Imperial College London

Applications of Machine Learning in medical research

QuanTII Summer Workshop

Guillem HURAULT

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Department of Bioengineering, Imperial College London

About me

- No background in T-cells, immunology or immunotherapy
- Completed a PhD in statistical machine learning to predict eczema (skin disease)
- Expertise in Bayesian modelling and time-series forecasting
- Post-doctoral researcher in the Tanaka group, Department of Bioengineering, Imperial College London
- The group mostly focus on mathematical modelling, systems biology, etc.

Group website: `https://rtanaka.bg-research.cc.ic.ac.uk/`

Personal website: `https://ghurault.github.io/`

What is Machine Learning?

The field of study that gives computers the ability to learn without being explicitly programmed.

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Supervised Learning

Unsupervised Learning

Reinforcement Learning

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Supervised Learning

Learning from labelled data (prediction)

- Neural networks
- Tree-based algorithms: CART, boosting, bagging, etc.
- Support Vector Machines
- Regression models: generalised linear models, regularised regression, splines, generalised additive models, Gaussian Processes, etc.

Unsupervised Learning

Reinforcement Learning

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Supervised Learning

Unsupervised Learning

Learning from unlabelled data

- Clustering
- Dimensionality reduction

Reinforcement Learning

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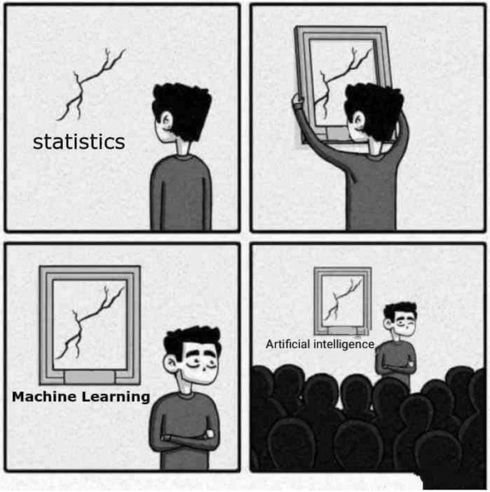
Supervised Learning

Unsupervised Learning

Reinforcement Learning

Learning how to make decisions

Machine Learning is mostly a buzzword



My work

- Eczema cannot be cured but can be managed with treatments
- Treatment responses vary from patient to patients
- Designing personalised treatment strategies is of high clinical relevance

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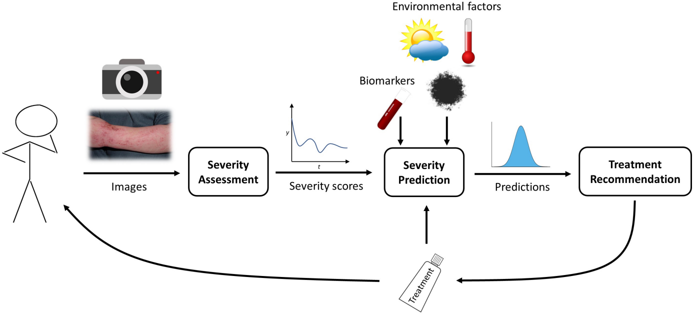
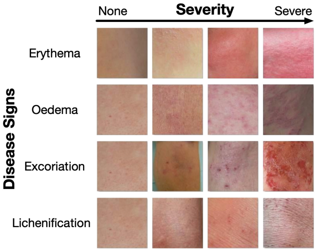


Assessing eczema from camera images[1]

- Patients need to visits clinic to have their eczema assessed
- Assessments can be biased
- We developed a computer vision algorithm to automatically detect and assess eczema from camera images



[1] K. Pan, G. Hurault, K. Arulkumaran, H. C. Williams, and R. J. Tanaka, "EczemaNet: Automating Detection and Severity Assessment of Atopic Dermatitis," in Machine Learning in Medical Imaging, Springer, Cham, 2020, pp. 220–230.

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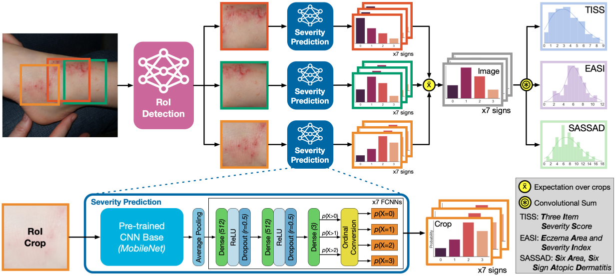

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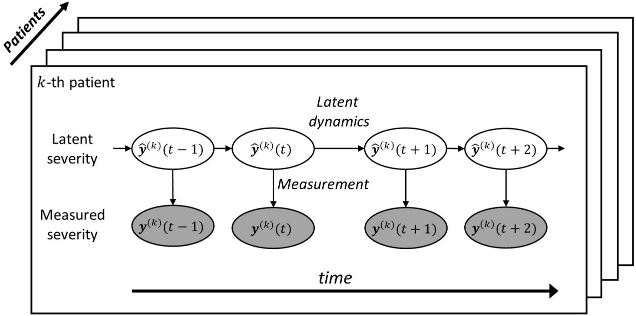
Predict eczema severity[2]



[2] G. Hurault et al., "EczemaPred: A computational framework for personalised prediction of eczema severity dynamics," Clin. Transl. Allergy, vol. 12, no. 3, p. e12140, Mar. 2022.

