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A Metabolic Energy Expenditure Model with a Continuous First Derivative and its Application to Predictive Simulations of Gait

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RESEARCH ARTICLE

A metabolic energy expenditure model with a continuous first derivative and its application to predictive simulations of gait.

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ABSTRACT
Whether humans minimize metabolic energy in gait is unknown. Gradient-based optimization could be used to predict gait without using walking data, but requires a twice differentiable metabolic energy model. Therefore, the metabolic energy model of Umberger et al. (2003) was adapted to be twice differentiable. Predictive simulations of a reaching task and gait were solved using this continuous model and by minimizing effort. The reaching task simulation showed that energy minimization predicts unrealistic movements when compared to effort minimization. The predictive gait simulations showed that objectives other than metabolic energy are also important in gait.

KEYWORDS
Metabolic Energy Minimization; Predictive Simulation; Gait

1. Introduction

Predictive gait simulations can provide theoretical explanations for features of human gait (Ackermann and van den Bogert 2010) and can be useful to predict the effect of an altered mechanical environment on human gait. If such predictions are accurate, simulations can aid design of exercise systems or prostheses (Van den Bogert et al. 2012; Koelewijn and van den Bogert 2016). In a predictive simulation, the muscle stimulations of a single gait cycle are found by minimizing an objective. This approach assumes that humans choose their gait such that a certain cost function is minimized (Bertram and Ruina 2001).

It is often assumed that metabolic energy is minimized in gait. Many gait parameters are chosen such that metabolic energy is minimized, such as walking speed (Ralston 1958), the ratio between step length and step frequency (Zarrugh et al. 1974), step width (Donelan et al. 2001) and vertical movement of the center of mass (Ortega and Farley 2005; Gordon et al. 2009). Selinger et al. also found that people adapt their step frequency when the metabolic energy optimum is changed using an exoskeleton, such that a different step frequency is optimal (Selinger et al. 2015).

If minimal metabolic energy is the true objective of human gait, predictive simulations should minimize metabolic energy. Several models exist that describe metabolic

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energy expenditure as a function of muscle activation, length and velocity (Umberger et al. 2003; Bhargava et al. 2004; Lichtwark and Wilson 2005; Houdijk et al. 2006). These models can be used as an objective for a predictive simulation. Simulations that minimize metabolic energy will allow verification of the objective of metabolic energy minimization in gait. Furthermore, this objective could be combined with other objectives, such as head movement or stability, to analyze how these factors influence the human's gait pattern.

Previously, Anderson and Pandy (2001), Sellers et al. (2005), and Miller et al. (2011); Miller (2014) created simulations of walking by minimizing metabolic energy without defining an analytical gradient. This required gradient-free optimization algorithms (Sellers et al. 2005; Miller et al. 2011; Miller 2014) or shooting (Anderson and Pandy 2001). Gradient-free optimization algorithms are known to be slow (Sellers et al. 2005). Shooting requires a forward simulation for each optimization variable to determine the gradient with respect to that optimization variable, and so is slow as well. Therefore, their simulations required thousands of CPU hours (Anderson and Pandy 2001; Miller 2014), sometimes to find only simple control profiles (Miller 2014). The solutions were not periodic gait cycles (Anderson and Pandy 2001; Miller 2014), and often data was used to create an initial guess (Miller et al. 2011; Miller 2014), which might influence the final solution.

Predictive simulations can be solved faster using direct collocation, which also allows for more complex control inputs, and ensures that the resulting gait cycle is periodic (Ackermann and van den Bogert 2010; Lin and Pandy 2017). This approach adds one-step dynamics between collocation nodes to the constraints, instead of using forward simulations. This creates a large-scale problem with many optimization variables and constraints, for which analytical gradients can be defined, which speeds up the optimization significantly (Ackermann and van den Bogert 2010). However, existing metabolic energy models cannot be used as objective, since the first derivative with respect to muscle states is not continuous. Therefore, this paper proposes a version of an energy expenditure model with a continuous first derivative. The model described by Umberger et al. (2003) and Umberger (2010) was selected since it is based on mammalian muscle data, includes the nonlinear relationship between energy output and muscle activation (Umberger et al. 2003), and is widely used due to its implementation in OpenSim (Delp et al. 2007).

Currently, an objective based on effort, or muscle activation, is often used with direct collocation (Ackermann and van den Bogert 2010; Van den Bogert et al. 2012; Koelewijn and van den Bogert 2016). Previous work showed that this objective can only predict the main features of gait (Ackermann and van den Bogert 2010).

Therefore, our goal is to investigate if it is possible to create a realistic gait cycle by minimizing metabolic energy. To do so, we have three aims:

(1) Create a version of the metabolic energy model by Umberger et al. suitable for optimization of movements
(2) Highlight the differences between optimization of metabolic cost and optimization of effort using a simple problem
(3) Compare a predictive gait simulation that minimizes metabolic cost to a predictive gait simulation that minimizes effort

We will show that the continuous version of the metabolic energy model correlates well with the original model over a range of walking and running speeds. We create predictive simulations of a single joint reaching task to highlight the differences between metabolic rate and effort minimizations. Finally, we present a predictive gait simulation that minimizes metabolic rate from a random initial guess, and compare to a predictive simulation that minimizes effort.

2. Methods

2.1. Adaptations to the Metabolic Energy Model

A metabolic energy expenditure model was created with a continuous first derivative. This model will be called the 'continuous model', while the original model is called the 'original model'. This section describes the changes that were made to the metabolic energy model described by Umberger et al. To review the original model, the reader is referred to Umberger et al. (2003) and Umberger (2010). The supplementary material describes the complete continuous energy model.

