The Optimisation of the energy-related cost function for the Delft Shoulder & Elbow Model

Master Thesis

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Abstract

For inverse-dynamic models cost functions account for the load sharing problem that arises when modelling the musculoskeletal system. This study focuses on the optimisation of the energy-related cost function integrated in the Delft Shoulder & Elbow Model and compares the translation of the obtained representation to results from *in vitro* measurements.

An existing data set containing electromyography (EMG) recordings of elbow flexors (m. biceps brachii, m. brachialis and m. brachioradialis) and extensors (m. triceps brachii and m. anconeus) was used. A grid search was performed over a range of [1, 120] for b_1 and [1, 60] for b_2 . The overall explained variance was calculated for each cost function, classifying the particular muscles in flexion and/or extension tasks where activity is expected. For the comparison to *in vitro* measurements the ratio of contraction dynamics and activation dynamics described by the cost function was determined under varying degree of force production over all muscles used for the analysis.

Optimal weight factors were obtained for $b_1 = 3$ and $b_2 = 50$. The contribution of the contraction dynamics compared to the activation dynamics was 60% at 50% of its maximal force generation and 78% at maximal force generation which compares to the *in vitro* measurements.

Keywords: Load sharing, EMG, Delft Shoulder & Elbow Model, cost function, optimisation

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Introduction

When applied in the inverse-dynamic mode, musculoskeletal models need cost functions to determine the relative and absolute contribution of individual muscles, or muscle parts, to a particular external force or moment. Generally, more than one muscle combination can, mechanically speaking, be used to exert this external force and humans appear to follow comparable musculoskeletal control principles in movement tasks. Given a particular force task, an inter-individually compatible pattern of load sharing occurs between muscles, while this does not seem to be mechanically necessary. It is, however, uncertain on what control principle load sharing between muscles occurs *in vivo* and how load sharing can be realistically simulated. Many different cost functions have been proposed (Tsirakos, Baltzopoulos et al. 1997), most of which were stress cost functions. These are based on muscle force and mostly lack physiological capabilities or functional properties. Validation has been proven difficult due to the fact that muscle force is not easily measured *in vivo* and that information on muscle contraction is often restricted to EMG patterns that is, the activation signal (Burden 2010; Hug 2010).

Especially for submaximal activities, it is often assumed that movements are performed minimising energy consumption (Hardt 1978; van der Helm 1991; Alexander 1997). Therefore, Praagman et al. (2006) proposed an energy-related cost function that is based on physiological parameters regarding energy consumption.

When looking into the processes of muscle contraction it becomes apparent that it is very sophisticated and gaining insight on how these processes are related to each other over different activation levels is not evident. Physiological muscle energetic measurements have led to the belief that three processes account for all the energy consumed during the stimulation of the muscle: (1) the attachment-detachment phases of the cross-bridge cycle; (2) the pumping of Ca²⁺ ions back into the lumen; and (3) the restoration of the Na⁺ ions after stimulation. From *in vitro* isometric single fibre measurements a general distribution was obtained: 60-75% for cross-bridge cycling and 25-40% for ion turnover (Rall 2005; Barclay, Woledge et al. 2007). Up until now it is unclear how these processes are related to each other under different degrees of stimulation leading to conflicting experimental results

(Stienen, Zaremba et al. 1995; Zhang, Andersson et al. 2006; Barclay, Lichtwark et al. 2008). However, it seems most likely that the distribution from cross-bridges and ion turnover will lead towards 50-50 at 50% of activation (Barclay and Loiselle 2007; Barclay, Woledge et al. 2007). That said, the true energetic principle is not fully understood and it is difficult to derive a valid energy-related cost function. Praagman et al (2006). divided the energy related processes into a contraction dynamics part, representing the cross-bridge cycling, and an activation dynamics part, consisting a description of the ion turnover and choosing weight factors in such a way that the two processes reached a 50-50 contribution at 50% and this implies a 1:2 ratio for contraction dynamics and activation dynamics at maximal activation.

