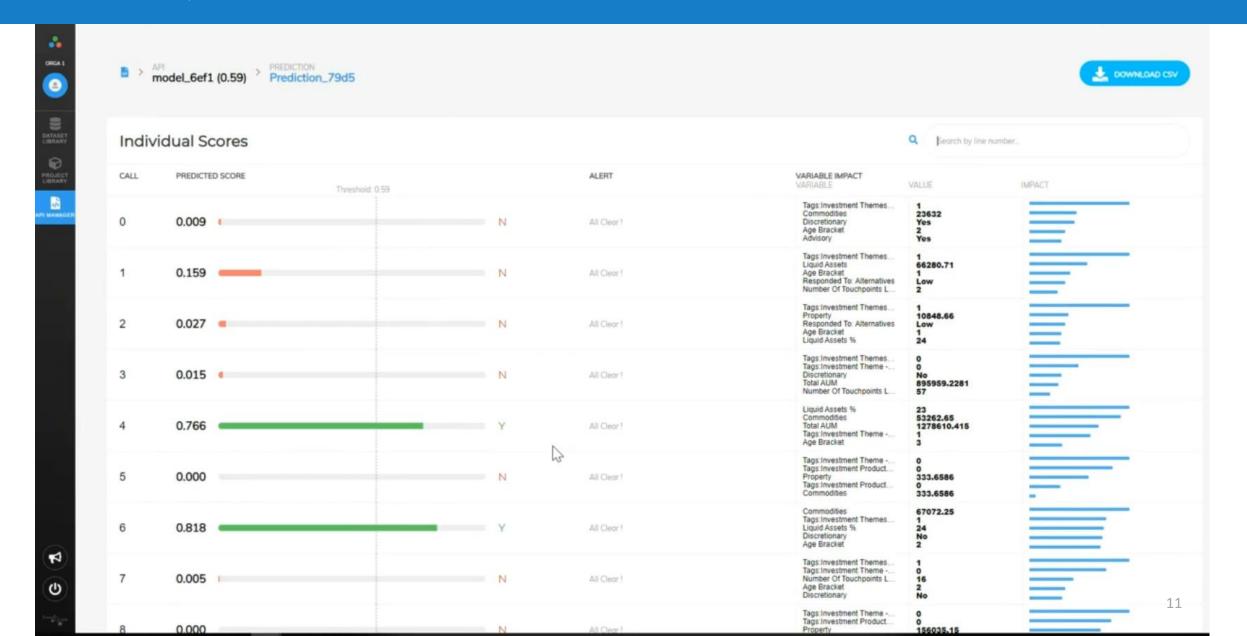


# Easily generate predictive models



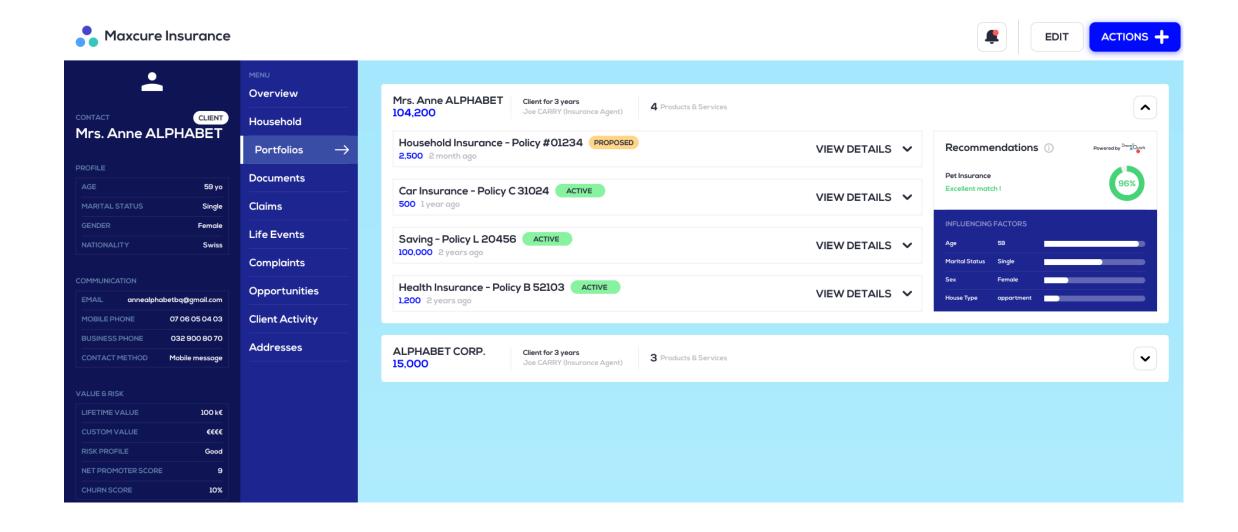


## **Create actionable predictions**





# Integrate with existing business apps





# Why is this interesting for (former) physicists?

Automatically training neural networks on tabular data

Explainable AI: "opening the black-box"

- Fairness of Al systems
- Robustness of Al systems
- Challenges for AI systems in production

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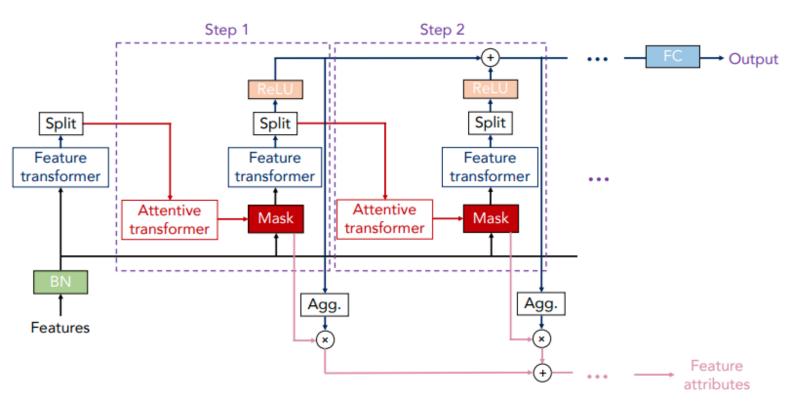
#### **Neural networks for tabular data**

- Most popular applications of neural networks focus on "unstructured" data (images, text, audio, video)
- Tabular data is actually less "structured" than e.g. images
- Most of the AI community still uses standard ML methods (boosting algorithms, random forests, etc) for tabular data
- We've found that neural networks are competitive if
  - Design suitable architectures (not necessarily very deep)
  - Find a reasonable grid for hyperparameter search [patent pending]
