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Accuracy of Optimized Branched Algorithms to Assess Activity-Specific PAEE

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Abstract

PURPOSE—To assess the activity-specific accuracy achievable by branched algorithm (BA) analysis of simulated daily-living physical activity energy expenditure (PAEE) within a sedentary population.

METHODS—Sedentary men (n=8) and women (n=8) first performed a treadmill calibration protocol, during which heart rate (HR), accelerometry (ACC), and PAEE were measured in 1-minute epochs. From these data, HR-PAEE, and ACC-PAEE regressions were constructed and used in each of six analytic models to predict PAEE from ACC and HR data collected during a subsequent simulated daily-living protocol. Criterion PAEE was measured during both protocols via indirect calorimetry. The accuracy achieved by each model was assessed by the root mean square of the difference between model-predicted daily-living PAEE and the criterion daily-living PAEE (expressed here as % of mean daily living PAEE).

RESULTS—Across the range of activities an unconstrained *post hoc* optimized branched algorithm best predicted criterion PAEE. Estimates using individual calibration were generally more accurate than those using group calibration (14 vs. 16 % error, respectively). These analyses also performed well within each of the six daily-living activities, but systematic errors appeared for several of those activities, which may be explained by an inability of the algorithm to simultaneously accommodate a heterogeneous range of activities. Analyses of between mean square error by subject and activity suggest that optimization involving minimization of RMS for total daily-living PAEE is associated with decreased error between subjects but increased error between activities.

CONCLUSION—The performance of *post hoc* optimized branched algorithms may be limited by heterogeneity in the daily-living activities being performed.

Keywords

Obesity; exercise; metabolism; simulated annealing; daily-living tasks

INTRODUCTION

Paragraph Number 1

In recent years obesity and its associated pathologies have reached remarkable prevalence in western societies (13), particularly those of North America (15). As might be expected, the physiological explanations for this escalating rate of overweight and obesity have focussed on a general behavioural shift toward a positive daily energy balance (13) due, in part, to a general waning of habitual physical activity (32). Importantly, the magnitude of this positive energy balance is relatively small - on the order of $100 - 400 \text{ kJ.day}^{-1}$ ($\sim 25-100 \text{ kcal.day}^{-1}$) (13). Such a small difference (approximately 5% of daily energy expenditure) is difficult to assess in the free-living circumstance, and likely contribute to the difficulty in implementing prescriptions for systematic and population-wide prevention of weight gain. Consequently, there is a need to develop methods to accurately estimate daily physical activity energy expenditure in order to develop effective weight management programs.

Paragraph Number 2

A variety of approaches have been used to measure free-living physical activity energy expenditure (PAEE). Some have been accurate but impractical (e.g. doubly labelled water and indirect calorimetry), while other more practical techniques, such as accelerometry (ACC) and heart rate (HR), have proven less accurate when used on their own (2,7,9). By combining heart rate and accelerometry, a series of investigations (1,12,20,22,23,27) have attempted to exploit the observation that the two measures are most accurate in different ranges of physical activity intensity (PAI - $\text{kJ.kg}^{-1}.\text{min}^{-1}$). Accelerometry has been shown to be more accurate at low to moderate intensities (2,10,20,33) while heart rate accurately estimates energy expenditure at higher intensities of activity (7,24,26). By taking a dual measurement approach, it is possible to achieve marked improvements in predictive accuracy, while retaining relative practicality in the methods. However, a caveat of all techniques that estimate PAEE from HR-PAI or ACC-PAI (including the dual methods described above) is that they have traditionally required subject-specific calibration to remove the negative effect of inter-individual variability on estimation accuracy. In the applied context, this process requires each prospective user to undertake a calibration protocol prior to using the device, and as such, techniques involving subject-specific calibration are much less applicable than techniques involving a more general population-based calibration.

Paragraph Number 3

Validation of techniques using population-based calibration of the HR-PAI, and ACC-PAI relationships, have been provided by the investigations of Brage *et al.* (4) and Crouter *et al.* (10). Crouter *et al.*, describe a two-regression model for predicting PAEE from accelerometry, which distinguishes between various types of activity by applying thresholds based on the variability of the accelerometer signal in order to better estimate intensity. Brage *et al.* (4) used a branched algorithm (BA) analysis model, which applied a series of thresholds to predict PAEE from calibration regressions for both heart rate and accelerometry. Both of these techniques improved the precision with which it was possible to estimate PAEE among adults with group calibration, and in doing so, have demonstrated the potential utility of branched analytic techniques for estimation of free-living PAEE. Several recent studies (5,28,30) have shown that the BA approach proposed by Brage *et al.* (2004) improves PAEE estimates in adults performing a variety of locomotor and daily-living activities, suggesting that this approach has broad applicability.

Paragraph Number 4

However, important questions remain regarding use of an optimized BA approach in estimating PAEE. This includes determining how constraining the optimization of BA parameters to more readily utilize HR as a predictor of PAI/PAEE at higher intensities, and ACC at lower intensities affects the accuracy achievable by optimized BA analyses. While the strategy of constraining the optimization is intuitive and adheres to current data suggesting that HR and ACC are effective in different ranges of PAI, it is possible that such constraints limit the accuracy that can be obtained. In addition, optimized BA analyses used by Brage et al.(4), and others have primarily been used to obtain an estimate of total PAEE during a protocol consisting of a variety of activities. Only one study has examined the activity-specific accuracy of optimized BA analyses. Thompson et al. (30) reported good agreement between estimated and criterion PAEE for a variety of low-moderate intensity daily-living activities (e.g. sweeping) using BA analysis. However, this study used the device manufacturers default HR/PAI and ACC/PAI relationships, rather than subject-specific calibrations. Quantitative comparison of the activity-specific PAEE estimation error achieved by BA analyses and other techniques is needed in order to improve our ability to accurately estimate daily energy expenditure.