While integrated in the Delft Shoulder & Elbow Model (DSEM), a 3D inversedynamic model of the complete shoulder and elbow mechanism (Van der Helm 1994; van der Helm 1997), it became apparent that the energy-related cost function led to more realistic predictions of muscle activation for measurements performed in a single position compared to a well-known stress cost function. For a larger range of isometric force conditions and elbow angles these findings were not only confirmed, but the energy-related cost function turned out to be more sensitive to tuning of morphological parameters (Praagman 2008). Still predictions for some conditions did not correspond with the experimental data. In the work by Praagman et al (2008), the weight factors for the two energy consuming processes that were built into their cost function were chosen arbitrarily. This implies that the relative contribution of both processes might work out to be suboptimal and improvements may be possible.

An optimised energy-related cost function will represent an objective for an inverse musculoskeletal model to account for load sharing. From a modelling point of view, this objective gives in how the energy related processes relate to each other within the skeletal muscle for a varying degree of force production.

The purpose of the current study was, starting from the work by Praagman et al (2008), to find the optimal weight factors for an energy-related cost function and thus the optimised description of the energy related processes within the skeletal muscle.

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In order to obtain these optimal weight factors a method was devised to compare the predicted outcome of the DSEM to the activation levels of individual muscles from an existing data set. The results were analysed for a wide range of weight factors. The optimal weight factors were chosen and translated into how this representation describes physiology.

Method

The energy-related cost function

For a detailed description of how the minimisation of the summed energy consumption is elaborated and includes the energy related processes see (Praagman, Chadwick et al. 2006). The cost function optimised in the present study is the minimisation of the summed energy consumption:

$$\text{minimise}\sum_{i=1}^{n} \dot{E}_{\text{m}i} = \sum_{i=1}^{n} \dot{E}_{fi} + \dot{E}_{ai}$$

In which E_m represents the muscle energy consumption and is based on the energy consuming processes in the muscle:

- 1. Detachment of cross bridges (\dot{E}_{fi}) also known as contraction dynamics.
- 2. Retrograding of the ions (\dot{E}_{ai}) also known as activation dynamics.

The simplified representation eventually leads to the following:

$$J_{E} = MIN\left(\underbrace{a_{1} \cdot F_{mi} \cdot lf_{opt}}_{contraction \ dynamics} + \underbrace{m \cdot \left\{b_{1} \cdot \frac{F_{mi}}{PCSA_{i} \cdot \sigma_{max} \cdot f_{l}\left(l_{mi}\right)} + b_{2} \cdot \left(\frac{F_{mi}}{PCSA_{i} \cdot \sigma_{max} \cdot f_{l}\left(l_{mi}\right)}\right)^{2}\right\}}_{activation \ dynamics}\right)$$

In which a_1 , b_1 and b_2 are constants or weight factors. $F_{m/}$ is the force produced by the *i*-th muscle; If_{opt} is the optimal fibre length of the *i*-th muscle; m is the muscle mass; PCSA_i is the physiological cross-sectional area of the *i*-th muscle and $f_i(I_{mi})$ is the normalised force-length relation. The σ_{max} was defined as 100 N/cm², a value derived from previous simulation studies done with the Delft Shoulder & Elbow model

(DSEM) (Veeger, Rozendaal et al. 2002). F_{mi} and $f_i(I_{mi})$ are dependent on the activation the muscle is subjected to. Praagman et al chose values of 100 for b_1 and 4 for b_2 leading to a 50-50 contribution from the linear and non-linear terms at 50% of activation and 33-67 contribution at maximal activation.

The cost function was implemented in the DSEM. Parameters for the model were obtained from a cadaver study (Klein Breteler, Spoor et al. 1999). The model generates among others the muscle forces of each individual muscle of the shoulder and elbow from the kinematic data as well as the external forces and moments that form the input.

