

TITLE

An Optimization-Based Simultaneous Approach to the Determination of Muscular, Ligamentous, and Joint Contact Forces Provides Insight into Musculoligamentous Interaction

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Abstract

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6 Typical inverse dynamics approaches to the calculation of muscle, ligament and joint
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8 contact forces are based upon a step-wise solution of the equations of motion. This
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10 approach is therefore limited in its ability to provide insight as to the muscular,
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12 ligamentous and articular interactions that create joint stability. In this study, a new
13
14 musculoskeletal model of the lower limb is described, in which the equations of
15
16 motion describing the force and moment equilibrium at the joints of the lower limb
17
18 are solved simultaneously using optimization techniques. The new model was
19
20 employed to analyse vertical jumping using a variety of different optimization cost
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22 functions and the results were compared to more traditional approaches. The new
23
24 model was able to find a solution with lower muscular force upper bounds due to the
25
26 ability of the ligaments to contribute to moment equilibrium at the ankle and knee
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28 joints. Equally, the new model produced lower joint contact forces than traditional
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30 approaches for cases which also included a consideration as to ligament or joint
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32 contact forces within the cost function. This study demonstrates the possibility of
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34 solving the inverse dynamic equations of motion simultaneously using contemporary
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36 technology, and further suggests that this might be important due to the
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38 complementary function of the muscles and ligaments in creating joint stability.
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50 Keywords: musculoskeletal modelling, muscle force, joint contact force, ligament
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52 force, inverse dynamics
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Introduction

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4 Inverse dynamics analyses have been widely employed within bioengineering to
5 improve the understanding of movement⁴⁰. To this end, the combination of inverse
6 dynamics and optimization techniques has been used to calculate inter-segmental
7 forces and moments, muscle forces, joint reaction forces and ligament forces⁴⁰. In
8 particular, the traditional approach to calculating the kinematic and kinetic quantities
9 of interest in lower body musculoskeletal models is well established and is generally
10 based upon a standard order of operations³ (or “pipeline”; Figure 1). Firstly, the inter-
11 segmental forces and moments are calculated by an inverse dynamics analysis based
12 upon a free body diagram of the segments that incorporates the external forces, the
13 linear accelerations of the segments and the rotational kinematics. Secondly, a
14 description of the musculoskeletal geometry of the model is added, which provides
15 detail as to the line of action and moment arms of the muscles. It is then common to
16 assume that the muscles are the sole contributors to the inter-segmental moments, thus
17 an indeterminate problem can be formulated that describes the contribution of each
18 muscle element to the inter-segmental moments previously calculated. In addition, in
19 some models additional constraints are included to further specify the kinematics or
20 kinetics of a given joint. For instance, at the shoulder joint the scapula can be
21 constrained to be in contact with the rib cage or the resultant glenohumeral joint
22 contact force can be compelled to point within the perimeter defined by the labrum to
23 prevent dislocation of the joint (see, for example⁶). This indeterminate problem can
24 then be solved using optimization techniques to give individual muscle forces. The
25 optimization problem is often formulated based upon a consideration of muscular
26 loading alone, and thus neglects a consideration as to the loading of other structures.
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1 Next the individual muscle forces are incorporated within the segmental free body
2 diagram in order to calculate the internal joint contact forces. Finally, it is frequently
3 assumed that the ligaments provide the restraint to the calculated internal joint shear,
4 thus the ligamentous force can be calculated by consideration of the internal forces
5 acting in the free body diagram.
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13 The standard approach to the inter-segmental inverse dynamics analysis is to employ
14 the Newton-Euler iterative method^{40,44}. Firstly, inter-segmental forces are calculated
15 in the laboratory fixed global coordinate frame (GCS). Secondly, the Euler equations
16 of rotational motion are used to calculate the inter-segmental moments in the body
17 fixed segmental coordinate frame (LCS). Traditional inverse dynamics therefore
18 entails multiple coordinate transformations which increase the computational
19 demands of the method. Dumas and colleagues¹⁸ have recently described an
20 alternative approach to the inverse dynamics analysis based upon the use of unit
21 quaternions and wrench notation which allows the complete analysis to be performed
22 in the GCS, thereby greatly reducing the computational complexity of the problem.
23 Recent research has demonstrated that the method of Dumas and colleagues is
24 computationally equivalent to the traditional approach⁸ and thus this alternative
25 formulation presents new opportunities for the analysis of movement. For instance,
26 Cleather and colleagues^{11,10} have recently demonstrated that the equations of motion
27 describing moment equilibrium given by Dumas and colleagues can be modified to
28 include the muscle forces in a musculoskeletal model of the lower limb. This results
29 in an indeterminate problem that can be solved using optimization techniques and
30 gives a more accurate representation as to the function of the biarticular muscles.
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1 The step-by-step approach described in Figure 1 does not recognise the interaction
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3 between muscles and ligaments in establishing moment equilibrium. In the first
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5 place, at the optimization stage it is assumed that the ligaments do not contribute to
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7 the inter-segmental moments observed at the joints. Then, later in the pipeline,
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9 indicative ligament forces are calculated based upon the imperative for force
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11 equilibrium again based upon the assumption that these forces do not alter the
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13 previously established moment equilibrium. This assumption may be valid for some
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15 ligaments, for instance, the cruciate ligaments could be reasonably considered to pass
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17 through the centre of rotation of the knee however, other ligaments are well placed to
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19 contribute to the moment equilibrium of the lower limb. Thus a major limitation of
20
21 the traditional approach to inverse dynamics is that it precludes an exploration of
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23 musculoligamentous interaction.
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31 The pipeline described in Figure 1 has evolved to simplify the computational
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33 complexities in determining muscle, ligament and joint reaction forces in the
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35 indeterminate musculoskeletal system. This is achieved by partially uncoupling the
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37 function of muscles and ligaments to allow the sequential determination of first
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39 muscle, then joint reaction and finally ligament forces. In reality, the musculoskeletal
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41 system is an integrated whole, and a more realistic representation could be achieved
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43 by formulating equations of motion that fully recognize the potential for
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45 musculoligamentous interaction, and by solving these equations simultaneously²⁴. To
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47 this end, the method of Dumas and colleagues¹⁸ has great utility for posing the
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49 equations of motion in a computationally friendly manner. The purpose of this study
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51 was therefore to demonstrate the feasibility of using existing technology to
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53 simultaneously solve the equations of motion during vertical jumping using
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1 optimization techniques. It was postulated that this approach would permit a more
2 physiologically realistic representation as to the function of the musculoskeletal
3 system than can be achieved by the sequential process represented in Figure 1. A
4 secondary aim was to explore the sensitivity of the solution to the choice of cost
5 function, and in particular the effect of employing cost functions based upon
6 considerations of different tissue loadings (muscular, ligamentous or bony).
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16 **Materials and Methods**

