Population Modeling By Examples III

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ABSTRACT

This review paper contains examples of population modeling that was collected through self introductions sent to the population modeling mailing list. It is the third review this group composes collaboratively. The paper forms a definition of a complex field spanning many disciplines by examples. The purpose of the paper it to further map the field and support future cross over and synergy between population modelers.

**Keywords:** Population Modeling, Definition, Multi Disciplinary, Classification.

# INTRODUCTION

Modelers are capable of modeling many phenomena to great accuracy. Examples of such models can be found in many technical engineering fields where models are very predictive. However, when moving towards more complex systems such as biological systems or behavior, we still have not perfected tools to model phenomena to great accuracy. Specifically, our capabilities to model populations are still limited although growing.

Tools to better model populations of many sorts have been suggested though the years. In the distant past differential equations were used, yet recently with advances in computing other computational techniques such as microsimulation and agent based modeling have been suggested. Techniques continue to improve and can be applicable to many types of population modeling.

To help bring together population modeler from multiple disciplines the Inter Agency Modeling and Analysis Group (IMAG) (IMAG, Online), that Is composed of government officers, created working group that can be composed of researches worldwide. The group has a project site in SmiTK (SimTk, Online) and a mailing list (PopModWkGrpIMAG-news, Online) and in the last few years the group recruited many population modelers to join the mailing list and introduce their work. The initial thought was to define a complex field that span disciplines such as healthcare, transportation, emergency response and many other fields. Towards that end the working group stated assembling review paper that edited self introductions of the authors and formed a map of the field by examples.

The first review paper (Population Modeling Working Group, 2015) was focused on establishing a definition of population modeling that was defined as “Modeling a collection of entities with different levels of heterogeneity”. The variety of types of modeling and techniques was great. In the second review paper (Smith? et. al., 2016) the group extended the work to bring more examples and map the field and to start forming a map of the field. This third paper extends this map by providing additional examples. The paper will continue by introducing members that introduced their work publicly to the mailing list in chronological order of introduction. The texts were edited for brevity and format.

# Examples

## Bishal Paudel – Vanderbilt University, USA

Quaranta's group at Vanderbilt University (Vanderbily, Online) uses systems biology approach to understand how cancer cells respond to therapies. BRAF-mutated melanoma was used as a model system. Their response dynamics in different targeted, and chemo therapies, were investigated. finding that the drug response behavior of these cells are complex and non-linear. High -throughput assay was developed to dissect the non-linearity in response dynamics and attribute it to non-genetic heterogeneity present within cell lines. Recent data suggest cells might be rapidly switching between different epigenetic states to evade the apoptosis, and eventually develop resistance. To understand the phenotypic state transitions, a simple three-state model was developed to describe the response dynamics we see in experimental data. We are in the process of identifying molecular signatures of such states, with a hope to calibrate the model, and be able to predict cancer cells response dynamics before they eventually develop some sort of resistance.

## Carl Asche - University of Illinois, USA

Focuses on the use of comparative effectiveness research and cost-effectiveness analysis in health care decision making (University of Illinois, Online). Specifically busy in utilizing predictive modeling techniques to help reduce hospital no-shows and readmissions (Asche et. al. 2014).

## Vivek Balaraman - Human Centric Systems Research Group in TCS Research, India

Conducting work in the area of grounded fine grained behavioral models of human populations with current focus on modeling work teams and groups within organizations (Singh et. al., 2016). Grounded means that ideally the model elements have to be grounded in observations and studies and not assumed. Fine grained means that multiple behavioral dimensions are investigated such as personality or affect influence decision making. This is done using 3 techniques: 1) conducting studies on the ground using surveys as well as other data collection techniques, 2) mining past literature for useful empirical results in a context. 3) working towards using serious games to capture behavior. Through these processes a behavior patterns repository is populated with the intention to provide in time foundational elements to build behavior models of entities in a context (Patel et. al. 2016). The business use of this work is to help understand existing behavior of organizations, allow what-if analysis of hypothetical situations as well as a sandbox to test out behavior change interventions.

