Ollscoil Chathair
Bhaile Átha Cliath
Dublin City University

CA685 - Practicum Project

MCM - Masters in Computing (Major in Data Analytics)

“Interpretable Machine Learning for the Structure Odour Relationship”

Project by: Denis Kealy

Supervised by: Dr. Martin Crane

Interpretable Models for Investigating Smell

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PROJECT INTRODUCTION

A quick word about the scope, background and goals of the project

“

Think multidisciplinary!

Problems by definition, cross many academic disciplines.

- LUCAS REMERSWAAL

DOMAIN

- Biology
- Chemistry

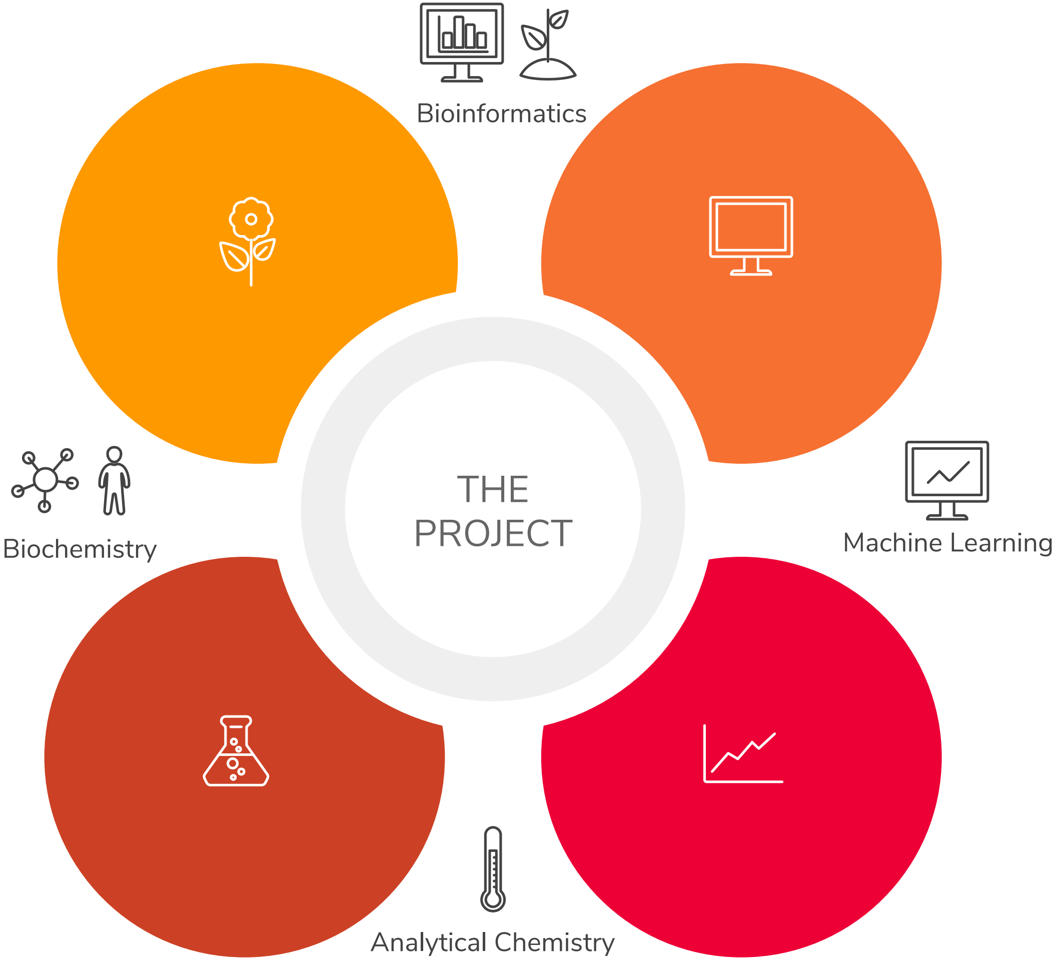
APPROACH

- Statistics
- Computer Science

Biology
Computer Science
THE PROJECT
Chemistry
Statistics

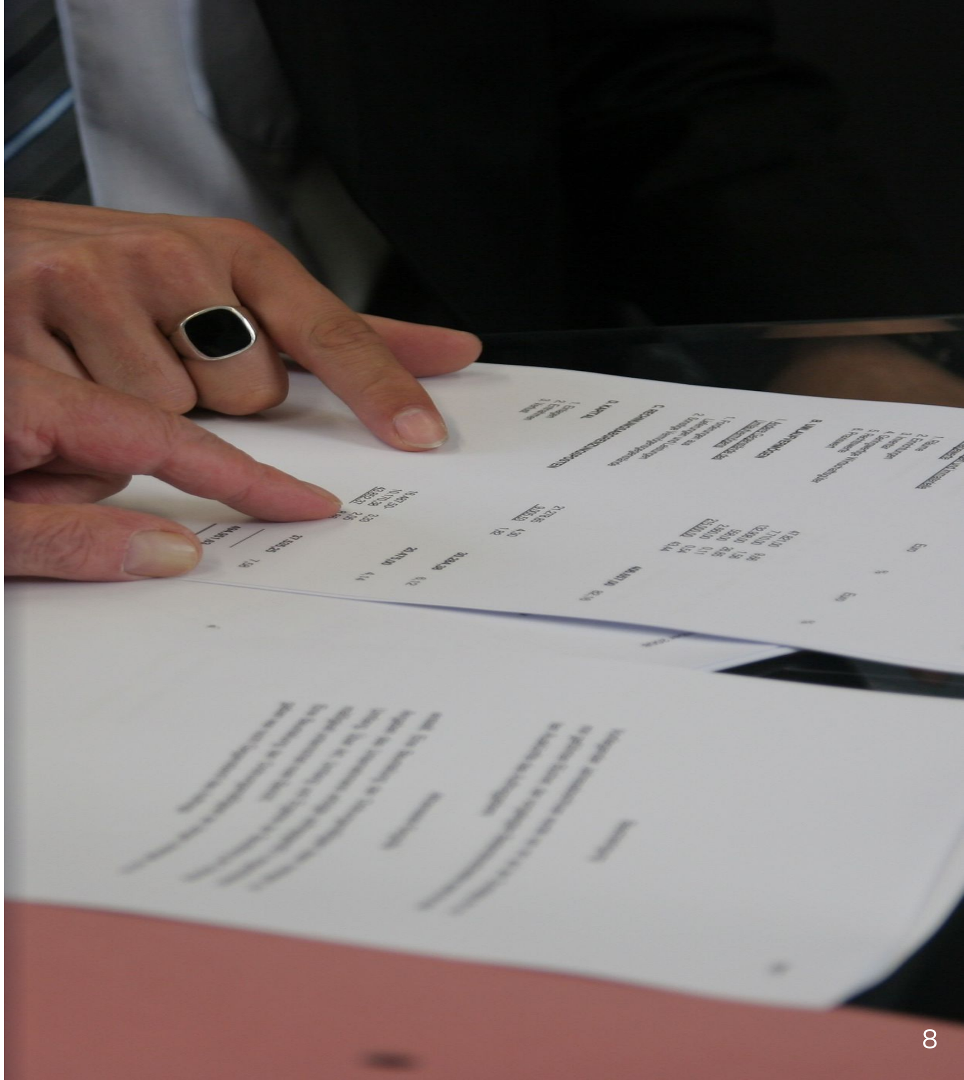
STRUCTURE ODOUR PROBLEM

... At the intersection of many disciplines



So we are on the same page!

