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Recent Advances in Group-Based Trajectory Modeling for Clinical Research

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Abstract

Group-based trajectory modeling (GBTM) identifies groups of individuals following similar trajectories of one or more repeated measures. The categorical nature of GBTM is particularly well suited to clinical psychology and medicine, where patients are often classified into discrete diagnostic categories. This review highlights recent advances in GBTM and key capabilities that remain underappreciated in clinical research. These include accounting for nonrandom subject attrition, joint trajectory and multitrajectory modeling, the addition of the beta distribution to modeling options, associating trajectories with future outcomes, and estimating the probability of future outcomes. Also discussed is an approach to selecting the number of trajectory groups.

Contents

INTRODUCTION

A trajectory describes the course of one or more repeated measures—whether a behavior, status, symptom, or biomarker—over age or time. Methods for identifying and analyzing trajectories abound. Among the most popular in clinical psychology and medicine is group-based trajectory modeling (GBTM) (Nagin 1999, 2005), which is also called growth mixture modeling (Muthén 2001). GBT models are designed to identify a finite number of clusters of individuals following similar trajectories. The categorical nature of GBTM is particularly appealing in clinical psychology and medicine, where patients are often classified into discrete diagnostic categories.

In 2010, the *Annual Review of Clinical Psychology* published "Group-Based Trajectory Modeling in Clinical Research" (Nagin & Odgers 2010). Since the appearance of that review there has been an exponential growth in applications of GBTM in clinical psychology and medicine. PubMed reports 101 citations to GBTM in 2010. By the close of 2022 that count had grown to 858.

The purpose of this review is to highlight advances in GBTM that either have appeared since the 2010 review or, in our judgment, have underappreciated relevance to clinical research. These include accounting for the impact of nonrandom subject attrition, joint trajectory and multitrajectory modeling, the addition of the beta distribution to modeling options, associating trajectories to future outcomes, and estimating the probability of future outcomes. Also discussed is an approach to selecting the number of trajectory groups. Before turning to these topics, we offer a brief history and overview of GBTM. For fuller elaboration, readers are referred to Nagin & Odgers (2010) and Nagin (1999, 2005).

A BRIEF HISTORY AND OVERVIEW OF GROUP-BASED TRAJECTORY MODELING

As noted, GBTM is designed to identify clusters of individuals following approximately the same trajectory of the measure(s) of interest. The unit of observation is typically an individual, but there are applications to organizations (Hasan 2012) and spatial units (Weisburd et al. 2004). Whatever the unit of observation, estimation of GBTM requires longitudinal data on that unit

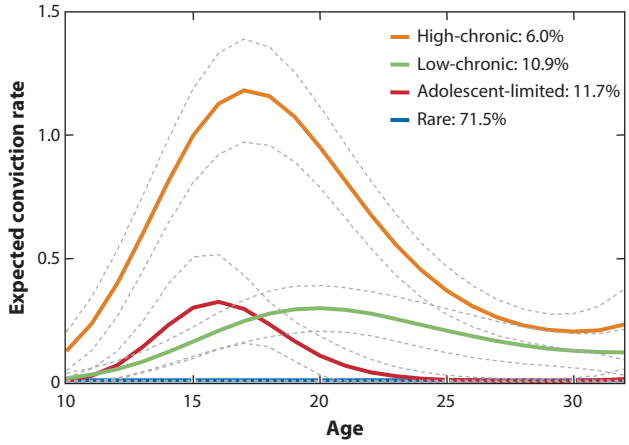

Figure 1

Four-group trajectory model of expected conviction rate with 95% confidence intervals (Cambridge Study in Delinquent Development; Farrington & West 1990).

of observation and consistent assessment of the measure of interest on the same scale. For expositional convenience, hereafter we refer to the unit of analysis as the individual or patient.

Figure 1 reports the first application of GBTM in a domain far from clinical psychology and medicine: criminology (Nagin & Land 1993). For this initial application, GBTM was applied to data from the Cambridge Study in Delinquent Development, which tracked 411 British males born in 1953 (Farrington & West 1990). The trajectories are based on the annual total number of convictions of each individual from ages 10 to 32. Four distinctive trajectory groups were identified: The largest group, estimated to compose 71.5% of the overall cohort, followed a trajectory of no convictions or at most one conviction from ages 10 to 32. A second group, called the adolescent-limited group, followed a rising and then falling trajectory over adolescence. This group was estimated to compose 11.7% of the overall cohort. The two final groups, called the high- and low-chronic groups, followed trajectories of active offending throughout the observation period. They were, respectively, estimated to compose 6.0% and 10.9% of the overall cohort. Since this inaugural application in criminology, GBTM came to be applied widely in developmental psychology, then clinical psychology, and, in the past decade, medicine.

Regardless of application domain, the most fundamental outputs of a GBTM are the shapes of the distinct trajectory groups and the probability of trajectory group membership, which measures the proportion of the population following each distinct trajectory group. As discussed below, from these quantities another fundamental quantity, the posterior probability of group membership (PPGM), can be calculated; it measures the probability that a specific individual follows each of the trajectories. Trajectories are typically specified to follow a polynomial function over age or time of an order specified by the user.

Technically, a GBT model is an example of a finite mixture model. The fundamental concept of interest is the distribution of repeated measures conditional on age or time—that is, the distribution of outcome trajectories denoted by $P(Y_i \mid Age_i)$, where the random vector Y_i represents individual i's longitudinal sequence of repeated measures, and the vector Age_i represents individual i's age when each of those measurements is recorded. Trajectories can also be defined by time—for example, time from treatment. GBTM assumes that the population distribution of trajectories arises from a finite mixture of unknown order J. The likelihood of the observed data Y_i for each

individual i, conditional on the number of groups, J, may be written as

$$P(Y_i|Age_i) = \sum_{j=1}^{J} \pi^j \cdot P(Y_i|Age_i, j; \beta^j), \quad 1.$$

where π^j is the probability of membership in group j, and the conditional distribution of Y_i given membership in group j is indexed by the unknown parameter vector β^j, which among other things determines the shape of the group-specific trajectory. For a given group j, conditional independence is assumed for the sequential realizations of the elements of Y_i and y_{it} over the T periods of measurement. Thus, we may write

$$P(Y_i|Age_i, j; \beta^j) = \prod_{t=i}^{T} p(y_{it}|age_{it}, j; \beta^j), \quad 2.$$

where $p(.)$ is the distribution of y_{it} conditional on membership in group j and measurement at time t (for a discussion of the conditional independence assumption, see Nagin 2005, chapter 2).[1] If desired, the group size parameter π_j can be specified to vary conditionally as a multinomial function of baseline covariates. For elaborations, readers are referred to Nagin (2005) and Nagin & Odgers (2010).

One of the most valuable outputs of GBTM, beyond the trajectories themselves and the probability of trajectory group membership, is the posterior probability of group j membership (PPGMj). As implied by the adjective "posterior," the PPGMj is a postestimation quantity. It is calculated according to Bayes's rule based on the maximum-likelihood parameter estimates, $\hat{\beta}^j$ and $\hat{\pi}^j$:

$$\hat{P}(j|Y_i) = \frac{\hat{P}(Y_i|j)\hat{\pi}_j}{\sum_j^J \hat{P}(Y_i|j)\hat{\pi}_j}. \quad 3.$$

That is, for each individual i, the PPGMj calculates the probability that the individual's observed longitudinal sequences of trajectory measurements, Y_i, are the outcome of each trajectory group j. Thus, across trajectory groups for each individual i, the posterior probabilities sum to 1. Returning to the introductory example of GBTM based on the data from the Cambridge Study in Delinquent Development, for an individual with a sustained high level of convictions over time, the PPGM for each of the two chronic groups would be high, and for the never/occasionally offending group it would be low. Conversely, for an individual with no convictions or perhaps only a few, the magnitude of these posterior probabilities would be reversed.

