Article

SMMR
STATISTICAL METHODS IN MEDICAL RESEARCH

Statistical Methods in Medical Research
2018, Vol. 27(7) 2015–2023

DOI: 10.1177/0962280216673085
journals.sagepub.com/home/smm
SAGE

Group-based multi-trajectory modeling

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Abstract

Identifying and monitoring multiple disease biomarkers and other clinically important factors affecting the course of a disease, behavior or health status is of great clinical relevance. Yet conventional statistical practice generally falls far short of taking full advantage of the information available in multivariate longitudinal data for tracking the course of the outcome of interest. We demonstrate a method called multi-trajectory modeling that is designed to overcome this limitation. The method is a generalization of group-based trajectory modeling. Group-based trajectory modeling is designed to identify clusters of individuals who are following similar trajectories of a single indicator of interest such as post-operative fever or body mass index. Multi-trajectory modeling identifies latent clusters of individuals following similar trajectories across multiple indicators of an outcome of interest (e.g., the health status of chronic kidney disease patients as measured by their eGFR, hemoglobin, blood CO_2 levels). Multi-trajectory modeling is an application of finite mixture modeling. We lay out the underlying likelihood function of the multi-trajectory model and demonstrate its use with two examples.

Keywords

Longitudinal analysis of multiple outcomes, group-based trajectory modeling, latent class analysis, trajectories of multiple disease biomarkers

1 Key messages

- **Background:** Conventional statistical practice generally falls far short of taking full advantage of the information available in multivariate longitudinal data on the course and interrelationship of different indicators of disease progression. More often than not, indicators of interest are analyzed in sequence rather than jointly.
- **What we offer:** Multi-trajectory modeling, an extension of the univariate group-based trajectory modelling (GBTM), is designed to overcome this limitation. It does so by defining a trajectory group in terms of trajectories for multiple indicators not just one indicator.
- **Implication:** Group-based multi-trajectory modeling is a flexible statistical tool that compactly and transparently represents the interrelationship of multiple clinically relevant indicators.

The importance of longitudinal multivariate data in the clinical and public health sciences cannot be overstated. Disease development and progression result from an intricate interplay of biological pathways producing complex, interdependent, measurable signals.[1] Identifying and monitoring multiple disease, biomarkers and other clinically important factors such as comorbidities affecting the course of a disease, behavior, or health status is of great clinical relevance.

Conventional statistical practice generally falls far short of taking full advantage of the information available in multivariate longitudinal data on the course and interrelationship of different indicators of disease progression.

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More often than not, indicators of interest are analyzed in sequence rather than jointly. Several multivariate techniques allowing for joint-trajectory modeling have lately emerged.[2,3] These approaches can roughly be classified by whether latent classes are used to model co-dependences among repeated measures. Group-based dual-trajectory modeling[4,5] is one of the currently available latent class techniques.

Group-based dual-trajectory modeling is a specific form of GBTM.[4] GBTM is a statistical method that is designed to identify a finite number of groups of individuals following similar trajectories over age or time of a single outcome or behavior. Growth mixture modeling is another closely related method.[6,7] Two key outputs of the GBTM are the shape of the trajectory, typically defined by a polynomial function of age or time, and probability of trajectory group membership.

Dual group-based trajectory modeling is a generalization of the basic univariate GBTM that allows analysis of the interrelationship of two outcomes or biological signals that jointly evolve (e.g., measures of acute inflammation such as fever and leukocytosis), are comorbid (glomerular filtration rate and hemoglobin A1C) or are related over different phases of the life course (e.g., childhood body mass index (BMI) and adult hypertension). The joint model estimates group-based trajectories for the two outcomes of interest and links them with a table of conditional probabilities measuring the probability of following a specific trajectory for outcome 2 given the individual is following a specified trajectory for outcome 1.