Data collection

The experimental data were collected in a study described by Praagman et al., 2008 and comprised the raw EMG measurements of four flexors: m. biceps brachii caput breve (BB), m. biceps brachii caput longum (BL), m. brachialis (BA) and m. brachioradialis (BR); and four extensors: m. triceps brachii caput longum (TR), m. triceps brachii caput mediale (TM), m. triceps brachii caput laterale (TL) and m. anconeus (AC). The subject was seated in a chair with elbow flexed at a fixed angle and forearm horizontal and in a neutral position without an elbow or arm support. Subjects had to generate pure moments around the elbow joint (flexion (FL) and extension (EX)) and radio-ulnar joint (pronation (PR) and supination (SU)), as well as combinations of these moments (flexion-supination (FS), flexion-pronation (FP), extension-supination (ES) and extension-pronation (EP)). The subjects held a special tool with their right hand, consisting of a stick with a horizontal bar on top to which on several positions weights (0.75, 1.5, 3 or 4.5 kg) could be applied (directly or through a pulley), enforcing the external moments the subject had to withstand (Figure 1). This resulted in flexion/extension moments around 5, 10 and 15 Nm and pro/supination moments around 1, 2 and 3 Nm. Subjects were instructed to hold the tool in a fixed position keeping the bar horizontal. Feedback was given by means of a horizontal cord in front of the subject. A full set of 49 flexion/extension and pro/ supination moment combinations were measured. The moment combinations protocol was repeated at four different elbow angles: 70°, 90°, 110° and 130° of flexion (where 0° is full elbow extension), leading to a total of 196 trials per subject. A detailed description of the experimental set up and data can be found in (Praagman 2008).



Figure 1: Experimental set-up. Subject was sitting on a chair with the elbow flexed and forearm in a horizontal and neutral position. The subject had to hold the tool with his right hand, keeping the bar on top horizontal (A). Visual feedback on the position of the tool was given by a horizontal cord. Flexion moments were enforced by hanging weights right under the stick while extension moments were enforced by loads applied to the middle of the bar using a pulley system. Pro/supination moments were imposed by hanging weights on different distances left or right from the stick (B) (Praagman 2008).

Data processing

The raw EMG measurements were categorised for each muscle and each task. The EMG signals were band-pass filtered at 20-500 Hz, corrected for offset and rectified using a Hilbert transform over the period of force production (Myers, Lowery et al. 2003). Peak EMG values of individual muscle were normalised to the EMG measured from maximal voluntary contraction (mvc) measurements, giving a value between 0-1 for each muscle.

The orientations of the skeletal elements were calculated from the measured 3D coordinates (van der Helm 1996). The 3D orientation together with the external

forces and moments were put in the DSEM. The cost function optimises the model resulting in predicted forces of all individual shoulder and elbow muscles.

Optimisation method

Changes of weight factors b_1 and b_2 lead to variations of the energy-related cost function. To obtain the optimal cost function, a grid of these weight factors was constructed. The range was chosen between the most extreme interpretations using scatter plots of the measured processed EMG compared the force generated from the DSEM as these form the basis of the analysis. From these results the ranges of [1, 120] for b_1 and [1, 60] for b_2 were chosen under the assumption that the optimised weight factors would be present.

This study tries to obtain the optimal weight factors for the energy-related cost function. Between the variations of the cost function it is unlikely that the model will produce more what are called false positives/ false negatives, which describes whether activity is measured while the model does not predict activity and vice versa, while large numbers of results around 0,0 will have a confounding effect on the actual relationship between activation and predicted force. Therefore, the relationship for the flexors and extensors was determined by classifying the particular muscles in flexion and/or extension tasks where activity is expected.

Statistics

A linear regression was performed to evaluate the relationship between EMG and the generated forces from DSEM by means of a variance coefficient (R^2). A high R^2 (=1) is obtained when the measures are perfectly related. To acquire the optimised cost function the mean over all of these individual variance coefficients was calculated and the highest value results in the most optimal weight factors.