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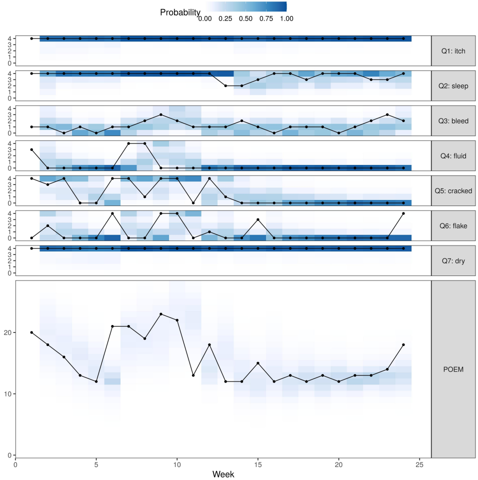

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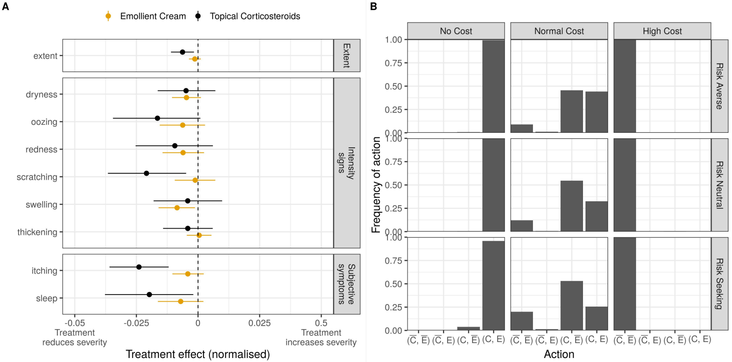
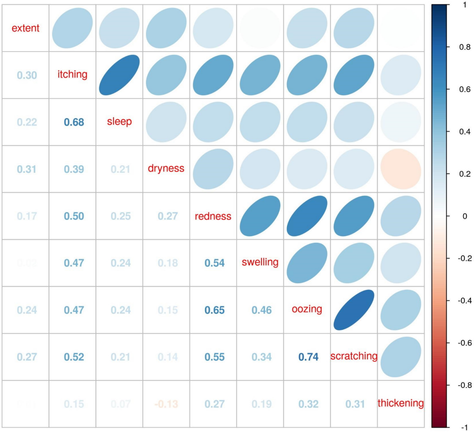
Making personalised treatment recommendations

- Turning predictions into actions
- Decision-making under uncertainty (Bayesian decision theory)



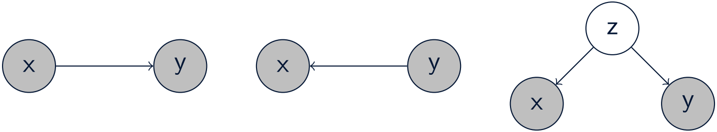
Finding a lower dimensional representation of eczema severity data

The data shows strong correlations



Finding a lower dimensional representation of eczema severity data

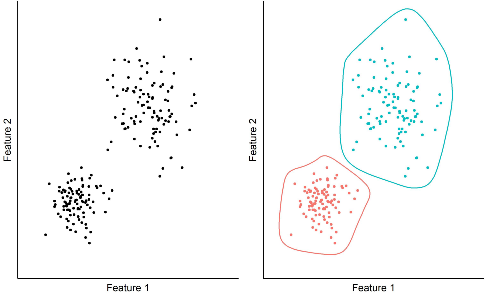
Mechanisms that could explain these correlations



Finding a lower dimensional representation of eczema severity data

A principled dimensionality reduction could

- Help us understand the data better (interpretability)
- Separate patients into different subgroups (clustering)
- Provide computational benefits



Questions?

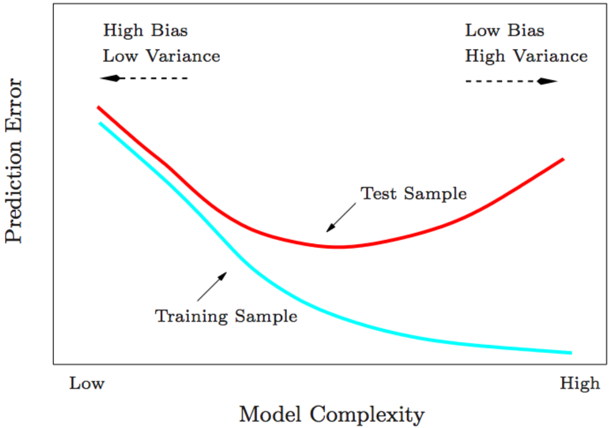
Machine Learning is mostly concerned with predictions

This is different from statistical modelling, where the goal can be:

