

## What smell?



### BUILDING A PREDICTIVE MODEL OF AXILLARY MALODOUR

Unilever / University of Nottingham

#### The need

The intensity of underarm odour is a direct product of the bacteria resident there. Unilever has made great progress in understanding which bacteria are responsible for which malodour products. The DNA from a sample of bacteria from the underarm can be sequenced to give a complete picture of the microbial community. These microbial communities vary greatly from sample to sample. The challenge is to use this rich source of information to model malodour numerically and also to justify this model scientifically.

The project aimed to construct complex mathematical algorithms to aid in the development of an *in silico* kinetic model of axillary (underarm) malodour.

#### The outcomes

The project addressed two significant deficiencies in Unilever's current prototype model.

First (and most importantly) we addressed the requirement for an algorithm that can relate traditional culture-based microbiological data with modern microbiomics-type data. Modern data capture is radically different and an algorithm is needed to factor this in so that we can convert such data to absolute bacterial numbers.

Second, we required an algorithm that could relate aroma threshold levels for odour molecules with clinical malodour scores. The existing model could

not compare the objective data with the subjective data from the expert underarm sniff-assessors.

The outcomes of this project have highlighted new and creative ways in which microbiomics data can be used to understand axillary malodour. It has demonstrated that there may be value in non-traditional ways of using multivariate data in predictive models.

Much insight into the ecology of bacterial communities can be found in the microbiomics data now becoming available which may result in new ways of constructing ecological models of microbial communities.

*"Zofia did an excellent job of absorbing and understanding the wealth of microbiological data ... She brought a real freshness of thought to the area, and we're delighted that she's decided to pursue her career doing similar work with one of our main external collaborators."*

**Gordon James, Unilever**

## Technical summary

The project was envisioned to combine the new form of microbiomics data and kinetics data on malodour producing metabolic pathways using a systems biology approach. However, the complexity of the data was underestimated. Microbiomics data is multi-dimensional. The DNA of each sample is exhaustively sequenced, resulting in a complete picture of the species of bacteria present. However, each sample corresponds to a single observable which is the mean malodour score (MMS).

Principal component analysis (PCA) and k-means clustering revealed the presence of a number of subgroups. The ecologies between subgroups were markedly different while the ecologies of samples within a subgroup were surprisingly consistent.

Common approaches to modelling trends between multi-dimensional data and a single observable include multivariate regression techniques such as partial least squares (PLS) regression. However, it was found that by pre-clustering the data surprisingly simple predictive trends were found between the abundance of bacteria and malodour. These trends involve an average of only three genera from a total choice

of over 40 genera of bacteria. These trends differed in form, for example sometimes logarithmic or non-logarithmic abundances of genera. PLS regression captures the relative importance of rarer types of bacteria, but does not allow for the malodour of different samples to follow different types of trends with common bacteria. Subsequent tests of the algorithm showed that it is a useful approach in predicting malodour.

The insight into the ecology of these bacterial communities may lead to new directions in experimental work and modelling approaches to the problem of axillary malodour. It is tempting to suppose that together with experimental work, microbiomics data may help build ecological models of bacterial communities by clarifying the laws of competition and co-operation operating in these communities.



*"I have greatly enjoyed my experience of working as an intern at Unilever. ... the microbiomics data offered many opportunities for creative investigation of the malodour problem. I was free to look at the problem independently which has helped develop my own research interests."*

**Zofia Jones**  
University of Nottingham

*"It was pleasing to see the progress that was made and how the direction of the internship evolved. [The project] brought her valuable new skills and new research interests, as well as experience of a challenging area of systems biology which is likely to influence her research strongly. The interactions with Unilever were stimulating and the results are, I hope, of value to them."*

**John King**  
University of Nottingham

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Unilever



## Project Details

### **Partners**

Unilever  
University of Nottingham

### **Project investment**

£13,000

### **Intern**

Zofia Jones

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