- Definitions
- Aims of the Project
- Previous Work



DEFINING A FEW TERMS

Machine Learning

- Interpretable
- Explainable / XAI
- Deep Learning
- Hyperparameter
- XNN
- Completeness & Accuracy
- AI, IA & AIA

Our Sense of Smell

- Olfaction
- Neuron
- Receptor
- GPCR
- Limbic system
- Neo-cortex
- Swipe card model

Chemical Structure

- SOR vs SAR
- Odorant
- Ligand
- Ligand-Receptor Binding
- Chemical Descriptors
- Chirality

PROJECT AIMS

The goals of the project & the contribution to knowledge.

PROJECT AIMS

Investigate Smell

Prior interest & promising new results

Generalised Methods

A solution that is not specific to this problem

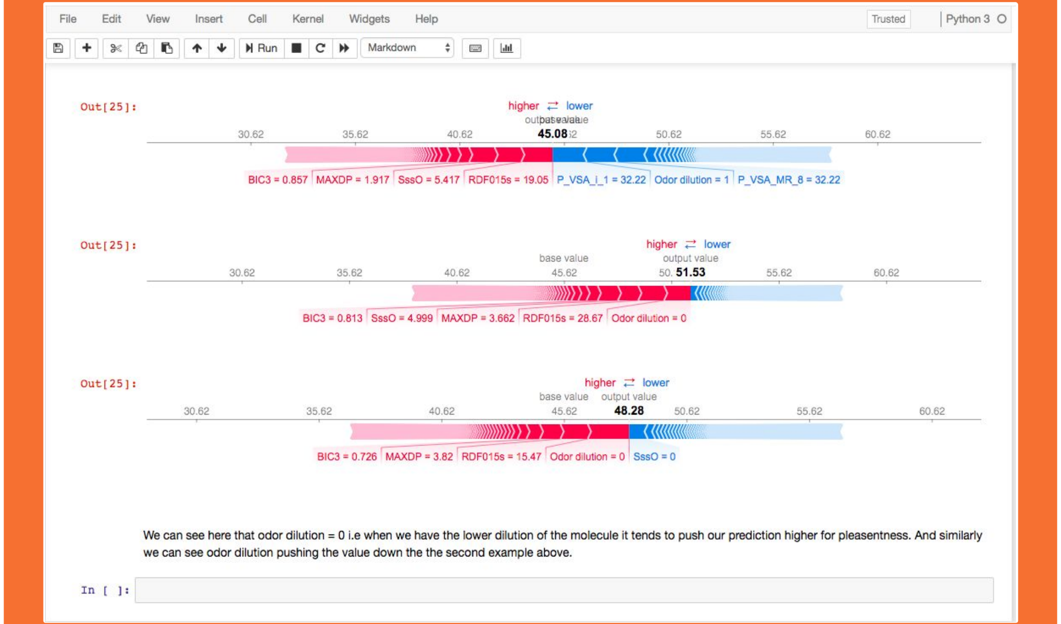
Learn

To investigate new techniques and gain

Experience with existing ones

FINAL GOAL

Demonstrate a generalised methodology for investigating this problem and similar problems.



We can see here that odor dilution = 0 i.e when we have the lower dilution of the molecule it tends to push our prediction higher for pleasentness. And similarly we can see odor dilution pushing the value down the the second example above.

PREVIOUS WORK

If I have seen further than others, it is by standing upon the **shoulders of giants**.

- Isaac Newton

PREVIOUS WORK

Domain Knowledge

- Olfactory System
- SOR Studies
- Geonomics
- Proteomics
- New imaging technologies...

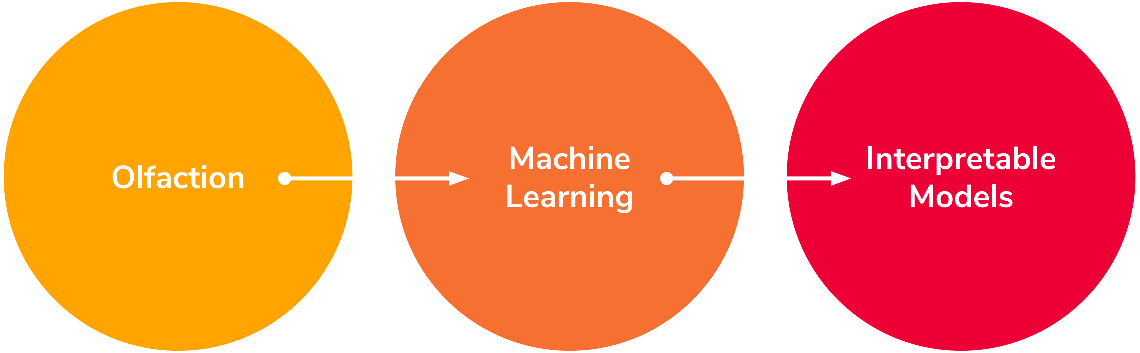
Previous Methods

- Odour Networks
- DREAM Machine

  Learning Tasks
- Neural Networks
  - E-nose
  - Fly Brain

Novel Interpretations

- LIME
- SHAP
- AIA



BACKGROUND

Some background about the problem, the data, and the available techniques

OUR SENSE OF SMELL

INTRINSICALLY COMPLEX

FULL OF COMPLEX INTRICACIES

INFLUENCES OUR CONSCIOUSNESS

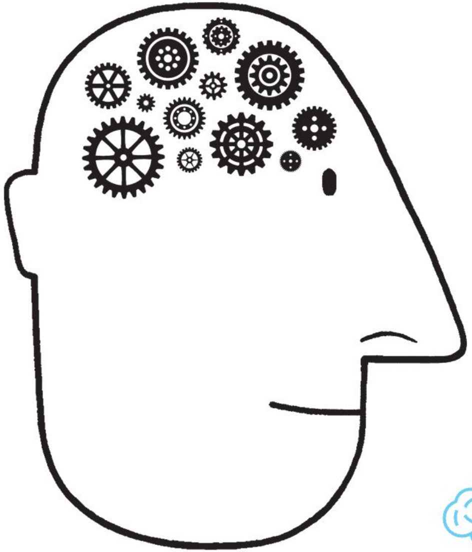
INFLUENCES OTHER SENSES

PREDICTIVE OF COGNITIVE DECLINE

INSPIRING ARTIFICIAL OLFACTION

POTENTIAL BENEFITS FOR:

