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The use of predictive models to optimize risk of decisions☆

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ABSTRACT

The purpose of this paper is to set up a mathematical framework that risk assessors and regulators could use to quantify the "riskiness" of a particular recommendation (choice/decision). The mathematical theory introduced here can be used for decision support systems. We point out that efficient use of predictive models in decision making for food microbiology needs to consider three major points: (1) the uncertainty and variability of the used information based on which the decision is to be made; (2) the validity of the predictive models aiding the assessor; and (3) the cost generated by the difference between the *a-priory* choice and the *a-posteriori* outcome.

1. Introduction

Predictive food microbiology focuses on the responses of foodborne bacteria to their environment. Sufficiently accurate predictions on bacterial growth and survival can reduce the need for microbiological testing of food, making product formulation and risk assessment much cheaper and more efficient, and ultimately improving microbiological food safety (Ross and McMeekin, 2003). The knowledge gained in the *c.a.* 30 years-long history of the discipline has been implemented in practical decision-supporting software packages, to be used by a range of stakeholders, including industrialists, academicians and regulation officers. Various predictive models are available for different foodborne pathogenic as well as spoilage organisms to help quantitative microbial risk assessment of food (Whiting and Buchanan, 2001; Koutsoumanis et al., 2016).

Practical users face the question to what extent they can rely on the predictions generated by predictive tools, for which one of the most used examples is the ComBase Predictor (ComBase, 2016). Overestimating the growth potentials of pathogenic bacteria can result in food waste and economic loss, while underestimation can have even more serious health- or reputation-related implications (Guillier et al., 2016). Prediction errors can originate from (i) biological and environmental variability; (ii) the uncertainty of the information (observations) on which the predictions are based; and (iii) the inaccuracy of the mathematical models and assumptions used.

Predictive models are predominantly based on simplifying assumptions and observed data. There is no recipe or algorithm to decide whether those simplifying assumptions are valid or allowed; they are accepted if observations validate them (empirical considerations) and they can be embedded in fundamental theories of science (mechanistic reasons). Empirical models are less applicable for extrapolation than mechanistic ones. However, to some degree, all predictions are extrapolations. Mathematical models exist in an ideal Platonian space, from which the applications to future scenarios are inferences. The experimental conditions of the observations, on which the models are based, can rarely be repeated exactly, due to the "*panta rhei*" Heraclitean principle: "*One cannot step into the same water twice*".

It is relatively easy to test whether a prediction is a mathematical extrapolation; i.e. whether it is outside the range of observations (Baranyi et al., 1999). It is much more difficult to decide whether, for instance, a set of measurements on a proxy organism can be applied to the "real one". An example for this is applying observations on *Listeria innocua* to infer the kinetics of *Listeria monocytogenes*. Similarly: are certain environmental conditions like food structure, native flora, processing background, etc. negligible? It is also an open question what details of experimental results should be used for a practical predictive tool. Namely, the higher its resolution, i.e. the more explanatory factors and in wider ranges are considered, the less robust the predictive model will be, more pruned to be affected by random errors. Finding a trade-off between resolution and robustness is a central question in predictive modelling (Ratkowsky, 1993).

While acknowledging the importance of such concerns, decision makers may come across even more complex questions when using predictive packages. Should a decision solely rely on predictions, which normally represent the expected value of a response variable in question? A simple method to correct predictions by a "bias factor" was proposed by Ross (1996), refined by Baranyi et al. (1999). It is

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evident, for example, that conservative (cautious) decisions are useful when the price of the prediction error is high. In fact, as we show below, one faces three major challenges when making decisions based on microbial risk assessment:

i) The accuracy (uncertainty and variability) of observations used for developing the predictive model is not necessarily known or easy to estimate;
ii) Available software packages are primarily based on empirical models and can generate markedly different predictions especially close to extrapolation regions;
iii) It is not straightforward to decide what measure of dissimilarity between prediction and actual response should be used. The cost (either measurable financially, or in damage of reputation, or severity of illnesses, or in decrease of influence or power, etc.) assigned to their individual components are frequently on mixed and asymmetric scales, which makes a combined optimization difficult.

In this paper we explain, backed by examples, why predictive models should be used in combination with a cost-benefit assessment. We point out that a correct strategy does not necessarily focus on the most probable event, but on mitigating the implications of wrong decisions that can randomly and/or sooner or later inevitably occur.

2. Theory and examples

It is commonly accepted and frequently cited (WHO/FAO, 2009) that risk assessment consists of four steps: hazard identification, dose-response assessment, exposure assessment and risk characterisation. Microbial risk itself is defined as the probability of an event and the severity of its known or potential adverse health effects. Therefore, mathematically, risk is a two dimensional vector variable assigned to an event. Its components are the probability and the severity of the event. Sometimes the product of the two is called the risk, which can be considered as the "expected severity" of the event. The severity can be quantified by various ways: e.g. number of death/hospitalization; missed working hours; cost of treatments, etc.

The focus of this paper is *not* the above interpreted risk, assigned to an *a-posteriori* event, but the risk of an *a-priory* decision, that we also call choice or bet in what follows. We will suggest and exemplify a formal mathematical definition for the risk of a decision. Its construction aims at the use of predictive microbiology in decision making, when for example a risk assessor needs to provide a recommendation or a regulatory unit or a health worker needs to choose: against what possible future events should be protective measurements introduced.