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20 In this study a previously described^{9,11,10} musculoskeletal model of the right lower
21 limb was employed to explore the use of a new approach to the determination of
22 muscle, ligament and joint contact forces by optimization techniques. The model
23 consists of a 3D description of four linked rigid segments representing the foot, calf,
24 thigh and pelvis. The data analysed in this study pertains to vertical jumps performed
25 by twelve athletic male subjects (mean age 27.1 ± 4.3 years; mean mass 83.7 ± 9.9
26 kg). The data set was acquired using a Vicon motion capture system (Vicon MX
27 System, Vicon Motion Systems Ltd, Oxford, UK) synchronised with a Kistler force
28 plate (Kistler Type 9286AA, Kistler Instrumente AG, Winterthur, Switzerland). The
29 raw data was captured at 200 Hz and consisted of the position of reflective markers
30 placed on key anatomical landmarks^{36,37} and the ground reaction force. The raw data
31 was filtered using a fifth order Woltring⁴¹ filter prior to analysis. The model is
32 specified by the translations and rotations that describe the position and orientation of
33 each segment, which are calculated using the method of Horn²¹.
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56 The musculoskeletal geometry used in the model is taken from the data set of Klein
57 Horsman and colleagues²² whereas the anthropometry is taken from de Leva¹⁷. The
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1 patella position and orientation is defined to be a function of the knee flexion angle
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3 where the data of Klein Horsman et al. is used to find the location of the patellar
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5 origin and the work of Nha et al.²⁵ to specify the patellar rotation. The model of Klein
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7 Horsman et al. provides a series of via points for each muscle element or ligament that
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9 specify its path. These via points include the origin and insertion of the element, but
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11 are also used to model the wrapping of muscle over bone by compelling certain
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13 muscle elements to pass through one or more fixed points. This anatomical
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15 information is used to find the line of action and moment arm of the muscle or
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17 ligament, where the line of action is considered to be the vector from the effective
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19 insertion to the effective origin, and the moment arm the vector from the centre of
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21 rotation to the effective insertion. The effective origin and insertion are defined in
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23 Figure 2. Table 1 presents the particular ligaments modelled in this study that were
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25 taken from the work of Klein Horsman et al., and details as to the upper bounds of the
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27 ligaments that were assumed. Further details as to the description of musculoskeletal
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29 geometry in the lower limb model are described in more detail elsewhere^{9,11}.
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38 The method of Dumas and colleagues¹⁸ is used to formulate the equations of motion
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40 of the lower limb model. Firstly, the inter-segmental forces can be calculated based
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42 on the traditional Newtonian iterative approach (Figure 3a):
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$$\hat{S}_i = m_i(\hat{a}_i - \hat{g}) + \hat{S}_{i-1} \quad (1)$$

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51 Next, considering the internal forces acting on each segment (Figure 3b) yields:
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$$\sum_{j=1}^U F_j \cdot \hat{p}_{ji} - \sum_{j=1}^U F_j \cdot \hat{p}_{j(i-1)} + \sum_{j=1}^V L_j \cdot \hat{q}_{ji} - \sum_{j=1}^V L_j \cdot \hat{q}_{j(i-1)} + \hat{J}_i - \hat{J}_{i-1} = m_i(\hat{a}_i - \hat{g}) \quad (2)$$

Where $\hat{J}_0 = \hat{S}_0$

The joint reaction forces are considered to act through the joint centres of rotation (which are defined to be located at the intersections of the linked rigid segments). Similarly, the rotational moments are taken around the joint centres of rotation. A consideration of the rotational movement at each segment (Figure 3c) gives:

$$\begin{aligned} \sum_{j=1}^U F_j \cdot \hat{r}_{ji} \times \hat{p}_{ji} - \sum_{j=1}^U F_j \cdot \hat{r}_{j(i-1)} \times \hat{p}_{j(i-1)} + \sum_{j=1}^U b_{ji} F_j \cdot \hat{d}_i \times \hat{o}_{ji} + \sum_{j=1}^V L_j \cdot \hat{s}_{ji} \times \hat{q}_{ji} - \sum_{j=1}^V L_j \cdot \hat{s}_{j(i-1)} \times \hat{q}_{j(i-1)} \\ = m_i \hat{c}_i \times (\hat{a}_i - \hat{g}) + \ddot{\hat{\theta}}_i + \dot{\hat{\theta}}_i \times I_i \dot{\hat{\theta}}_i + \hat{d}_i \times \hat{S}_{i-1} + \hat{M}_{i-1} \end{aligned} \quad (3)$$

$b_{ji} = 1$ for biarticular muscles that cross but do not attach to segment i ;

$b_{ji} = 0$ for all other muscles

$\hat{M}_i = 0$ for $i > 0$

Equation 1 is determinate and thus can be solved directly whereas the remaining equations of motion (Equations 2 and 3) are indeterminate. In this application, the musculoskeletal geometry taken from the Klein Horsman et al.²² data set comprises 163 different muscle elements and 14 ligaments. In combination with the articular contact forces this results in 186 unknown variables. Applying Equations 2 and 3 to the foot, calf and thigh segments in 3D gives a system of 18 equations. This system is solved with an optimization approach using the optimization toolbox of Matlab (version 7.5; The Mathworks, Inc, 2007) employing a cost function adapted from the work of Raikova²⁸:

$$\min_{F_j, L_j, J_j} f = k_1 \sum_{j=1}^U \left(\frac{F_j}{F_{\max_j}} \right)^{n_1} + k_2 \sum_{j=1}^V \left(\frac{L_j}{L_{\max_j}} \right)^{n_2} + \sum_{i=1}^W \left(\sum_{j=1}^3 (k_3 J_j)^{n_3} \right)_i \quad (4)$$

The first term in Equation 4 is based on the cost function of Crowninshield and Brand¹² which is thought to maximise muscular endurance. It is equivalent to minimizing muscle stress, as maximum muscle force is the product of the physiological cross sectional area ($PSCA_j$; taken from the Klein Horsman et al.²² data set) and the maximum muscle stress ($MS=3.139 \times 10^5 \text{ N/m}^2$; taken from Yamguchi⁴³ and doubled to represent the fact that the subjects are from a young athletic population).