The virtue of this form of joint-trajectory modeling is that it highlights heterogeneity in the linkage between trajectories of distinct outcomes that are thought to be related by a common underlying etiological process. Its downside is that it is a balky form of analyses for relating trajectories for more than two outcomes. While in principle the joint-trajectory model can be expanded to more than two outcomes, the number of conditional probability tables linking the different outcomes quickly becomes unmanageable. A joint model involving three outcomes requires three tables of conditional probabilities to link the trajectories of each of the outcomes. A four-outcome model requires six such tables of conditional probabilities.

This paper demonstrates an alternative to the joint model, called the multi-trajectory model, which is designed to avoid the problem of the proliferation of conditional probability tables that accompanies analyses relating trajectories for more than two outcomes. It does so by defining a trajectory group in terms of trajectories for multiple not just one outcome.

Figure 1 illustrates the method for three physiological measurements for 535 male subjects of the Dunedin, New Zealand Multidisciplinary Health and Development Study. Using a model, selection procedure described below a five-group model emerged as the preferred model. Each trajectory group is defined by a trajectory for three outcomes: mean arterial blood pressure at ages 7, 11, 18, 26, 32, and 38, a measure of lung capacity called the FEV1/FVC ratio, where FEV1 and FVC stand for Forced Expiratory Volume in 1 second and Forced Vital Capacity, measured at ages 9, 11, 13, 15, 18, 26, 32, and 38, and BMI measured at ages 3, 5, 7, 9, 11, 15, 18, 21, 26, 32, and 38. Group 1, which is estimated to constitute 30.9% of the sampled population, overall does as well or better than the other groups across the three measures. Its trajectory of arterial blood pressure is similar to those for Group 2 (36.5%) and Group 3 (15.2%) and distinctly lower than the trajectories for Group 4 (14.3%) and Group 5 (3.1%). Group 1's FEV1/FVC ratio is also similar to that of Group 2. What distinguishes these two groups is their BMI trajectories. Group 1 stays within the normal range through age 38 whereas group 2 moves into the overweight range in adulthood. Group 3 is distinguished by its having a distinctly lower lung capacity trajectory than all the other groups. Group 4 and Group 5 are distinguished by their blood pressure and BMI trajectories. While their blood pressure trajectories start off at about the same level as those of the other groups, by age 38 both groups have markedly higher blood pressure than the others. Similarly, the BMI trajectories of all the groups start off at about the same level but by adulthood Group 4 is well past the threshold for being overweight and Group 5 is in the obese range.

The remainder of this paper is organized as follows. Section 2 lays out the likelihood function for the multi-trajectory model. Section 3 discusses model selection and evaluation. Section 4 illustrates the method with another example and in this context discusses model estimation in more detail. Section 5 concludes.

2 The multi-trajectory likelihood function

This section lays out the generalization of the basic GBTM to the multi-trajectory format. We begin with the specification of the basic model in which each group is defined by a trajectory for a single outcome.

The group-based approach for modeling developmental trajectories is intended to provide a flexible method for identifying distinctive clusters of individual trajectories within the population and for profiling the characteristics of individuals within the clusters. Thus, whereas the hierarchical and latent curve methodologies model population