Umberger et al. (2003); Umberger (2010) introduced a metabolic energy model that is an expansion of the Hill type muscle model. The metabolic rate over all muscles, W, is calculated in W/kg by averaging the energy expenditure rate for each muscle over time and summing over all muscles:

$$W = \frac{1}{TM} \sum_{j=1}^{n_{mus}} \int_0^T \dot{E}_j(t) m_{mus(j)} \, \mathrm{d}t, \tag{1}$$

where T is the duration of the motion, M is the mass of the subject and $m_{mus(j)}$ the mass of muscle j. The metabolic cost in J/kg/m can be found by dividing the metabolic rate by the speed of the motion.

The energy rate, $\dot{E}$, normalized to the muscle mass, is equal to the sum of the heat rate from the activation of muscles and its maintenance, $\dot{h}_{AM}$, the heat rate due to shortening and lengthening of muscles, $\dot{h}_{SL}$, and the mechanical work rate, $\dot{w}_{CE}$:

$$\dot{E} = \dot{h}_{AM} + \dot{h}_{SL} + \dot{w}_{CE}. \tag{2}$$

The activation-maintenance heat rate has a continuous derivative. However, the shortening-lengthening heat rate has three discontinuities. The different heat rate formulas used for shortening and lengthening velocities cause the first discontinuity. The shortening coefficients are based on a study by Barclay et al. (1993), while the lengthening coefficient is based on experimental data (Umberger et al. 2003; Umberger 2010).

This discontinuity was removed by creating a separate shortening and lengthening velocity. The shortening velocity is nonzero and negative when the velocity, $\bar{v}_{CE}$, is negative and equal to zero when the velocity is positive. The lengthening velocity is nonzero and positive when the velocity is positive and zero otherwise. Then, the heat rate for the shortening and lengthening velocity are summed, since one of them will be zero. The shortening velocity, $\bar{v}_{CE(S)}$, and lengthening velocity, $\bar{v}_{CE(L)}$ are determined using the following smooth functions:

$$\bar{v}_{CE(S)} = \frac{1}{2}\left(\bar{v}_{CE} - \sqrt{\bar{v}_{CE}^2 + \varepsilon^2}\right), \tag{3a}$$

$$\bar{v}_{CE(L)} = \frac{1}{2}\left(\bar{v}_{CE} + \sqrt{\bar{v}_{CE}^2 + \varepsilon^2}\right), \tag{3b}$$

where ε is a small number.

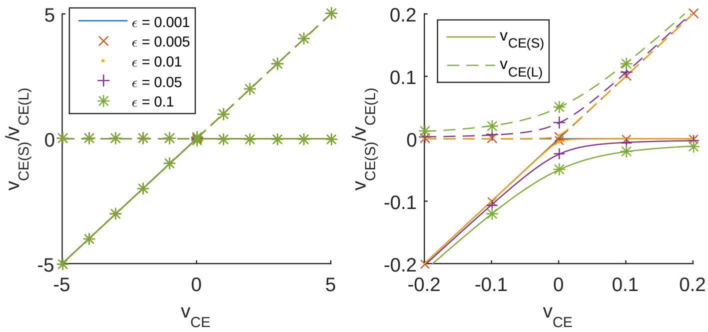

Figure 1.: Illustration of the shortening and lengthening velocity as a function of the contractile element velocity.

Figure 1 shows the shortening velocity, $\bar{v}_{CE(S)}$, and the lengthening velocity, $\bar{v}_{CE(L)}$, as a function of the contractile element velocity to illustrate their values. The right graph shows in more detail how the function is made continuous around zero velocity.

Two additional discontinuities in the first derivative are caused by the dependency of the shortening-lengthening heat rate changes on activation and stimulation. The heat rate is dependent on $A(t)$, which is equal to stimulation, $u(t)$, if the stimulation is larger than the activation, $a(t)$, and dependent on the average between the activation and stimulation if the stimulation is smaller than the activation, which can be described as follows:

$$A(t) = \begin{cases} u(t) & \text{if} \quad u(t) > a(t) \\ \frac{a(t)+u(t)}{2} & \text{if} \quad u(t) < a(t). \end{cases} \tag{4}$$

This equation can be rewritten to the following continuous version:

$$A(t) = u(t) + \frac{1}{2}\left(\frac{a(t)-u(t)}{2} + \sqrt{\left(\frac{a(t)-u(t)}{2}\right)^2 + \varepsilon^2}\right), \tag{5}$$

where ε is the same in equation 5 and equations 3a and 3b for simplicity.

The final discontinuity is the relationship between $A(t)$ and the shortening-lengthening heat rate. This relationship is quadratic for shortening (Buschman et al. 1995, 1996, 1997), but no information was available for lengthening (Umberger et al. 2003). Umberger et al. used a linear relationship. There is no evidence for a linear or a nonlinear relationship, though Umberger et al. claimed that this relationship is likely nonlinear as well (Umberger et al. 2003). A quadratic relationship is used for lengthening to make the relationship continuous, since this is the simplest nonlinear relationship.

2.2. Model Comparison using Simulated Gait

The correlation between the original and the continuous metabolic energy model was determined using simulations of walking and running. The correlation used metabolic cost, which is the metabolic rate normalized to speed. These simulations were found using an objective of muscular effort and tracking of gait data, using a procedure

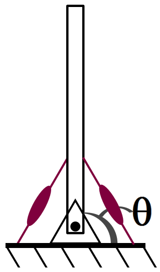

Figure 2.: Sketch of the arm, operated by muscles.

identical to the one used by Van den Bogert et al. (2012).

Simulations were used from 20 virtual subjects, randomly sampled with mean ($\pm$ SD) height of 176 $\pm$ 5.3 cm and weight of 73.5 $\pm$ 6.2 kg. Dimensions and inertial properties were taken from Winter (2005). All muscle parameters were varied around their original value with a standard deviation of 5% of the original value (see Van den Bogert et al. (2012)). For each virtual subject, gait simulations were generated at four different speeds, walking at 1.3 m/s and 1.8 m/s, and running at 3.6 m/s and 4.3 m/s.