Assume that a set of information quantified by an $\mathbf{x}$ random variable (an n-dimensional vector) is available on the past behaviour and the present state of a system. A decision maker needs to put forward a guess $\mathbf{b}$ (also called choice or "bet" in what follows) on a future event in the system, which is quantified by an m-dimensional random variable, $\mathbf{y}$. To help the decision, an $\mathbf{y} \approx \mathbf{g}(\mathbf{x})$ mapping or algorithm (the predictor), based on a mathematical model, is available that allows the estimation of the $\mathbf{y}$ outcome. Our focus is the error that $\mathbf{b}$ is not necessarily equal to $\mathbf{y}$. The objective is to find a $\mathbf{b}_{\mathbf{opt}}$, the "best bet", which is optimal from a certain point of view.

Obviously, any $\mathbf{b}$ choice, if based on a reasonable strategy, should depend on (i) the available information expressed by $\mathbf{x}$ (measurements, observations, with their probability distributions); (ii) the way how the $\mathbf{y}$ outcome and its probability distribution depends on the past and present of the system (this is approximated by the $\mathbf{g}(\mathbf{x})$ predictor); (iii) the implications if the outcome is different from the guessed one.

Therefore, the typical elements of our task are:

i) Quantify the uncertainty of the information available;
ii) Determine a mathematical model to estimate the outcome $\mathbf{y}$ as a function of the past behaviour and the present state of the system;
iii) Assign cost to the error generated by the difference between $\mathbf{b}$, the a-priori decision (bet) and $\mathbf{y}$, the in-fact to be happening *a-posteriori* outcome.

All these variables could also contain time-dependent components, in which case they are stochastic processes (dynamic, $\mathbf{x}(t)$, $\mathbf{b}(t)$, $\mathbf{y}(t)$ variables rather than just static ones). The available information can be a collection of measurements such as data on (possibly time-dependent) bacterial concentrations, or growth/death rates as a function of environmental factors.

The predictor $\mathbf{g}(\mathbf{x})$ is *unbiased* if the expected value of $\mathbf{g}(\mathbf{x})$ is equal to the expected value of $\mathbf{y}$. A well-known example for such predictor is when $\mathbf{x}$ is a set of independent, identically distributed measurements and the $\mathbf{g}(\mathbf{x})$ mapping is the procedure of taking their arithmetical average. A reasonable $\mathbf{b}$ bet on the result of the next measurement could be this arithmetical average. Note that this number may not be measured, therefore the bet could always be wrong, if for instance the set of possible outcomes consist of discrete values that do not include the calculated average; still the expected difference between the bet and the outcome could be smaller than betting on an outcome that can really occur.

For an example, for the simple $m = 1$ case, consider a "head or tail" trial, with not necessarily equal probabilities for the two possible outcomes, scored by 0 and 1, respectively. What is the best bet for the result of the next toss if the cost of a wrong bet depends on the difference between the bet and the actual outcome? Note that the decision can nominate any real number, not only 0 or 1.

We will see that if the aim is to minimize the expected cost of the error and this cost is proportional to the squared distance between the bet and the outcome, then the "best bet" is the average of the so-far observed experimental results. So though this strategy can never bring a correct prediction, since the decision is a number between 0 and 1, while a single outcome is either 0 or 1; still, in the long run, it leads to minimizing the loss due to wrong decisions.

That $\mathbf{g}(\mathbf{x})$ should be unbiased, i.e. the expected value of $\mathbf{g}(\mathbf{x})$ should be equal to the expected value of $\mathbf{y}$, is a rather trivial requirement. Could we impose more restrictions on $\mathbf{g}$? For example, what would be the "best bet" if we introduced asymmetric penalties for under- and over-estimations?

Below we define the risk of a decision. Let $\mathbf{b}$ be a bet on the $\mathbf{y}$ outcome. Introduce a

$$c(\mathbf{b}, \mathbf{y}) : \mathrm{R}^{\mathrm{m}} \times \mathrm{R}^{\mathrm{m}} \Rightarrow \mathrm{R}$$

cost function to quantify the price we would pay for a decision error, where R is the set of real numbers and R^{m} is the set of m-dimensional vectors with components from R. Define the risk of decision $\mathbf{b}$ as the expected cost caused by the difference between $\mathbf{b}$ and the outcome $\mathbf{y}$, where the expectation (an integral) is calculated as $\mathbf{y}$ runs through its possible values with p_y probability distribution:

$$Risk(\mathbf{b}) = \mathrm{E}(c\mathbf{b}, \mathbf{y}) = \int c(\mathbf{b}, \mathbf{y}) dp_y$$

We claim that this definition for the risk of the decision $\mathbf{b}$ is suitable for our purposes. The same idea is used for example in pattern recognition (Devroye et al., 1996).

Fig. 1 demonstrates well the main point this paper addresses; while traditional microbial risk assessment focuses on the *risk of future events*, we concentrate on the *risk of a decision* to be taken *before* those events.