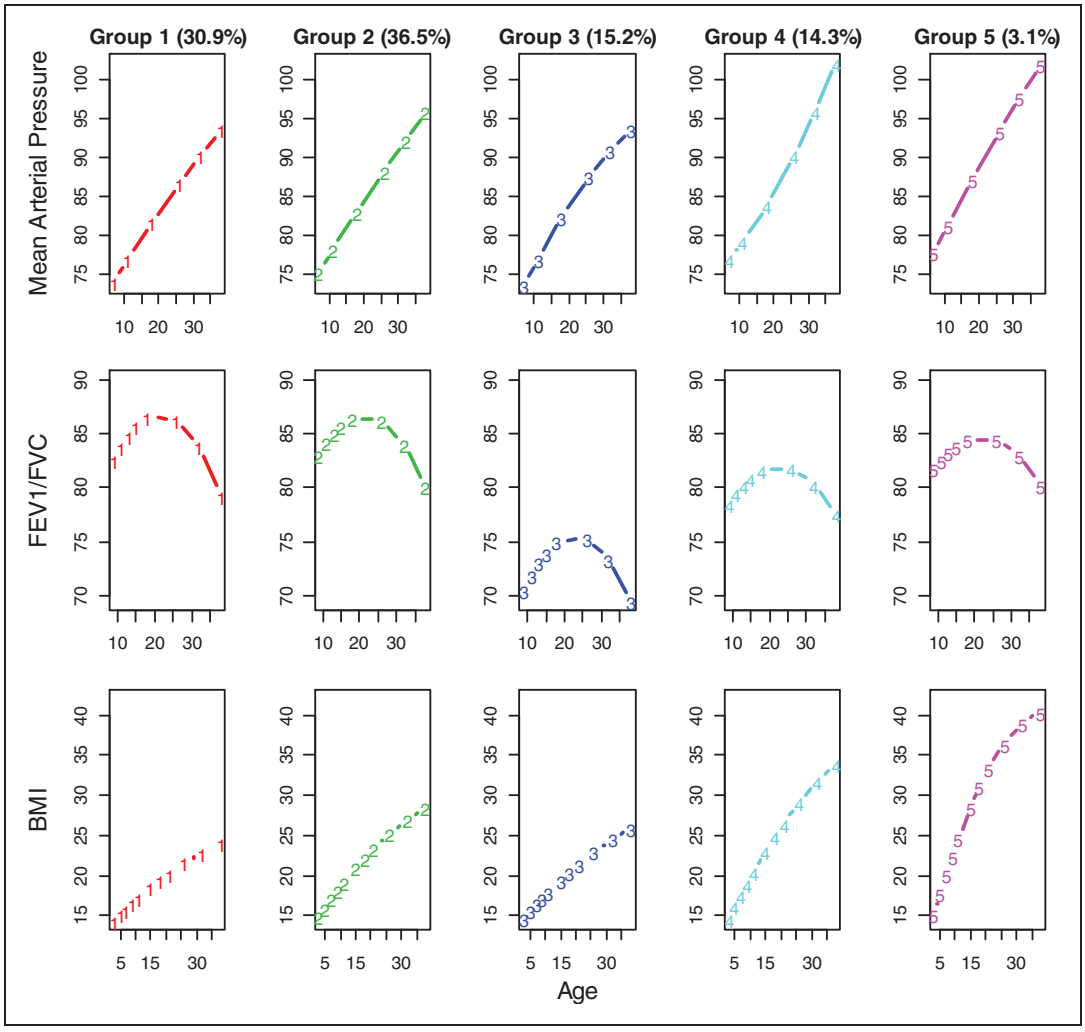

Figure 1. Male multi-trajectory model (Dunedin Health and Development Multidisciplinary Study).
FVC: forced vital capacity; FEV: forced expiratory volume; BMI: body mass index.

variability in growth with multivariate continuous distribution functions, the group-based approach utilizes a multinomial modeling strategy. Technically, the GBTM is an example of a finite mixture model. Maximum likelihood is used for the estimation of the model parameters. Two versions of software are available for estimating the models demonstrated in this paper. One version operates on the SAS platform and the other on the Stata platform. See Jones and Nagin.[8,9] The software for both versions can be freely downloaded at https://www.andrew.cmu.edu/~bjones/index.htm.