## Michael Thomas - Birkbeck University of London, UK

Focused on using multi-disciplinary methods to understand the brain and cognitive bases of cognitive variability, including behavioral, brain imaging, computational, and genetic methods (The Developmental neurocognition lab, Online). The interest is to use population modeling methods to understand the causes of variations in trajectories of cognitive development between children, from developmental disorders to giftedness.

One more recent computational approach is to simulate cognitive development in large populations of children and to include intrinsic (neurocomputational) and extrinsic (environmental) factors whose interaction produces variability in developmental trajectories across the whole population. This approach is used within several contexts. These include studying the causes of delay in developmental trajectories of language (Thomas & Knowland, 2014), investigating how socio-economic status effects may influence language development (Thomas, Forrester & Ronald, 2013), and investigating how population-wide individual differences can interact within pathological mechanisms in neurogenetic disorders such as autism (Thomas, Knowland & Karmiloff-Smith, 2011; Thomas et al., 2015).

Within a machine learning framework, artificial neural network architectures can be complemented with genetic algorithms, to stipulate a genetic level of description. The framework permits a consideration of the relationship between population variability at multiple levels of description, including genes, brain structure, brain function, and behavior. Examples of this work include simulation of genome-wide association analyses (Thomas, Forrester & Ronald, 2016), and simulation of developmental changes in the heritability of intelligence with age and their relation to differential rates of change of brain structure.

This multi-scale framework was used within a purely machine learning context to evaluate whether it may offer new methods for transfer learning (Stamate, Magoulas & Thomas, 2015).

## Nathan Geffen - University of Cape Town, South Africa

Dealing with different outcomes modeling various Sexually Transmitted Infections (STIs) in South Africa using equation-based (Frequency-dependent) models versus microsimulations (network models) (Johnson & Geffen, 2016).

In simulations of sexually transmitted infections how do we match agents with each other in sexual partnerships, and how does this affect the outcomes of simulations? If there is information (or assumptions) about who people are actually more likely to partner with, it may result in more accurate or realistic models and better insights into how infections spread.

The problem can be stated like this: given a set of agents, each representing a person or animal seeking a (sexual) partnership, find a set of partnerships such that every agent is paired with one and only one other agent. We need this assumption too: for any two agents a and b we have a distance function that calculates how realistic it is that a and b can become sexual partners. This distance function creates an ordering such that for any two potential partners, b and c, of a, we can calculate whether b or c is the more likely partner (perhaps with some arbitrary tie-breaking method). For example, the distance function might calculate that a 25 year-old heterosexual male living in Berlin is more likely to partner with a 25-year-old heterosexual female living in Berlin than a 45 year-old gay male living in Munich. but the latter in turn is more likely to partner with a 40-year-old gay male living in Munich than either of the first two individuals.

A matching algorithm was developed that tries to balance speed and quality (Gefen, Online). And it is currently explored how this affects the outcomes of a simulation.

## Pawel Topa - AGH University of Science and Technology, Poland

The "eVOLUTUS: project (Topa et. al. 2015) is a simulator of multiscale evolutionary processes tested on Foraminifera. The goal is to design a new algorithmic framework for testing and simulating evolutionary principles and their consequences in defined environments at various spatiotemporal scales. Due to biological complexity of organisms and their interactions with the environment, it has never been attempted to design such a numerical framework for the simulation of evolutionary patterns derived from the fossil record of real organisms. Foraminifera is a single-celled eukaryotes that occupy marine benthic and pelagic zones throughout the world and have an extraordinary fossil record throughout the Phanerozoic. This makes them an ideal model often used for testing general evolutionary hypotheses. Recent studies have shown that shell architecture and most prominent morphogenetic trends in shell development distinctly follow molecular phylogenetic patterns.

 We use approach named Individual Based Modelling in which modeler tries to present population of living organisms as being composed of discrete individual organisms. The model that uses IBM in natural way can be implemented using Agent-based Modeling computational paradigm (Topa & Faber, 2017). In order to model evolutionary processes we use the well known genetic operators: mutation and crossing over which are applied to the virtual genome consisted of parameters that govern agent (foraminifers) behavior. Selection is simply made by adaptation to environmental conditions in virtual habitat.