The posterior probabilities have many valuable uses. As described by Nagin (2005), they form the basis for several of the criteria for assessing the quality of fit for a particular GBT model. They can also be used to create profiles of the baseline characteristics of individuals following each of the trajectory groups. As discussed below, they also play a crucial role when associating trajectories with distal outcomes and when predicting future outcomes.

DETERMINING THE NUMBER OF TRAJECTORY GROUPS

Finite mixture modeling is used for two distinct purposes. One is to identify subpopulation characteristics in circumstances in which the population is composed of literally distinct groups that cannot be identified ex ante and thereby separately analyzed. For such applications, the number

[1]The applications reported in this review use trajectory estimation software that is freely available at **https://andrew.cmu.edu/user/bjones/traj**. That software is designed to operate on either the SAS or Stata statistical software platform. It provides four distributional options for $p(.)$—censored normal, zero-inflated Poisson, logit, and beta—but in general, there is no restriction on the form of $p(.)$.

of groups in the mixture, denoted *J*, is a theoretically well-defined quantity. A second use is to approximate the distribution of a characteristic of interest when the specific form of the population distribution is unknown (McLachlan & Peel 2004). For this type of application, *J* is less well defined.

As discussed at length by Nagin (2005), in the context of GBTM, few applications fit the first setting. Unlike some biological or physical phenomena, in which populations may be composed of literally distinct groups such as different types of animal or plant species, population differences in trajectories of behaviors or symptoms are unlikely to reflect such bright-line differences. To be sure, there are many taxonomic theories that predict different trajectories of development across subpopulations (e.g., Belsky et al. 1991, Kandel 1975, Loeber 1991, Moffitt 1993, Patterson et al. 1989), but the purpose of such taxonomies is practical—for example, to draw attention to differences in the causes and consequences of different trajectories within the population. They are not meant to suggest that the population is composed of literally distinct groups. As William Baumol (1992, p. 55) observed, "A well-designed model is, after all, a judiciously chosen set of lies, or perhaps more accurately put, partial truths about reality, which have been chosen so as to permit us to reason more effectively about some issue than we otherwise could."

The idea of using an approach such as a GBT model that relies on discrete grouping to describe the behavior of a population in which such distinctions do not literally exist is a standard procedure in nonparametric and semiparametric statistics (Follman & Lambert 1989, Heckman & Singer 1984, Lindsay 1995). This procedure is easily illustrated with an example. **Figure 2*a*** depicts the continuous distribution of some behavior *z* within a population. In **Figure 2*b***, this same

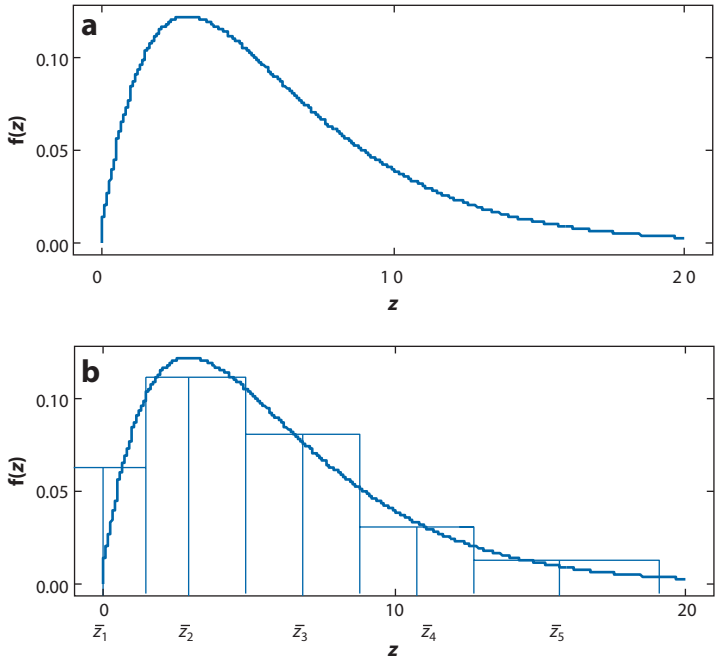

Figure 2

Use of a finite mixture model to approximate an unknown population distribution of trajectories. Panel *a* depicts a hypothetical unknown distribution, and panel *b* depicts the finite mixture model approximation. Figure adapted with permission from Nagin (2005); copyright 2005 by the President and Fellows of Harvard College. All rights reserved.

distribution is replicated and overlaid with a histogram that approximates its shape. **Figure 2*b*** illustrates that any continuous distribution with finite endpoints can be approximated by a discrete distribution composed of a finite number of "points of support" (i.e., the "pillars"). For any given number of points of support, maximum-likelihood estimation can be used to estimate two sets of parameters. The first identifies the location on the horizontal axis of each point of support. In **Figure 2*b***, these points are denoted by $\bar{z}_1, \bar{z}_2, \bar{z}_3 \ldots$, where $\bar{z}_j$ measures the average behavior of individuals at the *j*th point of support. A second set of parameters measure the proportion of the population, π_j, at each point of support (i.e., the "height" of the point of support). These proportions must sum to 1, but they are in general not equal. In GBTM, the estimate of π_j corresponds to the proportion of the population whose trajectory is best approximated by group *j*. If a third dimension were added to **Figure 2*b*** measuring the trend of $\bar{z}_j$ over time, each of these points of support would correspond to the trajectory groups depicted, for example, in **Figure 1**.

The capacity of finite mixture models to approximate unknown distributions is important because no theory in social, behavioral, or biomedical sciences predicts the exact form of the population. Instead, that distribution must be approximated in some fashion. Understanding that this approximation is the objective of GBTM has important implications for the selection of the number of trajectory groups. One is that a search for the true number of groups is a quixotic quest. In fact, in any given application it is most likely that there is no true number. The model is just an approximation of an unknown, likely continuous, distribution of measurements over time.

Another implication concerns the procedure used for specifying the number of groups, *J*. Notwithstanding the reality that there is no true number of groups, a common feature of model search procedures (cf. Muthén & Shedden 1999, Nagin 2005, van der Nest et al. 2022) is to optimize one or more statistics estimating goodness of fit to identify the optimal number of groups. Commonly used statistics include Bayesian information criteria, the Akaike information criterion, entropy, and the Lo–Mendell–Rubin statistic. Optimizing one or more of these statistics is only an initial step. In practice, the statistic commonly does not maximize but instead continues to improve as more groups are added. This is likely a reflection of a continuous underlying population distribution.

What then to do in this circumstance? Returning to the objective of GBTM—to identify distinctive features of the underlying distribution—a final chosen model should include the fewest groups necessary to capture distinctive trajectory clusters that are relevant to the research questions of interest. To be concrete, if the objective is to study the developmental course of conduct disorder, the selected model should be the model that identifies distinctive trajectories of conduct disorder. For example, a model that identifies a trajectory of chronically elevated conduct disorder and a trajectory that is initially elevated but then declines may be of interest, while a model that combines these two distinct trajectories may be less relevant. Such trajectories are typically compared with a trajectory of no or very few conduct disorder symptoms. Because most individuals in a population sample follow such a low- or no-conduct-disorder trajectory, this group is typically the largest group as measured by the probability of trajectory group membership. Once the distinctive elevated trajectories are identified along with the low-disorder group, adding still another trajectory group, even if the preferred model selection statistic improves, usually results in the splitting of the large low-conduct-disorder trajectory group in a fashion that distinguishes different forms of a low- or no-conduct-disorder symptom. Because such a distinction is unlikely to advance the study's research objective, we recommend the more parsimonious model. More generally, the aim of the model search process should be to identify the model with the smallest number of trajectory groups that captures distinctive features of the population distribution of trajectories that are relevant to the study's objectives.