The fundamental concept of interest is the distribution of outcomes conditional on age (or time); that is, the distribution of outcome trajectories denoted by $P(Y_i|Age_i)$, where the random vector Y_i represents individual i's longitudinal sequence of measurements and the vector Age_i represents individual i's age when each of those measurements is recorded. The group-based trajectory model assumes that the population distribution of trajectories arises from a finite mixture of unknown order J. The likelihood for each individual i, conditional on the number of groups J, may be written as

$$P(Y_i|Age_i) = \sum_{j=1}^{J} \pi_j \cdot P\left(Y_i|Age_i, j; \beta_j\right) \tag{1}$$

where π_j is the probability of membership in group j, and the conditional distribution of Y_i given membership in j is indexed by the unknown parameter vector β_j which among other things determines the shape of the group-specific trajectory. Typically, the trajectory is modeled with a polynomial function of age. For given j, conditional

independence is assumed for the sequential realizations of the elements of Y_i, y_{it}, over the T periods of measurement. While conditional independence is assumed at the level of the latent trajectory group, at the population level outcomes are not conditionally independent because they depend on a latent construct, trajectory group membership. See chapter 2 of Nagin[5] for a discussion of the conditional independence assumption.

Thus, we may write

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

where $p(.)$ is the distribution of y_{it} conditional on membership in group j and the age of individual i at time t. For the applications reported in this analysis, $p(.)$ is either the normal, censored normal, or Poisson distribution, but in general, there is no restriction on the form of $p(.)$.

In the multi-trajectory model framework, each of the J trajectory groups is defined by a set of trajectories for multiple outcomes. Let K denote the number of such outcomes with the random vector Y_i^k representing individual i's longitudinal sequence of measurements of the kth outcome and let $P_k\left(Y_i^k|Age_i, j; \beta_j^k\right)$ denote the distribution of that vector conditional on group j and the unknown parameter vector β_j^k.

It is assumed that, conditional on membership in the jth group, Y_i^k are independently distributed with $P_j(Y_i^1, Y_i^2, \ldots, Y_i^K) = P_{1j}(Y_i^1)P_{2j}(Y_i^2)\ldots P_{Kj}(Y_i^K)$. Note again that the k outcomes are not conditionally independent at the population level. Conditional independence as specified in equation (2) is assumed for each of the k outcomes. Thus, the likelihood for each individual conditional on number of groups J may be written as

$$\begin{aligned} P(Y_i^1, Y_i^2, \ldots Y_i^K|Age_i) &= \sum_{j=1}^{J} \pi_j \left[\prod_{k=1}^{K} P_k\left(Y_i^k|Age_i, j; \beta_j^k\right)\right] \\ with\ P_k\left(Y_i^k|Age_i, j; \beta_j^k\right) &= \prod_{t=1}^{T^k} p_k\left(y_{it}^k, j; \beta_j^k\right) \end{aligned} \tag{3}$$

To illustrate the specification of the likelihood, more concretely consider the case of the likelihood underlying the model reported in Figure 1. For this example, $K=3$ because each trajectory group is defined by three biomarkers—mean arterial blood pressure, FEV1/FVC, and BMI. For each of these biomarkers, $p_k(*)$ is assumed to follow the normal distribution. However, in general, $p_k(*)$ may follow different distributions across k.[a] Also, because the biomarkers were measured over different age ranges, the length of the Y_i^k vector varies across k (but not i).

Note that in the second part of equation (3) expressing the conditional independence assumption, the index T is superscripted with k. This detail has an important practical implication, namely that each of the k outcomes do not have to be measured over the same number of periods. We also note that the time frame for measurements can be any epoch length (e.g., years, hours, or minutes) and that trajectories can be defined in terms of time from an event, for example, the onset of cardiac arrest as in Elmer et al.[10] or time from the completion of surgery.[11]

3 Determination of the number of groups *J*

Finite mixture models are used for two distinct purposes.[12] One is to model populations that are thought to be composed of literally distinct groups. For applications of this type, there is no settled theory on the identification of the number of groups, j, that composes the population. The second use of finite mixture models is to approximate a continuous distribution functions. McLachlan and Peel[12] describe such use of finite mixture modeling as a "niche between parametric and nonparametric approaches to statistical estimation." When used in this fashion, there is no correct j to identify.