- HEALTH
- FRAGRANCE & FLAVOUR
- DIGITAL SCENT
- VIRTUAL REALITY



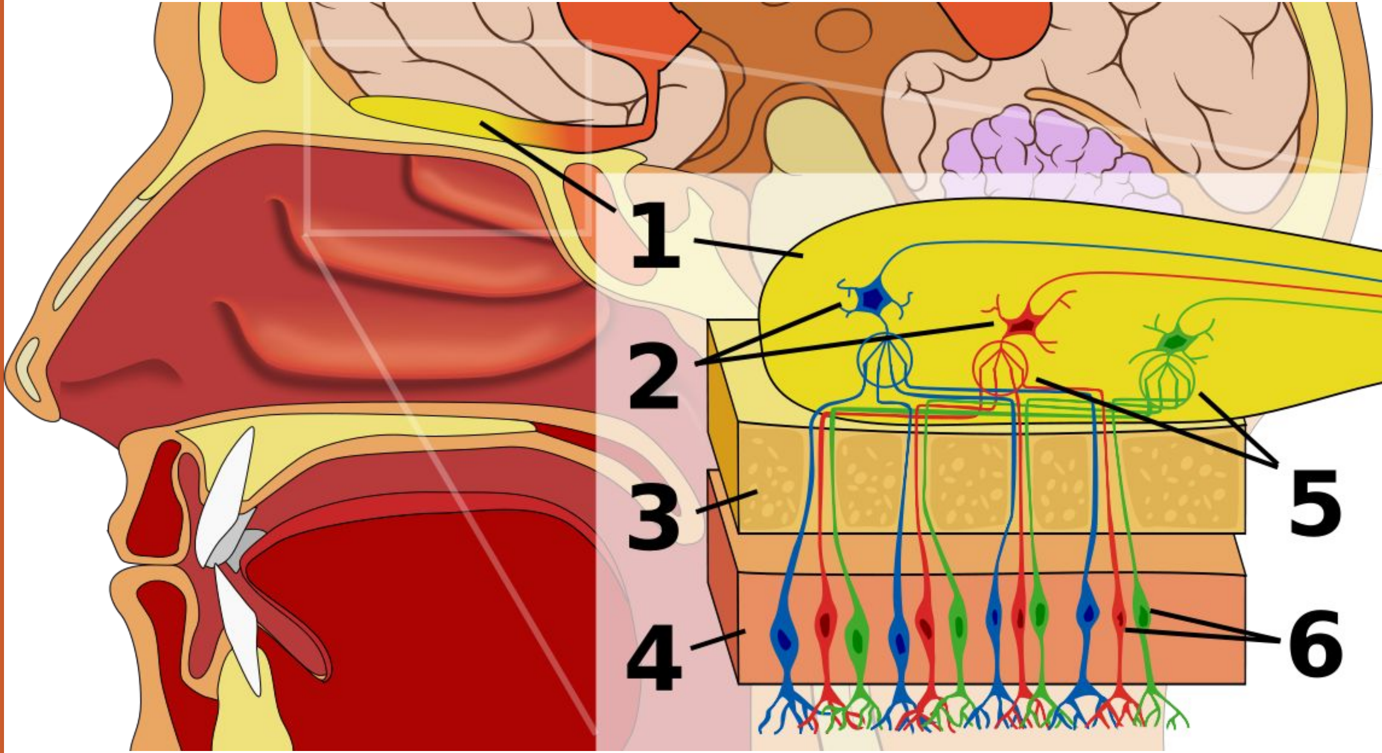
SMELL FACTS

What affects our sense of smell?

- Retro vs Ortho-nasal
- Mixing Compounds
- Culture & Language
- Familiarity
- Our Genes
- Time

HUMAN OLFACTORY SYSTEM

1. OLFACTORY BULB
2. MITRAL CELLS
3. BONE
4. EPITHELIUM
5. GLOMERULUS
6. OLFACTORY RECEPTORS NEURONS



STRUCTURE - ODOUR RELATIONSHIP

Can we predict:

- what a single molecule will smell of?
- what a SET of molecules will smell of?

Quantum Smell

- Structure doesn't tell the whole story
- Quanum properties seem to affect our sense of smell
- E.g. deuterated odorants & Drosophila Melanogaster

Swipe Card Model

- Structure plays a role, certainly, but other factors are at play
- Both chemical & physical properties of molecule are considered
- Combinatorial Encoding of Receptor Responses
- Cannot account for Chirality

STRUCTURE - ODOUR RELATIONSHIP (SOR)

VS

STRUCTURE - ACTIVITY RELATIONSHIP (SAR)

SOR

- Psychological Data

- Odour Panels
- Odour Descriptors
- Similarity Ratings
- Measure of conscious perception

- Many public databases
- Recent comprehensive dataset
- Highly predictive models recently published w/ best performance on this task to date

SAR

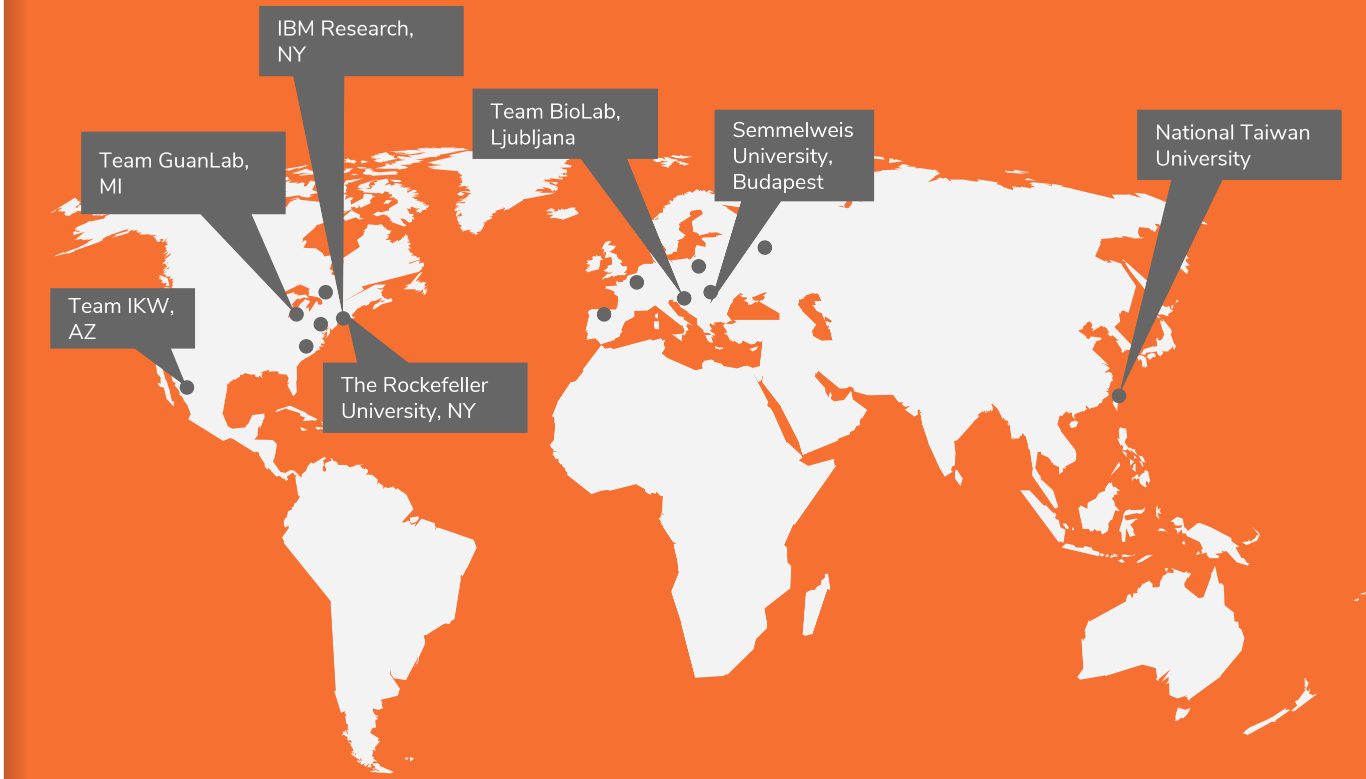
- Physiological Data

- Receptor Level (depolarisation of cell)
- Human Brain Imaging - e.g. fMRI, PET, CT scans
- Mice, Flies and Worms - in vivo, high granularity imaging
- Response levels & haplotypes for Human ORs
- Measure of biological activity