Paragraph Number 5

The primary purpose of this study was to develop and assess the accuracy (compared to indirect calorimetry) of algorithms to estimate activity-specific physical activity energy expenditure for sedentary *adults* using a dual (HR & ACC) measurement device and a series of six analytic models: 1) HR; 2) ACC; 3) Multiple linear regression of HR and ACC; 4) A *priori* branched analysis model of Brage *et al.* (4); 5) *Post hoc* branched analysis model of Brage *et al.*; 6) *Post hoc* branched analysis model without relative constraint of parameters determining HR-PAI and ACC-PAI weighting. We hypothesized that: 1) *post hoc* optimization of the branched algorithm parameters would provide a more accurate activity-specific estimation of PAEE than all other models, both across and within the various activities tested.

METHODS

Subjects

Paragraph Number 6—10 male and 10 female subjects were recruited for this study. All subjects were sedentary but otherwise free of musculoskeletal injury, cardiovascular risk factors (including obesity), or other contraindications to exercise. We used the Kriska Modifiable Activity Questionnaire (18) to confirm subjects were sedentary (less than 5 MET hours of activity per week for the year preceding participation in the study). All subjects provided written informed consent, which was approved by the Human Research Committee at the University of Colorado at Boulder.

Experimental Overview

Paragraph Number 7—Each subject first performed treadmill-based activity (calibration protocol), for construction of the HR-PAI and ACC-PAI relationships, which was followed by a series of structured activities designed to simulate common daily tasks (daily-living protocol). The accuracy of the various predictive models was tested on the basis of their ability to predict PAEE during the daily-living protocol. Two subjects of each sex failed to complete all aspects of one of the protocols, and were removed from all subsequent analyses, leaving 8 subjects in each group. Both protocols were performed on the same day of testing.

Measurements

Paragraph Number 8—To standardize postprandial status, all subjects were required to consume a nutritionally identical beverage (Ensure Plus™: 355 total kCal, 11g fat, 50g CHO, 13g protein) as their final meal at least 3 hours prior to arriving at the laboratory (11). Upon arrival, subjects were familiarized with the experimental equipment before being fitted with a 5-lead electrocardiogram and with 3 experimental devices:

1. Wireless device with simultaneous measurement of heart rate and accelerometry (WHA).
2. Polar S-510 heart rate monitor (Polar).
3. Actigraph GT1M-Lynx activity monitor (ACT).

Paragraph Number 9—While the WHA was the source of data used for analyses, we chose to include the Polar and Actigraph devices as references for the accuracy of WHA, which had yet to be compared to analogous devices, and also to provide a backup data source in the event of signal loss from WHA. As such, all three devices were synchronized for each test. The WHA is pre-commercial, but two identical prototypes were acquired from Triage Wireless Inc. (San Diego, CA). The device employs an ADXL103 uniaxial accelerometer oriented for optimal sensing of vertical acceleration, with a functional range of ± 1.7 g. The acceleration signal was low-pass filtered with a cut-off frequency of 32 Hz and sampled via a 10-bit A/D converter at 250 Hz. The sensitivity of the accelerometer was 0.64 v/g (0.065 v/m/s²). The movement measured by the accelerometer was summed over a one-minute epoch and counts/min were determined by counting the number of times acceleration was increasing and exceeded a pre-set threshold. Heart rate was measured at the chest by conventional removable strap coupled to a waist-mounted processing unit. The WHA chest strap was always worn superior to the Polar chest strap, and was checked for signal prior to and after mounting the Polar. All other details of the technology used for monitoring heart rate and acceleration remain proprietary. We mounted the wireless dual device monitor and the Actigraph at the level of the left hip at the anterior axillary line (33) with the Actigraph fixed superficially to WHA. The Polar receiver was worn on the wrist. Subjects then performed the calibration protocol, which was followed by at least 15 minutes of seated rest before continuing with the daily-living protocol.

Paragraph Number 10—During both protocols, criterion energy expenditure was assessed through indirect calorimetry via measures of expiratory gas concentrations and inspiratory ventilation. Expired gases were fed into a 5 L mixing chamber and sampled continuously by a Perkins-Elmer 1100 mass spectrometer (Boston, MA). Inspiratory ventilation was measured with a Hans-Rudolph pneumotachometer and differential pressure transducer (model MP45-14, Validyne engineering, Northridge, CA). The analog signal from the pressure transducer was conditioned externally (amplified and filtered - model MC1-3-871, Validyne engineering, Northridge, CA), before being interfaced with a Dell GX1 personal computer via analog-digital conversion and the previously validated (3) TrueMax 2400 software (ParvoMedics, Sandy, UT). Prior to and directly following each testing session this system was calibrated with known gas fractions and volumes. The post-calibration was used to check for drift over the course of the tests. In no testing session was this degree of drift outside the sensitivity of the calibration procedure itself (3%).

Paragraph Number 11—Final values of energy expenditure were calculated from oxygen consumption and respiratory exchange ratio (RER), which did not exceed 1.0 for any minute of the analyzed testing. PAI was defined as the rate of energy utilization (above rest) per 1-minute epoch, while PAEE was defined as the total energy expended by each subject over the entire daily-living protocol. During all tests subjects breathed a hyperoxic gas mixture,

which was calculated to counterbalance the elevation at the laboratory (25 % O₂, 0.03 % CO₂, N₂ balanced), and therefore simulate a sea-level $P_{I}O_2$ ($\approx$ 59 torr). This was done to enhance the applicability of our findings, and has previously been applied in our laboratory (6).