$$\min_{F_j} f = \sum_{j=1}^U \left(\frac{F_j}{F_{\max_j}} \right)^{n_1} = \sum_{j=1}^U \left(\frac{F_j}{PSCA_j \times MS_{\max}} \right)^{n_1} = \frac{1}{MS_{\max}^{n_1}} \sum_{j=1}^U \left(\frac{F_j}{PSCA_j} \right)^{n_1} \quad (5)$$

The advantage to calculating muscle forces by using a cost function based upon maximal muscle force is that it provides a simple and consistent way in which to include the ligaments in the optimization (the second term in Equation 4), as the failure strength of the ligaments is known from the literature^{26,30,34} and represents the force upper bound for the ligaments, which could therefore be considered to be comparable to the force upper bound for the muscles. Thus the optimization seeks a solution which both minimizes muscle stress, while seeking to minimize the force in the ligaments relative to their failure limits. If the maximum muscle force is also assumed to be the failure limit of a muscle, the optimization can be characterized as seeking a solution which minimizes the likelihood of any of the tissues approaching

1 their failure limits, and that there is no bias towards ligamentous or muscular failure.
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3 Finally the third term in the cost function represents an imperative to also minimize
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5 the joint reaction force²⁸.
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10 The coefficients k_1 , k_2 and k_3 and the exponents n_1 , n_2 and n_3 are chosen to alter the
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12 characteristics of the cost function. In this study, five different cases were considered
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14 and are presented in Table 1, along with their nomenclature. In particular, by setting
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16 the value of the coefficients k_1 , k_2 and k_3 to either 0 or 1, the cost function can be
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18 altered by removing selected terms. In this way, the four different cases can be
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20 derived. Case 1, includes only the first term of the cost function, and thus is a
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22 solution based upon muscle considerations only and is most analogous to the
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24 traditional approach (muscles only – MO). Similarly, Case 2 only includes the second
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26 term of the cost function, and is thus based solely upon ligament considerations and
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28 represents a movement strategy that is based upon the preferential recruitment of
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30 muscles to spare ligament loading (ligaments only – LO). Case 4 only includes the
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32 third term, and thus relates only to joint reaction force considerations would therefore
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34 be predicted to predict the lowest overall muscle and joint activations (joint reaction
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36 force only – JO). Case 3 includes both the first and second terms of the cost function
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38 (which are given equal weight) and thus relates to both muscle and ligament
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40 considerations and was chosen to represent the competing imperatives of muscular
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42 and ligament loading (muscles and ligaments – ML). This concept is discussed in
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44 more detail later. Finally, Case 5 includes all terms in the optimization, and thus
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46 represents the imperative to minimize muscular, ligamentous and joint loading (ALL).
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48 The coefficients k_1 , k_2 and k_3 can also be used to weight the relative importance of
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50 muscle, ligament or joint reaction force considerations to each other, and the
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1 appropriate weighting is an important aspect was not explored in this study. The
2 exponents n_1 , n_2 and n_3 are higher than those typically employed in the literature^{19,35}
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4 however, it has been suggested that the use of higher powers gives a physiologically
5
6 more realistic solution^{4,29}, and in particular that the muscular activation to external
7
8 load relationship is linear at higher powers²⁹.
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16 The ligament and joint contact forces presented in this study are those calculated in
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18 the optimization procedure (\hat{L}_j and \hat{J}_i respectively). The moments presented are
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20 directly calculated as the sum of the cross products of the individual muscle or
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22 ligament moment arms with the particular force derived from the optimization
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24 solution. The forces and moments calculated in this study were compared to those
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26 presented by Cleather and colleagues^{10,11}. Their analysis is based upon the same data
27
28 set of 12 vertical jumps, but employed a different approach to the calculation of
29
30 muscle forces. In particular, Cleather and colleagues present forces and moments for
31
32 the traditional approach (TRAD) and for an optimization based approach similar to
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34 that employed in the present work but comprising only muscle elements (that is no
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36 ligaments or contact forces including in the optimization algorithm; BI). The
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38 differences in muscle and joint forces and muscle moments were analyzed using a one
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40 way ANOVA with post hoc Tukey's HSD tests where alpha was set to 0.05 a priori.
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49 **Results**

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53 The optimization was successful in producing a solution for all cases. Table 3
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55 presents the muscle forces calculated in the five different cases in comparison to the
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57 previous results of Cleather and colleagues^{10,11} (TRAD and BI). The peak total
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1 activation of the muscle model was significantly lower for JO than all other cases ($p <$
2 0.05), a difference that was commensurate with significantly lower activation of
3 gastrocnemius, hamstrings and glutes. Total activation of the muscle model was of
4 similar magnitude for all other cases. The most notable difference at the muscle level
5 was the fact that in all cases the monoarticular plantar flexors had a significantly
6 greater level of activation than that reported previously. Those cases which included
7 a consideration as to muscle stress in the cost function (MO, ML and ALL) showed a
8 trend towards increased activation of the biarticular musculature, and in particular the
9 activation of gastrocnemius in MO was significantly greater than LO, JO, TRAD and
10 BI.
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26 When taken as a whole the magnitude of the peak joint contact forces were
27 consistently lower than that reported previously^{10,11}, although this difference only
28 reached a significant level for JO (Table 4). Notably, MO produced higher contact
29 forces than TRAD and BI, although this difference was not significant. The highest
30 ligament forces were also found in MO, although significant differences were only
31 found for the LCL, ACL and OPL. Ligament loading was smallest for LO and JO,
32 differences that were significant for LCL, ACL and OPL.
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45 Tables 5 and 6 present the peak non-sagittal plane moments created by the ligaments
46 alone, in each of the five cases. The ligaments principally provided adduction and
47 internal rotation moments at the ankle and knee and some abduction moment at the
48 knee. The ligaments of the hip produced minimal non-sagittal plane rotation
49 moments in all cases. Significant differences were only found for MO.
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Discussion