## Katherine Ogurtsova - DDZ, German Diabetes Centre, Düsseldorf, Germany

The center builds a diabetes model which will be suited to German settings, reflects German healthcare system structure, and established primarily on German data where it is possible. The plan is to use this model for cost-effectiveness analysis of population-based prevention programs. Currently the focus is on systematic literature review with the topic:: External validation of Type 2 diabetes models : definitions, approaches, implications and room for improvement. The objective is : to identify and critically appraise approaches that are used for external validation in the existing models of type 2 diabetes development and progression. The scope of the review is: 1) models of type 2 diabetes incidence and/or progression with or without complications, 2) built on simulation techniques on organ/systems, individual or cohort level.

## Jeff Shrager – Stanford, USA

Past work included multi-agent search problem, esp. focused on the question of pre-v.-post publication peer review (Shrager, 2010). Past work also created what was among the earliest, and almost certainly the most advanced, through-the-web programmable biocomputing engines (what they now call Software as a Service). Current work is focused on creating (and simulating) a new kind of clinical trial, called Global Cumulative Treatment Analysis (GCTA) (Shrager 2013), which amounts to operating an Air Traffic Control system over the whole biomedical system. The GCTA method uses Bayesian methods to adaptively (and so, theoretically, very efficiently) search the hugely combinatoric space, while treating each patient with the best validated knowledge to that moment.

## Christopher Fonnesbeck – Vanderbilt University. USA

Research interests center around the application of Bayesian computational methods to addressing epidemiological problems. The first of these is in the modeling of the effectiveness of interventions in the control of infectious disease outbreaks (Probert et. al., 2016). In particular, the goal is to estimate optimal policies for controlling outbreaks under uncertainty, and how information collected during the outbreak can be used to update the information state to improve future decisions, with an aim of reducing the severity or duration of the epidemic. Our approach allows for the recreation of past epidemics, and the exploration of the likely effects of alternative intervention strategies, as well as the value of reducing uncertainty in relevant parameters of the disease system.

Another research focus is meta-analytic modeling for evidence-based medicine (Fonnesbeck et. al. 2012). Bayesian hierarchical models are applied for evaluating comparative effectiveness across studies, because it allows information to be shared in a single analysis without completely pooling the information and ignoring heterogeneity. This paradigm allows multiple sources of independent information to be combined in a single analytic framework to provide information regarding a common set of parameters of interest.

An important aspect of work is in the development of computational tools for Bayesian modeling. The PyMC project (Salvatier et. al. 2016) was created in 2003. It is a Python library for probabilistic programming. PyMC implements modern algorithms for fitting Baysian models, including Markov chain Monte Carlo and variational inference, and makes it easy for applied statisticians and modelers to implement arbitrary models, fit them, and analyze their outputs without having to hand-code algorithms.

## Resit Akcakaya, Stony Brook University, USA

In the Akcakaya lab population models are used with dynamic spatial structure to study the effects of climate and landscape changes on species. The novelty of our approach is that it links climate change models, ecological niche (species distribution or habitat suitability) models, and demographic models to predict the extinction risk of species under global change. The development of this coupled niche-population modeling approach was based on our previous work on metapopulation models with dynamic spatial structure (Akçakaya et. al., 2013), which were applied to simulate the effects of landscape changes resulting from timber harvest and fires. The first applications of this modeling approach to climate change were developed in a series of workshops in 2007-2009. Later applications focused on incorporating predator-prey interactions and disease dynamics; these applications analyzed the effectiveness of conservation measures for the world's most endangered cat, which is impacted by climate change, and for one of the most threatened North American mammals, which is impacted by plague. These studies demonstrated that spatially structured prey-predator models allow realistic conservation planning that takes into account emerging threats such as climate change and infectious diseases.

One of the goals of these projects has been to contribute to the development of Red List Guidelines for identifying species threatened by climate change. To test the effectiveness of the Red List criteria as an early-warning system for climate change-related extinctions, we adapted the coupled niche-population modeling approach to simulate generic life-history types instead of particular species. The resulting analysis found that climate change causes high, but predictable, extinction risks, and that the Red List system would provide several decades of warning time for species that might go extinct because of climate change. In a related study, we combined the coupled niche-demographic models with recent advances in geochronological dating, palaeoclimate reconstructions and molecular techniques for retrospective modeling (Fordham et. al. 2016). Our preliminary results suggest that such long-term retrospective analyses will improve efforts to predict the likely effects of future climate and other environmental change on biodiversity, and target conservation management resources most effectively.

