Proceedings of the 2014 Winter Simulation Conference
A. Tolk, S. Y. Diallo, I. O. Ryzhov, L. Yilmaz, S. Buckley, and J. A. Miller, eds.

TOWARDS CLOSED LOOP MODELING: EVALUATNG THE PROSPECTS FOR CREATING RECURRENTLY REGROUNDED AGGREGATE SIMULATION MODELS USING PARTICLE FILTERING

Nathaniel Osgood

Department of Computer Science
176 Thorvaldson Bldg, University of Saskatchewan
Saskatoon, SK S7N 5C9,CANADA

Juxin Liu

Department of Mathematics and Statistics
106 Wiggins Road, University of Saskatchewan
Saskatoon, SK, S7N 5E6, CANADA

ABSTRACT

Public health agencies traditionally rely heavily on epidemiological reporting for notifiable disease control, but increasingly apply simulation models for forecasting and to understand intervention tradeoffs. Unfortunately, such models traditionally lack capacity to easily incorporate information from epidemiological data feeds. Here, we introduce particle filtering and demonstrate how this approach can be used to readily incorporate recurrently available new data so as to robustly tolerate – and correct for – both model limitations and noisy data, and to aid in parameter estimation, while imposing far less onerous assumptions regarding the mathematical framework and epidemiological and measurement processes than other proposed solutions. By comparing against synthetic ground truth produced by an agent-based model, we demonstrate the benefits conferred by particle filtering parameters and state variables even in the context of an aggregate, incomplete and systematically biased compartmental model, and note important avenues for future work to make such approaches more widely accessible.

1 INTRODUCTION

Despite the growing burden of chronic disease, infectious diseases still impose a heavy burden on length and quality of life worldwide. Such diseases are characterized by pronounced dynamics, being marked by patterns of change over time (Anderson and May 1991) such as the classic epidemic curves and patterns of waxing and waning. From the early days of infectious disease epidemiology (Defoe 2010) practitioners have placed great emphasis on deriving insight from empirical time series data capturing such patterns. Throughout the developed world, physicians are required to report incident cases of broad classes of notifiable diseases. Public health agencies from the local to international level monitor such data for several uses, including emerging outbreaks and monitoring trends in burden of endemic infections.

One of the most important potential uses of such time series data is as an aid to planning, particularly to help inform decision making regarding interventions. In the course of an outbreak, frequently public health agencies will carefully monitor incidence counts, and such data often figures directly into recurrent – for example, weekly – discussions concerning intervention options, whether they be targeted vaccination campaigns, advisories regarding hygiene or social distancing, or more heavy-handed measures such as recommendations for school or workplace closure.

While such empirical data offers great value for public health authorities, it is also associated with notable shortcomings. Incident case count data can be extremely noisy, particularly for contexts marked by smaller population or low incidence or diagnosis rates. The presence of such noise can confound ability to reliably infer trends and to assess with confidence the current epidemiological state of affairs.

More fundamentally, while time series data can aid assessment of the past and current situation, such data in isolation offer no direct capacity to predict what lies ahead. Among the foremost interests of public

978-1-4799-7486-3/14/$31.00 ©2014 IEEE

health authorities are understanding – in light of all available evidence, including recent data – both as to how an outbreak will play out in the status quo (in the absence of further intervention) and timely and robust evaluation of the tradeoffs between multiple intervention options. Unfortunately, neither of these insights are directly offered by the data in epidemiological time series.

To secure such insights regarding outbreak evolution, policy makers increasingly turn to complementing insight from such time series with modeling. While there are a variety of model types of relevance, the most popular and widely studied (Anderson and May 1991) modeling approach to inform decision making concerning both intervention options and epidemic evolution is based on *dynamic models*, whether they be aggregate in character (compartmental, System Dynamics), or individual-based (e.g., via agent-based methods). Over the past century (Kermack and McKendrick 1927), such modeling types – which captured the mechanics of transmission – have proven general and flexible vehicles for understanding how outbreaks and epidemics evolve, and for studying the impact of a variety of intervention strategies (Anderson and May 1991).

Unfortunately, dynamic models are also traditionally associated with an important set of shortcomings. While such models are often grounded by data – such as epidemiological time series data – the associated calibration processes often require much time and typically entail manual oversight or intervention. More significantly, such models often include omissions, simplifications and misestimates that inevitably lead the dynamic model predictions to diverge from empirical data. The presence of these shortcomings reflect many factors: Limited availability of data available to the modeler, approximations for certain processes, and the inevitable need to exclude a variety of processes and factors from the model. Moreover, there are a variety of effects involving the vagaries of weather, human behavior, economic behavior – often characterized stochastically in fine-grained models – whose prediction lies outside of even the most sophisticated existing models. As a result of such stochastic factors, systematic distortions, omissions, even highly articulated and precisely calibrated models – such as those sought in the MIDAS project and for national-level outbreak response planning – will inevitably begin to diverge from observed data. While dynamic models will often offer great predictive ability in the short-term, their medium- and long-term predictive capacity of even detailed models can be greatly impaired.

In short, public health planners are left with two terribly fallible tools. Epidemiological time series can give great insight into the current context, but can be highly noisy, and offer little guidance in isolation as to what to expect in the status quo or from interventions. Well-calibrated dynamic models can allow for highly accurate shorter-term projection of status quo or intervention scenarios, but offer longer-term projections that can be expected to diverge from empirical patterns and traditionally lack a reliable and automated means of keeping current with the latest in empirical data.