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6 In this study a new approach to the calculation of muscle, ligament and joint reaction
7 forces was presented which is based upon formulating a system of indeterminate
8 equations of motion containing all variables of interest, and then solving this system
9 with optimization techniques. This methodology allows a more complete description
10 of the equations of motion to be formulated, and therefore presents a basis for more
11 searching analyses of human movement.
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23 The inter-segmental moments calculated in this study are in agreement with those
24 previously presented in the literature^{2,23,38}. The previous literature relating to internal
25 joint loadings of the knee during jumping is sparse, and is mainly concerned with
26 jump landings however, recent work produced by Cleather⁷ suggests that the
27 magnitude of the joint contact forces during jumping and landing are similar. Studies
28 of jump landings suggest a tibiofemoral joint loading in the range of approximately
29 $17.0 \times BW^{31,32}$. The magnitude of the tibiofemoral joint loading found in this study is
30 over half as great as in these earlier works. Direct in vivo measurements of joint
31 loadings during activities of daily living in patient populations suggest a tibiofemoral
32 loading of $2.0 - 3.0 \times BW^{13,14,15,39}$, rising to $3.0 - 4.5 \times BW^{16}$ in sporting activities.
33 The range of tibiofemoral loadings suggested in this work therefore seems more
34 likely, and the authors would contend that the higher values found in the earlier works
35 are due to a lack of detail in early models. The ligament loadings predicted in this
36 study also seem reasonable when compared to their known failure limits. For
37 instance, this study suggests ACL and PCL loadings of around 250 – 420 N and 1,000
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1 – 2,000 N respectively, which compare favourably with failure limits derived from the
2 literature of 2,000 N^{5,26,42} and 4,500 N¹. Equally, in vitro measurements of ACL
3 loading during simulated jump landing suggest a loading of around 400 N, which is
4 close to the musculoskeletal model derived calculations of Pflum and colleagues²⁷.
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13 The most important limitation of the new method when compared to previous
14 approaches is the fact that in the new model the ligaments are modelled as active
15 force actuators which are able to produce, upon demand, any force up to their failure
16 limit, and without reference to their strain. This approach may at first appear to be
17 grossly unphysiological as a ligament is a passive tissue whose force production is a
18 direct consequence of the strain it experiences. Consequently the force in a ligament
19 should be predicated solely by the position of the joint it spans and thus determined
20 from the musculoskeletal geometry of the model prior to the optimization. This
21 approach is difficult in this type of large scale multi-body model however. The stress-
22 strain relationship of ligaments means that even small length changes can produce
23 large forces and therefore ligament models based purely upon strain considerations
24 tend to be highly sensitive to the specific ligament geometries and the determination
25 of segment positions. Practically, in models specified by generic ligament parameters
26 and based upon optical motion capture techniques, it is challenging to determine
27 changes in ligament length with the precision necessary to use them as inputs to the
28 optimization.
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55 Instead an optimization approach may represent an elegant solution to the problem of
56 determining ligament forces. The motor control strategy developed to perform a
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1 given movement will be chosen based on multiple physiological imperatives. Clearly
2 the articular geometry of a joint will be highly influential, however the motion of the
3 joint will also be guided by the action of muscles and the passive restraint of the
4 ligaments. The optimal movement strategy will therefore be one which is optimal
5 both in terms of the necessity for muscular force production, but also in optimizing
6 ligament strains. The optimal movement pattern may result in a cyclic tensile loading
7 of the ligaments to promote tissue health while preventing ligament strains from
8 exceeding a safe limit. It could be argued that the modelling approach taken in this
9 study can be characterized as capturing these imperatives of a motor control strategy.
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25 Of course, a more robust solution would also capture strain considerations within the
26 solution. For instance, it has been shown that the collateral ligaments of the knee are
27 slack at deeper knee flexion angles²⁰, an experimental finding that is also
28 demonstrated in this model as the collateral ligaments shorten with knee flexion
29 angle. However, in contrast with the ligament length data in the present model the
30 collateral ligaments are available as force actuators throughout the full range of knee
31 motion. The effect of this is that the current solutions sometimes predict a collateral
32 ligament recruitment that is not physiological. The remedy to this problem lies in
33 finding methods for incorporating length considerations within the solution. In a
34 preliminary study Cleather⁷ has demonstrated that strain considerations can be used to
35 specify further bounds for the optimization which improve the realism of the muscle
36 model. Alternatively, if ligament forces can be derived by other means (for instance
37 through more accurate length measurements derived from imaging techniques or the
38 use of alternative models), then these forces can be incorporated within the
39 optimization solution. For instance, Southgate³³ has recently incorporated ligament
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1 forces derived from a ligament model within an optimization procedure in order to
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3 evaluate muscular forces at the shoulder joint. This discussion should not detract
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5 from the principal argument of this paper, that optimization solutions to the inverse
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7 dynamic problem should incorporate all equations of motion, rather that future
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9 research should seek to populate the optimization problem with further detail (in the
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11 form of further constraints or equations) derived from kinematic and kinetic
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13 considerations.
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21 A pivotal question when employing this methodology is the appropriate choice of cost
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23 function for the ligaments. The cost function should both have a physiological
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25 meaning in representing the manner in which tension is likely to be controlled in the
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27 ligaments in isolation, but also in the representing the interaction between muscular
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29 and ligamentous forces. This work highlights various interesting questions. Firstly,
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31 what criteria are used to regulate the force experienced by the ligaments and how can
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33 these be best described by a cost function, given the assumption that motor control
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35 strategies are chosen to minimize the force in the ligaments? Secondly, what is the
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37 interaction between muscular and ligamentous forces during movement, and in
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39 particular, do muscle or ligament force considerations dominate motor control
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41 strategies? How can the relative weight of muscle or ligament considerations be
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43 reflected in a cost function, given an optimization approach to deriving force
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45 estimates?
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55 A further limitation of the present work is the lack of dynamic muscle modelling; that
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57 is, that the force generating capacity of the muscles is assumed to be constant and
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1 independent of the known force-length and force-velocity relationships. This
2 limitation may be particularly pertinent in high acceleration activities like vertical
3 jumping where the time taken to develop force may be an important determinant as to
4 the movement strategy employed. Equally a consideration of muscle dynamics is
5 important when considering the stability and musculoligamentous interaction at the
6 knee. Whereas muscles will require time to develop force in response to
7 perturbations, the ligaments are immediately responsive to position changes due to the
8 stress-strain relationship. Future work should therefore seek to incorporate muscle
9 dynamics within the optimization solution of this type of model.
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25 It is important to recognise that in the previous work of Cleather and colleagues¹¹, in
26 order for the optimization to produce a solution it was necessary to increase the upper
27 bounds for 6 of the 12 subjects, and for some subjects the necessary upper bound was
28 over double that used in this study. The increased upper bounds were utilized solely
29 by the small muscle groups and represented the difficulty in finding an equilibrium
30 solution in 3D (and in particular in the non-sagittal planes). This is a consequence of
31 the fact that the solutions of this type of model are highly sensitive to the number and
32 variability of force actuators available to the optimization algorithm⁹. In particular,
33 musculoskeletal models of the lower limb tend to have a limited number of muscle
34 elements that can provide non-sagittal plane rotations at the knee and it is common for
35 these types of models to constrain the knee to 1 DOF. The availability of the five
36 major ligaments of the knee (as well as ligaments of ankle and hip) as force actuators
37 within this model markedly increases the probability of finding an optimal solution
38 (and equally that this solution will have a lower overall level of activation). In this
39 study, the ability of the ligaments to provide rotational moments, ameliorated this
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1 problem, and it was possible to find a solution with upper bounds derived solely from
2 a consideration of physiological cross-sectional area. The physiological implication
3 of this finding is to emphasize the importance of the ligaments in creating joint
4 stability and may suggest that the maintenance of joint stability by muscular activity
5 alone, particularly at the knee, is challenging due to an insufficient number of
6 muscular moment arms with positions and orientations that can provide the required
7 stabilizing moments. Additionally it is important to recognize the role of the
8 ligaments in providing moments that are less optimally produced by muscle function
9 alone (which is a product of their position and orientation). The stability of the knee
10 is thus dependent on the synergy between muscles and ligaments and in particular
11 their relative musculoskeletal geometry.
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30 The results of this study suggest that the ligaments have a clearly delineated role in
31 creating stability at the ankle and knee during vertical jumping. Specifically, the
32 ligaments appear to be most consistently recruited in providing adduction and internal
33 rotation moments at these joints. This type of understanding as to the different roles
34 of the muscles and ligaments in creating joint stability can only be ascertained when
35 both structures are modelled as simultaneously contributing to force and moment
36 equilibrium, as demonstrated in this work.
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50 The joint contact forces predicted in JO are lower than those found in all other cases.
51 This is unsurprising in as much as the cost function in JO is solely based upon an
52 imperative to minimize joint contact forces. This is achieved by a commensurate
53 reduction in muscular cocontraction (when compared to the other cases) as indicated
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1 by the magnitude of the peak total muscle force. Equally, LO and JO relied less
2 heavily upon the recruitment of the ankle and knee ligaments to provide non-sagittal
3 plane rotation moments, which is again a consequence of the cost function based
4 imperative to reduce ligament or joint contact force loading. In contrast, MO
5 produced greater total activation, despite a muscle focussed cost function. This
6 somewhat counter-intuitive result is due to the fact that a cost function that minimizes
7 muscle stress can increase muscular activation due to the strong imperative for force
8 sharing among all involved musculature. These results demonstrate the key
9 sensitivity of muscle, ligament and joint contact forces to the choice of cost function –
10 and consequently the physiological imperatives that determine motor control
11 strategies. The use of a cost function similar to the one employed in this study allows
12 the exploration of these effects.