The metabolic cost of the simulations was calculated with the original and continuous model. These were compared using repeated measures correlation (Bakdash and Marusich 2017), since four data points were available for each subject. The correlation coefficient and its confidence interval were used to evaluate how well the continuous model agreed with the original model. This statistical analysis was performed in R.

2.3. Predictive Simulation of a Single Joint Reaching Task

Next, a predictive simulation minimizing metabolic rate was compared to a predictive simulation minimizing muscular effort. This comparison is done on a simple problem to highlight the different trajectories found with these objectives. This comparison is performed by looking at the differences in the optimal trajectory, metabolic rate, and muscle activation.

An arm, rotating around a single joint, controlled by two muscles, performs a reaching task in the horizontal plane. The task is to move 90 degrees and back in five seconds. Figure 2 shows the arm at $\theta = 90$ degrees. The two muscles are Hill-type muscles, with a contractile element with activation and contraction dynamics, a series elastic element, and a parallel elastic element, both modeled as nonlinear springs. Their properties were similar to muscle properties of a Brachialis muscle (Breteler et al. 1999) (see table 1).

The dynamics are formulated implicitly using state $x = [\theta \quad \omega \quad a_1 \quad a_2 \quad \tilde{l}_{CE(1)} \quad \tilde{l}_{CE(2)}]^T$, and control input $u = [u_1 \quad u_2]^T$ with angular velocity ω, activation a_j, stimulation u_j, and normalized fiber length $\tilde{l}_{CE(j)}$ for muscle j:

$$f(x(t), \dot{x}(t), u(t)) = 0, \tag{6}$$

Table 1.: Overview of muscle parameters used.

Activation Time	T_{act}	0.012 s
Deactivation Time	T_{deact}	0.0476 s
Maximum Force	F_{max}	1100 N
Optimal Fiber Length	$l_{CE(OPT)}$	7 cm
SEE slack length	$l_{SEE(slack)}$	5 cm
PEE slack length	$l_{PEE(slack)}$	8.4 cm
SEE stiffness	K_{SEE}	$1.76 \cdot 10^8$ N/m^2
PEE stiffness	K_{PEE}	77 N/m^2
Muscle length	l_0	12 cm
Moment Arm	d	2 cm
% Fast Twitch Fibers	FT	45 %

where:

$$f(x(t), \dot{x}(t), u(t)) = \begin{bmatrix} \dot{\theta}(t) - \omega(t) \\ \frac{M(t)}{J} - \dot{\omega}(t) \\ \dot{a_1}(t) - (u_1(t) - a_1(t))(\frac{1}{T_{act}}(u_1(t)+1) - \frac{1}{T_{deact}}) \\ \dot{a_2}(t) - (u_2(t) - a_2(t))(\frac{1}{T_{act}}(u_2(t)+1) - \frac{1}{T_{deact}}) \\ F_{SEE(1)}(t) - F_{PEE(1)}(t) - F_{CE(1)}(t) + bv_{CE(1)}(t)F_{max} \\ F_{SEE(2)}(t) - F_{PEE(2)}(t) - F_{CE(2)}(t) + bv_{CE(2)}(t)F_{max} \end{bmatrix}, \quad (7)$$

$$\text{and:} \quad F_{CE(j)}(t) = a_j(t)F_{max}f(l_{CE(j)}(t))g(v_{CE(j)}(t)). \quad (8)$$

where the torque, $M = F_{SEE}^T d$, is equal to the dot product of the vector of forces in the series elastic element (SEE), F_{SEE}, and the moment arms d. T_{act} and T_{deact} are the activation and deactivation time constants of the muscle, $F_{PEE(j)}$ is the force in the parallel elastic element (PEE), $g(v_{CE(j)})$ the force-velocity relationship and b is a small damping term equal to 0.001 s/m, used to aid the optimization. The SEE and the PEE are modeled as quadratic springs. The slack lengths and stiffness are given in table 1.

The following optimization problem was solved to find the optimal state and control trajectories, $x(t)$ and $u(t)$, to perform the reaching task over time T:

$$\begin{aligned} \underset{u(t)}{\text{minimize}} \quad & J = \textstyle\int_{t=0}^{T} c(x(t), u(t))\mathrm{d}t \quad 0 \le t \le T, & (9a) \\ \text{subject to:} \quad & f(x, \dot{x}, u) = 0 \qquad 0 \le t \le T, & (9b) \\ & \theta(0) = 0, & (9c) \\ & \theta(T/2) = \tfrac{\pi}{2}, & (9d) \\ & \omega(0) = \omega(T/2) = 0, & (9e) \\ & x(T) - x(0) = 0. & (9f) \end{aligned}$$

The objective to minimize metabolic rate is as follows:

$$J(x(t), u(t)) = \frac{1}{Tm_{pend}} \sum_{j=1}^{2} \int_{t=0}^{T} \dot{E}_j(t) m_{mus(j)} \, \mathrm{d}t, \quad (10)$$

where m_{pend} is the total mass of the pendulum.

The objective to minimize muscular effort is as follows:

$$J(x(t), u(t)) = \frac{1}{T} \int_{t=0}^{T} \sum_{j=1}^{2} a_j(t)^2 \text{ dt}. \tag{11}$$

These optimal control problems were solved using direct collocation, with 200 collocation nodes and a backward Euler formulation. The average between the upper and lower bounds was used as initial guess for the states, while a very small stimulation, 10^{-4} was used as initial guess for the controls. The bounds for the angle were $\theta_{min} = -5\pi$, and $\theta_{max} = 6\pi$, for the angular velocity $\dot{\theta}_{min} = -1000$ rad/s, $\dot{\theta}_{max} = 1000$ rad/s was used. The activation was founded between 0 and 1, and the normalized fiber length was bounded between 0 and 4. The problem minimizing metabolic rate was first solved using $\varepsilon = 10^{-2}$, and this solution was used as an initial guess for $\varepsilon = 10^{-3}$. IPOPT 3.11.0 (Wächter and Biegler 2006) was used to solve the optimization problem.