## Matthias Templ, Vienna University of Technology, Austria

The R package simPop (SimPop, Online) can be used to created synthetic population data needed for microsimulation tasks. It includes methods such as combinatorial optimization, iterative proportional fitting and updating, model-based regression methods to simulate data as well as some tools that are useful for demographers and economist that carry out microsimulations with data including age or income heaping problems. The aim is to simulate a population for all individuals, the data that are needed for time T\_0 where microsimulation methods are applied to carry on to T\_1, T\_2, ... The package is specialized for complex data from official statistics but is not limited to these data sets.

## Amit Huppert - Gertner institute, Israel

Two classical population dynamics examples that of interest in recent years are i) the unfolding of epidemics ii) predator prey interactions. In the case of infectious disease outbreaks the goal is to utilize data in order to first estimate the model parameters and conduct model selection. In the second phase, the selected model can be used to study different control methods with the aim of reducing and/or curtailing the outbreak in an optimal way (Yaari et. al. 2016). When studying ecological interactions there are many myriad theoretical studies that explore the role of spatial structures on predation and/or competition among different organisms. However, there are only sparse field studies that have validated, and quantified their predictions. In our work (Dattner et. al., 2017), we combine experimental results, which observed the temporal dynamic of the predatory bacterium, and its prey, in a structured environment composed of sand under various regimes of water content. By constructing a dynamic model, and estimated its parameters. The ability of the model to fit the data combined with realistic parameter estimates indicate that bacterial predation in the sand can be described by a relatively simple model, and stress the importance of prey refuge on predation dynamics in heterogeneous environments.

We developed and analyzed a set of novel dynamic models (Miller et. al., 2016) for multihost transmission. The model analysis reveals a new mechanism for disease amplification. In this mechanism the maximum disease risk is obtained when both host species are present in the community. The model expands on the previous understanding about the relationship between host diversity and disease risk by formulating the exact conditions under which diversity amplification, or dilution, would occur. Such formulation is able to account for the different and contradictory patterns often observed in nature. We have also extended the model to look at personal protection (PP) techniques, such as insecticide treated nets (ITN), repellents, and medications, include some of the most important and commonest ways used today to protect individuals from vector borne infectious diseases.

## Marco Ajelli, Northeastern University, USA & Bruno Kessler Foundation, Italy

Work in the Laboratory for the Modeling of Biological and Socio-technical Systems focused in the last decade on social mixing patterns – age mixing patterns in particular – and a variety of approaches has been used. Among them, diary-based surveys, use of wearable sensors, analysis of time-use data, and the development of synthetic populations of agents (Iozzi et. al. 2010).

In the latter category falls our work (Fumanelli et. al. 2012), where we estimated age-mixing patterns in 26 European countries through the simulation of a synthetic population of agents mimicking real-world contacts between individuals. To build the synthetic populations we relies on publicly available census and survey data on the main socio-demographic characteristics of each country (e.g., household size, age distribution by household size, schooling and employment rates by age). The resulting contact matrices describing the average frequency of “adequate” contacts that an individual of age i has with individuals aged j is derived by analysis of the contact network of the agents of the simulated population. The inferred contact matrices are validated by a detailed comparison with the matrices obtained in six European countries by the most extensive diary-based study on mixing patterns and against epidemiological influenza data.

This methodology allows a large-scale comparison of mixing patterns in Europe, highlighting general common features as well as country-specific differences. Clear relations were found between epidemiologically relevant quantities (such as reproduction number and epidemic size) and socio-demographic characteristics of the populations (e.g., average age of the population). This work provides a numerical approach for the generation of human mixing patterns, which is straightforward to apply to other countries as it is entirely based on routinely collected socio-demographic statistics. This approach could be instrumental for improving model accuracy, especially in the absence of specific empirical data on human mixing patterns.

## Dan Yamin, Tel Aviv University, Israel

The Laboratory for Epidemic Modeling and Analysis is focused on healthcare, predicting the spread of infectious diseases, as well as analyze population-level effectiveness and cost-effectiveness of potential intervention programs. In a broader context, there is interest in topics that can be modeled in the same manner as the spread of infectious diseases. These topics include cyber security and computer viruses, viral marketing, information spread, and even behaviors with social-contagion aspects such as imitation of facial expression, smoking habits and risk to become obese.