Two other considerations may influence final model selection. One is the size of the trajectory groups. Very small trajectory groups may simply reflect random data fluctuation. We therefore recommend against including groups with fewer than 30 individuals, calculated by multiplying the probability of trajectory group membership by the number of participants in the longitudinal study.

A second consideration is whether the model passes the adequacy tests laid out by Nagin (2005, chapter 4), which can be conveniently calculated with software developed by Klijn et al. (2015).

ADVANCES IN GROUP-BASED TRAJECTORY MODELING

We now highlight recent advances in GBTM and key capabilities that remain underappreciated in clinical research.

Nonrandom Attrition

We first highlight a capability of GBTM of particular relevance to clinical psychology and medical research: nonrandom attrition of subjects over time. Having nonrandom missing data due to dropout or loss to follow-up is a common problem in longitudinal research. The problem may be particularly severe in studies involving the elderly, the severely ill, or individuals with significant behavioral problems. Dropout may also disproportionately affect individuals from disadvantaged backgrounds. Whatever the cause, having data missing not at random may compromise the validity of research findings, particularly with respect to subgroups with high dropout rates.

The GBT models discussed thus far assume data are missing at random, as is common in most statistical methods. The GBTM extension by Haviland et al. (2011) was designed to account for nonrandom attrition. The Haviland et al. (2011) approach distinguishes two forms of missing data, as illustrated in **Figure 3**. The figure reports outcomes over six measurement occasions for four hypothetical study participants. Subject 1 has no missing assessments. Subject 2 has intermittent missing data. While assessments are missing in periods 4 and 5, an assessment is recorded in period 6, thereby indicating that the subject did not drop out. In the Haviland et al. (2011) extension, intermittent missing data are treated as missing at random. Subject 3 is an example of what Haviland et al. (2011) treat as nonrandom attrition (i.e., dropout) because there are no further assessments of this individual following assessment period 4. Finally, Subject 4 is an example of an

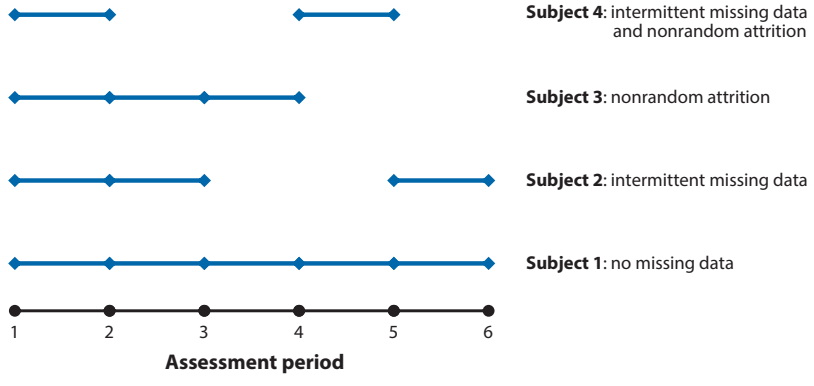

Figure 3

Two types of missing data—intermittent missingness and nonrandom attrition—for four hypothetical individuals in a six-period longitudinal study. Nonrandom attrition occurs for Subjects 3 and 4, who drop out before period 6. Figure adapted with permission from Haviland et al. (2011).

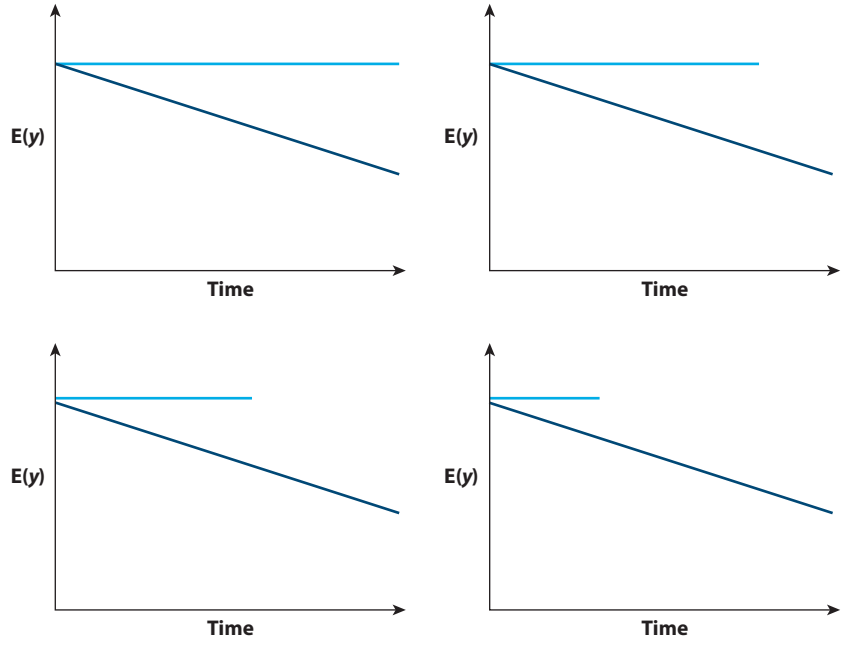

Figure 4

Two-group models with varying dropout probabilities for the group following the horizontal trajectory. Shorter trajectories denote higher dropout rates; E(*y*) denotes the expected value of the variable modeled by the trajectory. Figure adapted with permission from Haviland et al. (2011).

individual with both intermittent missing data and nonrandom attrition. Haviland et al. (2011) extend the basic GBTM by estimating trajectory group–specific dropout probabilities. This allows for the possibility that dropout rates may be higher for individuals following a trajectory of severe symptoms or illness compared with the dropout probability of individuals following trajectories of less severe symptoms or illness.

Based on simulations, Haviland et al. (2011) show that a model that does not account for dropout is most biased in its estimates of trajectory group size. This bias is most pronounced in circumstances where the groups are initially not well separated and there are large differences in the probability of dropout between groups. **Figure 4** illustrates this situation for a simple two-group model. In the initial period, both groups have the same mean trajectory value. Thereafter, the estimated trajectory for one group declines linearly, whereas the estimated trajectory of the other group remains unchanged. Further suppose for this stylized illustration that dropout is limited to the group following the unchanging trajectory. The shortened lengths of the constant trajectory in successive panels in **Figure 4** are meant to represent the effect on data availability of successively higher rates of dropout from the constant trajectory: Higher dropout rates will result in fewer and fewer individuals over time in the constant trajectory to support accurate estimation of its size and course. Because the trajectories separate over time, more data in each assessment period will make it easier statistically to detect their distinctive paths. However, as the per-period dropout rate from the flat trajectory increases, data for distinguishing it from the declining trajectory will become increasingly sparse. As a result, its presence will become increasingly difficult to statistically detect. These simulations demonstrate that as the dropout rate from the constant trajectory increases for the model without the dropout extension, the estimated size of the constant-trajectory group is progressively underestimated: It is estimated to be ever smaller than its actual size in the simulated

data. There is no such bias in the model with the dropout extension. Interestingly, dropout does not materially bias estimates of the trajectories themselves.

Haviland et al. (2011) apply the dropout model to data from the National Institutes of Health (NIH)-supported Chinese Longitudinal Healthy Longevity Survey (CLHLS), a four-wave survey conducted in randomly selected counties and cities in 22 Chinese provinces. The baseline sample, which was collected in 1998, included 8,805 individuals between ages 80 and 105. Haviland et al. (2011) focus on development of disability in this very elderly sample as measured by Katz's original Activities of Daily Living (ADL) scale (Katz et al. 1963). The inability to conduct one or more ADLs independently is considered a disability. The greater the number of inabilities, the more severe the disability.