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33 The new technique was capable of producing a viable solution for a variety of
34 different cost functions. The technique therefore has utility for improving the
35 understanding of human movement. In particular, the results of this study
36 demonstrate that an approach that captures the musculoligamentous interaction
37 involved in creating joint stability may result in solutions involving more realistic
38 maximum muscle forces and the calculation of joint contact forces that are lower than
39 have previously been reported. More importantly, this research demonstrates that
40 current technology permits the simultaneous solution of the equations of motion of
41 human activity. Future research should therefore seek to pose inverse dynamics
42 models in terms of the complete, simultaneous equations of motion in order to fully
43 explore the nature of joint stability.

Conflict of Interest Statement

There are no conflicts of interest.

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Definition of terms

| | | |
|----|-----------------|--|
| 1 | | |
| 2 | | |
| 3 | | |
| 4 | \hat{a}_i | linear acceleration of the centre of mass |
| 5 | | |
| 6 | | |
| 7 | \hat{c}_i | vector from the proximal joint to the segment COM |
| 8 | | |
| 9 | | |
| 10 | \hat{d}_i | vector from the proximal to the distal joint |
| 11 | | |
| 12 | f | cost function |
| 13 | | |
| 14 | | |
| 15 | F_j | magnitude of force in muscle |
| 16 | | |
| 17 | \hat{g} | acceleration due to gravity |
| 18 | | |
| 19 | | |
| 20 | i | segment/joint number (numbering from distal to proximal) |
| 21 | | |
| 22 | \hat{I}_i | inertia tensor |
| 23 | | |
| 24 | | |
| 25 | j | muscle or ligament number |
| 26 | | |
| 27 | | |
| 28 | \hat{J}_i | joint contact force at proximal end of segment |
| 29 | | |
| 30 | | |
| 31 | k_1, k_2, k_3 | cost function coefficients |
| 32 | | |
| 33 | L_j | magnitude of force in ligament |
| 34 | | |
| 35 | | |
| 36 | \hat{m}_i | mass of segment |
| 37 | | |
| 38 | | |
| 39 | \hat{M}_i | inter-segmental moment at proximal end of segment |
| 40 | | |
| 41 | | |
| 42 | n_1, n_2, n_3 | cost function exponents |
| 43 | | |
| 44 | \hat{o}_{ij} | line of action of biarticular muscle j about segment i |
| 45 | | |
| 46 | | |
| 47 | \hat{p}_{ij} | line of action of muscle j about joint i |
| 48 | | |
| 49 | | |
| 50 | \hat{q}_{ij} | line of action of ligament j about joint i |
| 51 | | |
| 52 | | |
| 53 | \hat{r}_{ij} | moment arm of muscle j about joint i |
| 54 | | |
| 55 | \hat{S}_i | inter-segmental force at proximal end of segment |
| 56 | | |
| 57 | | |
| 58 | \hat{s}_{ij} | moment arm of ligament j about joint i |
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An optimization based simultaneous approach

| | | |
|----|-------------------|---------------------------------|
| 1 | U | total number of muscles |
| 2 | | |
| 3 | V | total number of ligaments |
| 4 | | |
| 5 | W | total number of joints |
| 6 | | |
| 7 | $\dot{\theta}_i$ | angular velocity of segment |
| 8 | | |
| 9 | | |
| 10 | | |
| 11 | $\ddot{\theta}_i$ | angular acceleration of segment |
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Table 1. Ligaments included in the described model.

| Ligament | Joint | Upper bound (N) |
|-----------------------------------|-------|-----------------|
| Iliofemoral ligament (anterior) | Hip | 850 |
| Iliofemoral ligament (lateral) | Hip | 850 |
| Pubofemoral ligament | Hip | 450 |
| Ischiofemoral ligament | Hip | 450 |
| Anterior cruciate ligament (ACL) | Knee | 3000 |
| Posterior cruciate ligament (PCL) | Knee | 2000 |
| Medial collateral ligament (MCL) | Knee | 2000 |
| Lateral collateral ligament (LCL) | Knee | 4000 |
| Oblique popliteal ligament (OPL) | Knee | 1000 |
| Posterior tibiotalar ligament | Ankle | 850 |
| Tibiocalcaneal ligament | Ankle | 850 |
| Tibionavicular ligament | Ankle | 850 |
| Posterior talofibular ligament | Ankle | 850 |
| Calcaneofibular ligament | Ankle | 850 |