The core research lays the exploration of the dynamic between individuals in the population including use of tools such as Markov chains, statistics, differential equations modeling, game theory and network science, in an interdisciplinary way. For example, to evaluate the population effectiveness of an RSV vaccination program in the United States, and age-dependent transmission model was developed (Yamin et al. 2016 PNAS). Results demonstrated that vaccinating children younger than five years of age, will be the most efficient and effective way to prevent RSV infection in both children and older adults. In the same line, using theoretical epidemiological game model to find the optimal incentive for influenza vaccination, the findings suggested that for the benefit of the elderly greater incentives should be administered to the non-elderly than targeting the elderly themselves. Using network analyses as well as medical record examinations, results showed that individuals infected with influenza in previous year, were at an elevated risk to become infected in subsequent years, and thus should be prioritized for influenza vaccination. In light of these conclusions, the Israeli Ministry of Health updated the policy this year, and the largest HMO in Israel applied various intervention programs to promote vaccination among the targeted population. Another example is the development of a population model for Ebola disease based on methods from scheduling processes (Yamin et al., 2014). Results from this research demonstrated that Ebola can be eliminated if the World Health Organization will allocate the resources differently, by focusing on the isolation of infected individuals in critical condition within 4 days from symptom onset rather than isolating any case based on hospital capacity.

## Leandro Watanabe - The University of Utah, USA

The Mysers research group is active in Standard development. Standards are important for the ability to share and reuse models. The importance of modeling standards is higher than ever with the rising number of computer-aided design tools being developed because it grants interoperability between tools. In the systems/synthetic biology fields, the most widely used modeling language for simulation is the Systems Biology Markup Language (SBML, Online), which allows the representation of quantitative models. SBML has many features that allow the representation of chemical reaction networks, discrete event models, and ordinary differential equations models.

SBML supports extensions that increases the usability of the standard for different applications. The arrays package has been proposed to allow the representation of regular structures more concisely. The arrays package in SBML has been used for the representation of population models in the systems/synthetic biology domains within the iBioSim tool (iBioSim, Online). In particular, the arrays package was used to construct a lattice-based model of cellular populations to identify the behavior of genetic circuits in different cells when placed in an environment that allows cell-cell interactions (Watanabe & Myers, 2016). This is just one of the many applications of the arrays package, which could potentially be used for many other applications such as disease models.

## Ram Pendyala – Arizona State University, USA

PopGen (Synthetic Population Generator PopGen, Online) is a synthetic population generator that was developed in 2008 to support the development and implementation of activity-based microsimulation models for travel demand forecasting. The advent of activity-based microsimulation models of travel demand has provided the ability to simulate activity-travel patterns of individual travelers in time and space. The application of activity-based travel demand model systems requires the generation of synthetic populations whose attributes match those of the general population within small geographies (say, a traffic analysis zone, census tract, block group, or block). In (Ye et. al., 2009), we developed and introduced a heuristic iterative procedure known as the IPU (Iterative Proportional Updating) algorithm to facilitate the generation of a synthetic population that matches census data with respect to both household and person attributes. This algorithm has been implemented in PopGen, which is an open source synthetic population generator. In PopGen, the iterative proportional fitting (IPF) procedure is applied first to both household- and person-level control variables of interest to obtain the number of households and persons in each cell of the respective joint distributions. Appropriate rounding procedures are applied to obtain cell "constraints" that must be matched through the population synthesis process. The IPU algorithm computes weights for sample households such that household-level as well as person-level marginal distributions are matched as closely as possible.

In addition to developing the IPU algorithm, we also developed and implemented an entropy-maximization based approach to deriving weights for sample records such that both household and person attributes of interest are matched very closely. A relaxed formulation of this algorithm accommodates for data inconsistencies, which is often encountered when dealing with input data used for transportation demand forecasting. The PopGen software package incorporates both the IPU and entropy-maximization methodologies and the user can choose the method to be applied in any specific PopGen run. We have since enhanced the PopGen package to accommodate control variables at multiple geographic resolutions through an enhancement of the IPU algorithm. Current work focuses on the development of a full-fledged demographic and socio-economic evolution model system so that a base (current) year synthetic population can be aged through various lifecycle processes over time, thus enabling the generation of a future year synthetic population. In addition, we are implementing a cloud-version of PopGen to enable ease of use.