2.4. Predictive Simulation of Gait

Finally, a predictive gait simulation that minimizes metabolic energy was solved from a random initial guess, and compared to a predictive gait simulation minimizing effort. A sagittal plane musculoskeletal model was used with nine degrees of freedom: the position and orientation of the trunk, two hip angles, two knee angles, and two ankle angles. The multibody dynamics, muscle model, and ground contact model are described by Koelewijn and van den Bogert (2016).

The following optimal control problem was defined for a gait cycle of time T with speed $v = 1.325$ m/s:

$$\underset{u(t)}{\text{minimize}} \quad J = \tfrac{1}{TM} \textstyle\sum_{j=1}^{16} \int_{t=0}^{T} \dot{E}_j(t) m_j \text{ dt} \quad 0 \leq t \leq T, \tag{12a}$$

$$\text{subject to:} \quad f(x(t), \dot{x}(t), u(t)) = 0 \quad 0 \leq t \leq T, \tag{12b}$$

$$x_{sym}(T/2) - x(0) - \tfrac{1}{2} v T e_1 = 0. \tag{12c}$$

where equation 12c describes the periodicity constraint, and e_1 denotes a unit vector that describes which states should be displaced, such as the horizontal component of the trunk. Left/right symmetry was assumed, meaning that the states and controls of the left leg at time $T/2$ should be the same as the states and controls of the right side at time 0 and vice versa.

Three optimal control problems were solved to find the solution from a random initial guess. First, a problem was solved with $\varepsilon = 10^{-2}$ and first-order regularization (W_{reg}= 0.012, see supplementary material). This problem was less non-linear and therefore easier to solve from the random initial guess. The solution of this problem was used as an initial guess for a second problem, with less regularization (W_{reg}=$1.2 \cdot 10^{-4}$). The solution of this problem was used as initial guess for the final optimal control problem, with no regularization and $\varepsilon = 10^{-3}$. This process was repeated with fifty random initial guesses. The solution with the lowest objective was presented.

This solution is compared to a predictive simulation found with minimizing muscular effort, using the cost function described in equation 11. The same approach was used with the same two intermediate solutions with a regularization term, and fifty random initial guesses. Again, the solution with the lowest objective was used.

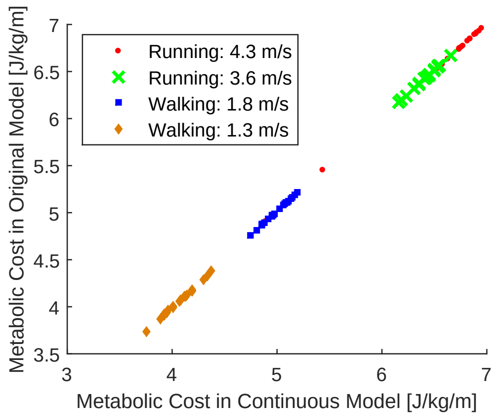

Figure 3.: Correlation between the continuous and original metabolic energy model for twenty virtual subjects for two walking speeds and two running speeds.

Direct collocation with 30 collocation nodes per half gait cycle was used to solve these problems, using IPOPT 3.11.0 (Wächter and Biegler 2006). More details on the solution method can be found in (Ackermann and van den Bogert 2010) and (Van den Bogert et al. 2012) and the supplementary material.

3. Results

3.1. Correlation

Figure 3 plots the metabolic cost of the predictive simulations, calculated with the continuous model versus the original model. The correlation coefficient was equal to 0.99, with a confidence interval of 0.99 to 0.99. The slope of the relationship between the original and continuous model found during the correlation analysis was 0.99. The RMS error was equal to 0.009 J/kg/m.

3.2. Predictive Simulation of a Single Joint Reaching Task

Figure 4 shows the reaching task that minimizes metabolic rate. The angle (top left figure) increases almost linearly from 0 degrees to 90 degrees, so the velocity is constant during most of the movement. This is due to the muscle stimulation (middle left figure), which is zero, except for a short burst around $t = 0$ s, $t = 2.5$ s and $t = 5$ s which was were the motion changes direction. The metabolic rate was 0.38 W/kg with the continuous model, and 0.26 W/kg using the original metabolic model.

Figure 5 shows the optimal solution that was found when minimizing effort. In this solution, the trajectory of the angle (top left figure) is smoother because the muscles are active during the full task, though the peak activation was lower (see middle left figure). The metabolic rate in this movement was 0.74 W/kg using the original metabolic model.