Calibration Protocol

Paragraph Number 12—Subjects first performed 30 minutes of supine rest. The final 10 minutes were used for assessment of supine energy expenditure, ACC, and HR, which were used analogously to RMR as an anchor for all predictions and measures of PAEE. While these measures of resting EE, ACC, and HR are distinct from the sleeping-based measures applied by Brage et al. (2004), previous work suggests that they offer a good approximation of true resting metabolism (8). Subjects then walked and jogged on a treadmill, performing a series of six, six-minute stages, with no rest separating them. Women began walking at 0.68 m/s (1.5 mph) and men at 0.90 m/s (2.0 mph). The speed was increased by 0.23 m/s (0.5 mph) for each new stage. We chose different speed profiles for men and women to normalize the range of relative physical activity intensity across the sexes. This normalization was effective as demonstrated by the peak HR achieved during the protocol, which reached 79 % for both men (range: 72–84) and women (range: 72–83). During pilot testing, at least 2 individuals of each sex exhibited discomfort walking at the highest two speeds. As such, we chose to remove variability in the ACC-PAEE regressions associated with differential gait choice by requiring all subjects to jog for the final two stages of their test. The test was terminated in the event that the subject's HR reached 85% of his or her age predicted maximum, or if any ECG abnormalities were present. Peak heart rate for this protocol across sexes was 78% of age-predicted maximum on average, and ranged from 68% – 84%. Average HR, ACC, and PAI were taken from the final 3 minutes of each stage and used in the individual and group calibration procedures.

Daily-Living Protocol

Paragraph Number 13—Subjects were required to perform six activities for six minutes each. We constructed a specialized experimental arrangement to allow three-dimensional movement during all activities. The activities were designed to be representative of daily-living movement patterns. Only the cycling and stair-stepping tasks involved a regulated pace, primarily to prevent subjects from exceeding the predetermined HR limit of 85% of their age predicted maximum. The activities were:

1. Cycling (1.25 W.kg⁻¹, 60rpm)
2. Sweeping (freely paced)
3. Vacuuming (freely paced)
4. Stacking (freely paced with a variety of household objects between 0.1kg and 5kg, moved a maximum horizontal distance of 1.5m and maximum vertical distance of 1m.)
5. Stair-stepping (5 vertical metres per minute)
6. Shoveling (freely paced)

Paragraph Number 14—The order of these activities was randomized other than for cycling, which was always performed first, and shoveling, which was always performed last. This was done to allow experimenters sufficient time to move these large pieces of equipment to and from the area of activity, and therefore minimize any break in activity. The activities were performed continuously and the time separating each from the next (for movement of equipment) was always less than 10 seconds. The initial 3 minutes of the

protocol were not used in the final analysis so as to limit any unmeasured anaerobic contribution to metabolism.

Analyses

Paragraph Number 15 Device Comparisons—To compare the WHA to devices with established experimental utility, we analyzed and compared WHA heart rate and accelerometer records to the synchronized records of the Polar and Actigraph devices. These assessments were made across all subjects for all conditions of the experiment. Paired Student's *t*-tests were used to compare mean differences, while Pearson product-moment correlations were used to assess association between the two measurement devices for each of the two dependent variables (ACC and HR). Bland-Altman plots were used to assess inter-instrument differences. Finally coefficients of variation were used to assess the total variability inherent to each device's measure/s of HR and/or ACC.

Paragraph Number 16 Calibration regressions

The origins for the HR-PAI and ACC-PAI relationships were set as supine HR and supine energy expenditure (HR-PAI), or supine ACC and supine energy expenditure (ACC-PAI), so as to prevent dilution of the PAEE estimates by energy expenditure not associated with activity. Similar to Brage *et al.*, 2004, HR, and mass-normalized PAI data were fit to a second order polynomial while ACC and mass-normalized PAI data were fit to 2 linear relations; one for ACC values below a flex point, which was forced through the origin, and one for ACC values above a flex point, which was not forced through the origin. For results involving individual calibration, ACC-PAI and HR-PAI regressions were constructed for each subject, while for group calibration results, they were fit to the combined data of all subjects in the analysis.

Paragraph Number 17 Estimation of Daily-Living PAEE

We used six analytic models to investigate our hypothesis; that an optimized branched algorithm would provide the most accurate assessment of PAEE across and within each activity of daily-living. These models were applied to ACC and/or HR data collected during the daily-living protocol to calculate an estimate of PAI for each minute of activity. The estimated values for minutes 4–36 were then summed to arrive at a compound model-estimated PAEE. This was done for each subject, and the precision of the estimate was calculated as the square root of the mean squared difference between the subjects' criterion PAEE and their predicted PAEE (the root mean square, RMS). To assess the degree to which these compound measures of error were due to estimation accuracy for each activity, we partitioned the model-predicted and criterion PAEE by activity for all models. RMS was then calculated for each activity within the various predictive models. In this context, only the sum of the final four minutes of each activity were used to arrive at model-predicted and criterion PAEE, so as to avoid inaccuracy in criterion PAI and HR due to transition between activities. It should be noted here, that the optimization procedures were only performed on the compound measure of PAEE, and not on any subset of activities.

1. HR prediction: We applied a Flex HR model to estimate PAEE, modified to employ our second-order regression of HR-PAI. This regression was used for HR values above HR-FLEX, which was defined as the average of supine HR and the HR recorded during the slowest walking speed (25). PAI was assumed to equal 0 below HR-FLEX.
2. ACC prediction: ACC estimation also involved a Flex type analysis. For ACC values below ACC-FLEX (defined as 50% of the ACC-value at the lowest walking

speed) the origin-anchored ACC-PAI relation was used, while for values above ACC-FLEX, the unanchored ACC-PAI relation was used.

3. Multiple regression prediction: HR and ACC data from the calibration protocol were fit via multiple linear regression to provide non-branched equations simultaneously relating HR and ACC to PAI. These relationships were anchored through the origin, and only included first order terms for HR and ACC.
4. Branched Algorithm *a priori* prediction: We applied the branched algorithm of Brage *et al.*, (Figure 1) with a set of parameters determined prior to analysis. All *a priori* parameters excepting X were determined as described by Brage *et al.* (4). We used a much greater X parameter because the WHA recorded accelerometer counts on a much larger absolute scale than the CSA (now Actigraph) device used by Brage *et al.* (4). For Y and Z parameters, individual HR values were used for the individual models and group mean HR values were used for the group model. The *a priori* parameters are listed below:

X: 10,000 (slightly less than mean WHA output during cycling)

Y: Mean of the HR values for the highest walking and slowest running speeds

Z: Flex HR (individual and group) (25)

P₁: 1, P₂: 0.5, P₃: 0.5, P₄: 0

5. Branched Algorithm constrained *post hoc* optimization: We applied the same branched algorithm as above, but optimized the parameters on the basis of the precision with which they estimated daily-living PAEE (the optimal set of parameters gained the lowest RMS). The simulated annealing technique was used for parameter optimization, and is described in further detail below. For this model we constrained our *post hoc* optimization within fixed ranges for the various parameters, and in particular we constrained the weighting parameters P₁₋₄ relative to one another, in a fashion similar to Brage *et al.* (4). As for the *a priori* parameters we used a different range (solution space) for the X-parameter than was used by Brage *et al.* (4), because the absolute scale of ACC data retrieved from the WHA is much greater than that of their CSA device.