Not surprisingly for such an elderly study population, the main form of dropout from the study was death. By the latest available wave of data collection in 2005, 69% of study participants had died. The Haviland et al. (2011) application was restricted to individuals who were similar in age at baseline, 90–93 years old, and excluded individuals who dropped out of the study for reasons other than death. The illustrative application was based on the three-group model. All trajectories are rising as expected—aging limits the capacity to carry out ADLs, but one from an initially high level of disability, another from a medium level, and a third from a low level. Consistent with simulation results, there were no material differences in the trajectories themselves between the models with and without dropout correction. There were, however, differences in the proportion of the sampled population following each trajectory as measured by the probability of trajectory group membership. The differences were due to marked differences in the probability of dropout due to death across trajectory groups. In the high-disability trajectory, the probability of dropout due to death between measurement occasions was 0.64, whereas for participants following the low-disability trajectory, that probability was nearly 50% smaller at 0.34. Consequently, probability of membership in the high-disability trajectory was 0.13 for the model without the dropout correction and 0.21 for the model with the correction. The counterpart probabilities for the low-disability trajectory were 0.27 for the model without the correction and 0.20 for the model with the correction.

While beyond the scope of this review, there is an extended discussion by Haviland et al. (2011) of the implications of dropout due to death versus dropout due to participants' exiting the study but remaining alive. The distinction is clinically important because participants who drop out due to death are no longer in the population under study, whereas those who drop out for other reasons remain in the population. This difference has important implications for extrapolating study findings to the clinically relevant population: the living.

Joint Trajectory and Multitrajectory Modeling

Development and progression of psychiatric disorders and other diseases typically result from an intricate interplay of complex, interdependent, and measurable signals (Ritchie et al. 2015). Thus, describing the trajectories of multiple measures of illness severity and/or mediators of disease progression as they evolve together over time is essential. Conventional statistical tools often do not take full advantage of available information in multivariate longitudinal data to study such relationships. In this section, we demonstrate two generalizations of GBTM, joint trajectory modeling and multitrajectory modeling, which are designed to address this need.

Joint Trajectory Modeling

The joint trajectory model, which was first reported by Nagin & Tremblay (2001) and is described in greater detail by Nagin (2005, chapter 8), links trajectories for two different repeated

measures, *i* and *j*, that are thought to be interrelated. It has three key outputs: (*a*) the polynomials describing the trajectory groups for both measures, (*b*) the probability of membership in the trajectory groups of *i* (p_i) and *j* (p_j), and (*c*) conditional probabilities linking *i* and *j*; $p_{i|j}$ and $p_{j|I}$; and the joint probabilities of trajectories *i* and *j*, p_{ij}. The conditional probabilities are the key advance of the joint trajectory model. Compared with the use of a single summary statistic to measure the association of two repeated measures, the conditional probabilities provide a far more detailed and varied summary of the interconnections between the measurements under study.

Joint trajectory modeling can be used to analyze the relationship between metrics that evolve contemporaneously over time (e.g., depression and alcohol use) or that evolve over different time periods that may or may not overlap (e.g., prosocial behavior in childhood and school achievement in adolescence).

The joint trajectory model can also be used to analyze the connection between the behaviors of distinct individuals who are thought to influence each other. We illustrate joint trajectory modeling with such an example with a summary of the finding of Loughran et al.'s (2017) analysis of the intergenerational transmission of substance use. The study uses longitudinal data on 427 parent–child dyads from Rochester, New York. Longitudinal data on substance use were available for generations 2 and 3 (G2 and G3), for whom the frequency of alcohol and marijuana use was assessed annually from ages 14 to 18.

Figure 5 shows the substance use trajectories for G2 and G3. Across generations, the substance use trajectories, which Loughran et al. (2017) label low, moderate, and chronic, are very similar in shape and size. As measured by the probability of trajectory group membership, the low trajectory is by far the largest for both generations, and the chronic trajectory is the smallest.

Figure 6 reports the conditional probabilities of trajectory group membership for G3 given their parents' G2 trajectories. Loughran et al. (2017) color-coded the entries according to whether the child follows the parent's childhood trajectory (continuity), the child follows a trajectory of lower substance use than the parent's childhood trajectory (resilience), or the child follows a trajectory of higher substance use than the parent's childhood trajectory (escalation). For individuals whose parents followed the low trajectory in their childhood, the great majority, 74%, also follow the low trajectory (i.e., continuity). For those whose parents followed either of the two higher trajectories in their childhood, the dominant pattern is resilience. Escalation is unusual.

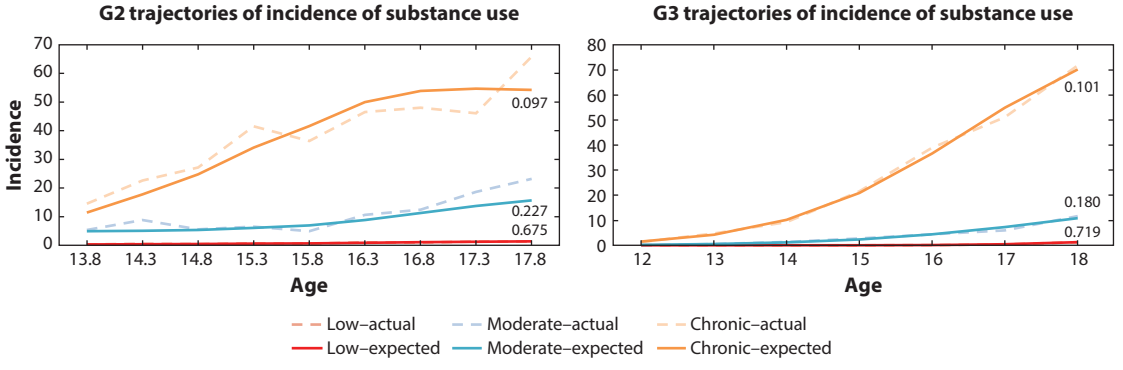

Figure 5

Intergenerational continuity in the actual and predicted incidence of substance use (Rochester Youth Development Study). Trajectory group probabilities are shown for each group on the right-hand side of each subpanel. The G2 trajectories are for the parents, and the G3 trajectories are for their children. Figure adapted with permission from Loughran et al. (2017).

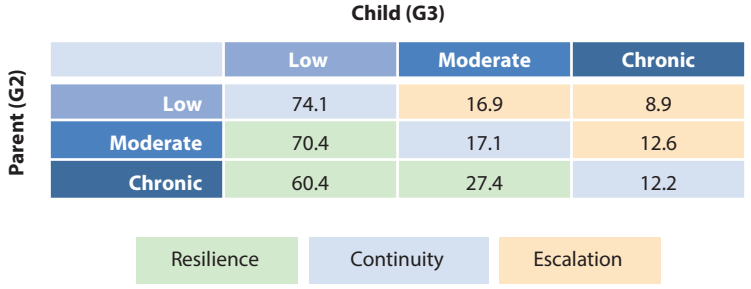

Figure 6

Transition conditional probabilities, *P* (G3|G2), linking parent (G2) substance use trajectory to child (G3) substance use trajectory. Continuity denotes the child following the same trajectory as the parent, resilience denotes following a trajectory of lower use than the parent, and escalation denotes following a higher use trajectory than the parent. Figure adapted with permission from Loughran et al. (2017).

This model can be extended to analyze whether the conditional probabilities linking trajectories across *i* and *j* vary as a function of individual characteristics. For this extension, the conditional probabilities are specified to follow the conditional logit distribution. This extension is illustrated with an analysis reported by Loughran et al. (2017) that examines the effect of parental substance use when the G3 child was age 10 on the conditional probabilities linking the child's G3 trajectory given the parent's G2 trajectory.

Figure 7 reports the probability of the G3 child following the chronic trajectory conditional on parental substance use or not when the child is age 10 and on the trajectory followed by the parent during their childhood. The analysis shows that parental substance use when the child is 10 is associated with a material increase in the probability of the child following the chronic trajectory for parents who followed the moderate or chronic trajectory in their childhood but not for parents who followed the low trajectory in their childhood.