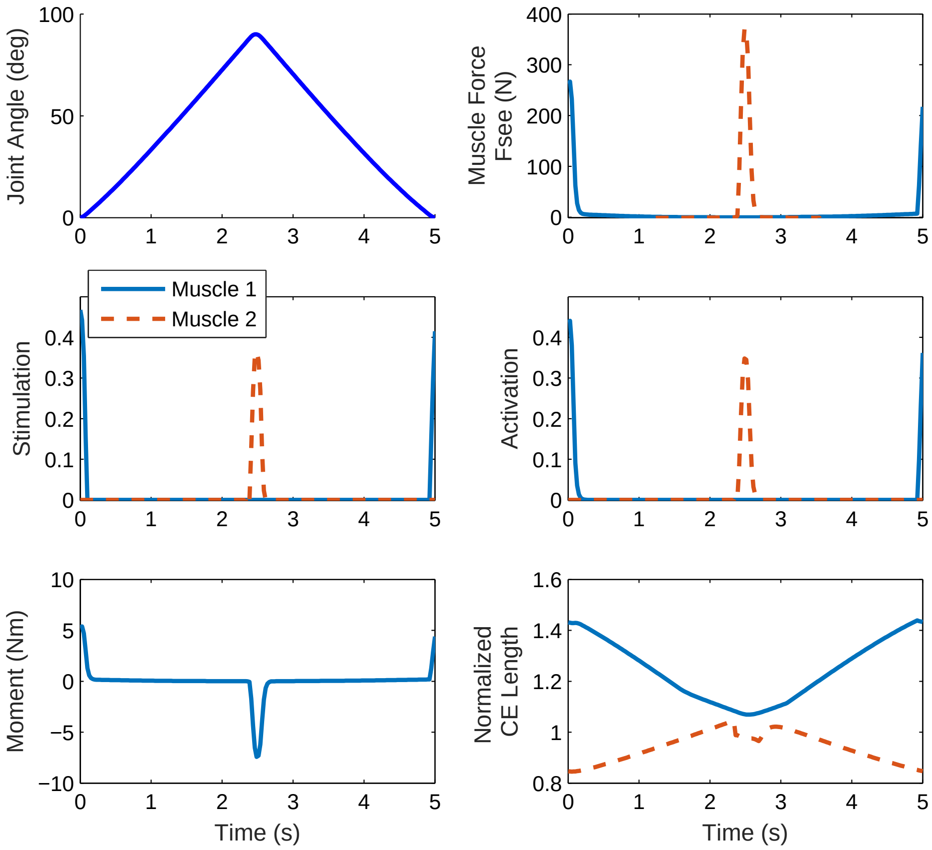

Figure 4.: Optimal trajectory for the single arm reaching task, minimizing metabolic energy.

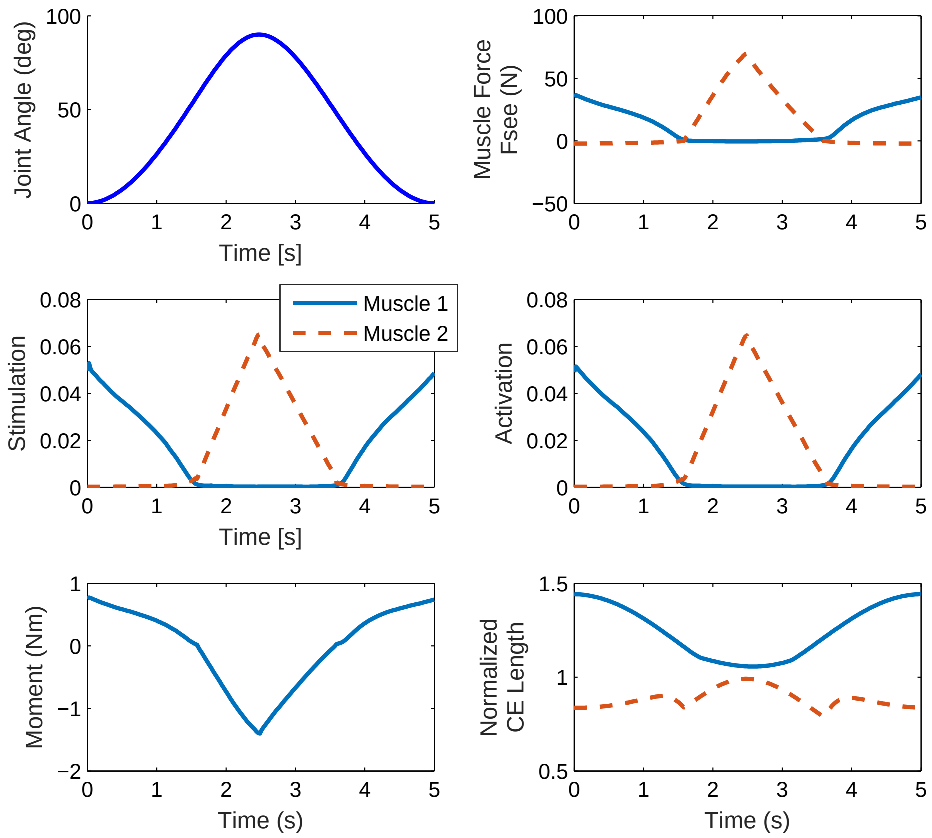

Figure 5.: Optimal trajectory for the single arm reaching task, minimizing effort.

3.3. Predictive Simulation of Walking

50 optimal control problems for gait were solved from random initial guesses minimizing metabolic rate and 50 were solved minimizing muscular effort. The optimization minimizing metabolic rate took about 90 minutes, while the optimization minimizing effort took about 10 minutes computer with an Intel Core i5-3210M CPU at 2.5 GHz clock speed. For the problems minimizing metabolic rate, five solved, one exceeded the maximum number of iterations, and the restoration phase failed for all others. The lowest objective, i.e. metabolic rate determined using the continuous model, was 1.50 W/kg. The metabolic rate of this solution determined using the original model is 1.43 W/kg.

When minimizing effort, 45 problems solved, four were terminated because an infeasible problem was detected, and one failed in the restoration phase. The metabolic rate of the solution with the lowest effort is 2.68 W/kg. This is also the lowest metabolic rate of all solutions that minimized effort.

Figure 6 shows joint angles, moments and muscle forces and activations of the solutions with the lowest objective. The stance phase is highlighted on the horizontal axis. Stick figure animations of these results are added in the supplementary material. The shaded area shows normal walking data from Winter (1991). The vertical peak ground reaction force at heel strike was larger than normal for both solutions. The horizontal peak ground force was twice as high as normal at heel strike. The stance phase was shorter than normal for both solutions.

The range of the hip angle was close to normal for both solutions, only the peak flexion angle in the minimum-effort solution deviated more than a standard deviation. The knee angle of the minimum-energy solution was within normal range, except for the smaller peak flexion angle. The peak knee flexion angle in the minimum-effort solution was larger than normal during stance and smaller than normal during swing. The peak ankle dorsiflexion angle was smaller than normal for both solutions, while the minimum-effort solution had a very high plantarflexion angle at push-off.