X: 0 to 12,000 (at integer increments)

Y₁: -5.0 to 5.0 (at increments of 0.1), Y₂: -250 to 250 (at integer increments),
Compound Y: 0 to 250

Z₁: -5.0 to 5.0 (at increments of 0.1), Z₂: -250 to 250 (at integer increments),
Compound Z: 0 to 250 $0.0 \leq P_4 < P_3 < P_2 < P_1 \leq 1.0$ (at increments of 0.01)

6. Branched Algorithm unconstrained *post hoc* optimization: As for model 5, except that the regression weighting parameters ($P = \{P_1, P_2, \dots, P_4\}$) were not constrained relative to one another (i.e. each could have any value between 0 and 1.0 for any iteration).

Paragraph Number 18 Optimization by Simulated Annealing—To determine *post hoc* parameters used in the branched algorithm, we applied a Simulated Annealing (SA) technique for combinatorial optimization. This technique searches for a global optimum by applying principles central to statistical mechanics and the annealing process of solids (16,17), and has been applied to large-scale multi-dimensional problems in physiology (21).

Paragraph Number 19—Generally, SA involves random reconfiguration of a set of inputs (branched algorithm parameters), which are then applied to an objective function

(RMS calculation of the BA PAEE estimate). As these random reconfigurations proceed, the annealing algorithm records the lowest RMS achieved and the configuration that achieved it. Simultaneously the number of possible configurations that can be “reached” during the next reconfiguration shrinks, and as such, the algorithm “cools” toward a global optimum. While a theoretically perfect implementation of Simulated Annealing is guaranteed to retrieve the globally optimal configuration, practical implementations generally arrive at solutions that closely approximate the global optimum (31).

Paragraph Number 20—The specific details of our SA implementation are as follows:

1. Initial temperature (c_0) = 100. Justification: During pilot analyses the largest difference between any two RMS values in 1,000,000 random parameter reconfigurations was $4.9805 \text{ kJ.kg}^{-1}$. With this value representing the maximal difference (i.e. maximal ΔC_{ij}) likely for any application of the Metropolis criterion [$\exp(-\Delta C_{ij}/c_i)$], we chose an initial temperature ($c_0 = 100$) that would allow an acceptance probability of 0.95.
2. Length of Markov chains: Each temperature was maintained for 100,000 successive reconfigurations of the branched algorithm parameters. Pilot testing suggested that stability in ΔC_{ij} (an indication of quasi-equilibrium) occurred at approximately 3,000 reconfigurations for the highest temperature, and 10,000 at temperatures < 5 . As such we consider our algorithm to have implemented a relatively conservative cooling schedule.
3. Decrement in the control parameter was achieved by the simple asymptotic relation [$c_i = c_j - (c_j/1000)$]. We chose this protocol because a potential weakness of simulated annealing appears at lower temperatures where linear cooling schedules tend to underemphasize the need for local search (insert numerical recipes in C reference, Press).

The termination criterion for our algorithm was satisfaction of two conditions: 1) no improvement in the lowest RMS for 300,000,000 consecutive parameter reconfigurations 2) no improvement in the lowest RMS for at least 3000 consecutive search space adjustments (temperature decrements). At this point the algorithm ceased reconfiguration of the parameters, and returned the set of parameters that obtained the lowest RMS value.

Statistical Treatment

Paragraph Number 21—Mean differences in PAEE as calculated by the various analytic models were assessed via repeated measures ANOVA. Pair-wise differences were highlighted with Tukey’s HSD *post hoc* test. Pearson product-moment correlations were used to calculate relationships and coefficients of determination (r^2) for each analytic model with criterion PAEE. Significance was assessed at $\alpha < 0.05$ for all analyses.

RESULTS

Device Comparisons

Paragraph Number 22 Heart Rate—The WHA device provided mean HR values that were not different to the Polar for all subjects performing any daily-living activity ($p = 0.49$) or treadmill speed ($p = 0.29$), and also at rest ($p = 0.27$). The two devices were also very well correlated during the treadmill activity ($r = 0.995$), and only slightly less so during the daily-living activities ($r = 0.925$). The likely reason for this latter result is the more homogeneous HR data observed during the daily-living activities (mean range for all tasks = $14.1 \text{ beats.min}^{-1}$) as compared to the treadmill activity (mean range for all speeds = $58.1 \text{ beats.min}^{-1}$). Bland-Altman analyses of the treadmill and daily-living HR data (not shown)

indicate good agreement and very little bias between the devices (treadmill: $y = -0.0040x + 0.064$, RMS = 1.46, 95 % limits of agreement = +2.58, -2.16; daily-living: $y = -0.0062x + 0.8745$, RMS = 2.19, 95 % limits of agreement = +3.18, -2.98).