Table 2. Parameters used within the optimization cost function for the four different cases considered in this study (Cases 1-5), and for the previous work of Cleather and colleagues¹¹.

| Case | k_1 | k_2 | k_3 | n_1 | n_2 | n_3 |
|-----------------------------|-------|-------|-----------|-------|-------|-------|
| 1. Muscles Only (MO) | 1 | 0 | 0 | 30 | - | - |
| 2. Ligaments Only (LO) | 0 | 1 | 0 | - | 30 | - |
| 3. Muscles + Ligaments (ML) | 1 | 1 | 0 | 30 | 30 | - |
| 4. JRF Only (JO) | 0 | 0 | 1 | - | - | 2 |
| 5. ALL | 1 | 1 | 10^{-4} | 30 | 30 | 30 |
| 6. TRAD | 1 | 0 | 0 | 30 | - | - |
| 7. BI | 1 | 0 | 0 | 30 | - | - |

Note: although the TRAD and BI cases use comparable cost functions, the optimization problem is formulated differently (see Cleather et al.¹¹ for more details).

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An optimization based simultaneous approach

Table 3. Peak muscle forces (\times BW) calculated during vertical jumping for selected muscles ($^n = p < 0.05$, when compared to Case n; $* = p < 0.05$, for the comparison with all cases).

| | Biarticular | | | Monoarticular | | | Total | Total (+ Ligaments) |
|------------------------|-------------------------|---------------|-------------------------|---------------------------|---------------|-----------------------|------------------|------------------------|
| | Gastroc | Rec Fem | Hamst | Sol + Tib P | Vastus | Glutes | | |
| 1. Muscles Only | $2.0 \pm 1.3^{2,4,6,7}$ | 0.5 ± 0.4 | 1.1 ± 0.3^4 | $6.5 \pm 1.3^{6,7}$ | 2.6 ± 0.4 | 3.0 ± 1.1^4 | 16.1 ± 3.3^4 | 19.5 ± 4.5^4 |
| 2. Ligaments Only | 1.0 ± 0.5^1 | 0.4 ± 0.2 | 1.0 ± 0.3^4 | $6.6 \pm 1.2^{6,7}$ | 2.5 ± 0.4 | 2.4 ± 0.8 | 15.1 ± 2.9^4 | 17.0 ± 3.7^4 |
| 3. Muscles + Ligaments | 1.2 ± 0.6^4 | 0.5 ± 0.2 | 1.0 ± 0.3^4 | $6.6 \pm 1.2^{6,7}$ | 2.6 ± 0.5 | 2.6 ± 0.8^4 | 15.6 ± 2.6^4 | 18.7 ± 4.3^4 |
| 4. JRF Only | $0.4 \pm 0.3^{1,5}$ | 0.4 ± 0.3 | $0.5 \pm 0.3^{1,2,3,5}$ | $6.2 \pm 1.2^{6,7}$ | 2.2 ± 0.4 | $1.4 \pm 0.4^{1,3,5}$ | $11.0 \pm 1.6^*$ | $11.9 \pm 2.0^*$ |
| 5. ALL | 1.3 ± 0.8^4 | 0.5 ± 0.3 | 1.0 ± 0.3^4 | $6.6 \pm 1.2^{6,7}$ | 2.5 ± 0.4 | 2.6 ± 0.8^4 | 15.3 ± 2.3^4 | 18.2 ± 3.6^4 |
| 6. TRAD | 0.7 ± 0.3^1 | 0.2 ± 0.1 | 0.7 ± 0.3 | $4.4 \pm 1.0^{1,2,3,4,5}$ | 2.3 ± 0.4 | 2.3 ± 0.8 | 15.6 ± 2.7^4 | - |
| 7. BI | 0.7 ± 0.4^1 | 0.4 ± 0.4 | 0.8 ± 0.5 | $4.4 \pm 1.1^{1,2,3,4,5}$ | 2.2 ± 0.4 | 2.4 ± 1.1 | 15.8 ± 3.8^4 | - |

Note: total represents the peak forces for all force actuators combined (for muscles alone and for muscles + ligaments).

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An optimization based simultaneous approach

Table 4. Peak joint contact forces and ligament forces (\times BW) calculated during vertical jumping ($^n = p < 0.05$, when compared to Case n; $* = p < 0.05$, for the comparison with all cases).

| Case | AF | TFJ | HF | MCL | LCL | ACL | PCL | OPL |
|------------------------|---------------|----------------------------|----------------------------|---------------|----------------------------|----------------------------|---------------|------------------------------|
| 1. Muscles Only | 9.1 \pm 2.5 | 8.5 \pm 1.9 ⁴ | 6.9 \pm 2.2 ⁴ | 0.4 \pm 0.2 | 1.6 \pm 0.7 ⁴ | 0.5 \pm 0.2 ⁴ | 2.2 \pm 1.5 | 0.7 \pm 0.4 ^{2,4} |
| 2. Ligaments Only | 8.7 \pm 1.6 | 6.8 \pm 1.7 ⁴ | 5.4 \pm 1.0 ⁴ | 0.3 \pm 0.1 | 1.0 \pm 0.6 | 0.3 \pm 0.2 ⁴ | 1.1 \pm 0.8 | 0.2 \pm 0.3 ^{1,3} |
| 3. Muscles + Ligaments | 9.0 \pm 1.6 | 7.4 \pm 2.1 ⁴ | 5.5 \pm 1.0 ⁴ | 0.4 \pm 0.2 | 1.2 \pm 0.8 | 0.5 \pm 0.4 ⁴ | 1.7 \pm 0.9 | 0.7 \pm 0.5 ² |
| 4. JRF Only | 7.5 \pm 1.5 | 4.2 \pm 0.6* | 3.4 \pm 0.8* | 0.3 \pm 0.2 | 0.7 \pm 0.4 ¹ | 0.0 \pm 0.1* | 1.3 \pm 0.9 | 0.2 \pm 0.4 ¹ |
| 5. ALL | 9.0 \pm 1.5 | 7.4 \pm 2.0 ⁴ | 5.5 \pm 0.9 ⁴ | 0.3 \pm 0.3 | 1.3 \pm 0.8 | 0.6 \pm 0.4 ⁴ | 1.7 \pm 0.9 | 0.6 \pm 0.5 |
| 6. TRAD | 9.1 \pm 1.8 | 8.1 \pm 2.0 ⁴ | 5.8 \pm 1.3 ⁴ | | | | | |
| 7. BI | 9.0 \pm 1.8 | 8.0 \pm 1.9 ⁴ | 6.0 \pm 1.3 ⁴ | | | | | |