The hip and knee moments of the minimum-energy solution showed brief bursts, separated by periods where there was no moment at all. Also, the knee extension moment during stance was absent in this solution. The knee and hip moment of the minimum-effort solution changed more gradually and were nonzero throughout. The ankle moment had an extra early peak in the stance phase for both solutions. The hip moment of both solutions are similar to normal walking data, while the minimum-effort solution had a shift in time. The knee moment of the minimum-energy solution was unrealistic, while the minimum-effort solution had a knee moment similar to normal.

The Vasti and Hamstrings were not used at all in the minimum-energy solution and neither was the Tibialis Anterior during heel strike. The peak force in the Iliopsoas, Gluteals, and Soleus was higher in the metabolic rate solution, while the peak Gastrocnemius force was higher in the minimum-effort solution. In general, the metabolic rate solution showed short bursts of large activity, compared to longer activity with smaller peaks for the minimum-effort solution.

4. Discussion

The original and continuous version of the metabolic energy expenditure model correlated very well (R=0.99). Also, the slope of the relationship was equal to 0.99, and the intercepts were less than 0.1, meaning that the continuous model matched the original

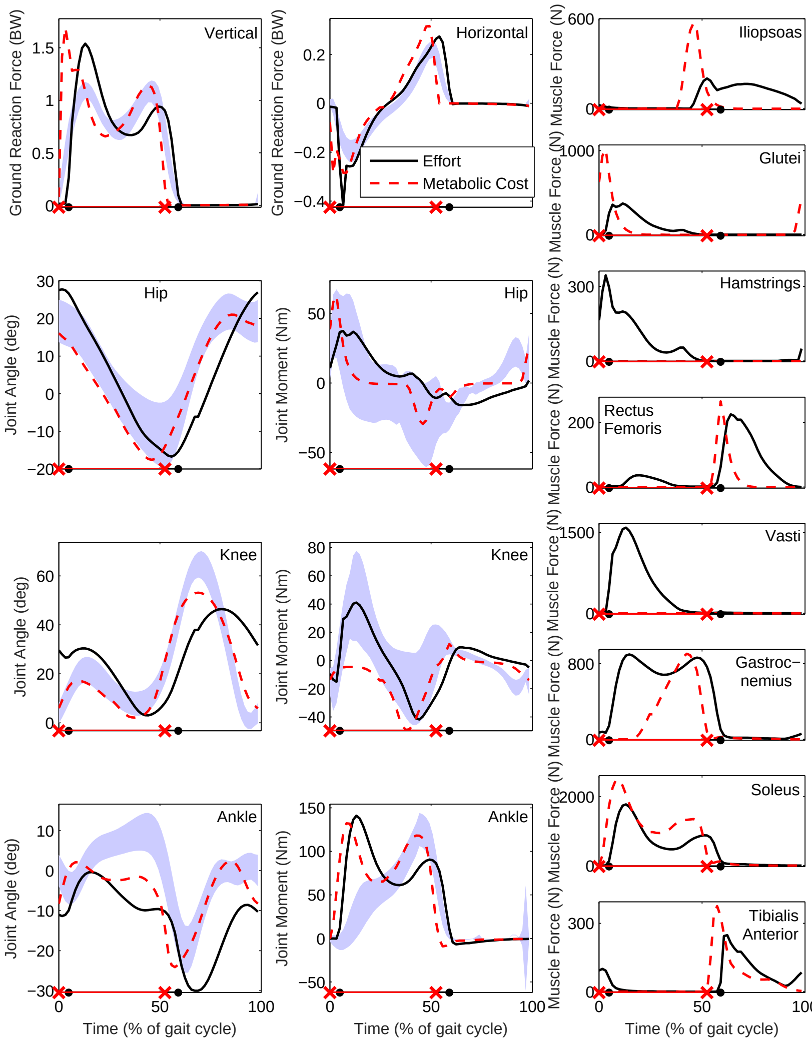

Figure 6.: Joint angles (flexion/dorsiflexion positive), joint moments (extension/plantarflexion positive), and muscle forces for predictive gait simulations that minimize metabolic energy expenditure (red, dash) and effort (black, solid). The shaded area shows data from Winter (1991). The stance phase of both solutions is highlighted on the horizontal axis (crosses for minimum-energy solution and dots for minimum-effort solution.

model very well. Therefore, the changes in the continuous model, the separate shortening and lengthening velocity and the handling of the activation and stimulation, only had a small effect on the metabolic energy expenditure calculation. Therefore, this model is suitable for solving predictive simulations.

However, for the predictive simulations, the difference between the metabolic reported by the original model and the continuous model was larger than in the regression comparison. There was a 5% different for the predictive gait simulation, and a 30% difference for the reaching task. The fiber velocity was small in the simulations that minimize metabolic rate, since this minimizes muscle work and shortening-lengthening heat rate. Therefore, when the muscle is lengthening, the shortening velocity $\bar{v}_{CE(S)}$ (equations 3) will make a significant contribution to the shortening-lengthening heat and vice versa. Additionally, the muscle work w_{CE} is smaller due to the smaller velocities, meaning that the shortening-lengthening heat rate also has a larger contribution to the total energy rate. The effect on the reaching task is larger since the energy rate, $\dot{E}$, is about ten times lower throughout the motion, while the same number for ε was used. The effect was even larger with a larger value of ε.