Past research has sought to address this quandary. Some authors have applied the long-established and well-codified (Gelb et al. 1974) extended Kalman Filtering as a tool for creating a consensus estimate from empirical data and model predictions. While capable of performing updates to both state and parameter estimates (Qian et al. 2014) Kalman Filtering is hamstrung by several factors. The first is heavy reliance on strong distributional assumptions concerning both processes noise and measurement error – assumptions that can prove highly problematic in cases with low counts of incident infection. Secondly, in the presence of non-linearity, the Kalman Filter reliance on a linearization-based approximate can in some cases lead to strong divergence of the estimate from the underlying situation. Thirdly, the covariance matrix estimate of model state cannot be readily translated into similar dispersion estimates around arbitrary model outputs. Finally, the Kalman Filter relies upon the capacity to formulate the dynamic model as a series of state equations. While this approach works well with classic compartmental models, it is incompatible with the growing numbers of models using agent-based and other formulations.

We leverage here well-studied computational statistics techniques to demonstrate and evaluate a technique that combines the best features of empirical data and dynamic models while mitigating the characteristic weaknesses of both. The approach uses sequential Monte Carlo methods in the form of particle filtering (Andrieu et al. 2010) to combine insights from noisy empirical data (on the one hand) and dynamic models that exhibit growing systematic errors, omissions, and stochastic divergence over time (on the other) to yield a more reliable consensus estimate. Like Kalman Filtering (Gelb 1974) this consensus estimate takes into account the relative reliability of empirical data and the model, and considers the fact that the dynamic model is likely to exhibit growing inaccuracy over time. However, in contrast to Kalman Filtering, the approach here is not hampered by strong distributional assumptions concerning process and measurement error, does not assume that the dynamic model is formulated using state-equations, and –in contrast to the restrictive MLE estimates and covariance provided by the Kalman Filter – provides samples from the posterior over model states and arbitrary model outputs. While particle filtering has been applied to a wide variety of previous domains, it is seen very few previous applications in the public health area in general, and in infectious disease prevention and mitigation (Dukic et al. 2012). In addition to introducing the technique to additional segments of the infectious disease modeling community, we contribute here – using synthetic ground truth data – the first evaluation of the application of the approach to the public health area of which we are aware.

The balance of the paper is organized as follows. Section 2 provides a general introduction to the particle filter. Section 3 discusses the dynamic model and the simple particle filter formulation used for this study. Section 4 describes the experimental setup used to evaluate the performance of the particle filter for this study, and introduces the experiments conducted. Section 5 presents the results from those experiments. Section 6 discusses the formulation used here and the implications of the experimental findings and concludes.

2 INTRODUCTION TO PARTICLE FILTERING

Particle filtering is a popular numerical method for optimization problems in general state space methods, especially in non-linear non-Gaussian scenarios. The state space model provides a flexible framework for modeling one or more time series of the form $\{y_t\}_{t=1:T}$ and has two major components: (1) the observation equation for the probabilistic model of y_t conditional on the state variable x_t, denoted by $g(y_t|x_t)$ and (2) the state equation characterizing the evolution of the state variables, which is a Markov process for $x_t|x_{t-1}$, ,denoted by $p(x_t|x_{t-1})$. In general, the state variables will be *latent*, meaning that they cannot be directly observed. Please note that for ease of presentation, our discussion suppresses explicit mention of the parameters in the two model parts. That is, within this presentation, we assume that the parameters are known. For estimation of both latent variables and unknown parameters, please see Andrieu et al. (2010) for some recent work.

A main challenge is to find efficient methods for on-line estimation for the state variables when the observation y_t comes in one or more sequences, and in the context of stochastics in state evolution. Work half a century ago recognized that an important restricted case of this problem termed the linear state space model is amenable to treatment by simpler methods: Specifically, when both $g(y_t|x_t)$ and $p(x_t|x_{t-1})$ are linear Gaussian conditional distributions (i.e., when both process stochastics and measurement errors are characterized by Gaussian errors), the computationally frugal Kalman filter (Gelb 1974) can be shown to be offer optimal estimation of the posterior $p(x_t|y_{1:t})$. Such methods – which provide MLE mean and covariance estimates of system state – can be heuristically generalized via linearization to handle non-linear non-Gaussian distributions in the form of the Extended Kalman Filter (Gelb 1974), although the resulting estimates are no longer provably optimal, and can be subject to significant estimation error. A more flexible method without that avoids reliance on either Gaussian error assumptions or the local linearization technique is the particle filter, proposed by Gordon et al. (1993).

Particle filters aim to obtain a numerical approximation of the joint distribution $\{p(x_{1:n}|y_{1:n})\}_{n=1:T}$ sequentially. The technique achieves significant computational economies by its recursive formulation, in which samples for later points of time are dependent on the estimates of the samples derived for earlier time points. Such a formulation is of particular importance in the context of process stochastics, which generally make intractable naïve sampling from the latent distributions of state variables over time by application of Markov Chain Monte Carlo algorithms.

Before giving the algorithm details, we first briefly introduce *importance sampling* method**,** which is closely related to particle filtering method. Like other Monte Carlo techniques, particle filtering focuses on *sampling* from a distribution – that is, drawing values from the sample space of the distribution with a frequency proportional to their probability density. Suppose that we wish to sample from target distribution $p(x)$, but that this is difficult. One can sample $\{x^{(i)}\}_{i=1}^{n}$from an importance proposal distribution $q(x)$, which retains the key features of p(x). Then the target density can be approximated by $\hat{p}(x) = \sum_{i=1}^{n} w\left(x^{(i)}\right)\delta_{x^{(i)}}(x)$, where $w(x) = p(x)/q(x)$ and is called *importance weight* and $\delta_{x^{(i)}}(x)$ is the delta-Dirac mass located at $x^{(i)}$.