Multitrajectory Modeling

One of the main strengths of joint trajectory modeling is that it highlights heterogeneity in the linkage between trajectories of distinct metrics in the form of a table of conditional probabilities rather than a single summary measure of association such as a correlation. Its downside is that it is a bulky form of analysis for relating trajectories across more than two types of repeated measures.

Current parent substance use G3 age 10

	Low	Moderate	Chronic
No	0.07	0.07	0.06
Yes	0.07	0.11	0.14

Figure 7

Probability of transitioning to a chronic child trajectory depending on parent substance use trajectory and parent substance use when the child is age 10. Parental substance use when the child is 10 is associated with an increased probability of the child following the chronic trajectory if their parent followed the moderate or chronic trajectory but not if their parent followed the low trajectory. Figure adapted with permission from Loughran et al. (2017).

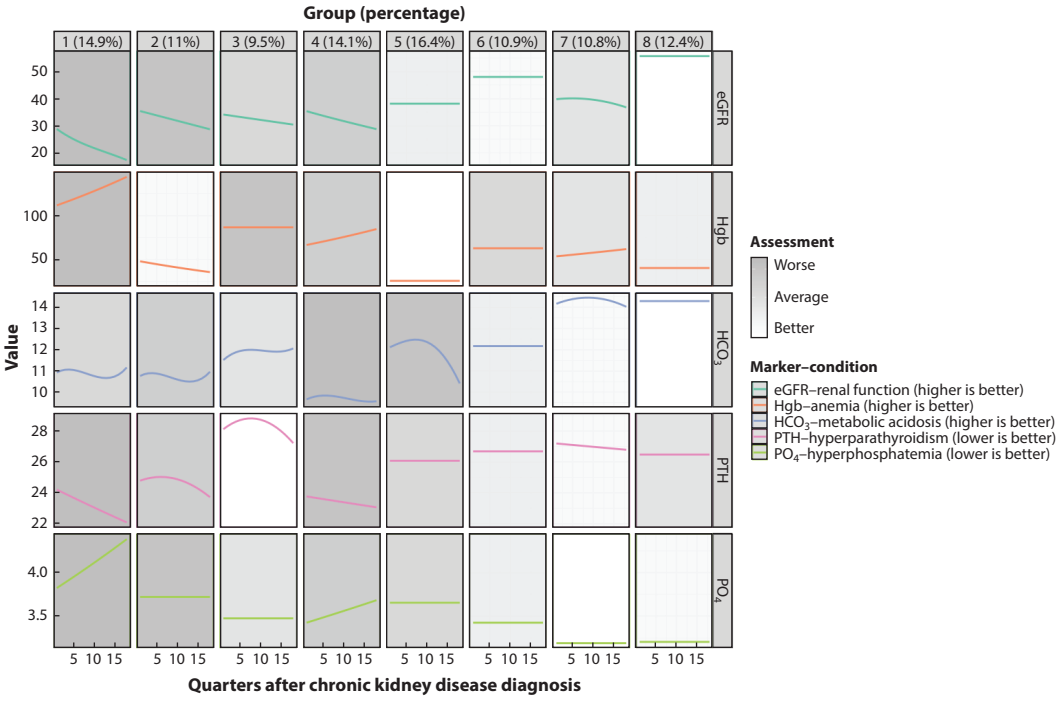

Figure 8

Eight-group multitrajectory model of kidney functioning (as indicated by eGFR) and comorbidities of chronic kidney disease. Trajectories show that poor eGFR is associated with elevated levels of comorbidities in the quarters following a stage III chronic kidney disease diagnosis. Abbreviations: eGFR, estimated glomerular filtration rate; HCO_3, bicarbonate; Hgb, hemoglobin; PO_4, phosphate; PTH, parathyroid hormone. Figure adapted from Burckhardt et al. (2016).

While in principle a joint trajectory model can be expanded to higher-dimensional settings, the number of conditional probability tables quickly becomes unmanageable. A joint trajectory model involving three metrics requires three tables of conditional probabilities; a four-metric model requires six such tables. Multitrajectory models are designed to avoid the problem of the proliferation of conditional probability tables by defining each trajectory group in terms of multiple measurements assessed over time.

Figure 8 illustrates a multitrajectory model applied to the study of the course of chronic kidney disease (CKD). The data used to estimate the model were extracted from the records of a large nephrology practice and include 1,944 patients diagnosed with stage III CKD between January 2009 and November 2012. Time zero is the time of diagnosis with stage III CKD, and each included biomarker is averaged by quarter thereafter[2] (for details of the analysis, see Burckhardt et al. 2016). An eight-group model was chosen as preferred based on a combination of statistical and clinical considerations. Each of the eight trajectory groups is defined by the evolution of five markers of CKD severity and its complications: estimated glomerular filtration rate, a standard measure of renal function; hemoglobin and serum bicarbonate, both of which can fall over time as a complication of CKD; and parathyroid hormone and serum phosphate, both of which can become elevated as a complication of CKD.

[2]The one exception is patients already diagnosed with stage III CKD at the outset of the measurement window. For these individuals, time zero is the outset of the measurement window, quarter 1 of 2009.

Background shading in **Figure 8** reflects the ranking of each trajectory compared with the others. This highlights that Groups 1–4 have generally worse biomarker values compared with Groups 5–8. Reflecting underlying disease heterogeneity, trajectory group membership is associated with markedly different frequencies of CKD progression. By the end of the observation period, the prevalence of stage IV CKD and dialysis dependence among Group 1 members is 54.4% and 37.4%, respectively, whereas no Group 8 members progress to stage IV CKD or became dialysis dependent. Groups 2–7 follow in a continuum between these two extremes. For details regarding the specification of the likelihood function of the multitrajectory model and a discussion of model selection, readers are referred to Nagin et al. (2016).

Associating Trajectory Group Membership with Future Outcomes

A common goal of research in both psychology and medicine is to estimate the probability of a future clinical event given data known in the present. When the available data have a structure amenable to longitudinal modeling, GBTM can be an excellent tool to achieve this goal. For example, one may wish to predict whether individuals with persistently severe symptoms of depression on the Patient Health Questionnaire-9 (PHQ-9) after starting a certain antidepressant have a higher chance of suicide in the next year than patients who exhibit a trajectory of falling PHQ-9 scores. Similarly, as illustrated for the CKD multitrajectory model, it is plausible that patients who follow trajectories of worsening biomarkers of kidney function have a shorter time to hemodialysis dependence. GBTM can be used to test these hypotheses quantitatively.

Creating the linkage requires specifying the distribution of the outcome variable, which in principle can be any distribution. Current software supports three distributions: logit, Poisson, and normal. Because trajectory group membership is uncertain for each individual i, the linkage between the trajectory and the future outcome is performed by regressing the outcome on the PPGMs for each individual. For a normally distributed outcome, y, this is estimated via the following regression equation:

$$y = \beta_0 + \beta_1 \text{PPGMj} + \ldots \beta_J \text{PPGMj} + \varepsilon,$$

where ε is an independent and identically distributed normal random variable.[3] For binary and count outcomes, the equivalent form of the regression is expressed in terms of the logit link function and the natural logarithm of the Poisson rate parameter (typically denoted by λ), respectively. We illustrate this capability with two examples using data from a Montreal-based longitudinal study. The first links trajectories of physical aggression to sexual activity, and the second links multitrajectories of different types of substance use to long-term social and economic outcomes.