Comparison to physiology

To get an impression whether the obtained optimised cost function compares to the values obtained by the *in vitro* single fibre measurements described in the literature the contribution of the contraction dynamics and activation dynamics were determined for a particular task and run through the DSEM. Here, it was expected that the chosen task would address fully activated muscles as well as submaximal activated muscles and will result in a description of how the dynamic processes are related to each other for varying degree of force production.

Results

Predicted muscle forces from the DSEM were plotted against the measured EMG for the cost function used by Praagman et al (weight factors $b_1 = 100$ and $b_2 = 4$) are shown in Figure 2. The explained variance was calculated over the particular task the muscle is expected to be active. For BL, BB, BR and BA the flexion tasks were chosen and for TR, TL, TM and AC the extension tasks. The figures show a false negative outcome for BL and a large scatter is observed for BB resulting in a low variance coefficient. The predicted muscle force for BR is low even though the muscle is active during the force production tasks and BA shows a regression line with an intersection with the x-axis that is a lot higher than 0. The extensor muscles show overall good linearity. This indicates that the predicted forces comply with the activity the muscle produces.





Figure 2: the explained variance (R^2) and regression line (blue) for the flexors and extensors determined by classifying the particular muscles in tasks where activity is expected, for flexors that is flexion pronation (FP)/flexion supination (FS) and extensors extension pronation (EP) and extension supination (ES), for the energy-related cost function with weight factors $b_1 = 100$ and $b_2 = 4$.

The mean was calculated over all explained variance results of individual muscle for a whole grid of weight factors. Figure 3 shows the outcome of the grid

search. In this 3D bar chart the weight factors are plotted on the x and y axis respectively and the height of the bar chart corresponds to the mean of all the R^2 of the individual muscles classified in particular tasks. The overall explained variance varies between the 0.1 for the least optimised cost function to 0.31 for the optimal weight factors. When zooming in on the grid search (Figure 4) a clear rise is visible of the overall variance up until a range of combinations for weight factors. Increasing either of the weight factors beyond this range deteriorates the cost function slightly. The maximal overall explained variance is obtained at the cost function with weight factors $b_1 = 3$ and $b_2 = 50$ and results in a value of 0.31. Compared to the weight factors used by Praagman et al. this is an increase from 0.28.

The overall results were divided into the contribution of the extensors and of the flexors (Figure 5 & 7). The variance for the flexors varies between the 0.1 and 0.2 for the most optimal weight factors; for the extensors between 0.2 and 0.45. For both classifications the same shape of the plot becomes apparent when zooming in on the grid (Figure 5 & 8). The explained variance rises until a combination of weight factors is reached and increasing these weight factors more does not improve the predicted muscle forces from the DSEM any further. For the extensors these values decrease while increasing the weight factors beyond this combination. For the flexors the maximal explained variance is 0.19 and obtained at $b_1 = 10$ and $b_2 = 58$ compared and is an increase from 0.40 to 0.45 at $b_1 = 3$ and $b_2 = 50$.



Figure 3: Outcome of the grid search. Weight factors b1 and b2 are varied and the height of the bar corresponds to the mean explained variance over all of the muscles.



Figure 4: surface plot of the mean explained variance over all the muscles for weight factor b1 ranging from 1:10 and b2 from 1:60



Figure 5: Outcome of the grid search for the flexor muscles. Weight factors b1 and b2 are varied and the height of the bar corresponds to the mean explained variance over all flexors (BL, BB, BR, BA).



Figure 6: surface plot of the mean explained variance over the extensors for weight factor b1 ranging from 1:10 and b2 from 1:60



Figure 7: Outcome of the grid search for the extensor muscles. Weight factors b1 and b2 are varied and the height of the bar corresponds to the mean explained variance over all extensors (TR, TL, TM, AC).