The particle filter derives the first part of its name from the fact that it maintains a set of particles representing an approximation to the distribution of the state variables whose evolution is described by the process model. Each such particle is associated with a *weight* (reflecting the probability of occurrence of that particle) and a *state*, as defined by the state variables associated with the process model. Other than the possibility of being replaced by a copy of another particle, the state associated with a given particle evolves completely independently of the state of other such particles.

The general particle filter algorithm leverages the approach of importance sampling (Murphy 2012) and can be summarized as follows. Let N be the number of particles.

1. At time $t = 1$, for $i = 1,2,\dots,N$
   (1) Sample $X_1^{(i)}$ from $q_1(x_1|y_1)$;
   (2) Compute a *weight* for each particle $w_1^{(i)} = \frac{p(x_1)g(y_1|x_1)}{q(X_1^{(i)}|y_1)}$.
   Normalize the weights $W_1^{(i)} = \frac{w_1^{(i)}}{\sum_{i=1}^{N} w_1^{(i)}}$.
2. At time $t \geq 2$, perform a recursive update as follows
   (1) Advance the sampled state by sampling $X_t^{(i)} \sim q_t(x_t|y_t, X_{1:t-1}^{(i)})$ and set $X_{1:t}^{(i)}$=$(X_{1:t-1}^{(i)}, X_t^{(i)})$;
   (2) Update the weights to reflect the probabilistic and state update models $w_t^{(i)} = w_{t-1}^{(i)} \frac{p(X_t^{(i)}|X_{t-1}^{(i)})g(y_t|X_t^{(i)})}{q(X_t^{(i)}|y_{t,}X_{t-1}^{(i)})}$.
   Normalize the weights $W_t^{(i)} = \frac{w_t^{(i)}}{\sum_{i=1}^{N} w_t^{(i)}}$.
3. Resampling step:

   For any time t, if the effective sample size is too small (i.e., the variance of the weights is too high, $\frac{1}{\sum_{i=1}^{N}(W_t^{(i)})^2}$<K), resample $X_t^{(i)}$ and set $W_t^{(i)} = \frac{1}{N}$. Here K is a threshold value for the variation of the weights.

Please note that the resampling step is used to mitigate a well-known drawback in which variance of the state estimates increases as time evolves (see an example in Section 3.3 in Doucet and Johansen (2009)). The idea of resampling is to remove the particles with low weights and duplicate the particles with high weights. Because it is driven by weights reflecting fitness of a particle, recurrent resampling tends to lead to a sort of "survival of the fittest" of particles within the particle filter.

Another fact worth noting is that formula for updating weights based on a new measurement y_t can be simplified to $w_t^{(i)} = w_{t-1}^{(i)} g(y_t|X_t^{(i)})$ if one choses $q\left(X_t \middle| y_{t,}X_{t-1}\right) = p(X_t|X_{t-1})$. In this case, the state update process between measurements proceeds in a process that does not explicitly consider later measurements. The weight update occurring at each measurement point then simply multiplies the weight associated with each particular by the likelihood of observing the measured data conditional on the state of that particle. This approach – termed the Condensation algorithm (Isard and Blake 1998) and used in our example below – offers significant benefits in that the process model can be formulated independent of the vagaries of measurement, but can be highly inefficient in cases in which measurements occur infrequently when compared to the speed at which the state diverges due to the stochastic process (Murphy 2012).

3 MODEL FORMULATION

Within this study, we present an example application of a particle filter for a simple compartmental (System Dynamics) transmission model for a communicable illness, and then evaluate the performance of that particle filter when operating using synthetic empirical data produced by a much more complex situation whose ground truth is precisely known. We present here the formulation of the compartmental model and the accompanying particle filter; discussion of additional components involved in the generation of the empirical data and evaluation is deferred until the next section. We took advantage of the hybrid modeling capabilities of AnyLogic by simultaneously running both the particle filtered System Dynamics implementation and the ground truth model as two parts of a single overarching model within in AnyLogic 6.8.1.

Beyond the standard formulation of the particle filter (in terms of resampling, etc.) the application of the particle filter to the model presented here includes 3 components, described in following sub-sections.

- **Dynamic model**: An aggregate System Dynamics (compartmental) infection transmission model.
- **Probabilistic model**: A probabilistic model specifying the likelihood of observing the specified empirical data for a given point in time in light of the state of that dynamic model at that same point in time
- **Measurement update rule**: A measurement update rule specifying how the weight of the particle is updated in light of the probabilistic model

3.1 Dynamic Model

We describe here our dynamic model to be used with the particle filter. The state equations for the model are given as follows:

$$\dot{S} = -\frac{Poisson\left(cS\left(\frac{I}{S+E+I+R}\right)\beta\Delta t\right)}{\Delta t}$$

$$\dot{E} = \frac{Poisson\left(cS\left(\frac{I}{S+E+I+R}\right)\beta\Delta t\right)}{\Delta t} - \frac{E}{\tau}$$

$$\dot{I} = i = \frac{E}{\tau} - \frac{I}{\mu}$$

$$\dot{R} = \frac{I}{\mu}$$

It is notable that the model includes a stochastic process associated with incidence of infection. This process reflects the small number of cases that occur over each small unit of time (Δt). As a result, the model exhibits multiple possible trajectories. Compartmental parameters are specified in the following table 1:

Table 1: Insert Table caption here.