- Bonus: ensembling of neural networks and standard ML



## **TabNet: Attentive Interpretable Tabular Learning**

[S.O. Arik & T. Pfister, arXiv September 2019]



- Sparse learned feature selection
- Sequential multi-step architecture (each step contributes to a portion of the decision)
- Attentive transformer ensures different steps learn from different features
- Non-linear processing of selected features (=> model capacity)

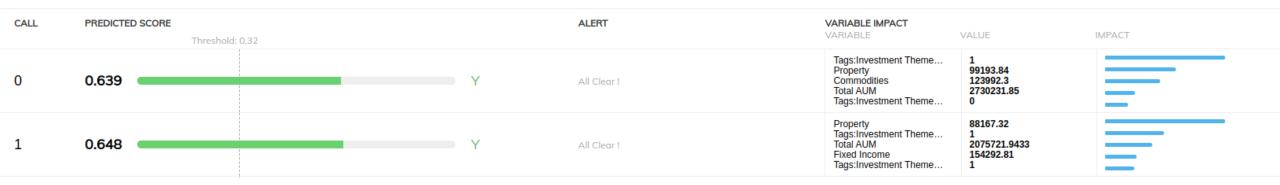
- Original publication by Google Cloud AI team: <a href="https://arxiv.org/abs/1908.07442">https://arxiv.org/abs/1908.07442</a>
- Open-source (pytorch) implementation by DreamQuark: <a href="https://github.com/dreamquark-ai/tabnet">https://github.com/dreamquark-ai/tabnet</a>





# **Explainable Al**

- Understanding model decisions is a requirement for our users
  - Business users must have confidence in models before deploying them
  - Regulations require that decisions based on algorithms be made "understandable by non-experts"
  - For marketing use cases, explanations also make decisions actionable