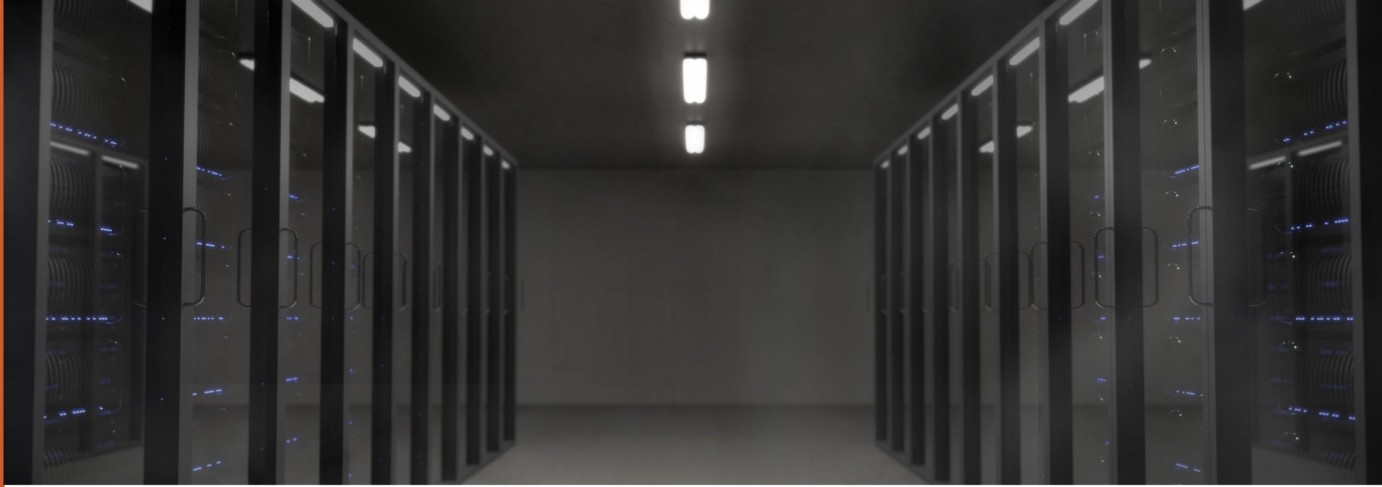
- Not enough data to study population level responses
- Some available data from outdated studies

Olfaction DREAM Challenge

- **The Rockefeller University:** Data collected in 2014
- **Team GuanLab** - winner of individual sub challenge
- **Team IKW** - winner of population sub challenge
- **Team BioLab** - runner up for population sub challenge


IBM Research, NY
Team GuanLab, MI
Team BioLab, Ljubljana
Semmelweis University, Budapest
National Taiwan University
Team IKW, AZ
The Rockefeller University, NY

DATA



PSYCHOLOGICAL DATA

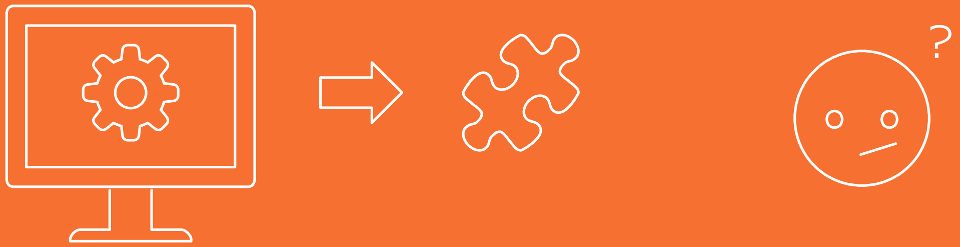
- 55 Subjects
- 480 Molecules
- 2 Dilutions
- Responses (0-100)
- 3 Mandatory Fields
  - Pleasantness
  - Intensity
  - Familiarity
- 19 Optional Fields e.g.
  - Fish
  - Fruit

CHEMICAL/PHYSICAL DATA

- 4884 features
- Describes Molecular Shape
- Describes Molecular Vibrational Frequencies
- 476 molecules (4 missing)
- Compiled using DRAGON software
- Top 20 descriptive features for each target published

INTERPRETABLE MODELS

- Interpretability vs Completeness
- Natural Interpretation
- Post-hoc
- Local vs Global
- Model Specific/Agnostic
- Improve Trust & Discovery



OUTPUTTING A PREDICTION

OUTPUTTING A JUSTIFICATION OR EXPLANATION

METHODS

Pre-processing, training & evaluation methods

METHODS OVERVIEW

Research

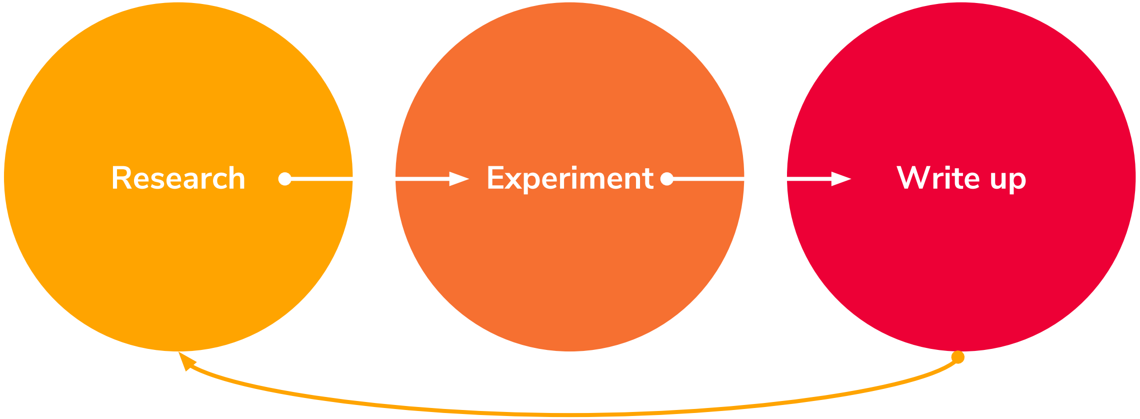
- Olfactory System
- Machine Learning Methods
- Interpretability Methods

Experimentation

- Data Collection
- Network Analysis
- Training, training, training…
- Evaluation

Documentation

- Code - Jupyter Notebooks
- Blog
- Presentation & Report



METHODS

Preprocessing

PREPROCESSING

- Cleaning Data
- Dilution/Concentration
- Calculating Mean Responses
- Combining Data
- Hidden Test Set Split
- Persists Datasets

METHODS

Training Overview

TRAINING MODELS

- Baseline Modelling - 22 Targets
    - Default Hyperparameters
    - 10 Algorithms Tested
    - 5-fold Cross Validation