Variable Name	Notation	Value	Units
Mean Latent Period in Weeks	τ	0.42857 (*i.e.*, 3 days)	Week
Total Population Size	N	*1000*	Person
Probability of Infection Transmission Given Exposure	β	0.005	Unit
Mean Time to Recovery in Weeks	μ	1	1/Week
Contacts per Week	c	375	1/Week

The model runs for 31 weeks. Numerical integration is carried out using the Euler method with a time step of 10^{-5}. Primary model outputs examined here are susceptibles, the incidence case rate (in Persons/Week), and the count of infectives.

3.2 Particle Filter

3.2.1 Particle Characteristics

Recall that each particle for a particle filter at time t (X_t) is associated with a complete copy of the system state at that point in time. In this case, each particle at a point in time is associated with a value for each state variable (S, E, I, R). Dynamic models are typically approximations to more complex underlying situations, and often quantities commonly treated as fixed within such models (e.g., contact rate) evolve over time (e.g., as an infection spreads from core areas of a scale-free network to more peripheral regions). In order to investigate the capacity to use particle filtering to adapt to values of parameters whose effective values evolve over the course of a simulation, we further associate each particle with a value for the parameter *c*. Each particle in such scenarios is thus associated with a vector $[S, E, I, R, c]^T$.

3.2.2 Weight Update Rule

The particle state evolves over time. For this simple implementation of the particle filter, we make use of the previously contributed condensation algorithm (Isard and Blake 1998) in which the state at time t (X_t) is simply generated by sampling from the stochastic process model $p(X_t|X_{t-1})$ – that is, using the notation of the previous section, $q(X_t|y_t, X_{t-1}) = p(X_t|X_{t-1})$. In concrete terms for our example, this means that between measurements at times $t-1$ and t, we simply simulate forward each particle according to the state equations specified above. For the condensation algorithm, the weight update rule for a new datum received at measurement time t simply involves multiplying the existing weight by the likelihood of observing that datum (in our case, the number of reported cases within a week) given the system state associated with that particle; that is, using the notation above, $w_t^{(i)} = w_{t-1}^{(i)} g(y_t|X_t^{(i)})$.

In the cases where the effective sample size falls below 25% of the nominal sample size, resampling from particles is performed in accordance with Step 3 of the particle filtering algorithm presented in Section 2.

3.2.3 Likelihood Function

In the example model, observations provide weekly counts of individuals leaving the latent and incubation state and developing symptoms and becoming infective. In the model, we ignore the lag effects, and treat this as given by the rate of the "Incubation" flow (measured in incident individuals per week becoming cases, and abbreviated as i_t). Following Dorigatti et al. (2012), we treat the likelihood of observing y_t individuals within that week given an estimated weekly count of incident individuals i_t as follows:

$$p(y_t|x_t) = p(y_t|i_t) = \binom{y_t + r - 1}{y_t} p^{y_t}(1-p)^r$$

where $p = \frac{i_t}{i_t + r}$ is the probability that a given reported case is in fact a true incident case and r is a dispersion parameter. This formulation associates a non-zero probability density of observing reporting cases both above and below the posited number of actual cases (as captured by the stock and flow model). We note that in addition to the desire to approximate an important real-world processes involving case identification, use of a negative binomial (rather than a classic binomial) formulation is important for the robustness of the particle filtering in the context of process models stochastics. A more obvious alternative likelihood formulation – applied by the authors in the context of MCMC (Osgood and Liu 2015) – would treat the likelihood of observing a given count of reported cases in light of the particle as given by a binomial draw from i_t incident cases. While conceptually simple, a likelihood formulation causes problems because it exhibits 0 probability of yielding a reported cases count greater than the posited rate of those undergoing incubation associated within that particle. Situations where all particles are associated with rates of incubation smaller than the empirically observed data can trigger weights identically equal to zero across all such particles, causing a singularity during weight renormalization. This consideration provides a strong motivation for the negative binomial formulation used here.

4 EVALUATING PARTICLE FILTER PERFORMANCE

Given the highly aggregate character of the dynamic model described in section 3.1, the literature provides much reason to wonder (Kneeling and Eames 2005) about the degree to which – with particle filtering or without – that model is capable of robustly and reliably estimate model state using data arising from a far more complex underlying epidemiological process. Such concerns are magnified in the context of systematic biases in aggregate model parameters that frequently result from incomplete knowledge of the situation. While aggregate models can frequently be calibrated to characterize data arising from epidemiological processes (Rahmandad and Sterman 2008), such calibrated models may not accurately capture intervention tradeoffs, and reliably performing such calibration is difficult and burdensome when modelers initially lack empirical data and such data accumulates incrementally over time. In this section, we seek to investigate the capacity of particle filter to mitigate the effects of aggregation and biases in the aggregate model to estimate current epidemiological state.

While the particle filter described in the previous section can be applied to data from real-world outbreaks, it is difficult to assess the resulting accuracy improvements absent additional data concerning the underlying epidemiological situation – data that are often unavailable or infeasible to obtain. To more rigorously evaluate the effectiveness of that particle filter, we sought to construct a carefully designed test context in which the underlying epidemiological situation (the "ground truth") is precisely known, but which – like the external world – exhibits far more complex underlying dynamics than are depicted in the dynamic model.

Specifically, we evaluated the particle filter introduced above by comparing its estimates of 3 outcomes (count of susceptibles, the incidence case rate (in Persons/Week), and the count of infectives) against corresponding quantities drawn from an agent-based transmission model representing the richer underlying epidemiological processes. That "ground truth" model is discussed next.