Heckman and Singer[13] built upon the approximating capability of finite mixture models to construct a nonparametric maximum likelihood estimator for the distribution of unobservables in hazard models. Their motivation was that theory rarely provides theoretical guidance on the population of distribution of unobserved individual differences, yet statistical models of duration data were sensitive to the assumed form of the distribution of such differences. Their proposed estimator finessed the problem of having to specify a distribution of unobserved individual differences by approximating the distribution with a finite mixture model. The Heckman and Singer application served as the inspiration for GBTM. As described in its first application in

Nagin and Land[14] and elaborated in Nagin,[5] theory does not provide guidance on the specific form of the distribution of developmental trajectories. Thus, GBTM is a device for approximating the unknown population distribution of trajectories. From this perspective, the latent trajectory groups should not be thought of as literally distinct groups but rather as clusters of individuals following approximately the same trajectory. The objective GBTM is not to identify the true number of trajectory groups because there is no true number. Instead it is to identify the distinct features of the data. These features can be thought of as longitudinal latent strata. Conventional fit statistics such as the Bayesian Information Criterion (BIC) and Akaike Information Criterion can play a useful role in identifying such features. Indeed, Klijn et al.[15] have developed R-based software that compares the performance of alternative GBTMs based on various well-known fit statistics as well as model diagnostics described in Nagin.[5] However, model choice cannot be left to mechanical application of fits statistics and model diagnostics. Models must also be evaluated on their substantive interest. This admonition is particularly important in the multi-trajectory context in which model selection requires identification of a substantively useful model over multiple measurement dimensions.

4 Another application

The second illustrative example is based on data from a Montreal-based longitudinal study of 1037 males. The first wave of measurements was made in 1984 when the boys were in kindergarten. Four outcomes are modeled in the multi-trajectory model: childhood physical aggression based on teacher assessments at ages 6, 10, 11, 12, and 13, incidents of violent delinquency and incidents of drug use based on self-reports at ages 13, 14, 15, 16, and 17 and number of self-reported sexual partners at ages 13, 14, 15, 16, and 17. Physical aggression, which is measured on a psychometric scale, was modeled as following the censored normal distribution where the censored minimum was set at the scale minimum and the censored maximum at the scale maximum. Number of sexual partners, incidents of violent delinquency, and incidents of drug use were modeled as following the Poisson distribution.

As noted, model search is particularly challenging in the multi-trajectory application domain because each trajectory group is a representation of the course over time or age of multiple outcomes. The first step in the search involved estimating trajectory models with varying number of groups for each of the outcomes separately. The objective was not to identify the preferred model for each outcome separately but instead to clarify the types of distinctive trajectories that it was important be represented in the multi-trajectory model. With two exceptions, trajectories were assumed to follow a quadratic function of age because cubic terms were rarely significant. The two exceptions involved number of sexual partners and physical aggression. For both behaviors, initial analyses revealed that there were individuals who, respectively, were sexually abstinent or who according to teachers were never physically aggressive. Higher order polynomials are not required to characterize inactivity. To accommodate the inactive individuals, the models for sexual activity and physical aggression included a zero-order trajectory to account for these individuals.

Models for up to six groups were estimated for each outcome. For violent delinquency, BIC increased with the addition of groups. For drug use, BIC continued to improve up to five groups and was nearly identical for the five- and six-group models. For number of sexual partners and physical aggression, BIC was maximized with the four group model. Based on this search, we concluded that at least a five-group multi-trajectory model was required. While the six group multi-trajectory model had a better BIC score than the five-group model, the six group model did not include a group that was substantively distinct from those in the five-group model. Also, the five-group model captured the distinctive trajectories for each outcome revealed in the first stage analysis. In the interest of parsimony, our preferred multi-trajectory model included five groups.