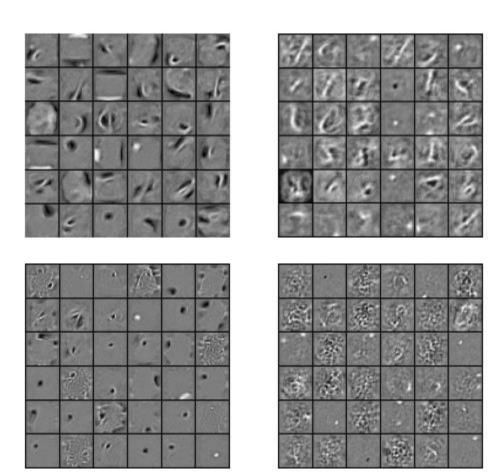


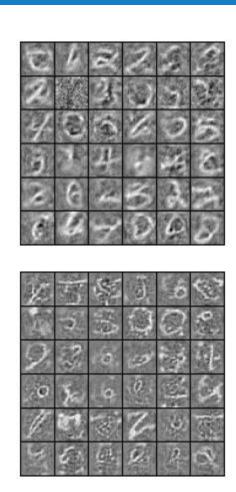
- Also much academic interest around this research topic
  - DARPA XAI program: <a href="https://www.darpa.mil/program/explainable-artificial-intelligence">https://www.darpa.mil/program/explainable-artificial-intelligence</a>

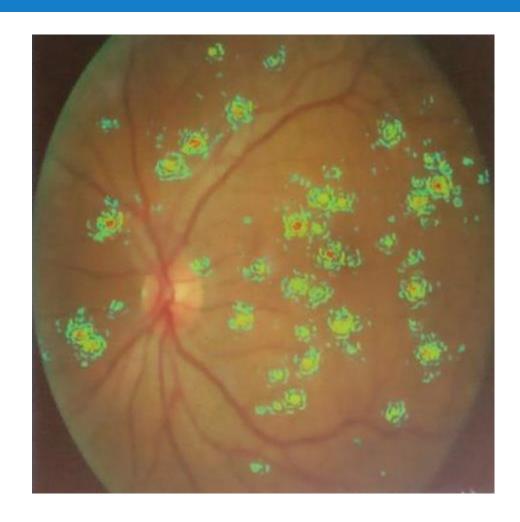
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# **Explaining Convolutional Neural Networks: saliency maps**