4.1 Agent-Based Ground Truth Model

We constructed an agent-based transmission model with a population size identical (1000) to that of the aggregate model. Within the ABM, agents representing individual people were scattered according to a spatial Poisson process across a space of size 500 by 500. Experiments were conducted to evaluate the accuracy of the particle filter when agents were connected by four different types of networks: Distance-based, scale free, small world (with 95% of connections local), and Poisson. Parameters for all networks were set to yield a similar number (30) of connections per agent. The behavior of each agent was characterized by a probabilistic process. Specifically, a single index infective began in the infective state; all remaining agents began in a Susceptible state. Infective agents sent "exposure" messages to a neighbor (selected with uniform probability from their immediate connections) 350 times per week (50 times per day). Each such exposure event between an infective and susceptible conferred a probability of 0.01 of infection. A memoryless transition process was followed when proceeding from the latent ("Exposed") to the infective state, and from the infective to the recovered states, with rate constants identical to that used in the aggregate model; as in the aggregate model, time in those states was thus exponentially distributed, with respective mean resident times being identical in the two models.

Every week, two observer processes (Railsbeck and Grimm 2011) were undertaken. The first of these processes was used to generate the synthetic regular (noisy) reporting counts treated as empirical data within the particle filtering. Within that process, we assumed that each case emerging from latency and incubation into the infectious state would present for care and be reported. Reflecting the presence of further measurement noise, we further assumed that individuals not in the infectious state exhibit a certain probability per week of presenting for care with symptoms that would be erroneously reported as incident cases of illness.

While the first type of observer process associated with this model provided synthetic empirical data to be used by the particle filter, the second type of observer process was used to collect ground truth data for *evaluation of the accuracy of the particle filter*. Specifically, every week we collected across the population a count of susceptibles, infectives, exposed, and incident cases within the past week; these values were then used in the particle filter to compare to respective aggregate quantities.

To evaluate the performance of the particle filter under a variety of conditions, we ran scenarios for each network type (mentioned above). Because some of the networks involved in the agent-based "ground truth" model exhibit heterogeneity in connection counts – and, by extension, in the effective contact rate over time – for each such network, we further considered handling the contact rate *c* in the aggregate model in four different ways when performing particle filtering: As fixed at some incorrect value (375), as fixed at some correct value (350), as drawn from a continuous uniform distribution between 20 and 1200, or drawn initially from that range and then allowed to vary over time according to multiplicative random walk as described in Section 3.2 and with per-unit-time standard deviation 10.

Thus, for each combinations of the 4 network types, we ran 6 scenarios: Two baseline scenarios without particle filtering (one for a case of a correctly estimated contact rate, one for a biased contact rate), and then 4 with particle filtering (fixed correct contact rate, fixed biased contact rate, contact rate drawn from a distribution, and contact rate drawn from a distribution and then allowed to evolve according to a random walk). For each of these 24 scenarios, we ran an ensemble of 100 realizations.

The primary metric examined for the scenarios was a measure of discrepancy between the aggregate model estimates and the ground truth (as produced by the ABM model). The discrepancy metric was chosen to penalize both bias and dispersion in the aggregate simulation model results when compared with the ground truth value. Specifically, each week, we sampled 1000 times from the particles, where – in accordance with importance sampling practice – the probability of selection of a given particle was treated as proportional to its weight. For each such sample, we computed – and summed into a single number – the square of the differences between the value of the S, E, I, R state variables in the aggregate model and count of individuals who are in the corresponding disease state in the ABM. This number was normalized by the count of observations [31] and the count of particles sampled in each such observation [1000]. Once discrepancies were computed for all weeks, a square root was taken to yield a quasi-linear discrepancy measure.

In light of the stochastic nature of the aggregate model, we compared discrepancies associated with each scenario using per-scenario boxplots and non-parametric hypothesis testing between scenarios. For hypothesis testing, 1-Sided Mann-Whitney U Tests were performed to assess whether a given scenario using a specific network in the ground-truth model yielded discrepancies significantly below those of one or more reference scenarios for the same network. We specifically sought to examine the statistical significance differences observed in results between particle filtering scenarios and their corresponding scenarios absent particle filtering (but with the same network). Again within the context of identical ground-truth networks, we further sought to compare the statistical significance of the difference particle filtering with a distribution of contact rates against particle filtering with a correct contact rate, and of a particle filter with a distribution of contact rates and with a random walk in contact rates against a corresponding particle filter without a random walk.

5 RESULTS

Figures 1-4 each present boxplots showing discrepancies from ground truth of each scenarios for a particular network type. In each plot, the vertical axis shows the accumulated discrepancy, and successive columns indicate the scenario in the following order: A) No Particle Filtering with a biased contact rate estimate, B) No Particle Filtering with a correct contact rate estimate, C) No Particle Filtering drawing the contact rate from a uniform distribution (with an expected value different than the true contact rate), D) particle filtering with a biased contact rate estimate, E) particle filtering with a correct contact rate estimate, F) particle filtering with a drawing the contact rate from the same uniform distribution, and, finally, G) a similar particle filtering scenario where the initial contact rate is drawn from the same distribution, but then evolves according to a random walk. The final two cases are the only ones in which *c* serves as state variable of the particle filter differing across particles.