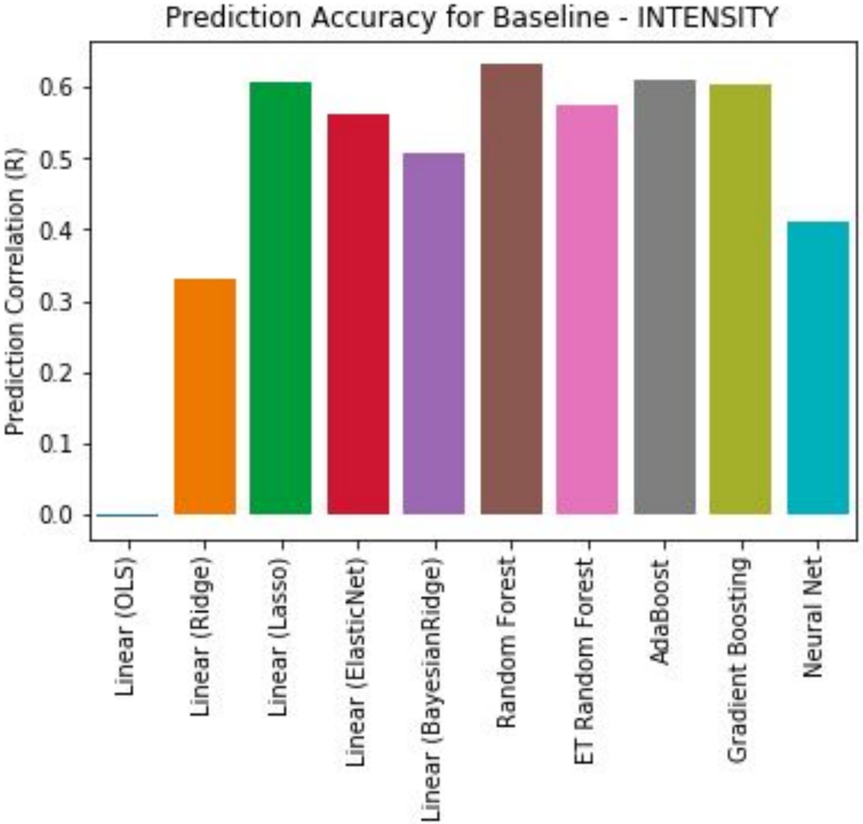
- Hyperparameter Tuning
    - Random Grid Search
    - 5 Algorithms Tested
    - 3-Fold Cross Validation

- Final Approach - 8 Targets, 3 set of models
    - Regularized Linear Models (L1)
    - Random Forest with & without reduced features

METHODS

Baseline Predictions

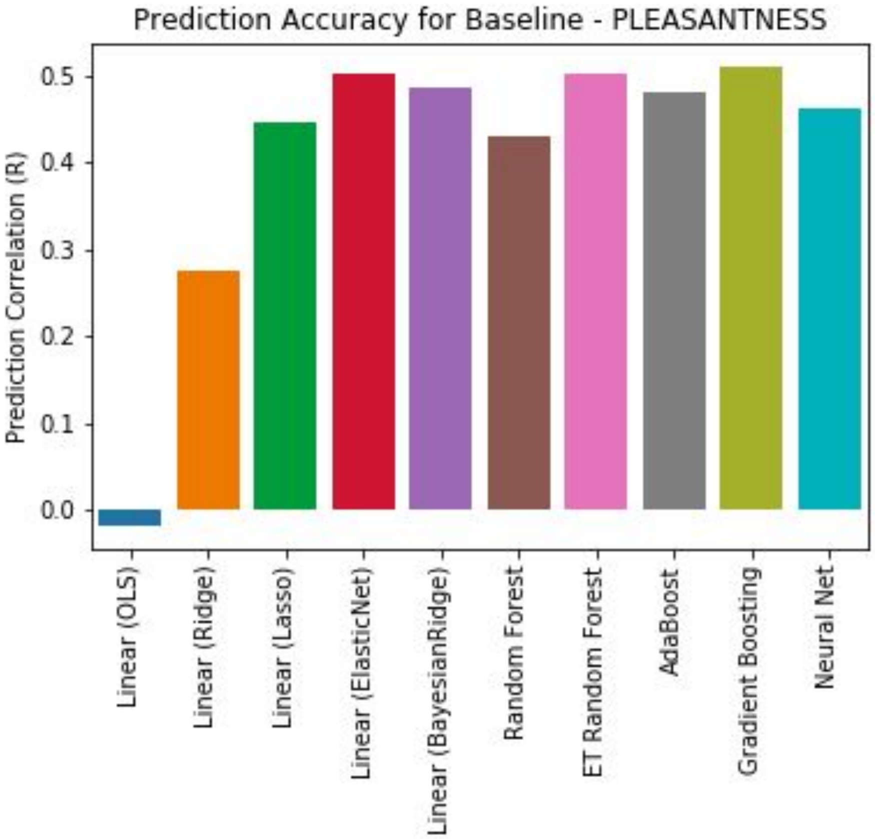
BASELINE MODELS - INTENSITY



METHODS

Baseline Predictions

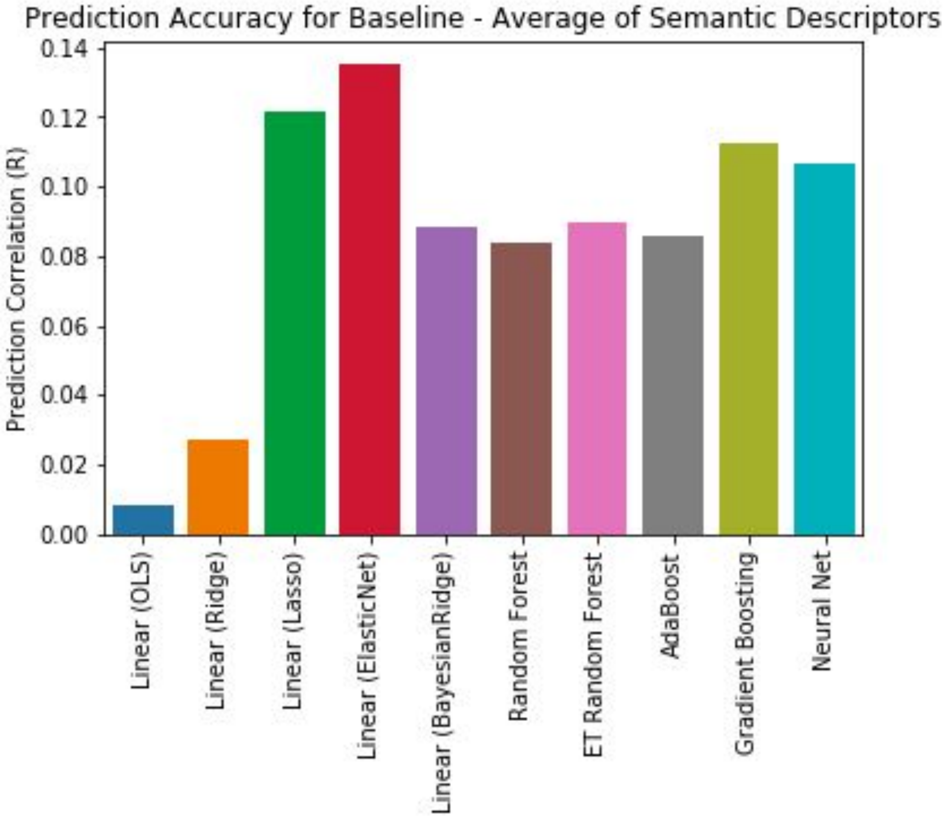
BASELINE MODELS - PLEASANTNESS



METHODS

Baseline Predictions

BASELINE MODELS - SEMANTIC DESCRIPTORS



METHODS

TRAINING MODELS

- Hyperparameter Tuning - Random Grid Search
- Testing Feature Spaces
  - Reduced Features
  - Principal Components
  - Mean vs Raw Responses
  - Imputation & Masking
- Reducing the considered Targets and Algorithms
- Evaluation & Comparison
  - Pearson R for each target/model pair
  - More details in Results