Table 5. Peak internal/external rotation moments (\times BW) created by the ligaments during vertical jumping ($^n = p < 0.05$, when compared to Case n).

| Case | Ankle | | Knee | | Hip | |
|------------------------|------------------------------|-----------------|------------------------------|-----------------|------------------------------|------------------------------|
| | Internal | External | Internal | External | Internal | External |
| 1. Muscles Only | 0.20 \pm 0.09 | 0.07 \pm 0.04 | 0.60 \pm 0.27 ⁴ | 0.07 \pm 0.05 | 0.09 \pm 0.05* | 0.01 \pm 0.01 ⁴ |
| 2. Ligaments Only | 0.20 \pm 0.11 | 0.05 \pm 0.03 | 0.38 \pm 0.21 | 0.05 \pm 0.05 | 0.02 \pm 0.01 ¹ | 0.00 \pm 0.00 |
| 3. Muscles + Ligaments | 0.23 \pm 0.12 | 0.06 \pm 0.03 | 0.43 \pm 0.26 | 0.06 \pm 0.04 | 0.04 \pm 0.03 ¹ | 0.01 \pm 0.00 |
| 4. JRF Only | 0.16 \pm 0.10 ¹ | 0.04 \pm 0.04 | 0.29 \pm 0.15 ¹ | 0.04 \pm 0.03 | 0.01 \pm 0.01 ¹ | 0.00 \pm 0.00 ¹ |
| 5. ALL | 0.23 \pm 0.12 | 0.06 \pm 0.03 | 0.43 \pm 0.26 | 0.06 \pm 0.04 | 0.04 \pm 0.02 ¹ | 0.00 \pm 0.00 |

Table 6. Peak ad/abduction moments (\times BW) created by the ligaments during vertical jumping ($^n = p < 0.05$, when compared to Case n).

| Case | Ankle | | Knee | | Hip | |
|------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|------------------------------|
| | Add | Abd | Add | Abd | Add | Abd |
| 1. Muscles Only | 0.15 \pm 0.07 | 0.09 \pm 0.10 | 0.25 \pm 0.12 | 0.20 \pm 0.11 | 0.08 \pm 0.08 | 0.09 \pm 0.13* |
| 2. Ligaments Only | 0.12 \pm 0.08 | 0.05 \pm 0.03 | 0.16 \pm 0.10 | 0.13 \pm 0.08 | 0.03 \pm 0.02 | 0.01 \pm 0.01 ¹ |
| 3. Muscles + Ligaments | 0.14 \pm 0.07 | 0.09 \pm 0.08 | 0.21 \pm 0.12 | 0.15 \pm 0.11 | 0.06 \pm 0.09 | 0.03 \pm 0.03 ¹ |
| 4. JRF Only | 0.10 \pm 0.08 | 0.02 \pm 0.02 | 0.17 \pm 0.12 | 0.14 \pm 0.08 | 0.02 \pm 0.03 | 0.00 \pm 0.00 ¹ |
| 5. ALL | 0.14 \pm 0.07 | 0.09 \pm 0.08 | 0.21 \pm 0.12 | 0.15 \pm 0.10 | 0.05 \pm 0.04 | 0.02 \pm 0.02 ¹ |

Figure Legends

Figure 1. Traditional approach to the calculation of muscle, ligament and joint contact forces.

Figure 2. Diagram depicting the effective origin and insertion of a muscle element. The filled rhomboids represent muscle via points, whereas the dotted boxes enclose the via points that are considered to be located in a given segment. The effective origin is the most distal via point in the proximal segment and the effective insertion is the most proximal via point in the distal segment.

Figure 3. Nomenclature used to describe segmental kinematics and kinetics.

Table Legends

Table 1. Ligaments included in the described model.

Table 2. Parameters used within the optimization cost function for the four different cases considered in this study (Cases 1-5), and for the previous work of Cleather and colleagues¹¹ (Cases 6 and 7).

1 Table 3. Peak muscle forces (\times BW) calculated during vertical jumping for selected
2 muscles ($^n = p < 0.05$, when compared to Case n; * = $p < 0.05$, for the comparison
3 with all cases).
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10 Table 4. Peak joint contact forces and ligament forces (\times BW) calculated during
11 vertical jumping ($^n = p < 0.05$, when compared to Case n; * = $p < 0.05$, for the
12 comparison with all cases).
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20 Table 5. Peak internal/external rotation moments (\times BW) created by the ligaments
21 during vertical jumping ($^n = p < 0.05$, when compared to Case n).
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27 Table 6. Peak ad/abduction moments (\times BW) created by the ligaments during vertical
28 jumping ($^n = p < 0.05$, when compared to Case n).
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Figure 1. Traditional approach to the calculation of muscle, ligament and joint contact forces.

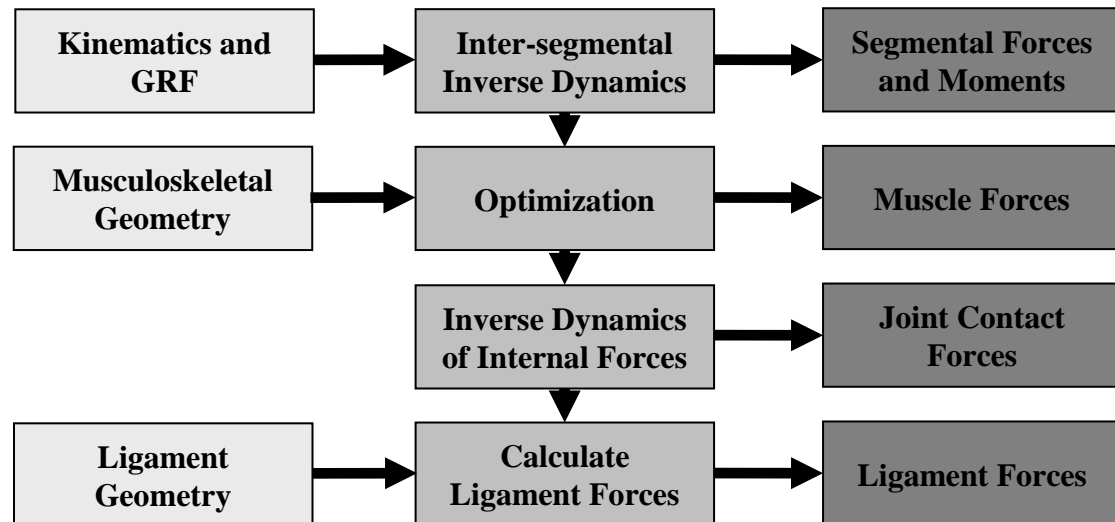


Figure 2. Diagram depicting the effective origin and insertion of a muscle element. The filled rhomboids represent muscle via points, whereas the dotted boxes enclose the via points that are considered to be located in a given segment. The effective origin is the most distal via point in the proximal segment and the effective insertion is the most proximal via point in the distal segment.