Paragraph Number 23 Accelerometry—At rest, during walking or running at any treadmill speed, and during any activity of daily-living, the WHA device recorded much greater absolute ACC values than the Actigraph (all $p < 0.0001$). However, because accelerometer counts are arbitrary indicators of movement, the reliability of the ACC measure is of much greater importance than its absolute value. The WHA measure of ACC (WHA_{ACC}) was well correlated to that of the Actigraph during the treadmill activity ($r = 0.959$), and like the HR comparison, only slightly less so for the daily-living activity ($r = 0.872$). Again the homogeneity of the data during the daily-living tasks (mean ranges for all tasks = 7640 counts.min⁻¹) is the likely explanation for this difference (treadmill mean range for all speeds = 10944 counts.min⁻¹). The regression relating the two ACC devices during treadmill activity was: $\text{WHA}_{\text{ACC}} = 89.45 \cdot \text{Actigraph} + 10180$. When expressed relative to the total measured ACC, the variability of WHA_{ACC} was much less than that of the Actigraph. During the treadmill activity the coefficients of variation for WHA_{ACC} ranged from 4.0 % to 9.8 % depending on speed, while for the Actigraph they were as high as 51.5% of the mean ACC value at 2mph. The Actigraph was also more variable during the daily-living activities with its mean coefficient of variation across all tasks being some 6 times greater than the mean coefficient of variation for WHA ($p < 0.01$). Although the algorithm used to calculate WHA_{ACC} counts/min from acceleration remains proprietary, we used published ACC data for walking and running (5) to estimate that the relationship between WHA_{ACC} counts/min and acceleration was $A \text{ (m/s}^2\text{)} = 0.000047(\text{CPM})$.

Subject Characteristics

Paragraph Number 24—Pertinent subject characteristics are described in Table 1. $\text{VO}_{2\text{max}}$ was calculated as a function of individual HR- VO_2 relations from the calibration protocol, and age-predicted maximal HR according to the equation of Tanaka and Seals (29).

Group Calibration Equations

Paragraph Number 25—Group calibration equations are provided in Table 2. All equations apply net (measured – supine) HR and/or WHA_{ACC}. Not shown in Table 2 is the first order coefficient used to model PAI from ACC values below ACC-FLEX, which was equal to 7.57×10^{-3} . Group mean activity-specific ACC, HR and PAI data are provided in Table 3.

Model Comparisons: (See Figure 1)

Paragraph Number 26 HR—The HR model significantly overestimated criterion PAEE among men and women ($p < 0.01$). The root mean square error values for HR were 59 % of the mean criterion PAEE for the individually calibrated model, and 63 % for the group-calibrated model. HR predicted energy expenditure was significantly correlated with criterion energy expenditure ($r^2 = 0.60$, $p = 0.04$).

Paragraph Number 27 ACC—In both men and women the ACC model significantly underestimated mean energy expenditure ($p < 0.01$). Root mean square values represented 53 % (individual calibration) and 64 % (group calibration) of mean criterion PAEE. Interestingly the ACC models were not associated with criterion PAEE, with the individually calibrated model appearing completely unrelated ($r^2 = 0.001$).

Paragraph Number 28 Multiple Linear Regression—MLR was a more accurate predictor of PAEE than HR or ACC alone. While group-calibrated MLR significantly overestimated criterion PAEE ($p = 0.04$) and individually calibrated MLR did not, it is unlikely that this represents inaccuracy attributable to group calibration because error in the mean prediction afforded by group calibration was less than that for individual calibration (Figure 1). Furthermore, the group-calibrated MLR model offered the lowest prediction error of any non-optimized model with an RMS equal to 26 % of mean criterion PAEE. Neither calibration method allowed MLR-predicted PAEE to be significantly correlated to criterion PAEE (individual calibration, $r = 0.38$; group calibration, $r = 0.64$).

Paragraph Number 29 A priori Branched Algorithm—The *a priori* branched analyses overestimated criterion PAEE whether they involved group or individually calibrated regressions ($p > 0.05$). RMS error was intermediate in these two models at 42 and 45 % of criterion PAEE for individual and group calibration, respectively. Only the individually calibrated model achieved significant association with the criterion measure ($r = 0.75$). In an additional analysis to partially replicate the later paper by Brage et al., (5), we performed these analyses with the following modifications to the *a priori* parameters ($P_1 = 0.9$, $P_2 = 0.5$, $P_3 = 0.5$, $P_4 = 0.1$). These analyses improved the mean estimate (individual calibration = 8.06 vs. 8.39 kJ.kg⁻¹; group calibration = 8.33 vs. 8.69 kJ.kg⁻¹) and RMS measured precision (individual calibration = 36 % of criterion PAEE; group calibration = 39 %)

Paragraph Number 30 Post hoc Branched Algorithm—Post hoc optimization of the branched algorithm parameters offered the most accurate models for prediction of daily-living PAEE, with unconstrained optimizations resulting in more accurate estimates than constrained optimizations. Estimates from the constrained and unconstrained models were not significantly different to mean criterion PAEE. The constrained and unconstrained optimization RMS errors for individual calibration were 16 % and 12 %, respectively. Under group calibration those errors rose to 18 % with constraint and 14 % without. Estimates afforded by all optimized models were significantly correlated to criterion PAEE ($r = 0.74$ to 0.81).

Paragraph Number 31—The optimized BA parameters are shown in Table 4, and indicate that when the branched algorithm is constrained so that $P_4 < P_3 < P_2 < P_1$, the number of branches reachable by the algorithm is much fewer than for the unconstrained algorithm. As can be observed in Figure 1, the effect of this constraint is relatively slight whether assessed as a difference in mean model accuracy, or RMS indicated estimation error.

Activity-Specificity of Model Estimations

Paragraph Number 32—When parsed by activity, measures of mean criterion PAI indicate that bicycling was performed at the highest intensity, and was closely followed by stepping while all other activities were performed at significantly lower rates of energy expenditure (between 44% and 59% of bicycling PAI).