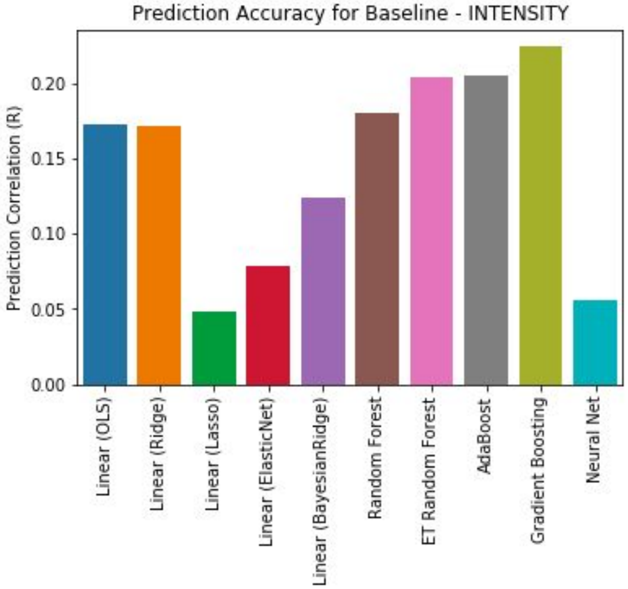
METHODS

Top 20 published features

Delta Error Method

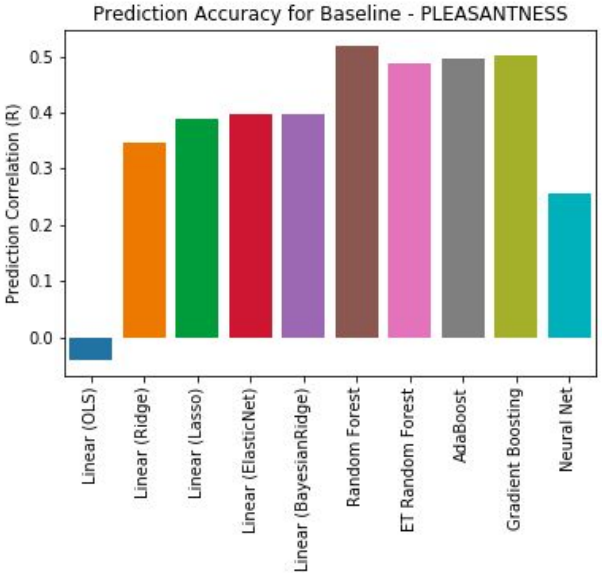
INTENSITY

- Predictions worse across the board
- Intensity predictions are difficult with reduced descriptors - DREAM



PLEASANTNESS

- Predictions worse for all except Random Forest
- Predictions improve for Random Forest Baseline