The five-group model also performed well on all of the tests of model adequacy laid out in Nagin[5] and implemented in Klijn et al.[15]; the average posterior probability for those assigned to a group based on the maximum posterior probability rule is greater than 0.95 which is far above the 0.7 threshold of acceptability; the proportion assigned to the group closely matches the estimated probability of group membership, and the odds of correct assign all exceeded 5 by a wide margin.

Figure 2 shows the preferred model. Group 1, which composes an estimated 18.2% of the population, is most distinctive with regard to these behaviors due to their low involvement in them all—they were not physically aggressive in their childhood and in adolescence were not violent or sexually active and used drugs at only a very low level. At the other extreme in this regard are the members of Group 5 who account for an estimated 12.4% of the population. They follow trajectories that are highest on all these measures of problematic youthful behavior. Group 2 (14.7%) and Group 3 (26.2%) are an interesting contrast. Both follow similar trajectories of modest but declining childhood physical aggression, neither engages in much violent delinquency in their adolescence, and

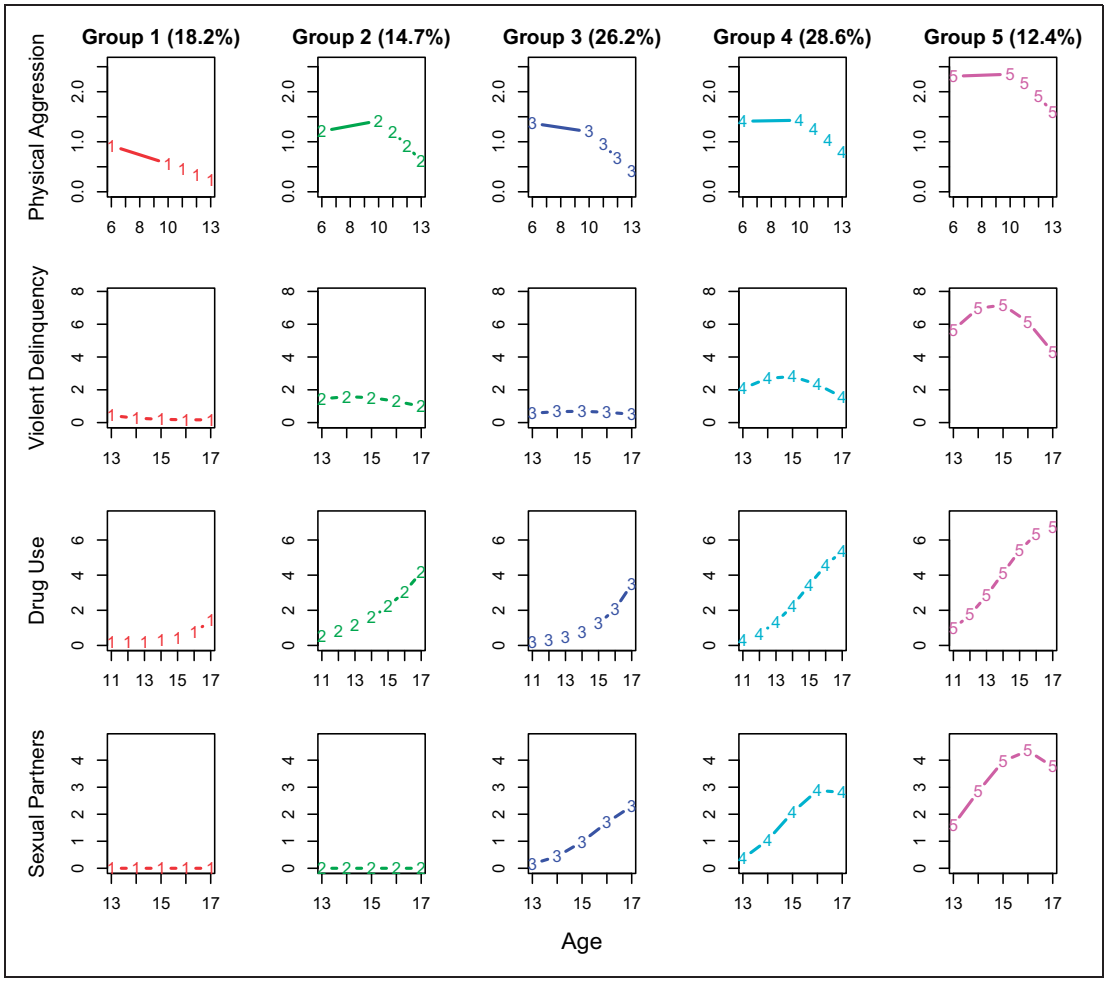

Figure 2. Multi-trajectory model (Montreal Experimental Longitudinal Study).

both follow similar trajectories of modest drug use. What distinguishes them is sexual activity. Group 2, like Group 1, is sexually inactive whereas Group 3 is sexually active but not nearly at the level of group 5. Group 4 (28.6%) is an interesting contrast to Group 3. Their trajectories of physical aggression, drug use, and sexual activity are all similar. Where they differ is in their violent delinquency. Group 4 engages in moderately high levels of violent delinquency whereas Group 3 does not.

The basic multi-trajectory model can be expanded in many useful ways. One is to add baseline predictors of trajectory group membership. In the basic model, probability of trajectory group membership is specified to follow the multinomial logistic function but with no predictors of trajectory group membership. Thus, in the basic model, π_j measures the unconditional probability of trajectory group membership for the jth group. The multinomial logit function readily accommodates the addition of predictors of probability of trajectory group membership. Let x_i denote a