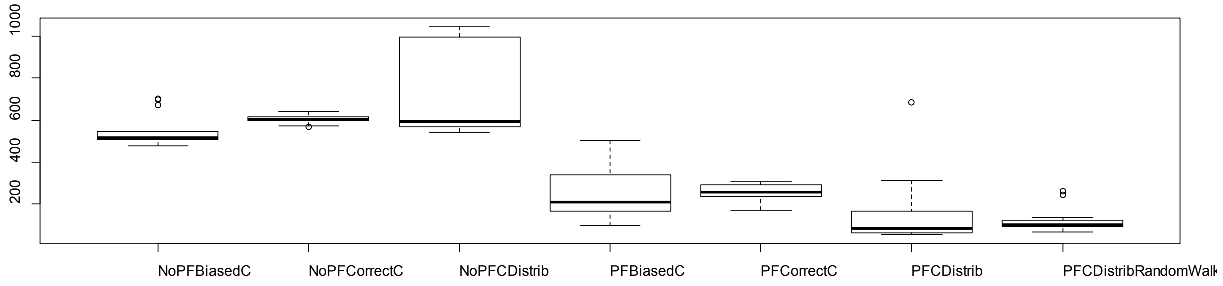

Figure 1: Scenarios for Scale Free Network.

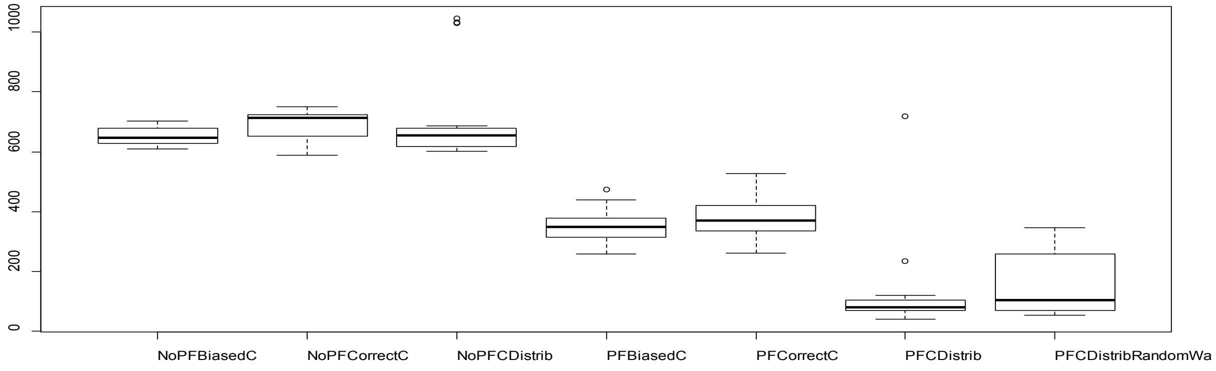

Figure 2: Scenarios for Random Network.

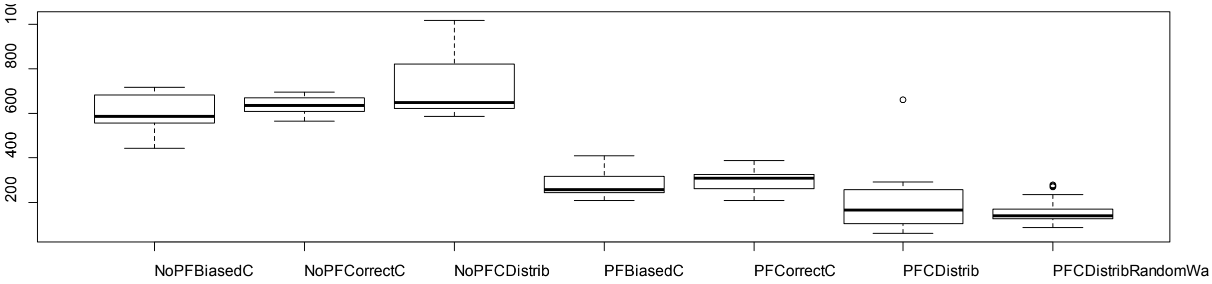

Figure 3: Scenarios for Small World Network.

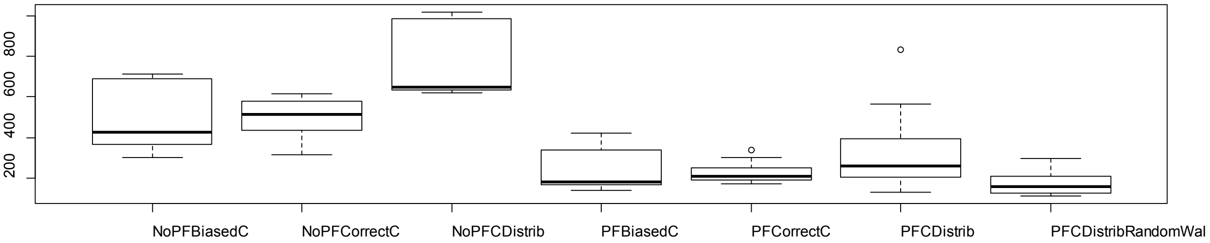

Figure 4: Scenarios for Distance-Based Network.

While results differ significantly by network type, a few general patterns can be discerned. Even for scenarios associated with a correct contact rate estimate (with or without the particle filter), a significant discrepancy was observed. This reflects the strong mediating influence of network structure on contagion (Keeling 2005, Keeling and Eames 2005), the limited capacity of random mixing to capture the effects of such structure, and the presence of significant stochastics within both the aggregate and ABM models.