The Montreal-based study began tracking about 1,000 ethnically French boys when they were in kindergarten in 1984. Among a multitude of variables, teachers evaluated the physical aggression of the boys at age 6 and again from ages 10 to 15 using a six-item scale. The four-group trajectory model and 95% confidence intervals for each group (see **Figure 9**) were first reported by Nagin & Tremblay (1999). One group accounting for an estimated 15% of the sampled population was consistently rated at the scale minimum. The largest group (54%) followed a declining quadratic trajectory starting at a modest level of physical aggression at age 6. A third group (27%) followed a similarly declining quadratic trajectory but started at a higher level at age 6. Finally, a small group estimated to account for about 5% of the sampled population followed a flat trajectory of sustained high-level physical aggression from ages 6 to 15. Appended to each trajectory is the

[3] Because the posterior probabilities must sum to 1, one trajectory group must serve as the reference group, which in the above equation is group $j = 1$.

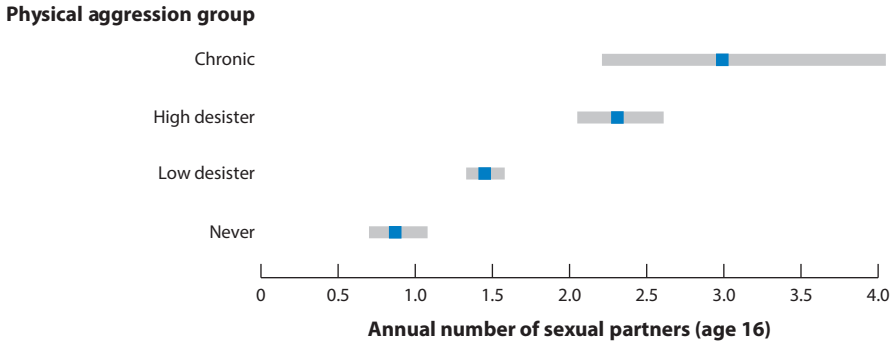

Figure 9

The linkage of trajectories of physical aggression from ages 6 to 15 with number of sexual partners at age 16. The trajectories demonstrate that higher physical aggression trajectories are associated with higher numbers of sexual partners at age 16.

estimated number of sexual partners at age 16 based on respondent self-reports. The estimates assume this count follows the Poisson distribution; 95% confidence intervals for the Poisson rate parameter estimates are also provided. As can be seen, the number of sexual partners increases steadily from a low of 0.87 for the lowest trajectory group to 3.0 for the high-chronic group.

The second example, also using the Montreal data, is reported by Vergunst et al. (2022) and is based on self-reported use of alcohol, tobacco, cannabis, and other illicit drugs from ages 13 to 17. These data were used to estimate the multitrajectory model depicted in **Figure 10**, which in turn was linked to a variety of social and economic outcomes. In this analysis, the regression predicting

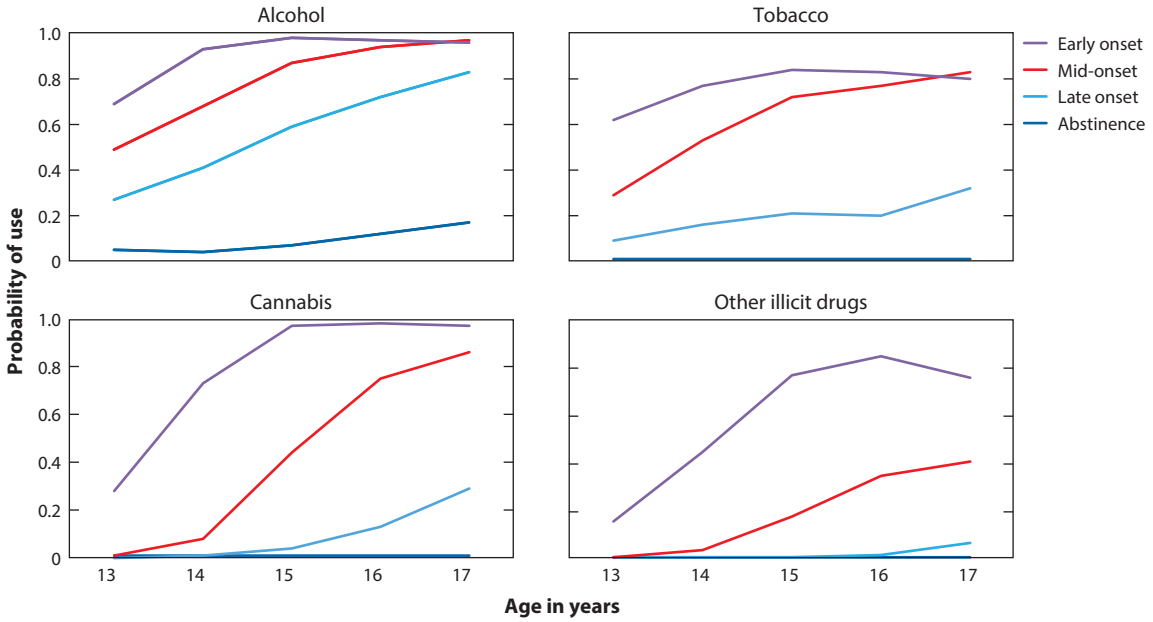

Figure 10

Multitrajectory model of alcohol, tobacco, cannabis, and other substance use from ages 13 to 17. Figure adapted with permission from Vergunst et al. (2022).

these outcomes from the multitrajectory group posterior probabilities also included a number of psychosocial measurements made during childhood (e.g., intellectual quotient). Compared with the late-onset polysubstance use group, there were few differences in later life outcomes in the abstinent multitrajectory group. There were, however, material differences between the late-onset group and the mid-onset and early-onset groups. For example, the early-onset group had materially higher rates of criminal conviction at ages 23–24 and welfare receipt over ages 19–37, and lower earnings at ages 33–37. They were also less likely to be married or cohabiting from ages 19 to 37.

Beta Distribution–Based Trajectories

Elmer et al. (2018) demonstrate an application of GBTM in which the repeated measurements forming the trajectories, Y, are specified to follow the beta distribution. It offers a flexible alternative to the normal distribution for modeling "badly behaved" continuous longitudinal data. Real-world data are often not normally distributed. This is particularly true of biomarker data, which are generally positive and right skewed, creating a need for alternatives to the Gaussian distribution (Albers et al. 2018). The primary advantage of the beta distribution is the flexible shape of the density function. The normal density function, even in its censored form, must follow some portion of its familiar bell-shaped curve, whereas the shape of beta distribution is far less constrained. A disadvantage of beta distribution is that the data under study must be transformable to a 0–1 scale. However, because biomedical data often have a known maximum value (e.g., the highest reportable value of a particular biomarker assay), as is also the case for psychometric scale data, or a highest value where differences are of clinical relevance, this transformation can often be accomplished simply by dividing through by the maximum possible or highest clinically interesting value.

The beta distribution can be parameterized several ways. One particularly useful form for GBTM was proposed by Ferrari & Cribari-Neto (2004). Let y denote a beta-distributed random variable:

$$P(y;\mu,\phi) = \frac{\Gamma(\phi)}{\Gamma(\mu\phi)\Gamma((1-\mu)\phi)}\, y^{\mu\phi-1},$$

where $0 < y < 1$, $0 < \mu < 1$, and $\phi > 0$. Under this parameterization, $\mathrm{E}(y) = \mu$ and $\mathrm{var}(y) = \mu(1-\mu)/(1+\phi)$. The parameter ϕ is known as the precision parameter because, for any μ, a larger value of ϕ results in a smaller $\mathrm{var}(y)$.

We demonstrate the beta distribution extension using electroencephalographic (EEG) data measured from comatose patients resuscitated from cardiac arrest. From these data, we extract a quantitative summary measure from the original waveform data, the suppression ratio, which estimates the proportion of a given epoch during which measurable cortical electrical activity is absent. For this example, we summarize this measure as the hourly median. Measurements are available for over 1,000 patients for up to 48 hours from admission to the intensive care unit. Across these patients, **Figure 11** shows a histogram of suppression ratios at hour 12, which bears no resemblance to the normal distribution. Overlaid on the histogram is the best-fitting beta distribution, which nicely captures its parabola-like form.