vector of predictors of trajectory group membership for individual i. With the addition of predictors, $\pi_j(x_i)$ measures the probability of membership in the jth group conditional on x_i. In the model with predictors of group membership probability, the parameters measuring the association of the predictor variables with trajectory group membership probability are estimated jointly, not sequentially, with the parameters specifying the shapes of the trajectory. Table 1 reports the parameter estimates of the group membership probability component of the likelihood function, in which a measure of the subject's hyperactivity and his family's adversity, both measured at baseline, are added as predictors of trajectory group membership.[b] Adversity is most strongly associated with membership in Groups 3, 4, and 5 compared to Group 1 (respective p-values are 0.04, 0.02, and <0.01). Hyperactivity strongest association is with Group 5 (p-value <0.01).

Table 1. Predictors of trajectory group membership.

Group Variable	Coefficient	T-score
Group 1	–	–
Group 2:		
Constant	−0.541	−2.23
Adversity	0.392	0.66
Hyperactivity	0.135	1.35
Group 3:		
Constant	0.049	0.25
Adversity	1.022	2.10
Hyperactivity	0.064	0.75
Group 4:		
Constant	0.094	0.49
Adversity	1.131	2.36
Hyperactivity	0.054	0.64
Group 5:		
Constant	−1.620	−5.74
Adversity	1.760	2.97
Hyperactivity	0.388	3.87

5 Conclusion

At the outset, we emphasized the importance to clinical practice of identifying and monitoring the various biomarker progressions and other factors in a patient's life circumstances that affect the course of a disease and of health status and behavioral patterns more generally. In this paper, we have presented a generalization of GBTM which is designed to address this need. It does so by defining a trajectory group in terms of trajectories for multiple outcomes not just one outcome. In so doing, the model generalization is intended to provide a statistical tool that compactly and transparently represents the interrelationship of multiple clinically relevant indicators.

Future methodological research on multi-trajectory modeling should focus on sharpening the guidelines for model selection and evaluation. While in our judgment the model selection processed used here is reasonable, as experience with multi-trajectory model grows, as we hope it will, that experience will undoubtedly form the basis for more specific guidance on this important first step in the analysis.