Erhan, Bengio et al. 2013

DreamQuark 2016



## **Explaining Recurrent Neural Networks: cell activations**

[Karpathy et al, 2015]

```
Cell sensitive to position in line:
                                                                                    Cell that turns on inside comments and quotes:
The sole importance of the crossing of the Berezina lies in the fact
                                                                                    / Duplicate LSM field information. The lsm_rule
that it plainly and indubitably proved the fallacy of all the plans for
                                                                                    static inline int audit_dupe_lsm_field(struct audit_field *df,
cutting off the enemy's retreat and the soundness of the only possible
                                                                                          struct audit_field 'sf)
line of action--the one Kutuzov and the general mass of the army
demanded -- namely, simply to follow the enemy up. The French crowd fled
                                                                                     int ret = 0;
at a continually increasing speed and all its energy was directed to
                                                                                     char "lsm_str;
/ " our own copy of lsm_str "/
lsm_str = kstrdup(sf->lsm_str, GFP_KERNEL);
reaching its goal. It fled like a wounded animal and it was impossible
to block its path. This was shown not so much by the arrangements it
                                                                                     if (unlikely(!lsm_str))
made for crossing as by what took place at the bridges. When the bridges
broke down, unarmed soldiers, people from Moscow and women with children
                                                                                      return - ENOMEM;
                                                                                     df->lsm_str = lsm_str;
/* our own (refreshed) copy of lsm_rule */
ret = security_audit_rule_init(df->type, df->op, df->lsm_str,
who were with the French transport, all--carried on by vis inertiae--
pressed forward into boats and into the ice-covered water and did not,
surrender.
                                                                                               (void **)&df->lsm_rule);
                                                                                        keep currently invalid fields around in case they
Cell that turns on inside quotes:
                                                                                        become valid after a policy reload. */
"You mean to imply that I have nothing to eat out of.... On the
                                                                                      if (ret == -EINVAL) {
contrary, I can supply you with everything even if you want to give dinner parties," warmly replied Chichagov, who tried by every word he
                                                                                      pr_warn("audit rule for LSM \'%s\' is invalid\n",
                                                                                       df->lsm_str);
spoke to prove his own rectitude and therefore imagined Kutuzov to be
                                                                                      ret = θ;
animated by the same desire.
                                                                                     return ret;
Kutuzov, shrugging his shoulders, replied with his subtle penetrating
smile: "I meant merely to say what I said.
                                                                                    Cell that is sensitive to the depth of an expression:
                                                                                    #ifdef CONFIG AUDITSYSCALL
Cell that robustly activates inside if statements:
                                                                                    static inline int audit_match_class_bits(int class, u32 *mask)
static int __dequeue_signal(struct sigpending *pending, sigset_t *mask,
siginfo_t *info)
                                                                                     if (classes[class]) {
 int sig = next_signal(pending, mask);
                                                                                      for (i = 0; i < AUDIT_BITMASK_SIZE; i++)
 if (sig) {
                                                                                       if (mask[i] & classes[class][i])
                                                                                        return 0;
  if (current->notifier) {
   if (sigismember(current->notifier_mask, sig)) {
                                                                                     return 1;
    if (!(current->notifier)(current->notifier_data)) {
     clear_thread_flag(TIF_SIGPENDING);
     return 0;
                                                                                    Cell that might be helpful in predicting a new line. Note that it only turns on for some ")":
                                                                                    char *audit_unpack_string(void **bufp, size_t *remain, si
  collect_signal(sig, pending, info);
                                                                                     if (!*bufp || (len == 0) || (len > *remain))
                                                                                      return ERR_PTR(-EINVAL);
 return sig;
                                                                                     /* of the currently implemented string fields, PATH_MAX

    defines the longest valid length.

A large portion of cells are not easily interpretable. Here is a typical example:
                                                                                     if (len > PATH_MAX)
/ * Unpack a filter field's string representation from user-space
                                                                                      return ERR_PTR(-ENAMETOOLONG);
 buffer. /
                                                                                      str = kmalloc(len + 1, GFP_KERNEL);
char *audit_unpack_string(void **bufp, size_t *remain, size_t len)
                                                                                     if (unlikely(!str))
                                                                                      return ERR_PTR(-ENOMEM);
                                                                                     memcpy(str, *bufp, len);
str[len] = 0;
 char *str;
 if (|*bufp || (len == 0) || (len > *remain))
  return ERR_PTR(-EINVAL);
                                                                                      bufp += len;
  * Of the currently implemented string fields, PATH_MAX
                                                                                      remain -= len;
    defines the longest valid length.
                                                                                      return str;
```



#### What about tabular data?

- Several approaches stand out in the community:
  - LIME [Ribeiro et al, 2016 & https://github.com/marcotcr/lime]
    - ➤ Model agnostic, generates and scores random points around an example
    - > Trains a simple (e.g. linear) model to reproduce this local behavior
  - SHAP [Strumbelj et al, 2014 & https://github.com/slundberg/shap]
    - ➤ Game theory approach: "connects optimal credit allocation with local explanations using the classic Shapley values from game theory"
  - **Permutation** Feature Importance
- DreamQuark method for individual explainability [patent pending]
  - For each ("local") prediction, use the neural network's underlying architecture to determine (locally) the most important variables for the model's decision
  - Decorrelate input variables in order to present more consistent explanations
- Definitely not the end of the story here, research is ongoing