Figure 8: surface plot of the mean explained variance over the extensors for weight factor b1 ranging from 1:10 and b2 from 1:60

The optimised cost function with weight factors $b_1 = 3$ and $b_2 = 50$ was run through the DSEM to relate the contraction dynamics $(a_1 \cdot F_{mi} \cdot lf_{opt})$ to the activation

dynamics (
$$m \cdot \left\{ b_1 \cdot \frac{F_{_{\text{min}}}}{PCSA_i \cdot \sigma_{_{\text{max}}} \cdot f_l(l_{_{\text{min}}})} + b_2 \cdot \left(\frac{F_{_{\text{min}}}}{PCSA_i \cdot \sigma_{_{\text{max}}} \cdot f_l(l_{_{\text{min}}})} \right)^2 \right\}$$
) under a varying

degree of force production by skeletal muscle. Results are shown in Figure 9. For a force production below 40% the contribution of the contraction is much higher van activation. This distribution gradually decreases to 60-40 when skeletal muscle generates 50% of its maximal force and increases up to 78-22 for maximal force.



Figure 9: the relation between the contraction dynamics and activation dynamics for the optimised cost function with weight factors $b_1 = 3$ and $b_2 = 50$ under a varying degree of force production.

Discussion

Inverse dynamic models use cost functions in order to account for the load sharing problem that arises when trying to model the musculoskeletal system. The exact principles that predict the individual muscle forces are unknown, making it difficult to find the right cost function. Previous work by Praagman et al. has shown that implementing the description of the energy consuming processes in a cost function led to improved results (Praagman, Chadwick et al. 2006). In the current study, the objective was to optimise the energy-related cost function by varying the weight factors in order to try and further understand the energetics of skeletal muscle and to further improve the Delft Shoulder and Elbow Model.

The optimisation

From an existing data set the mean explained variance of the obtained forces from DSEM and the measured activation were calculated over the individual muscles classified in particular tasks. For the optimised weight factors the average R^2 was 0.31. Compared to the weight factors chosen by Praagman et al. (2008) it is an improvement of 0.03, an increase of 10 percent. Here, the question rises whether this cost function is susceptible to optimisation. When looking at the overall results one can observe for very low weight factors (i.e. $b_1 = 1$ and $b_2 = 1$) the predicted force and measured activation are not related well. Once a combination of weight factors is reached any increase in these values does not significantly decrease the outcome of the analysis. The model generates errors when weight factors are high (i.e. $b_1 = 120$ and $b_2 = 60$) and it is recommended to choose weight factors below these extreme values.

If one looks at the magnitude of the overall outcome (Figure 3) it can be said that these values are low. This is mainly due to the outcome of the flexor muscles which are scattered as can be seen in Figure 2. However, m. anconeus does not show a very high explained variance either. Analysing the method used to determine the overall outcome starts with the EMG measurements obtained that were compared to the predicted forces from the DSEM. Although EMG measurements are a commonly used technique for validation, it has its drawbacks. One of the most important sources of error in interpreting surface EMG is what is known as crosstalk. It is defined as a contamination of the EMG signal by nearby muscle's activity. It is known that the amount of crosstalk depends on the thickness of the subcutaneous layer, the detection system and non-propagating signal components (Hug 2010). Crosstalk factors vary among test subjects and different poses the arm assumes at which the muscles are measured. Therefore, it is hard to quantify these factors but it probably improves the measured data when these are taken into account. Analysis of the explained variance for different angles showed that measurements done at 70° and 90° of flexion led to better results and this can be included when forming a new protocol for this kind of optimisation. The dataset was originally intended to compare the energy-related cost function with a well-known stress cost function. It was important to generate a large range of angles at which measurements were done as well as include a large range of external moments. For optimisation, a qualitative measurement for validation is of more importance than the extent of the dataset.