Figure 12 illustrates a three-group beta distribution model, which we also associate with survival to hospital discharge. EEG data are no longer collected when a patient either dies or awakens from coma, so the model incorporates the previously discussed extension to account for nonrandom subject attrition. As shown in **Figure 12**, the trajectories are highly predictive of survival to discharge.

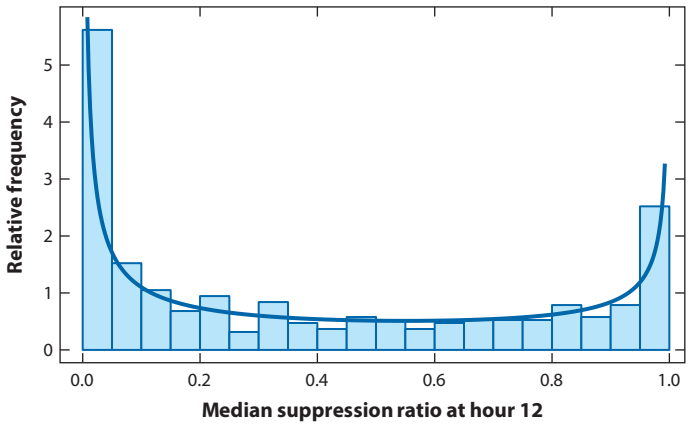

Figure 11

The beta distribution applied to the neurological activity of comatose cardiac arrest patients at hour 12 of electroencephalographic monitoring. The figure demonstrates that the flexible shape of beta distribution allows it to closely fit the distribution of the hour 12 data. Figure adapted from Elmer et al. (2018) (CC BY 4.0).

How well do these beta distribution–based trajectories fit the data? **Figure 12** also overlays the actual distribution of the suppression ratio data by trajectory group with the predicted distribution according to the beta distribution at hour 24. Inspection of **Figure 12** reveals that for each trajectory group, the actual and predicted values nicely correspond, even though across trajectory groups, the distributions of the suppression ratio are quite different. Trajectory Groups 1 and 2 have left-skewed suppression ratio distributions, whereas the distribution for trajectory Group 3 has an opposite right skew. Moreover, the left skews of Groups 1 and 2 are distinctly different, with Group 1's skew more extreme than Group 2's. The fit between the actual and predicted data distribution by trajectory group is similarly good for other hours.

Real-Time Prediction of Future Events

Early knowledge of the likely trajectory of an individual's illness and expected outcomes is a fundamental requirement for precision care. Improving the timeliness with which these can be known can facilitate early disease-modifying interventions and harm reduction and can help one avoid care that is likely to be futile. In this section, we demonstrate a method based on GBTM for making predictions about disease outcomes that can be updated in real time. Details are described by Elmer et al. (2018).

We illustrate the methodology using the beta distribution–based model linking trajectories of the suppression ratio after cardiac arrest with survival at hospital discharge described in the subsection above. The method builds from the key output of GBTM discussed above, PPGMj. Instead of calculating this value for each individual i after the entire vector of hourly suppression ratio measurements is available, PPGMj is instead calculated only on measurements up to hour $t' < T$ according to

$$\hat{P}(j|Y_i^{t'}) = \frac{\hat{P}(Y_i^{t'}|j)\hat{\pi}_j}{\sum_j^J \hat{P}(Y_i^{t'}|j)\hat{\pi}_j},$$

where $Y_i^{t'}$ is a vector of outcome measurements for $t \leq t' < T$.

To implement this in practice, the parameters of a GBT model are first estimated for a subset of subjects (i.e., training data) based on the entire measurement series, Y_i. In a second training

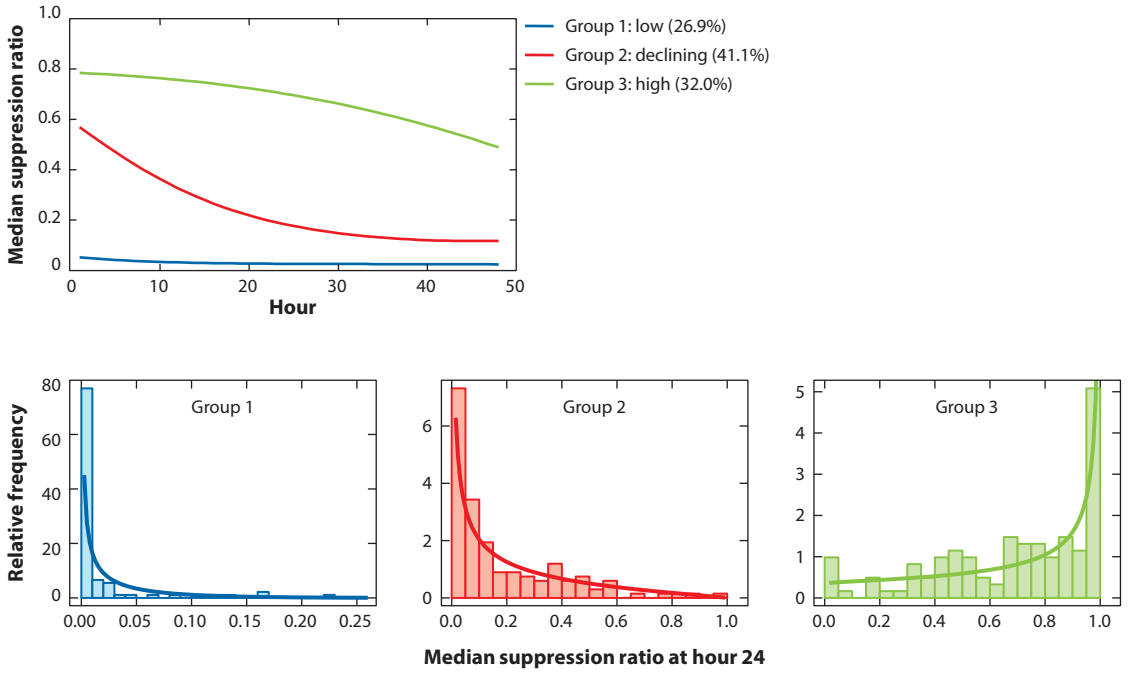

Figure 12

Three-group beta-based group-based trajectory modeling of the suppression ratio. The model demonstrates that the trajectory of the suppression ratio is closely associated with survival probability (0.666 for Group 1, 0.258 for Group 2, and 0.027 for Group 3), and the beta distribution–based model closely conforms with the hour 24 distributions of the suppression ratio across groups. Figure adapted from Elmer et al. (2018) (CC BY 4.0).

step, the future outcome of interest (in this case, survival to hospital discharge) is then regressed on the PPGMs. For future individuals (i.e., those in the test set), the PPGMj values are calculated only using the outcome measurement available at t'. Although the previously discussed examples of linking trajectories to outcomes jointly estimate the parameters for these two steps, joint estimation is improper in the predictive setting since, for future individuals, their eventual outcomes will be unknown at time t' when the PPGMs are estimated.

The predicted probability of a binary outcome for individual i at time t', $p_i^{t'}$, is based on the posterior probability calculations for i at t', $\text{PPGMj}_i^{t'}$, and the logit function parameter estimates of the outcome probability for each trajectory group j, $\hat{\alpha}_j$. The quantity $p_i^{t'}$ is calculated according to the following equation:

$$p_i^{t'} = \frac{e^{\left(\sum_j \text{PPGMj}_i^{t'} * \hat{\alpha}_j\right)}}{1 + e^{\left(\sum_j \text{PPGMj}_i^{t'} * \hat{\alpha}_j\right)}}.$$

In principle, this calculation can be extended to predict outcomes of any structure from $\text{PPGMj}_i^{t'}$.