Trajectory optimization problems were solved successfully on two musculoskeletal dynamic systems with muscles. In both the reaching task and the predictive gait simulation, when metabolic energy was minimized, the muscles had high activation levels for short time. This approach corresponds with the result of FitzHugh, who describes that when minimizing metabolic energy, the motor signal consists of three phases: maximal stimulation to accelerate the mass to the optimal velocity, an intermediate level to maintain the velocity and zero stimulation to have the mass slow down (FitzHugh 1977). The reaching task yielded the same result, except that the intermediate level is equal to 0 due to the absence of friction and gravity, while activation of the other muscle is required to slow the arm down. Accelerating and decelerating the mass happen as fast as possible. This was verified by repeating the optimization with 50 and 100 nodes, since the acceleration is limited by the number of nodes. With a smaller number of nodes, the peak acceleration was reduced, which indicates an impulsive control strategy.

When minimizing effort, or the squared muscle activation, the highest activation was much lower, while the muscles were activated longer compared to a solution that minimizes metabolic rate. When the square of the muscle activation is minimized, larger activation levels are penalized more heavily and smaller activation levels over a longer time are favored. However, this increases the required metabolic energy.

The solution that was found when minimizing effort is more similar to reaching movements that are observed in humans, where jerk is minimized (Flash and Hogan 1985), than minimizing metabolic rate. This might mean that metabolic energy is not minimized in reaching tasks. Another reason is that uncertainty, for example in the muscular control is not taken into account. The motion that was found by minimizing metabolic rate may be harder to control, because the timing and size of the activation burst should be exactly right. Therefore, this might not be optimal in practice, where there is uncertainty in the control and the environment.

Finally, predictive gait simulations minimizing metabolic rate and muscular effort were solved. To the authors' knowledge, this is the first work where a predictive gait simulation is solved minimizing metabolic rate, from a completely random initial guess, without using any data in the optimal control problem. The solution had realistic joint angles, except the ankle range of motion, which was lower than normal. The smaller range of motion was also reported by Miller (2014), who minimized metabolic energy using normal gait as initial guess. Contrary to Miller's study, in this work the model was able to predict knee flexion in early stance (Miller 2014).

The minimum-effort solution found large knee flexion in the stance phase, similar to Ackermann and van den Bogert (2010). A possible reason is that activation is minimized. To reduce the required activation, the largest muscle, the quadriceps, is recruited, and used at optimal fiber length, which is achieved at larger knee flexion.

The hip and knee moments of the minimum-energy solution showed brief bursts, separated by periods where there was no moment at all, causing the knee moment to be different from normal (Winter 1991). This result, as well as the smaller ankle range of motion could be caused by the lack of uncertainty in this model, similar to the reaching task. A walking motion with zero joint moments is unstable and hard to control in practice, and therefore will not be optimal when uncertainty is taken into account. However, a zero moment is optimal if stability is not an issue, since this requires no muscle activation. The lack of uncertainty also explains the smaller ankle range of motion. The smaller ankle range of motion was due to the model standing on the toe early in stance, which is unstable as well (see video in supplementary material).

It was observed that the Hamstrings and Vasti did not do any work in the optimal solution. A reason for this is that the metabolic energy model is normalized to muscle mass. Therefore, the objective of the optimization is proportional to the weight of the muscles, which means that it is optimal to avoid a muscle with a high mass. The unrealistic joint moment patterns might also be improved by taking into account uncertainty in the environment, since this might require more realistic joint moments and thus more work from the muscles.

Joint angles of the minimum-energy solution were more realistic than those of the minimum-effort solution, while the joint moments, especially in the knee, were more realistic in the minimum-effort solution. The minimum-effort solution also yielded a more realistic metabolic rate. The metabolic rate of both was lower than normal (4.0-4.3 W/kg, see Umberger et al. (2003)), possible since only eight muscles were used in a sagittal plane model. After comparing the minimum-energy solution with the minimum-effort solution, it cannot yet be concluded that either effort or metabolic rate is the objective that humans use to choose their gait. Therefore, further studies should consider adding other objectives, especially to take into account uncertainty in the model and dynamics, to find a more realistic human gait.

Five solutions with the lowest objectives were analyzed, and are presented in the supplementary material. The gaits found by minimizing metabolic rate were consistent. Four solutions had the same joint angles, joint moments, and muscle forces, while the fifth solution was different, since in early stance a knee extension moment was present instead of a hip moment. This implies that the reported result is similar to the global minimum of the problem. When minimizing effort, the five gaits with the lowest objective were dissimilar.

The objective of minimum metabolic rate solved from five out of 50 initial guesses. For most problems, the algorithm terminated with 'restoration phase failed'. The restoration phase tries to find decrease the constraint violation when the normal algorithm is not able to improve. In practice, the restoration phase can be called even when the constraint violation is small (Wächter and Biegler 2006). This likely happens due to the nonlinearity of the metabolic rate objective. However, the algorithm was fast enough to be able to attempt multiple random initial guesses. In most studies, an initial guess is used closer to the optimal solution, so it should be easier to successfully find an optimal solution.

In conclusion, we have adapted the metabolic energy model of Umberger et al. (2003) to be suitable for gradient based optimization. We showed that when metabolic energy is minimized on a single joint reaching task, the solution is less realistic than when effort is minmized. Then, the solution was similar to minimizing jerk. Finally, we successfully solved a predictive gait simulation minimizing metabolic energy from a random initial guess. The simulation was realistic in joint angles, but an effort objective was more realistic in joint moments. It is expected that a more realistic gait cycle will be found if uncertainty in the model and the dynamics is taken into account.

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References

Ackermann, M. and van den Bogert, A. J. (2010). Optimality principles for model-based prediction of human gait. *Journal of Biomechanics*, 43(6):1055–1060.

Anderson, F. C. and Pandy, M. G. (2001). Dynamic optimization of human walking. *Journal of Biomechanical Engineering*, 123(5):381–390.

Bakdash, J. Z. and Marusich, L. R. (2017). Repeated measures correlation. *Frontiers in Psychology*, 8.