For all networks, particle filtering reduced the discrepancy by several times compared to both the baseline case with a biased estimate of the contact rate and over the baseline case with a correct estimate of the contact rate. The occurrence of *any* type of particle filtering conferred a pronounced benefit – often by binary order of magnitude – even in the context of a fixed, bias contact rate. However, very significant additional benefit – often a factor of 2 or more – extended from use of particle filtering with a distribution of contact rates. Although not documented here, even if particles are initialized to a minimally informative distribution of contact rates (as here, uniformly distributed between 20 and 1200), the "survival of the fittest" associated with particle filtering's weighting and weight-based resampling tends to concentrate effective contact rates within a region of much tighter support. While commonly associated with state estimation, the particle filtering here performs a very effective form of parameter estimation.

By contrast, with the exception of the distance based networks – i.e., propinquity-enforcing networks where connections between two individuals are made only when those individuals lie within a certain distance of one another – very limited benefit extended from further incorporating a random walk in contact rates, beyond the basic provision of a distribution in in contact rates. For some networks (e.g., Poisson random and perhaps scale free), use of a random walk in contact rates appears to adversely affect results.

Table 2 reports the median discrepancy values for each scenario and network type in the underlying network. Table 3 indicates statistical significance of the differences between the particle filter results of a given network and corresponding (non-particle filtered) results for that same network. In all cases, the results were significant.

Table 2: Median Discrepancy by Scenario and Ground-Truth Network Type.

		No particle filtering			**With particle filtering**			
	Scenario	**Biased Contact Rate**	**Correct Contact Rate**	**Contact Rate Distrib.**	**Biased Contact Rate**	**Correct Contact Rate**	**Contact Rate Distrib.**	**Contact Rate Distrib. & Random Walk**
Underlying Network	**Scale-Free Network**	517.8	602.35	594.41	206.41	255.95	83.84	98.85
	Poisson Random Network	647.42	714.59	654.44	348.35	371.17	80.09	105.77
	Small World Network	584.28	633.26	648.75	258.14	308.61	167.42	137.73
	Distance Based Network	427.17	512.73	647.76	185.1	212.67	260.8	158.3

Table 3: Wilcoxon p-values for particle filtering scenarios when compared to stated reference scenarios.

	Correct Contact Rate	**Biased Contact Rate**	**Static Contact Rate Distribution**		**Contact Rate Distribution and Random Walk**		
Reference Scenario	Correct without PF	Biased without PF	Distrib. without PF	Correct c without PF	Distrib. without PF	Correct c without PF	Distrib. with PF
Scale-Free Network	7.254e-12**	5.078e-11**	2.706e-09**	1.969e-08**	7.254e-12**	7.254e-12**	0.8676
Poisson Random Network	7.254e-12**	7.254e-12**	8.792e-09**	3.685e-09**	7.254e-12**	7.254e-12**	0.9254
Small World Network	7.254e-12**	7.254e-12**	1.415e-09**	1.415e-09**	7.254e-12**	7.254e-12**	0.4521
Distance Based Network	1.451e-11**	1.442e-06**	2.706e-09**	3.455e-05**	7.254e-12**	7.254e-12**	0.000129**

6 CONCLUSIONS

In the increasingly rich data environment heralded as the era of "Big Data" and characterized by the "4 V's" – data velocity, volume, variety, veracity – a growing number of public health decision makers are grappling with the problem of leveraging structured understanding of the world in the context of incoming time series of data. While machine learning and classic statistical models form important elements in making sense of the growing volumes of available data, dynamic models provide a key element in delivering vale in this world due to their ability to capture causal theory and to address decision-making needs by virtue of their capacity to reason in the context of counter-factuals. The results shown in the previous section suggest that – over a variety of network types – particle filtering may be able to very significantly enhance the accuracy of model-based estimates of underlying epidemiological phenomena. These strengths persist even in the face of – and can help correct for – the distortions inevitably accompanying model aggregation (Osgood 2004) and significant and systematic misestimates of model parameters present within such models. Within the cases examined, particle filtering was able to aid not only in estimation of model state, but also in estimating model parameters, and – reflecting the presence of underlying heterogeneity and more complex epidemiological processes in the system from which data is drawn – adapting to evolution in the effective value of parameters that would otherwise be treated as static. It is notable that applying a contact rate distribution during particle filtering confers clear benefits for at least some network types; this allows more accurate contact rate estimates to emerge during the simulation, through the "survival of the fittest" process typical of the particle filter. By contrast, allowing that contact rate to evolve dynamically was associated with demonstrable benefit for only distance based networks.

It is notable that the particle filtering methods examined here were able to confer these benefits – including recurrent incorporation of newly emerging data – in a fully automated fashion. The results raise the tantalizing possibility that particle filtering may allow rough, quickly assembled aggregate models that are recurrently and automatically regrounded by emerging data may be able to serve as reliable projection and intervention-evaluation vehicles. This envisioned "closed loop" modeling can help reduce the chance that a model – once delivered – gathers dust, and instead enhances the chance that they will serve as living documents as part of an on-going decision support system offering reliable projection abilities even in the face of highly unexpected eventualities that lie outside the scope of the model.

The prospects of the approach are particularly attractive because of the conceptually straightforward nature of adapting models for use with the particle filter, and the simple implementation involved, and the notable generality of the method when compared with the stiff restrictions – distributionally, in terms of model formulation – associated with some other predictor-corrector methods. Just as it is accepted wisdom that even the best mental model of a route from one city to another would not allow one to drive that distance with one's eyes closed, so it may become accepted that it is suspect to rely upon a dynamic model to plan in a fashion that does not readily adapt to incoming data.