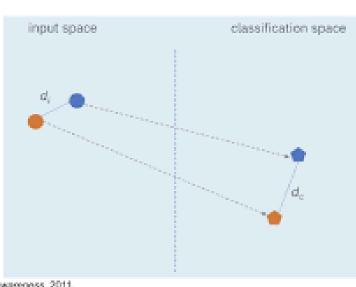
- What constitutes fairness?
  - Demographic blindness (training data is not correlated with demographics)
  - Demographic parity (outcomes are proportionally equal for all classes)
  - Equal opportunity (true-positive rates are equal for all classes)
  - Equal odds (true-positive and false-positive rates are equal for all classes)
- "impossibility theorems" of fairness, see e.g. [Zhao&Gordon, 2019]
- Equality of Opportunity in Supervised Learning [Hardt et al, 2016]
  - Pre-define sensitive groups before training a model
  - => ensure no discrimination against protected groups in the learned model



## **Individual fairness = Robustness ?**

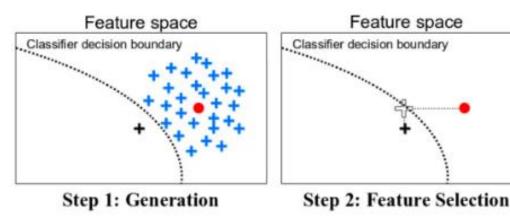
- Definition of individual fairness [Dwork et al, 2011]
   "similar individuals are treated similarly"
- In other words: a fair model is a robust model
- Difficulty: how do we define *similar* inputs?

Fairness Through Awareness



Dwork et al. Fairness Through Awareness, 2011

- Alternative approach: counterfactual explanations
  - => Find the "closest" neighbor which the model predicts differently

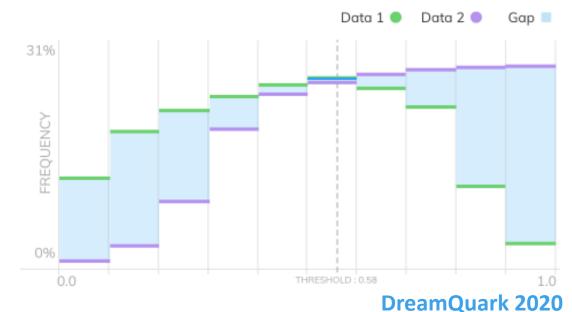


[Lauger et al, 2017]
Method of « growing spheres »
for selecting sparse conterfactuals