Barclay, C., Constable, J., and Gibbs, C. (1993). Energetics of fast-and slow-twitch muscles of the mouse. *The Journal of physiology*, 472:61.

Bertram, J. E. and Ruina, A. (2001). Multiple walking speed–frequency relations are predicted by constrained optimization. *Journal of Theoretical Biology*, 209(4):445–453.

Bhargava, L. J., Pandy, M. G., and Anderson, F. C. (2004). A phenomenological model for estimating metabolic energy consumption in muscle contraction. *Journal of Biomechanics*, 37(1):81–88.

Breteler, M. D. K., Spoor, C. W., and Van der Helm, F. C. (1999). Measuring muscle and joint geometry parameters of a shoulder for modeling purposes. *Journal of biomechanics*, 32(11):1191–1197.

Buschman, H., Elzinga, G., and Woledge, R. (1995). Energetics of shortening depend on stimulation frequency in single muscle fibres from xenopus laevis at 20 c. *Pflügers Archiv*, 430(2):160–167.

Buschman, H., Elzinga, G., and Woledge, R. (1996). The effects of the level of activation and shortening velocity on energy output in type 3 muscle fibres from xenopus laevis. *Pflügers Archiv*, 433(1-2):153–159.

Buschman, H., Linari, M., Elzinga, G., and Woledge, R. (1997). Mechanical and energy characteristics during shortening in isolated type-1 muscle fibres from xenopus laevis studied at maximal and submaximal activation. *Pflügers Archiv*, 435(1):145–150.

Delp, S. L., Anderson, F. C., Arnold, A. S., Loan, P., Habib, A., John, C. T., Guendelman, E., and Thelen, D. G. (2007). Opensim: open-source software to create and analyze dynamic simulations of movement. *IEEE transactions on biomedical engineering*, 54(11):1940–1950.

Donelan, J. M., Kram, R., et al. (2001). Mechanical and metabolic determinants of the preferred step width in human walking. *Proceedings of the Royal Society of London B: Biological Sciences*, 268(1480):1985–1992.

FitzHugh, R. (1977). A model of optimal voluntary muscular control. *Journal of mathematical biology*, 4(3):203–236.

Flash, T. and Hogan, N. (1985). The coordination of arm movements: an experimentally confirmed mathematical model. *Journal of neuroscience*, 5(7):1688–1703.

Gordon, K. E., Ferris, D. P., and Kuo, A. D. (2009). Metabolic and mechanical energy costs of reducing vertical center of mass movement during gait. *Archives of physical medicine and rehabilitation*, 90(1):136–144.

Houdijk, H., Bobbert, M., and De Haan, A. (2006). Evaluation of a hill based muscle model for the energy cost and efficiency of muscular contraction. *Journal of biomechanics*, 39(3):536–543.

Koelewijn, A. D. and van den Bogert, A. J. (2016). Joint contact forces can be reduced by improving joint moment symmetry in below-knee amputee gait simulations. *Gait & Posture*, 49:219–225.

Lichtwark, G. A. and Wilson, A. (2005). A modified hill muscle model that predicts muscle power output and efficiency during sinusoidal length changes. *Journal of Experimental Biology*, 208(15):2831–2843.

Lin, Y.-C. and Pandy, M. G. (2017). Three-dimensional data-tracking dynamic optimization simulations of human locomotion generated by direct collocation. *Journal of Biomechanics*.

Miller, R. H. (2014). A comparison of muscle energy models for simulating human walking in three dimensions. *Journal of biomechanics*, 47(6):1373–1381.

Miller, R. H., Umberger, B. R., Hamill, J., and Caldwell, G. E. (2011). Evaluation of the minimum energy hypothesis and other potential optimality criteria for human running. *Proceedings of the Royal Society of London B: Biological Sciences*, page rspb20112015.

Ortega, J. D. and Farley, C. T. (2005). Minimizing center of mass vertical movement increases metabolic cost in walking. *Journal of Applied Physiology*, 99(6):2099–2107.

Ralston, H. J. (1958). Energy-speed relation and optimal speed during level walking. *Internationale Zeitschrift für Angewandte Physiologie Einschliesslich Arbeitsphysiologie*, 17(4):277–283.

Selinger, J. C., OConnor, S. M., Wong, J. D., and Donelan, J. M. (2015). Humans can continuously optimize energetic cost during walking. *Current Biology*, 25(18):2452–2456.

Sellers, W. I., Cain, G. M., Wang, W., and Crompton, R. H. (2005). Stride lengths, speed and energy costs in walking of australopithecus afarensis: using evolutionary robotics to predict locomotion of early human ancestors. *Journal of the Royal Society Interface*, 2(5):431–441.

Umberger, B. R. (2010). Stance and swing phase costs in human walking. *Journal of the Royal Society Interface*, 7(50):1329–1340.

Umberger, B. R., Gerritsen, K. G., and Martin, P. E. (2003). A model of human muscle energy expenditure. *Computer methods in biomechanics and biomedical engineering*, 6(2):99–111.

Van den Bogert, A. J., Hupperets, M., Schlarb, H., and Krabbe, B. (2012). Predictive musculoskeletal simulation using optimal control: effects of added limb mass on energy cost and kinematics of walking and running. *Proceedings of the Institution of Mechanical Engineers, Part P: Journal of Sports Engineering and Technology*, pages 1–11.

Wächter, A. and Biegler, L. T. (2006). On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Mathematical Programming*, 106(1):25–57.

Winter, D. A. (1991). *Biomechanics and motor control of human gait: normal, elderly and pathological*. University of Waterloo Press.

Winter, D. A. (2005). *Biomechanics and motor control of human movement*. John Wiley & Sons.

Zarrugh, M., Todd, F., and Ralston, H. (1974). Optimization of energy expenditure during level walking. *European Journal of Applied Physiology and Occupational Physiology*, 33(4):293–306.