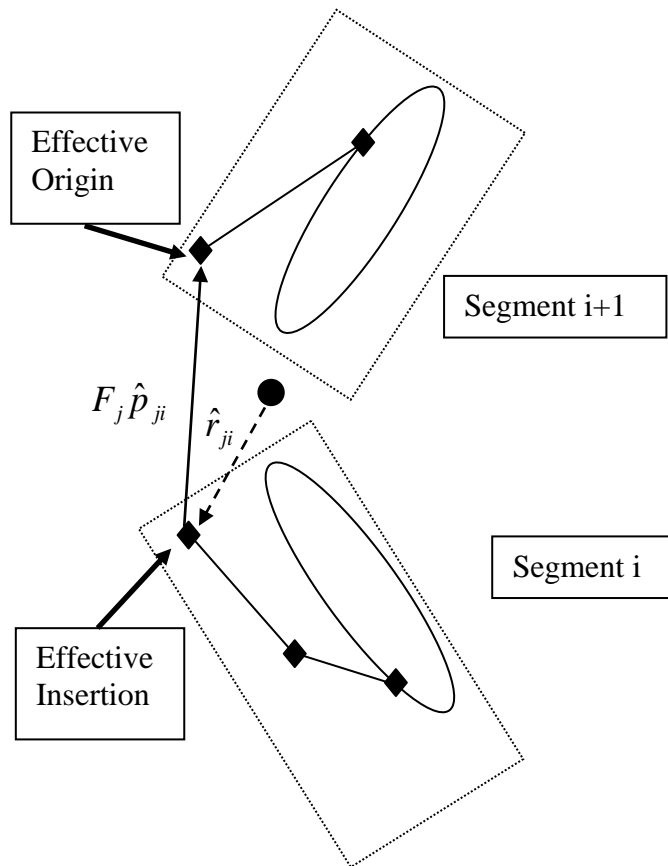


Figure 3. Nomenclature used to describe segmental kinematics and kinetics in Equations 1-3.

Figure 3a. Nomenclature related to Equation 1 (external force equilibrium).

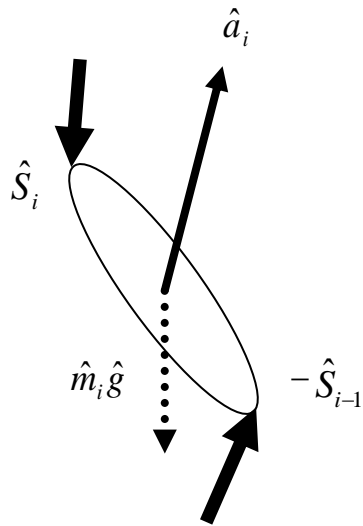
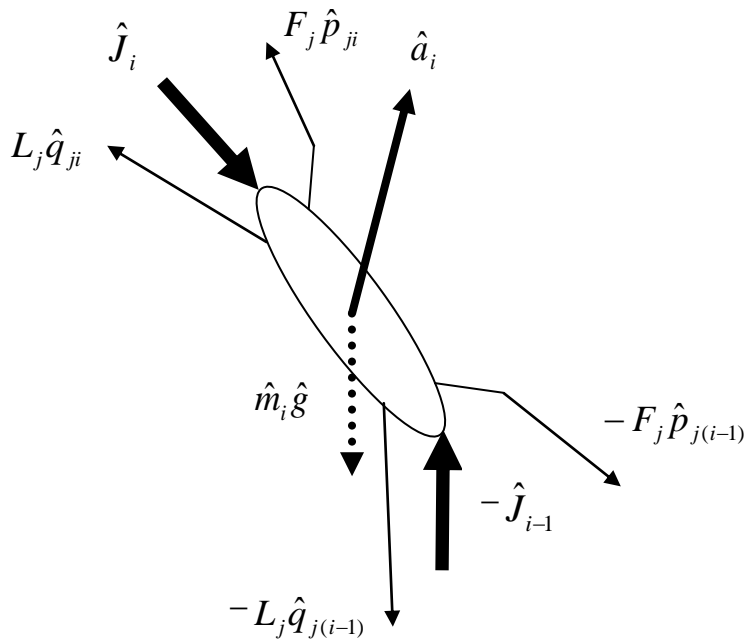
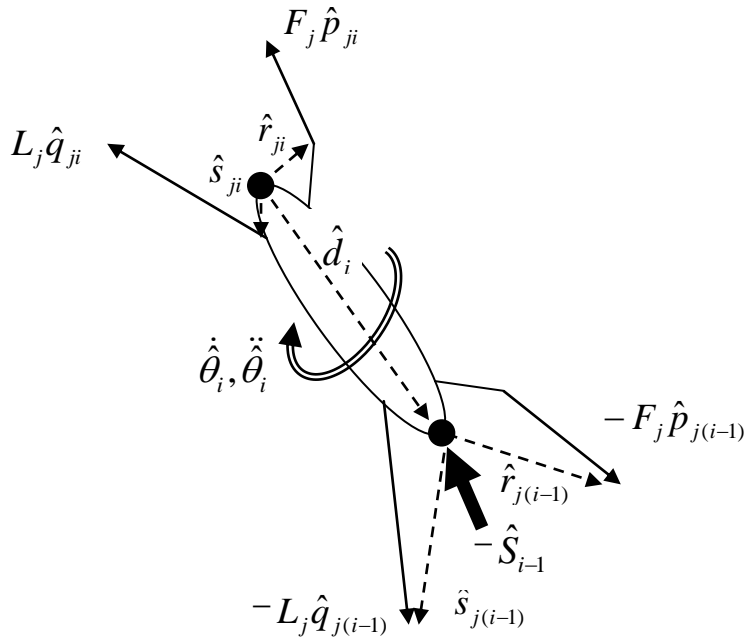


Figure 3b. Nomenclature related to Equation 2 (internal force equilibrium).



Note: the change in direction of the muscle forces represents the wrapping of muscle around bone and soft tissue and is modelled by the use of via points.

Figure 3c. Nomenclature related to Equation 3 (internal moment equilibrium).



Note: the change in direction of the muscle forces represents the wrapping of muscle around bone and soft tissue and is modelled by the use of via points.