Paragraph Number 33—Figure 2 displays fractional representations of model accuracy across the various activities in the daily-living protocol. Similar characteristics are apparent for these analyses across the two calibration techniques, and as such, group and individual calibration will be described together when referring to activity-specificity. ACC alone underestimated PAEE in all activities, particularly bicycling, but generally exhibited relatively little activity-specificity. HR alone exhibited more activity-specificity as it provided accurate prediction during stepping and bicycling, but substantially overestimated

PAEE associated with all other activities. The *a priori* branched model displayed similar activity-specificity as HR alone, albeit less extreme, suggesting that our determination of *a priori* parameters may have too heavily weighted the HR-PAI regressions. Multiple linear regression proved more versatile than HR and ACC alone, and compared well to the optimized branched algorithm analyses. Indeed during the higher intensity activities of stepping and bicycling, MLR provided a slightly more accurate estimate than either of the optimized models, although it did so in a more variable manner. Perhaps most interesting is the degree to which the optimized branched algorithm estimations varied in accuracy among the six activities, while exhibiting low variability within each activity.

Paragraph Number 34—To determine whether our expectation that optimization to total daily-living RMS would be associated with variation in estimation error between subjects rather than activities, we applied ANOVA (Subject $\times$ *Post hoc* model) to the estimation errors (model-predicted PAEE – criterion PAEE) for each subject performing each activity. Figure 3 shows that between mean square error for the subject factor was strongly and directly associated with RMS magnitude ($p < 0.01$). Conversely the between mean square error for activity was significantly and negatively associated with overall RMS error ($p < 0.05$). These analyses indicate that, within the optimized *post hoc* analyses, RMS measured error increased with increasing variability in the prediction error occurring between subjects, but decreased between activities.

DISCUSSION

Accuracy of the Branched Algorithm Analyses

Paragraph Number 35—Herein we provide evidence to support previous investigations showing that branched algorithm analyses are capable of providing substantial predictive improvement over less complex analytical techniques (4,14,28). Across calibration methods and with or without constraint of the BA, our data indicate that the PAEE prediction error (RMS) of multiple linear regression can be reduced by between 28 and 75 % through application of optimal branched algorithm parameters. These are comparable to the results obtained by Brage et al., (5), which ranged from 73 % (group calibration) to 84 % (individual calibration) improvement. Furthermore, the optimized BA improved mean predictive accuracy, as evidenced by decreases in the error of the mean prediction, by between 78 % and 82 % over MLR, and an absolute mean error as small as 0.17 kJ.kg^{-1} (2.5 % of mean criterion PAEE). This approaches the optimal results obtained by Brage et al., 2004 (0.2 kJ.kg^{-1} , 0.6%), and therefore indicates that our branched analyses are performing with relatively high precision. With these points noted, our current data are also likely constitute a conservative estimate of optimized BA precision given that our daily-living protocol did not include movements involved in the calibration procedure. In free-living adults, energy expended during walking represents a majority of the daily PAEE (19) and including walking in the daily-living protocol is likely to have considerably improved the precision of our daily PAEE estimates.

Paragraph Number 36—The data presented here also support those of Brage *et al.* (4), in suggesting that group level calibration can be used to similar effect as individual level calibration when optimized branched algorithms are used for the analysis. The mean RMS difference between the two calibration methods was only 2% across the unconstrained and constrained analyses. The observation that this finding corresponds closely with that of Brage et al.,(4) (who observed a mean difference of 2.3%), in the presence of markedly different subject populations, daily-living activities, and definitions of resting HR and energy expenditure, suggests that the utility of group calibration is a consistent and stable characteristic of optimized branched analyses. This finding is perhaps the most immediately

applicable as it suggests that it may be possible to apply BA parameters optimized for a representative sample, to the population at large. A key step required to firmly establish this assertion will be a large-scale crossover design study to assess the degree to which the parameters optimized to one sample are applicable to another of the same population.

Paragraph Number 37—While *post hoc* models exhibited better predictive precision than all other models, the *a priori* models only offered improvement over HR and ACC. It is clear from our *a priori* results that branched algorithm analyses may not be inherently more efficacious than other techniques, specifically multiple linear regression. Indeed, we considered our choice of *a priori* parameters to have strong theoretical justification, and empirical precedent (4,23,26–28), but found them to be less powerful than group-calibrated MLR in predicting daily-living PAEE. The reasons for this relatively poor performance are likely to centre on over-utilization of HR-based estimation of PAI, and ambiguity in determination of the X parameter, which was enforced by the very large scale of the ACC data recorded by the WHA device. We attempted to adjust for the latter effect by altering our *a priori* value for X, but this was clearly not sufficient to allow *a priori* algorithm performance to approach that of the *post hoc* optimized models. Additional modification of the *a priori* parameters to reflect those chosen by Brage *et al.*, in a later study, which involved a more heterogeneous population (5), did improve model precision but only to a modest extent that did not surpass that offered by group calibrated MLR.

Activity–Specificity

Paragraph Number 38—A primary objective of the current investigation was to assess the activity-specificity apparent among *post hoc* optimized branched algorithm analyses. To that end, we applied a series of daily living activities that are distinguished by their mechanical heterogeneity and by their tendency to pose a challenge to ACC-based measurement of physical activity. That is, most were primarily upper body, or in the case of bicycling, known to be dissociated from ACC-PAI relationships developed from other locomotor activities such as walking and running. To assess the degree to which these challenges may have limited model performance across and within the various activities, we parsed the estimation data by activity. These activity-specific analyses replicate established principles of physical activity quantification. Our data clearly show that HR tends to be more effective at estimating activity performed at higher intensities (as observed for stepping and bicycling), ACC prediction tends to underestimate PAI but generally improves at lower intensities, and MLR extends the effective intensity ranges of HR and ACC. The novel, and most important finding of these analyses is that even the most flexible analysis applied herein, the unconstrained individually calibrated BA, exhibited systematic errors in predicting PAEE for certain activities. The underestimation of bicycling PAI by this optimized model offers the best example of activity-specificity, and viewed in concert with the accuracy of HR-based estimation of bicycling PAI, suggests that optimizing the branched algorithm to minimize total daily-living RMS may significantly disadvantage it's accuracy for certain activities. This contention is supported by analyses indicating that, within the optimized models, the variability of prediction error between subjects is strongly positively associated with RMS-assessed precision, while the variability of prediction error between activities is strongly negatively associated with that precision (Figure 3). This suggests that increasing the precision of the *post hoc* optimized models across all activities is linked to decreased variability in the error of prediction between subjects, and increased variability in the error of prediction between activities. The first of these results is intuitive to the extent that minimising the magnitude of each subject's estimation error across all activities will decrease the RMS of these errors over all subjects, which was the sole criterion for optimization. The second result is less intuitive but perhaps more insightful in that it implies that, as RMS and between subject mean square error decrease, between