Acknowledgements

The authors thank Avshalom Caspi, Richie Poultin, and Terry Moffitt for making available data from the Dunedin, New Zealand Multidisciplinary Health and Development Study to illustrate the method. The authors also thank Jonathan Elmer, MD for numerous helpful comments.

Declaration of conflicting interests

The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

Funding

The author(s) received no financial support for the research, authorship, and/or publication of this article.

Notes

a. As discussed in Appendix 1, the software used to estimate the model assumed that these three measures followed the censored normal distribution. To disable the censoring component of the likelihood, the upper and lower bounds of censoring were set at values outside the range of the data.
b. In the basic model without predictors of trajectory group membership, the parameter estimates would include only those labeled as the "constant" in Table 1.

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Appendix 1

The models reported in this paper were estimable using software that is more generally designed to estimate GBTMs. It is freely available at https://www.andrew.cmu.edu/~bjones/index.htm. Two versions are available, one that operates on the Stata platform and the other on the SAS platform. Below are the command structures for the Stata and SAS versions that would be used to estimate the models reported in Section 4.

Stata

Model without predictors of trajectory group membership:

```
traj if nmiss<3, multgroups(5) var1(d13-d17) indep1(t5-t9) order1(2 2 2 2 2)/// model1(zip)///
var2(dro13-dro17) indep2(t5-t9) order2(2 2 2 2 2) model2(zip)///
var3(nbp13-nbp17) indep3(t5-t9) order3(0 0 2 2 2) model3(zip)///
var4(qcp84bat qcp88bat qcp89bat qcp90bat qcp91bat) indep4(t1-t5)///
order4(0 2 2 2 2) model4(cnorm) min4(0) max4(6)
```

where nmiss is a count of the number of missing assessments of the frequency of violent delinquency at ages 13 to 17 as measured by d13–d17, dro11–dro17 measure the frequency of drug use at ages 11–17, nbp13–nbp17 measure number of sexual partners at ages 13 to 17, qcp84bat–qcp91bat measure teacher ratings of physical aggression at ages 6, 10, 11, 12, and 13.

To generalize the model to include adversity and hyperactivity at baseline as predictors of trajectory group membership, the option, multrisk(advers84 qcp84op), is added to the above command structure.

The graphs of the resulting trajectory model are produced by the command:

```
multtrajplot, xtitle(Age/10) ytitle1(Violent Delinquency) ytitle2(Drug Use)/// ytitle3(Sexual
Partners) ytitle4(Physical Aggression) ylabel1(0(1)3) ylabel2(0(2)6) ylabel3(0(1)4)
ylabel4(0(1)3)
```

SAS

The SAS-based version of the above command structure for model estimation is as follows. Presently, there is no additional macro for graphing multi-trajectory modeling results; however, each individual model result can be plotted using the trajplotnew macro.

```
PROC TRAJ DATA=WORK.ONE OUT=OF OUTPLOT=OP OUTSTAT=OS OUTPLOT2=OP2 OUTSTAT2=OS2
  OUTPLOT3=OP3 OUTSTAT3=OS3 OUTPLOT4=OP4 OUTSTAT4=OS4;

    VAR d13-d17; INDEP t5-t9; MODEL ZIP; ORDER 2 2 2 2 2;
    VAR2 dro11-dro17; INDEP2 t3-t9; MODEL2 ZIP; ORDER2 2 2 2 2 2;
    VAR3 nbp13-nbp17; INDEP3 t5-t9; MODEL3 ZIP; ORDER3 0 0 2 2 2;
    VAR4 qcp84bat qcp88bat qcp89bat qcp90bat qcp91bat; INDEP4 t1-t5;
    MODEL4 CNORM; MIN4 0; MAX4 6; ORDER4 0 2 2 2 2;
    MULTGROUPS 5;
RUN;

%TRAJPLOTNEW(OP,OS)
%TRAJPLOTNEW(OP2,OS2)
%TRAJPLOTNEW(OP3,OS3)
%TRAJPLOTNEW(OP4,OS4)
```