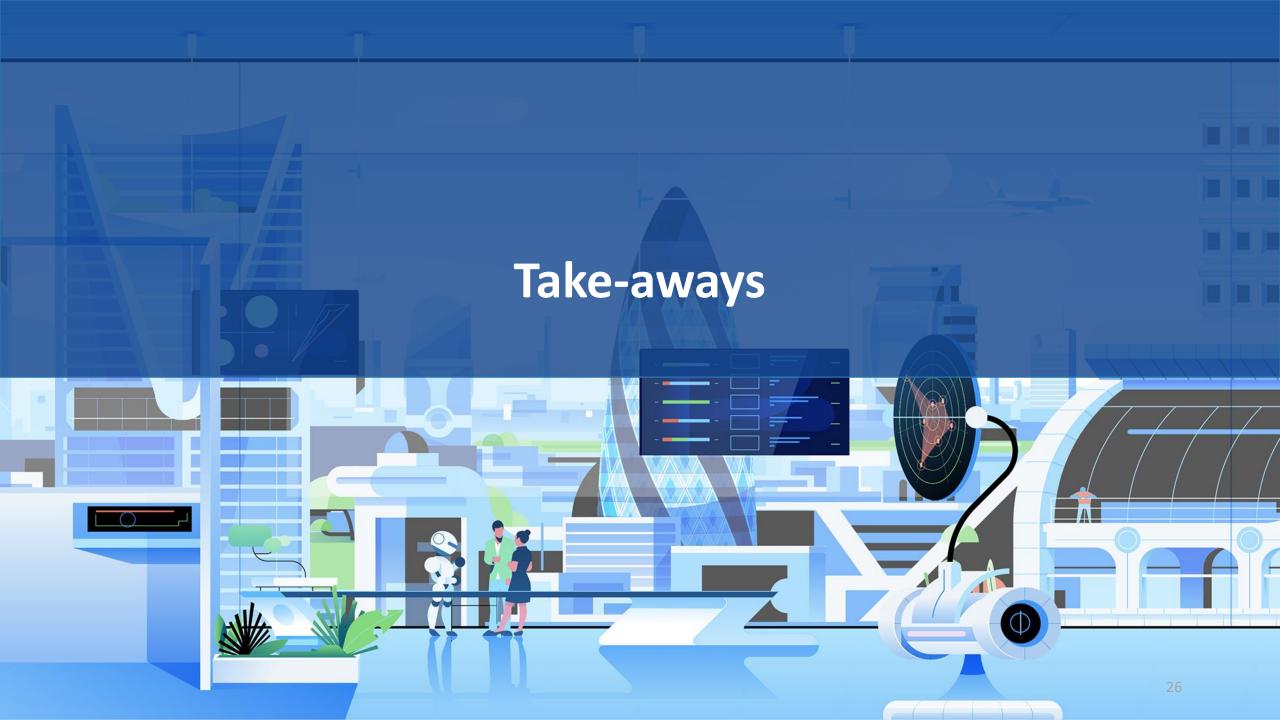


# Model stability in production

- Model performance (e.g. AUC, accuracy), even on test data, does not guarantee robustness and results in production
- => models bust me monitored in production, and eventually retrained
- Model stability (e.g. PSI)
- Data stability / data shifting
  - Does the distribution of datapoints in production match training data?
  - Train a simple model to distinguish test data vs train data
  - If successful, your data has shifted



• Possible added benefit: robustness of AI system against adversarial attacks





# **Key take-aways**

- Physicists can successfully transfer their skills and experience
- Innovation is possible in the industry, even as a small company
- As a private company: use open source software, develop proprietary code and file patents, but also publish open-source code
- Deep learning on tabular data is an emerging topic in AI community
- Beyond accuracy of models, challenges for both academia and industry
  - Explainable Al
  - Fairness
  - Robustness
  - Model stability and data stability







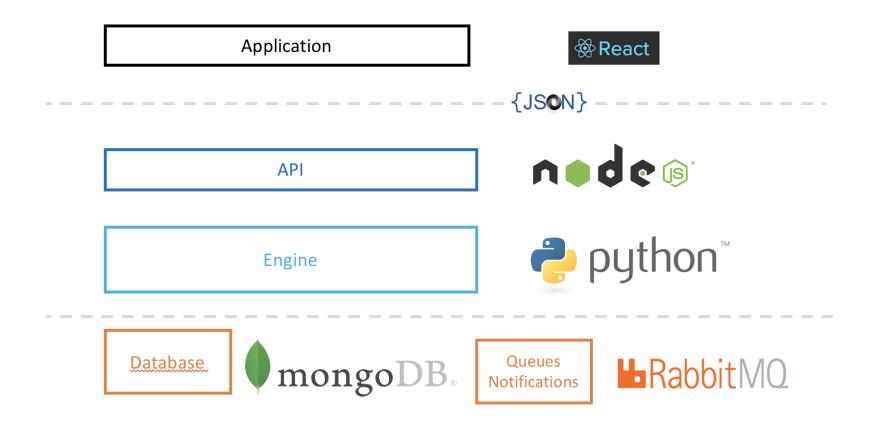
# Automated generation of optimized tabular networks for structured data [patent pending]

## Initial problem to solve:

- Neural networks are a "universal approximator", but typically require significant manual effort for each new dataset
- Many hyper-parameters: architecture, learning rate, regularization, etc
   => many-dimensional space for optimization, often carried out more or less manually
- Our solution to this problem, in a nutshell
  - Carry out training of a large number of models on a reduced dataset and/or for a small number of epochs, in order to gain "insights" on the dataset
  - => automatically deduce a reduced search space for hyperparameters
  - Optimize on this reduced search space using Bayesian methods



# Technology stack



• + systematic use of Docker + Kubernetes for deployment (both cloud and on-premise)



#### **Containerization: docker + kubernetes**

- Kubernetes: industry standard for container orchestration
- Deployment compatible with multiple cloud providers & on-premise

- Automated delivery of new releases
- Monitoring tools deployed as part of the product
- Easily manage many (independently scalable) micro-services