We illustrate this calculation at hour 15 for an actual individual for whom $\text{PPGM1}^{t'=15} = 0.000$, $\text{PPGM2}^{t'=15} = 0.372$, and $\text{PPGM3}^{t'=15} = 0.628$, and $\hat{\alpha}_1 = 0.689$, $\hat{\alpha}_2 = -0.920$, and $\hat{\alpha}_3 = -3.59$, which as reported in **Figure 12** translate into probabilities of survival to discharge of 0.666 for Group 1, 0.258 for Group 2, and 0.027 for Group 3. For this individual, predicted survival probability at hour 15 is thus $0.070 = e^{0.000*0.689+0.373*(-0.920)+0.628*(-3.59)} / 1 + e^{0.000*0.689+0.373*(-0.920)+0.628*(-3.59)}$. The predictive method can also assign 95% confidence intervals to the predicted probability to provide a metric for

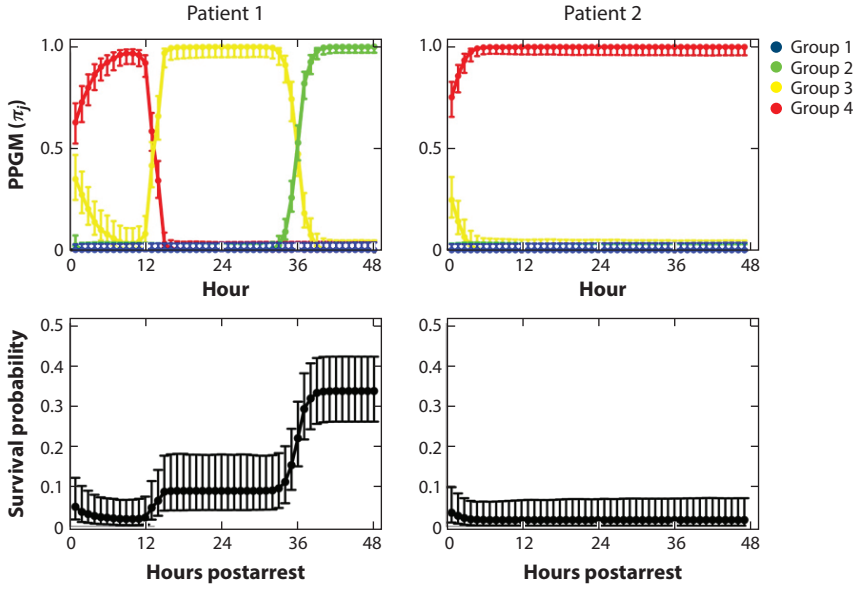

Figure 13

Patient-level data depicting hourly updates of posterior probability of trajectory group membership (PPGM) from a model of suppression ratio and seizure probability, accounting for propofol administration and baseline Pittsburgh Cardiac Arrest Category, for two patients. PPGMs are depicted in blue for Group 1, in green for Group 2, in yellow for Group 3, and in red for Group 4. The bottom subpanels depict the corresponding survival estimates for the patients.

judging the precision of the estimate, which for this individual is (0.048, 0.100). For details on the calculation of confidence intervals for this situation, readers are referred to Elmer et al. (2018).

The prognostication methodology can be applied with ease to PPGMs derived from more elaborate models. To illustrate, we make outcome predictions based on a four-group multitrajectory model defined by two EEG measures—hourly median suppression ratio and maximum estimated seizure probability, which we dichotomized at a threshold of 0.5.[4] Also included in the model as a time-varying covariate is the hourly dose of an anesthetic infusion propofol (which is used to treat seizures and which increases suppression ratio); a baseline severity measure of brain and cardiopulmonary dysfunction is included as well. For a discussion of adding baseline measurements and time-varying covariates to GBT models, readers are referred to Nagin & Odgers (2010).

The results for this model are illustrated in **Figure 13** for two actual patients.[5] For Patient 2, the trajectories of subsequent suppression ratio and seizure probability measures remain consistent with Group 4 membership, and the PPGMs and associated survival estimates are quite static. By contrast, Patient 1's suppression ratio and seizure probability improve over time, resulting in a

[4]Seizure probability can be represented in many forms. For the purpose of this illustration, we dichotomize it to being above or below 0.5. The trajectory itself is defined by a logit link measuring the probability over time that seizure probability exceeds the 0.5 threshold.

[5]For a prognostic method to be useful, it is important to demonstrate that the method has good prediction capacities for data not used in the estimation sample for the prediction model. The predicted probabilities shown in **Figure 13** are out-of-sample quantities and were calculated as follows. The sample was randomly divided into five equally sized groups. The model was iteratively estimated on four of the groups and then applied to the holdout group to calculate the prognostic predictions.

shift in the maximum PPGM from Group 4 to Group 3 by hour 15, and ultimately to Group 2 by hour 35. This results in a considerable corresponding increase in the patient's estimated survival probability over time. As it happened, Patient 1 did indeed survive, but Patient 2 did not.

The clinical implication of the outcome estimate, and the necessary certainty in outcome in terms of confidence at any time point and the stability of the estimate over time, depends on the clinical application. When a safe, potentially efficacious disease-modifying treatment is available (e.g., more intensive clinical follow-up for CKD patients deemed at risk of ultimately progressing to dialysis dependence), any nontrivial predicted outcome probability may be sufficient to intervene. By contrast, weightier treatment decisions, such as involuntary hospitalization for patients predicted to be at high risk of suicide, may require much more certainty. Regardless, by providing both point estimates for outcome probability and associated confidence intervals, clinicians and researchers have the full information needed to make these decisions based on context-specific values and preferences.

FUTURE DIRECTIONS

Current capabilities of GBTM make it an appealing option for analysis of longitudinal data sets. As its use becomes more widespread, additional investigation into model building and specification will help inform researchers as they distill potentially complex data into parsimonious yet informative models. For example, there are innumerable scales that measure the severity of psychological symptoms, protective factors, substance use, and concomitant medical comorbidities, with hundreds of medications and other clinical interventions that could be considered as time-varying covariates. Selecting the correct measures from which to build trajectories and choosing baseline risk factors and time-varying covariates can be informed by plausible hypotheses grounded in domain knowledge in a particular application. At the same time, model specification choices should result in an informative and clinically interesting final model with favorable statistical properties (e.g., a high proportion of subjects with accurate, early outcome predictions in the case of prognostication). Direct comparison with other available methodologies is also needed. However, because of the strengths of the methodology, we expect the trend of increasing applications of GBTM in biomedical research to continue.

SUMMARY POINTS

1. Group-based trajectory modeling is an application of finite mixture modeling designed to identify groups of individuals following approximately the same trajectory of one or more repeated measures of interest over age or time.
2. Because trajectory groups are not literal entities, the aim of the model search process is to identify the model with the smallest number of trajectory groups that still captures distinctive features of the population relevant to the study objectives.
3. Development and progression of psychiatric disorders and other diseases typically result from an intricate interplay of complex, interdependent, and measurable signals. Joint trajectory and multitrajectory modeling are designed to identify the trajectories of multiple measures of illness severity and/or mediators of disease progression as they evolve together over time.
4. Real-world data are often not normally distributed. This is particularly true of biomarker data, which are generally positive and right skewed, creating a need for an alternative to

the Gaussian distribution. The beta distribution modeling option is intended to address this need. Its primary advantage is the flexible shape of its density function.

5. Early knowledge of the likely trajectory of an individual's illness and expected outcomes is a fundamental requirement for precision care. Using a newly developed extension, group-based trajectory modeling can estimate the probability of an individual's trajectory group membership and/or the probability of a future clinical event given data known in the present, facilitating real-time outcome prediction.

DISCLOSURE STATEMENT

The authors are not aware of any affiliations, memberships, funding, or financial holdings that might be perceived as affecting the objectivity of this review.

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