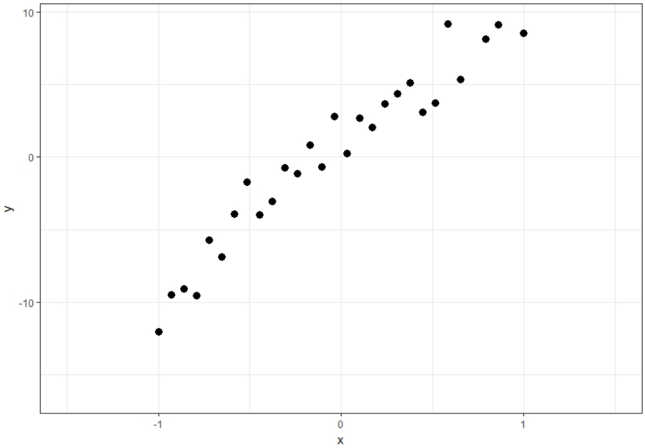
- Prediction
- Inference (explanatory modelling)
- Descriptive modelling

Machine Learning is mostly concerned with predictions

We want to learn models that generalise well to new data.

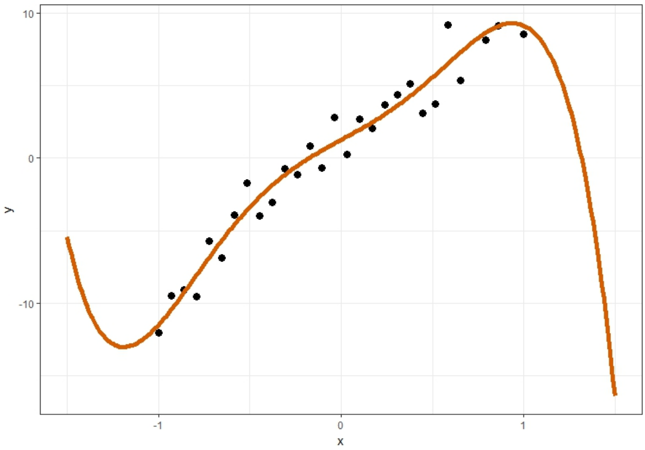


Overfitting



Linear data + noise

Overfitting



Fit with 5-th order polynomial

Statistical modelling or Machine Learning?

Prefer Machine Learning

- Prediction is the main goal
- High signal-to-noise ratio (e.g. computer vision, natural language processing)
- Big data
- Non-linear effects

Prefer statistical modelling

- Prediction is not the main goal (e.g. inference, interpretability, causality)
- Uncertainty is inherent (low signal-to-noise ratio)
- Small sample size
- Effects are mostly additive

Bayesian modelling

Bayes' theorem

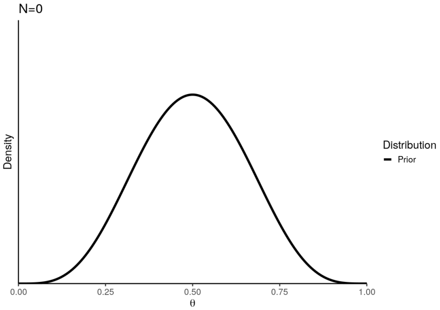
$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} \propto p(y|\theta)p(\theta)$$

- y represents data
- θ represents parameters
- $p(y|\theta)$ is the likelihood (the model)
- $p(\theta)$ is the prior
- $p(\theta|y)$ is the posterior
- $p(y) = \int p(y|\theta)p(\theta)d\theta$ is the evidence (normalisation constant)

Bayesian modelling

Example

- Coin flipping: what is $p(\text{Head}) = \theta$?
- Data: $x \in \{\text{Head}, \text{Tail}\}^N$
- Model: $x \sim \mathcal{B}(\theta)$ with prior $\theta \sim \text{Beta}(5, 5)$



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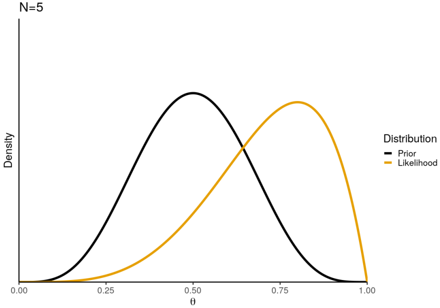

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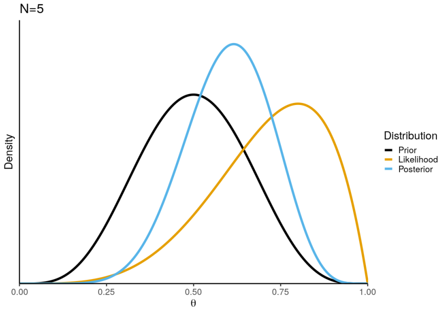

Why Bayesian modelling?

- Uncertainty quantification
- Flexible modelling framework[3]
- Prior knowledge
- Results are more intuitive

[3] C. M. Bishop, "Model-based machine learning," Philos. Trans. R. Soc. A Math. Phys. Eng. Sci., vol. 371, no. 1984, p. 20120222, Feb. 2013, doi: 10.1098/rsta.2012.0222.