activity mean square error (the variance of prediction error among the various activities and across all subjects) increases. In other words, it appears that optimization to minimize error in the prediction of all subjects' total daily-living PAEE occurs at the expense of accuracy in predicting PAEE for all activities. An intuitive strategy to improve BA performance that follows from these observations is to use branched analyses with a number of different sets of parameters each of which has been optimized to a specific activity. In practice these analyses would be most applicable in conjunction with algorithms capable of determining the activity being performed on the basis of the ACC and HR signals. We suggest that this avenue offers the potential for substantial further improvement in the prediction of PAEE by BA, which is otherwise likely to be hampered by the counteractive effects of activity heterogeneity.

Paragraph Number 39—Another important observation of the current study is that the use of a BA in which regression weighting (P) parameters were not constrained, improved the predictive precision of the model. While this improvement was relatively modest (RMS error was decreased by between 20 and 35% relative to constrained optimization) it was consistent across calibration methods, and data not shown here indicate that this principle holds within sample subsets separated by sex. This finding suggests that the desire to anchor the branched algorithm parameters to the well-established principle that HR and ACC best predict PAI in specific intensity ranges, may in fact counteract optimal BA performance. It is intuitive and certainly empirically established that prediction by HR-PAI is generally more effective at higher PAI, whereas ACC-PAI is more effective at lower PAI. However, imposing these principles as a necessity of parameter optimization may restrict the algorithm to an extent capable of limiting the precision achievable by the optimization process. Removing such constraint will certainly allow optimization to access unorthodox regression weighting for activities in which ACC or HR violate the principle that HR and ACC are effective at high and low ranges of PAI, respectively. This concept is best supported by our data describing utilization of the optimized P parameters. Constrained optimization tended to arrive at a solution that forced all data towards a single P parameter, which presumably represents the single weighting of HR and ACC that provides the lowest RMS across all activities. Along with the loss of the other weighting parameters, most of the power intended by branching became inaccessible, and the optimal solution was effectively reduced to an analysis theoretically similar to multiple regression, albeit constructed from daily-living rather than calibration data. It should be noted here that Brage et al., 2004 also utilized constrained optimization, and observed much more balanced algorithm behaviour, with optimal solutions allowing significant utilization of at least 2 regression-weighting parameters. There are 3 likely reasons for these observations:

1. We employed a mechanically heterogeneous range of activities compared to Brage *et al.*, 2004, which for the above mentioned reasons may limit the combination of parameters that can be simultaneously effective across the broader range of activity characteristics.
2. By utilizing a less physically active subject population we have substantially limited the reachable range of PAI, and therefore may have decreased the resolution of the branched algorithm for prediction of PAI and forced the algorithm toward a single regression-weighting parameter.
3. Our definition of resting HR and energy expenditure (EE) differed from those of Brage *et al.*, 2004, and because RHR is a central component of both the HR-PAI regressions, and the Y and Z parameters of the BA, it is possible that these differences underlie decreased flexibility within our constrained optimized branched analyses.

Paragraph Number 40—In contrast to constrained optimization, unconstrained optimization yielded an algorithm that allowed access to other P parameters, which is likely to have permitted improvement in BA precision by accounting for data that are not well described by the more generally appropriate constraint. Based on this finding we suggest that both unconstrained and constrained optimization be utilized in future studies applying BA to estimation of daily- or free-living PAEE, particularly if the activities involved are relatively varied. With this potential noted we also suggest that removing constraint upon the regression weighting parameters has potential to limit algorithm performance with orthodox data, and as such, the validity of any one set of unconstrained parameters will need to be comprehensively experimentally verified.

Conclusions

Paragraph Number 41—Here we have supported previous work by demonstrating the utility of branched algorithm analyses of HR and ACC in the assessment of daily-living PAEE. The current study also offers two novel insights regarding the behaviour of these analyses when applied to a challenging and heterogeneous range of daily-living activities:

1. The precision of *post hoc* optimized branched analyses may be enhanced by eliminating constraint on parameters involved in weighting the influence of HR and ACC in prediction of PAEE.
2. The precision of *post hoc* optimized branched analyses is limited by the opposing algorithm requirements of different activities, and is therefore impaired by heterogeneity in the range of activities being assessed.

Limitations

Paragraph Number 42—To temper these findings, there are several limitations to the current study:

1. The sample size is relatively small and as such does not offer the generalizability and robustness of a larger sample, which may be particularly important in comparing parameter optimizations achieved by non-linear optimization to those of other investigations.
2. While the WHA device offered reliable ACC data, the scale on which that data is recorded also impairs cross-study comparisons.
3. Our application of a slightly but importantly different definition of RHR from that of Brage et al., (4) likely contributes to differences in optimal parameter configurations between the two studies. This methodological difference may also have contributed to the very narrow branching exhibited by the constrained *post hoc* optimized BA models, but we suggest a more likely explanation for this observation is the very heterogeneous selection of daily-living activities applied here.

Future Directions

Paragraph Number 43—To extend the work detailed here, we suggest three directions that may allow further improvement in our ability to predict daily-living PAEE in general, and enhance the utility of branched algorithm analyses in particular:

1. Sufficient data now exist to warrant a large-scale crossover design study of *post hoc* BA optimization. Such an investigation has the potential to firmly establish group calibration as a strategy applicable to a broad population range, and therefore

to eliminate the requirement for individual calibration in both the research and clinical settings.

2. Future work should include both constrained and unconstrained optimization of BA parameters, particularly in circumstances where daily-living is likely to involve a broad range of activities.
3. The development of different sets of BA parameters optimized for common daily-living activities offers the potential for much greater algorithm flexibility, and should be a priority for future work. Simultaneous development of algorithms capable of determining activity on the basis of real-time HR and ACC data is clearly a complementary research goal of substantial potential benefit.