Next to an improved measurement protocol, the analysis for validation may also need to be looked into. It is generally accepted that, for isometric force production and when the EMG signal measured is sufficiently smoothed, there is a linear relationship between EMG amplitude and applied force (De Luca 1997). Therefore, it seems valid to compare the smoothed EMG measurements with the force output from the DSEM by means of an explained variance measure. It measures the strength of the relation between two variables. However, it does not necessarily measure the agreement between them. One may obtain a high explained variance when generated forces are high while no muscle activity is present. When scales of the measurements are changed it does not affect the explained variance, but it does affect the agreement. One way to account for this inconsistency is by measuring repeatability (Martin Bland and Altman 1986). Measuring agreement instead of a linear relationship might help to improve this irregularity. The main objective of the analysis then should be to produce a high measure for increasing force production while the muscle activation increases. Apart from repeatability, also the number of test subjects analysed should be more to get more reliable results.

Returning to the question whether this cost function is susceptible to optimisation. The grid search outcome has a distinct shape. This shape does not only arise for the overall results, also when classifying these for different angles and results for individual muscles show a similar shape (Appendix A). A particular range of weight factors give better overall explained variance and also there are cost functions that show a bad linear relationship for another range. The differences seem marginal for a large scope of weight factors; the shape implies that the cost function is susceptible to optimisation and improved measures an analysis may provide results with more significance.

Translation from cost function to physiology

For the comparison of the obtained optimised cost function to data from *in vitro* measurements found in literature the DSEM was used to generate the relationship between the contraction dynamics and activation dynamics. Although the final result looks promising, some caution is warranted. The data points in Figure 9 are the averaged data for the flexion and extension muscles at relative force production levels for a particular task. When looking at the raw generated data a large scatter is observed as well as data points that seem to follow an inverse exponential function that is not equivalent to the function described by the final result. As the activation dynamics is exponentially related to muscle activation it would imply that the relationship of activation dynamics and contraction dynamics obtained from individual muscle elements will not produce a lower contribution for the contraction dynamics at 50 percent of force production than at maximal force. Therefore, the weight factors of the cost function cannot accurately describe the whole spectrum of the relationship of the energy related processes by one muscle fibre.

The exponential relationship between the activation dynamics and muscle activation is presumably based on the energy consumed by ion turnover to be linearly related to stimulation frequency. However, a mammalian skeletal muscle model describing the movements of Ca^{2+} in the sarcomeres show that energy related to Ca^{2+} turnover is dependent on stimulation frequency as well as diffusion of the

calcium in the sarcomere (Baylor and Hollingworth 2003). If this is true, the exponential relationship for the activation dynamics and muscle activation may need to be revised resulting in a different optimisation of the model and translation from the optimised cost function to the physiological data.

Conclusion

From the overall mean explained variance grid search results shown in Figure 3 the most optimised weight factors for the energy-related cost function defined by Praagman et al. are $b_1 = 3$ and $b_2 = 50$. Implementing these factors in the function results in:

$$J_{E} = MIN\left(F_{mi} \cdot lf_{opt} + m \cdot 3\left\{\frac{F_{mi}}{PCSA_{i} \cdot \sigma_{max} \cdot f_{l}\left(l_{mi}\right)} + 50 \cdot \left(\frac{F_{mi}}{PCSA_{i} \cdot \sigma_{max} \cdot f_{l}\left(l_{mi}\right)}\right)^{2}\right\}\right)$$

The cost function describes the contribution of cross-bridge cycling is around 60% when skeletal muscle produces 50% of its maximum force after which it increases to around 75% at maximal force production over an average of all relevant muscle elements over the entire range of force production.

For an improved translation of the energy-related cost function integrated in the DSEM to the energy related processes from *in vitro* measurements the description of the energy consumption of the ion turnover related to activation level needs to include a diffusion coefficient resulting in a different description of the energy consumption of this process related to the force production.

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