RESULTS

Visualising and interpreting our predictions

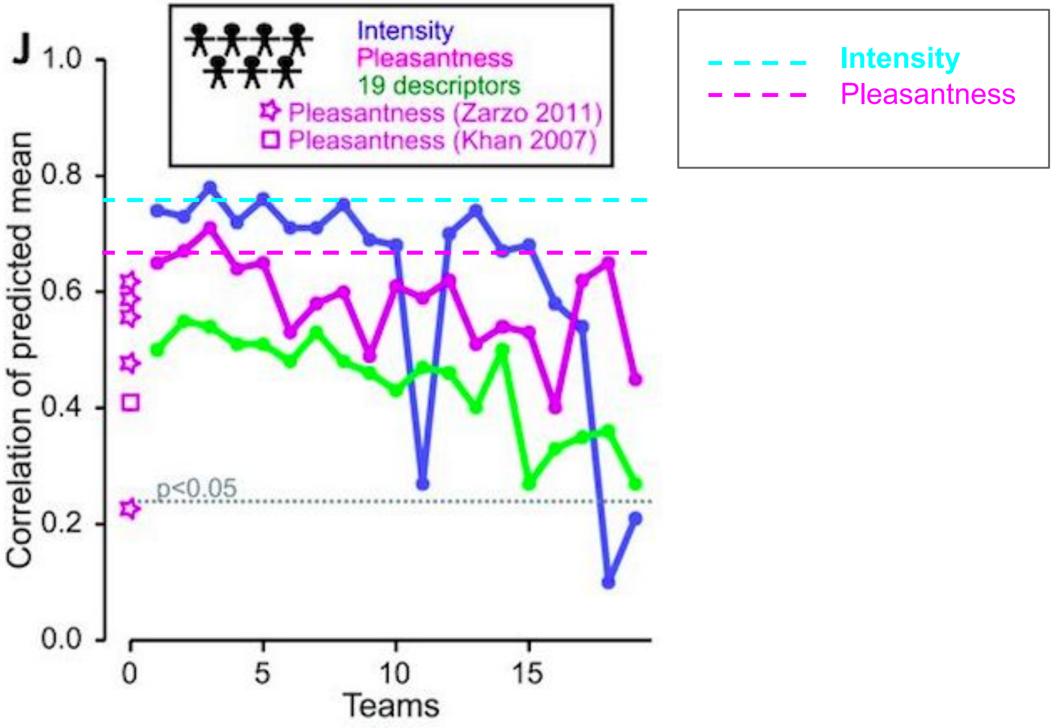
AI

PREDICTION ACCURACY

RESULTS

Predictions

PREDICTION CORRELATION - POPULATION

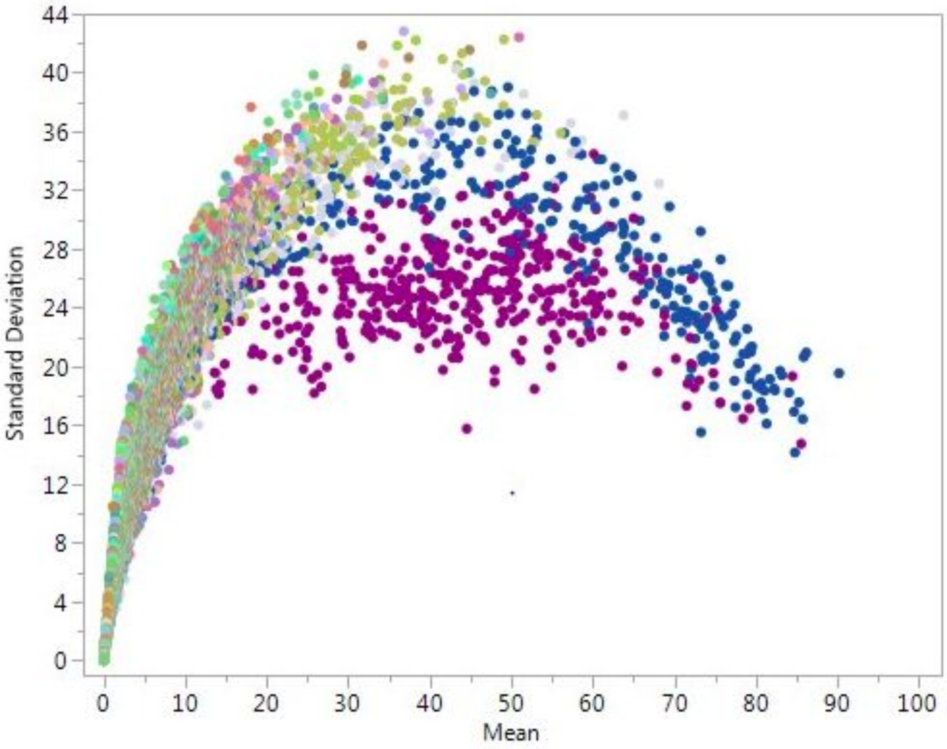


RESULTS

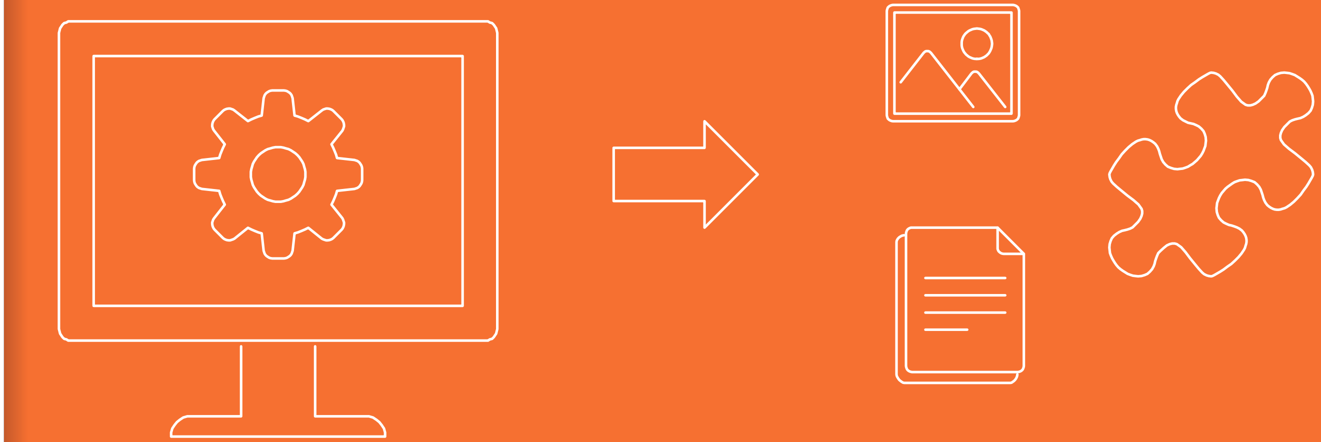
Residual Analysis

- shows that our error is largest around the mean
- This conforms to the observed data and previous analysis