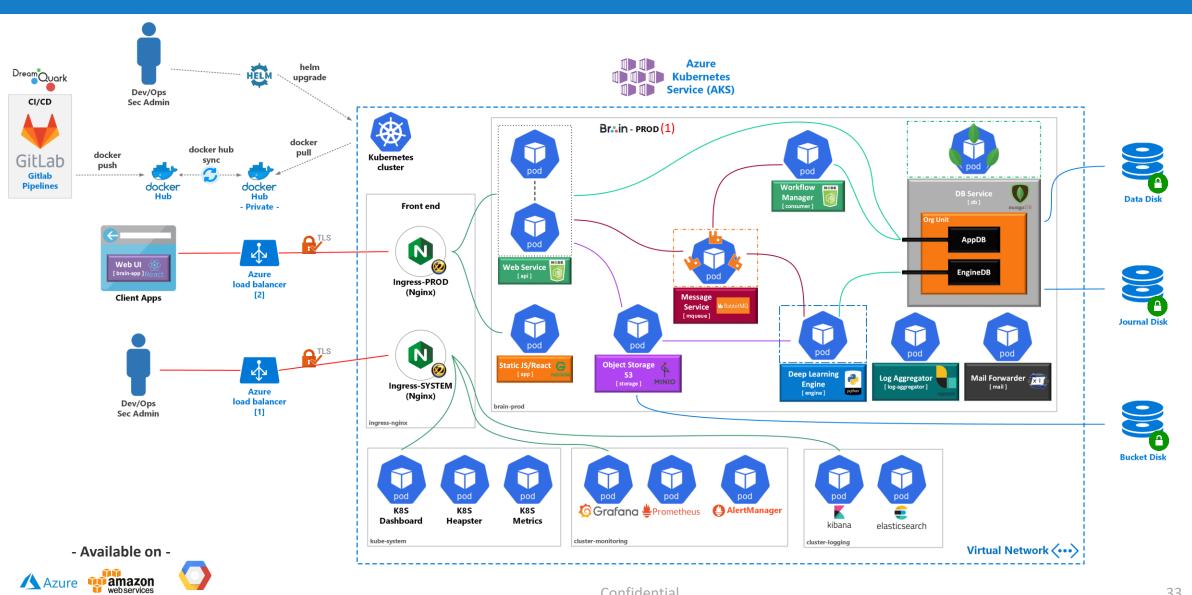






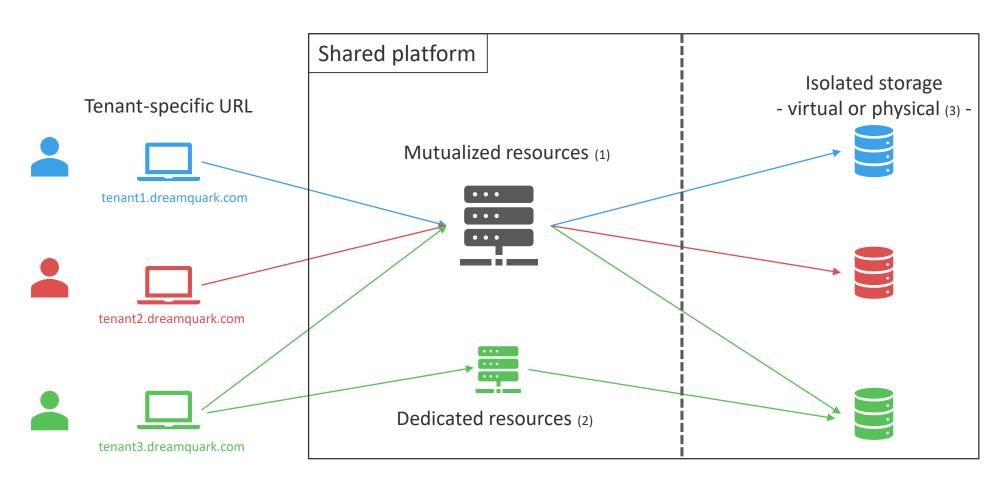
Google Cloud Platform

## **Architecture diagram**





## **Multi-tenant platform**



- 1. Instances of Brain microservices (API or engine)
- 2. Only instances of engine micro-services
- MongoDB: separated instances or separated databases

Sa Object Storage:
Separate Buckets or isolated "folders" in the same Bucket