Many priorities remain for future work. It will be important to evaluate similar, stylized models against more sophisticated "ground truth" models. Experience in applying particle filtering in other contexts also suggests that particle impoverishment may result from prolonged time series (Murphy 2012) while it remains unclear how strong this risk is in the context of stochastic processes, it merits investigation. In addition, the simple measurement updating scheme used here – based upon the condensation scheme (Isard and Blake 1998) – may perform poorly when used with much longer times between measurement updates. It is also not clear that an aggregate and biased model whose state is sampled via particle filtering will yield accurate estimates of intervention tradeoffs when used to evaluate policy scenarios. Finally, in some scenarios associated with high-variance random walks in the contact rate, we encountered conditions where round-off causes the weights of all particles to be treated as zero; implementation of a different approach to weight normalization will be required for such cases.

A distinct class of needs relates to software (and particularly API) support for particle filtering. While this technique offers sufficient generality to be used with a wide range of modeling architectures – System Dynamics, agent-based modeling, discrete event simulation, etc. – the requisite software support is often not present to make its application feasible. For example, most agent-based modeling packages and discrete event modeling lack APIs supporting creating a model stratified by particles. Given the memory demands associated with agent-based models, naïve attempts to apply particle filtering for such models could easily encounter severe difficulties. As a key final area of future work, we wish to advance the suggestion that creators of frameworks consider putting in place mechanisms for easily and transparently creating particle filters together with the models represented in those frameworks.

REFERENCES

Anderson, R. M., and R. M. May. 1991. *Infectious diseases of humans : dynamics and control.* Oxford ; New York: Oxford University Press.

Andrieu, C., A. Doucet, and R. Holenstein. 2010. "Particle Markov chain Monte Carlo Methods (with discussion)." *Journal of the Royal Statistical Society B*, 72:269-342.

Defoe, D. 2010. *A journal of the plague year.* Oxford University Press.

Dorigatti, I., S. Cauchemez, A. Pugliese, and N. M. Ferguson. 2012. “A new approach to characterising infectious disease transmission dynamics from sentinel surveillance: application to the Italian 2009–2010 A/H1N1 influenza pandemic.” *Epidemics*, 4(1), 9-21.

Doucet, A., and A. M. Johansen. 2009. “A tutorial on Particle Filtering and Smoothing: Fifteen years later.” *Handbook of Nonlinear Filtering*, 12, 656-704.

Dukic, V., H. F. Lopes, and N. G. Polson. 2012. “Tracking epidemics with state-space SEIR and Google Flu Trends.” Unpublished manuscript.

Gelb, A. and Analytic Sciences Corporation. Technical Staff. 1974. *Applied optimal estimation.* Cambridge, Mass.: M.I.T. Press.

Gordon, N. J., D. J. Salmond, and A. F. Smith. 1993. “Novel approach to nonlinear/non-Gaussian Bayesian state estimation.” In *IEE Proceedings F (Radar and Signal Processing)* (Vol. 140, No. 2, pp. 107-113). IET Digital Library.

Isard, M., and A. Blake. 1998. “Condensation—conditional density propagation for visual tracking.” *International journal of computer vision*, *29*(1), 5-28.

Keeling, M. J. 2005. “The implications of network structure for epidemic dynamics.” *Theoretical population biology,* 67(1), 1-8.

Keeling, M. J., and K. T. D. Eames. 2005. “Networks and epidemic models.” *Journal of The Royal Society Interface,* 2(4), 295-307.

Kermack, W. O., and A. G. McKendrick. 1927. A Contribution to the Mathematical Theory of Epidemics. *Proceedings of the Royal Society of London A,* 115(772), 700-721.

Murphy, K. P. 2012. *Machine Learning: A Probabilistic Perspective*. The MIT Press.

Osgood, N. D. 2004. “Representing Heterogeneity in Complex Feedback System Modeling: Computational Resource and Error Scaling. “ Paper presented at the *22nd International Conference of the System Dynamics Society*.

Osgood, N. D. and J. Liu. 2015. “An Introduction to Using Markov Chain Monte Carlo Approaches with Dynamic Models” accepted (with revisions) December 2013 for inclusion in Rahmandad et al., *Analytical Handbook for Dynamic Modelers*. Cambridge MA. MIT Press (forthcoming).

Qian, W., N. D. Osgood, and K. G. Stanley. 2014. “Integrating epidemiological modeling and surveillance data feeds: a Kalman filter based approach.” Accepted December 20, 2013 for oral presentation and publication in *Proceedings the 2014 International Social Computing, Behavioral Modeling and Prediction Conference* (SBP14).

Rahmandad, H., and J. D. Sterman. 2008. “Heterogeneity and Network Structure in the Dynamics of Diffusion: Comparing Agent-Based and Differential Equation Models. ”*Management Science,* 54(5), 998-1014.

Railsback, S. F., and V. Grimm. 2011. *Agent-Based and Individual-Based Modeling: A Practical Introduction.* Princeton University Press.

AUTHOR BIOGRAPHIES

NATHIANIEL OSGOOD is an Associate Professor in the Department of Computer Science at the University of Saskatchewan specializing in the creation and application of computational, data science and informatics tools to inform public health decision making received a Ph.D. in Computer Science from MIT. His email address is osgood@cs.usask.ca.

JUXIN LIU is an Associate Professor in the Department of Mathematics and Statistics at the University of Saskatchewan. She received a Ph.D. in Statistics from the University of British Columbia. Her email address is liu@math.usask.ca.