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Figure 1.

Total daily-living PAEE (kJ.kg^{-1}) as estimated under individual (open bars) and group (filled bars) calibration, and by accelerometry alone (ACC), heart rate alone (HR), multiple linear regression (MLR), an *a priori* branched algorithm (APBA), constrained *post hoc* optimized branched algorithm (C-PHBA), and unconstrained *post hoc* optimized branched algorithm (U-PHBA). Data are presented as mean PAEE, + RMS, and – SEM. * $p < 0.05$ both calibration methods vs. criterion PAEE, † $p < 0.05$ group calibration vs. individual calibration, # $p < 0.05$ group calibration vs. criterion PAEE

Figure 2. Mean estimation error expressed as a fraction of criterion PAEE for all daily-living activities and estimation models (accelerometry alone, ACC; heart rate alone, HR; multiple linear regression, MLR; an *a priori* branched algorithm, APBA; constrained *post hoc* optimized branched algorithm, C-PHBA; and unconstrained *post hoc* optimized branched algorithm, U-PHBA). Panel A provides data for individual calibration, and Panel B for group calibration.

Figure 3.

Root mean square error ($\text{kJ} \cdot \text{kg}^{-1}$) for estimation of total daily-living PAEE as a function of between mean square error by subject (filled symbols), and activity (open symbols), among the four optimized branched algorithm models. Both relationships were significant at $p < 0.05$.

Table 1

Descriptive characteristics for all subjects

Subject	Sex	Age (years)	BMI (kg·m ⁻²)	Mass (kg)	Height (m)	VO _{2max} (mL·kg ⁻¹ ·min ⁻¹)
1	F	18	25.2	63.0	1.58	23.6
2	F	33	21.2	57.0	1.64	23.6
3	F	18	24.5	76.2	1.77	26.8
4	F	48	25.6	64.5	1.59	20.0
5	F	35	17.5	45.5	1.61	26.4
6	F	33	28.7	68.8	1.55	21.5
7	F	23	20.5	63.0	1.75	21.8
8	F	20	21.4	52.2	1.56	26.9
9	M	31	29.9	90.5	1.74	27.7
10	M	23	21.0	64.5	1.75	31.9
11	M	20	24.6	88.0	1.89	26.7
12	M	19	25.0	74.5	1.73	32.7
13	M	18	22.2	75.2	1.84	33.4
14	M	27	25.7	83.5	1.80	27.5
15	M	27	22.4	73.5	1.81	33.8
16	M	21	24.9	86.3	1.86	35.3

Group calibrated regression coefficients for ACC-PAI ($\text{J.kg}^{-1}.\text{count}^{-1}$), HR-PAI ($\text{J.kg}^{-1}.\text{beat}^{-1}$), and J.kg⁻¹.beat⁻²), and MLR. Root mean square values (RMS) are presented to reference regression fit

Table 2

Group Calibrated Regression Coefficients							
	Intercept	ACC	HR	HR ²	FLEX	RMS	r ²
ACC	52	3.07×10 ⁻³			11568	5.5×10 ⁻²	0.84
HR	0		5.65	-2.58×10 ⁻³	9	4.8×10 ⁻²	0.89
MLR	0	3.64	1.28×10 ⁻³			4.0×10 ⁻²	0.92

ACC-PAI and HR-PAI coefficients are normalized to body mass: ACC-PAI ($\text{J.kg}^{-1}.\text{min}^{-1}.\text{count}^{-1}$); HR-PAI ($\text{J.kg}^{-1}.\text{min}^{-1}.\text{beat}^{-1}$), and $\text{J.kg}^{-1}.\text{min}^{-1}.\text{beat}^{-2}$). Root mean square values (RMS) and coefficients of determination (r^2) are presented to reference regression fit

Table 3

Accelerometer counts (ACC, counts.min⁻¹), heart rate (HR, beats.min⁻¹), and PAI (kJ.kg⁻¹.min⁻¹), for each daily-living activity. Data are presented as means (SEM)

	ACC	HR	PAI
Stepping	17990 (3220)	61.0 (4.9)	0.28 (0.02)
Sweeping	19060 (3210)	61.4 (5.9)	0.17 (0.01)
Stacking	12260 (2240)	55.1 (5.0)	0.16 (0.01)
Shoveling	12250 (1190)	57.8 (5.7)	0.19 (0.02)
Vacuuming	17630 (2560)	62.7 (5.8)	0.14 (0.01)
Bicycling	11420 (1310)	64.4 (4.0)	0.32 (0.02)

PAI data are normalized to mass (kJ.kg⁻¹.min⁻¹), while heart rate (HR, beats.min⁻¹), and accelerometer counts (ACC, counts.min⁻¹) are not. All data are presented as values above rest (supine) and as means (SEM).

Table 4

Optimal branched algorithm parameters and their utilization (%) for post hoc optimized BA models involving individual or group calibration, and constrained or unconstrained optimization. Braces indicate that the value of the compound Y or Z parameter was constrained to equal 0 because calculation for any feasible resting heart rate would provide a negative value.

Parameter	Constrained		Unconstrained	
	IC	GC	IC	GC
X	4069	1369	11980	9246
Y ₁	-5.0	2	1	0.3
Y ₂	-223	126	192	50
Z ₁	-4.8	-3.7	-1	-2.6
Z ₂	-204	-234	&1320	105
P ₁	0.49	0.65	0.52	0.38
P ₂	0.46	0.46	0.43	0.72
P ₃	0.33	0.38	0.31	0.27
P ₄	0.11	0.12	0.75	0.83
Utilization (1/2/3/4; %)	99/0/1/0	0/100/0/0	0/50/12/38	25/44/31/0

Braces indicate that the value of the compound Y or Z parameter was constrained to equal 0 because calculation for any feasible resting heart rate would provide a negative value.