OBSERVED MEAN VS STANDARD DEVIATION



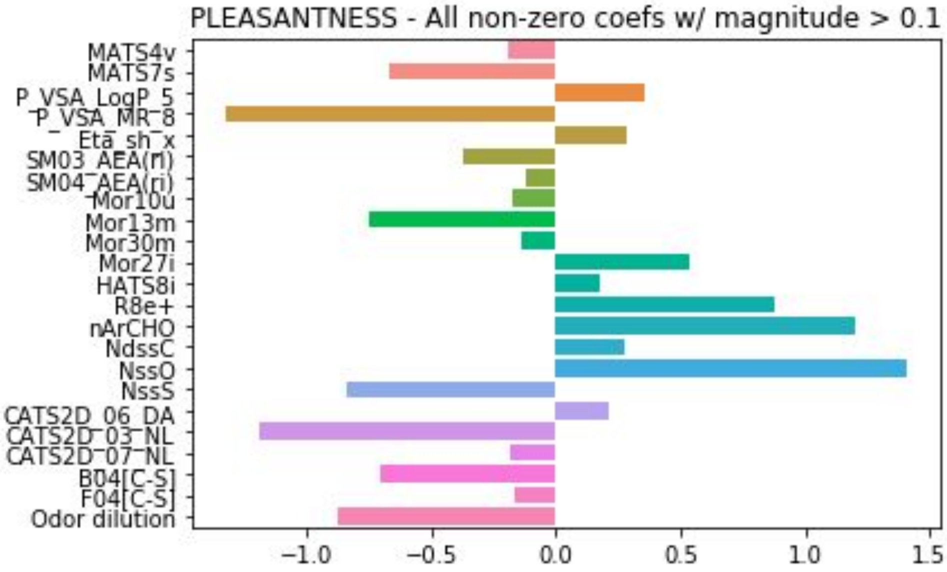
INTERPRET MODELS



RESULTS

Naturally Interpretable Global Explanation

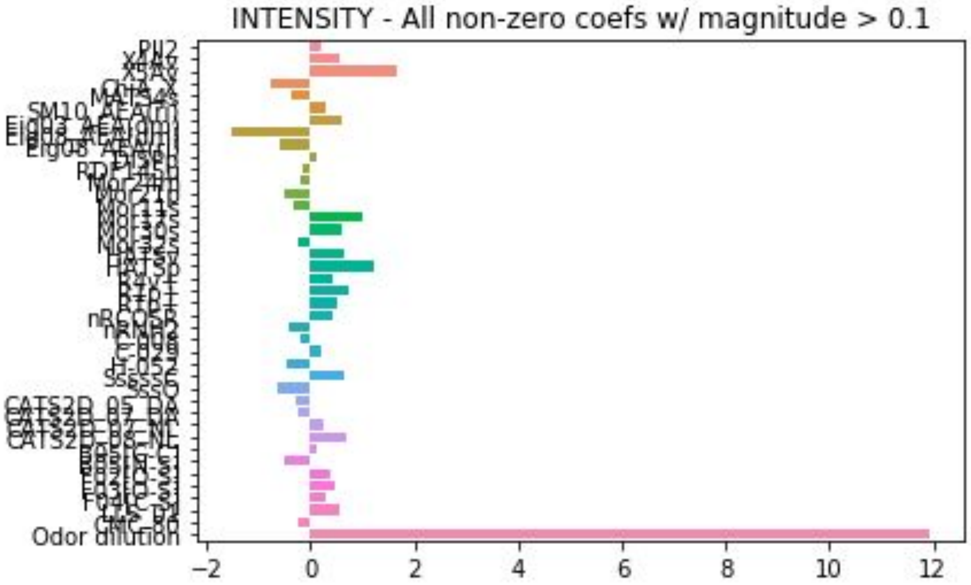
L1 REGULARISED LINEAR MODEL - PLEASANTNESS



RESULTS

Naturally Interpretable Global Explanation

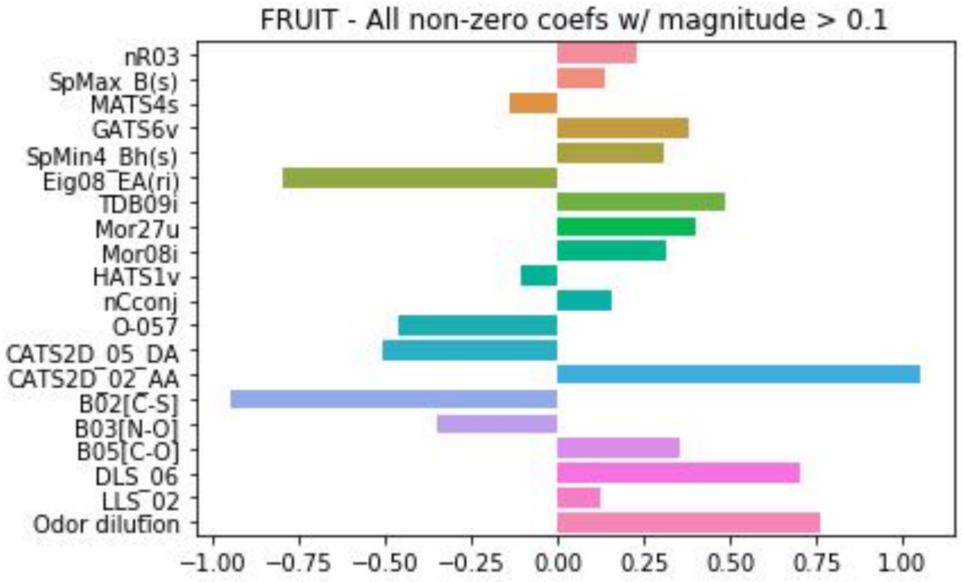
L1 REGULARISED LINEAR MODEL - INTENSITY



RESULTS

Naturally Interpretable
Global Explanation

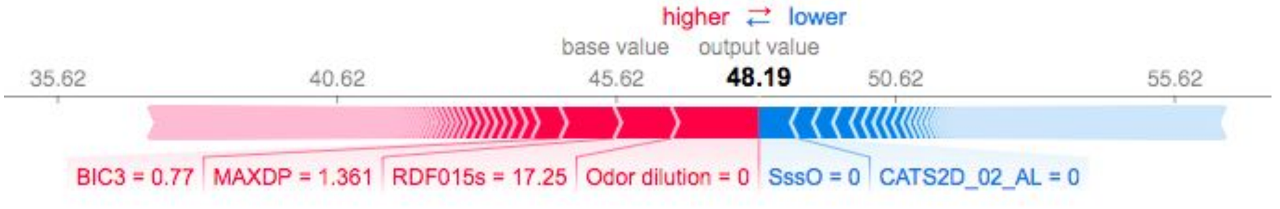
L1 REGULARISED LINEAR MODEL - FRUIT

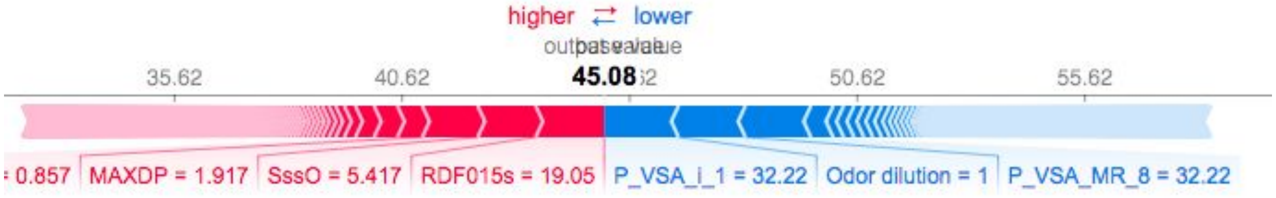


RESULTS

Local, Post-hoc Explanation

RANDOM FOREST & SHAP

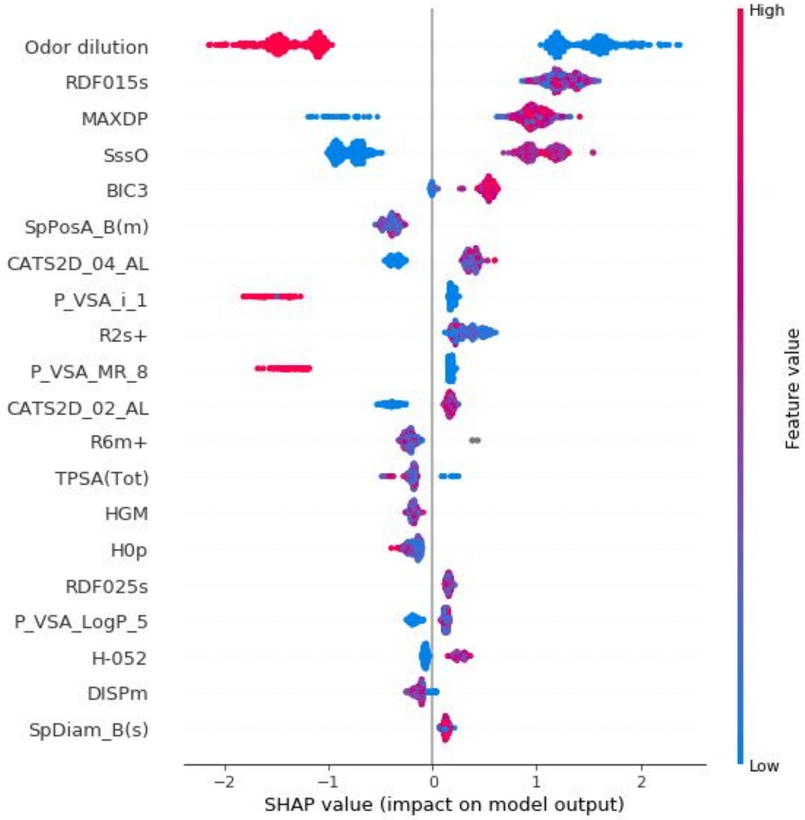




RESULTS

Global, Post-hoc Explanation

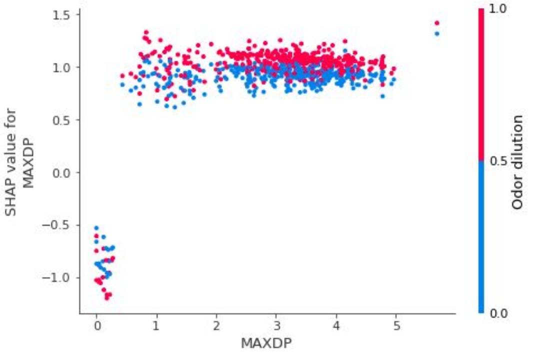
RANDOM FOREST & SHAP - PLEASANTNESS

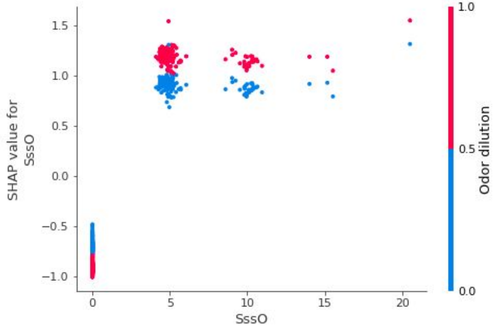


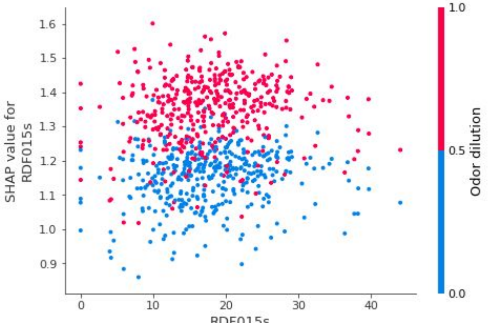
RESULTS

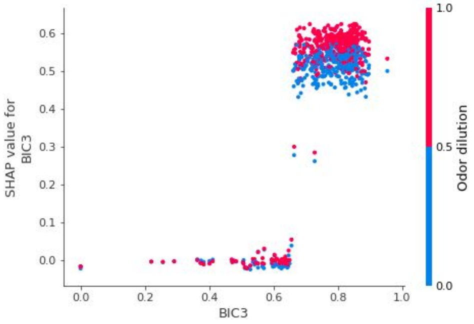
Post-hoc Explanations
- Feature Dependence

RANDOM FOREST & SHAP - PLEASANTNESS









DISCUSSION

Questions & Clarifications

REFERENCES

Similar work and resources for presentation