# Discussion

A summary of the work reported in this paper is reported in Table 1 that attempts to classify the work in a wider view of the entire field. This is the third review paper that the working group produces. Therefore it is possible to deduce trends in field development over a few years. In the first review paper, the main discussion was regarding definition of the field and whether cohort modeling or individual based modeling should be both included in the same group. By this review paper it is clear that many population modelers are now leaning towards individual based models such as microsimulation or agent based models. This is not surprising considering advances in computing in the last several decades.

To support example provided in this paper modifications were made to categories of use to Table 1: The word economics was added to the resource planning and allocation category since this is where health economist fall. Yet more importantly two new categories were added: behavior modeling, and tools categories. The last category seems to be very active and many tools are reported in this paper that span fields such as healthcare and transportation or are generic and non affiliated to a specific field of use. This is a promising development that may help cross over and fertilization between fields which may lead to future standardization which is already starting.

# Acknowledgments

Jacob Barhak edited this paper from contributions provided on the mailing list. WE thank all contributors to the discussions on the mailing list. Reviewer responses will be placed here.

Table 1: two-dimensional view of the organizational structure of this paper

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|  | **Managing disease spread** | **Resource planning & allocation, economics** | **Predicting drug effects** | **Risk assessment** | **Ecosystem management** | **Testing theory** | **Epidemiology and public health** | **Behavior modeling** | **Tools** | **Summary of methods** |
| Bishal Paudel  |  |  | √ |  |  |  |  |  |  | High throughput imaging, Image registration. |
| Carl Asche |  | √ |  | √ |  |  | √ |  |  | Cost effectiveness analysis |
| Vivek Balaraman  |  |  |  |  |  |  |  | √ |  | Agent Based modeling, surveys, Serious games |
| Michael Thomas |  |  |  |  |  |  | √ | √ |  | Machine learning, genetic algorithms |
| Nathan Geffen | √ |  |  |  |  |  | √ |  |  | Agent based modeling. Matching algorithms. Equation based models, microsimulation |
| Pawel Topa |  |  |  |  | √ | √ |  |  |  | Agent Based Modeling, Evolutionary Computations |
| Katherine Ogurtsova |  |  | √ |  |  |  | √ |  |  | Cost Effectiveness Analysis |
| Jeff Shrager |  |  | √ |  |  |  | √ | √ | √ | Machine Learning, Bayesian methods. |
| Christopher Fonnesbeck | √ |  |  |  |  |  | √ |  | √ | Markov Chain Monte Carlo, Baysian models, Meta Analysis, reinforcement learning |
| Resit Akcakaya |  |  |  | √ | √ |  |  |  |  | Coupled niche-demographic models; Matrix population models; Metapopulation models with dynamic spatial structure |
| Matthias Templ  |  |  |  |  |  |  |  |  | √ | Population Generation, iterative proportional fitting |
| Amit Huppert | √ |  |  |  | √ |  |  | √ |  | Predator Prey Models, Differential equations |
| Marco Ajelli |  |  |  |  |  |  | √ |  |  | Agent based models, synthetic populations |
| Dan Yamin | √ | √ | √ |  |  |  | √ |  |  | Cost Effectiveness, Markov Chains, Differential Equations, Game Theory |
| Leandro Watanabe |  |  |  |  |  |  |  |  | √ | SBML Arrays, Stochastic Simulation |
| Ram Pendyala  |  | √ |  |  |  |  |  |  | √ | Population generation, microsimulation |

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**THE POPULATION MODELING WORKING GROUP** is composed of researchers that gather together in the population modeling mailing list. The purpose of the group is to promote population modeling in multiple fields. The activities of the working group are reported annually at the Inter Agency Modeling and Analysis Group (IMAG) and MultiScale Modeling Consortium (MSM) meeting. IMAG is composed of government officials, yet the working group is international and composed of academics and industry members. The mailing list address is popmodwkgrpimag-news@simtk.org