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Curve fitting problem: torque–velocity relationship with polynomials and Boltzmann sigmoid functions

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Purpose: The aim of this study was to investigate the curve fitting and model selection problem of the torque–velocity relationship of elbow flexors and extensors in untrained females. The second goal was to determine the optimal models in different function classes and the best, among the optimal ones. Lastly, test the best models to predict the torque were tested. *Methods*: Using the polynomials (second – fourth degree) and Boltzmann sigmoid functions, and a different presentation of data points (averages, a point cloud, etc.), we determined the optimal models by both error criteria: minimum residual sum of squares and minimum of the maximal absolute residue. To assess the best models, we applied Akaike and Bayesian information criteria, Hausdorff distance and the minimum of the smallest maximal absolute residue and the predictive torque–velocity relationships of the best models with torque values, calculated beyond the experimental velocity interval. *Results*: The application of different error and model selection criteria showed that the best models in the majority of cases were polynomials of fourth degree, with some exceptions from second and third degree. The criteria values for the optimal Boltzmann sigmoids were very close to those of the best polynomial models. However, the predicted torque–velocity relationships had physiological behavior only in Boltzmann's sigmoid functions, and their parameters had a clear interpretation. *Conclusion*: The results obtained suggest that the Boltzmann sigmoid functions are suitable for modeling and predicting of the torque–velocity relationship of elbow flexors and extensors in untrained females, as compared to polynomials, and their curves are physiologically relevant.

Key words: *torque–velocity relationship, elbow flexors and extensors, Boltzmann sigmoid, polynomials, fitting function, model selection criteria*

1. Introduction

The classical fitting problem – fitting a smooth curve to a set of data points – has been studied extensively over the past 20 years by many techniques and theories. The fitting of the data of the form (x_i, y_i), $i = 1, 2, ..., n$ by a function $y = f(x, a_1, ..., a_s) \equiv f(x; a)$, depending on parameters (coefficients a_j, $j = 1, ..., s$), and the independent variable x, is frequently used in scientific and engineering work, either to determine the most probable values of the fitting coefficients, which may relate to some physically reasonable model of the process under study, or simply to permit the prediction of the most probable value of the dependent variable y for a given value of x, including those values where no data exist. Many methods obtain fitting or interpolating curves (functions) by minimizing error functions or computational geometric methods [2], [9]. The error function could be defined as follows:

(a) the sum of the square deviation of the fitting function of the mean values to be minimal [25];

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(b) the maximal deviation of the fitting function of the mean values to be minimal [6];

(c) the Hausdorff distance between the input data and the searched function to be minimal [5], [22].

In this study the problem for optimal fitting is being solved for experimental data received with isokinetic dynamometric measurements, focused on the nonlinear torque–velocity relationships at the elbow joint level, investigated in our previous research [20]. The importance of these relationships and their graphs as curves, is their informativeness in fundamental and applied studies in the area of the skeletal-muscular activity of the locomotor system. Explaining the approaches for fitting of the torque–velocity relationships is an essential element of studies on the behavior of these curves in:

– a change in the type of muscle contractions, in shortening (concentric) or in lengthening (eccentric);
– a change in the level of research, single-joint or multi-joint movements;
– changes in systemic exercise of certain muscle groups in various sports disciplines, which produce velocity specific strength gains, achieved by high-velocity or low-velocity strength training, etc.

In a number of practical papers on this classical subject in the field of biomechanics of the locomotor system, polynomial functions are mostly used in modeling of this relation. In this case, when approximating a set of data points, curve fitting is usually performed, but not interpolation and extrapolation, in order to avoid a high degree of polynomials. However, the data points are usually unordered and noisy. How to find a smooth curve from point cloud data still remains an active research problem. In most of the existing methods, the noisy data points are first smoothed out. And secondly, a curve is being fitted to the smoothed data points. In this connection, the following three approaches could be suggested:

– substituting the cloud of the data points with the mean value;
– substituting the cloud with minimum (min) and maximum (max) value;
– substituting the cloud with the mean value of min and max.

A variety of different procedures, such as reducing data points to a thinner set, using special maps of the cloud of points and using their image, clustering, etc., were also used to perform a curve fit. There are few data in the pertinent literature on comparative studies on the different approaches for presentation of data points and data processing in modeling the torque–velocity relationship.

By analyzing the experimental data points, we believe that the data cloud can be fitted by the model of one of the possible classes of models $M_1, ..., M_k$. In this paper, a model will refer to a function from some well-defined class of functions named a class of models [7], while model selection refers to the problem of using the data to select one model from the list of candidate classes of models $M_1, ..., M_k$. Selection refers to the process of estimating some quantity under each class model M_i and then comparing these quantities by applying model selections criteria such as Akaike information criterion (AIC) and Bayesian information criterion (BIC), [1], [3], [17] or some other less investigated, such as Hausdorff distance criterion (HDC) [5], [22] and minimum of their *MM* (MMR) [21], [22], in order to choose the best candidate.

Since the polynomial functions are widely applied in the modeling of torque–velocity relationship, they are given a special attention in the design of this study. For convenience, we presented them as separate sets or model classes, depending on their degree. The polynomial fitting problems have been an object of interest in various areas of research [11], [20]. However, their specificity in modeling of the torque–velocity relation also refers to possibilities of polynomials for predicting muscle torque or strength and behavior of muscle groups in a joint [8].

On the other hand, along with the polynomials, in some investigations such relationship was examined with the, so-called, sigmoid function, as it is represented as an "S"-shaped graph or sigmoid curve, based on the logistic functions [12], [20]. The hypothesis for the application of such a logistic function is based on the known S-shaped relationships between torque and velocity, especially when the muscles can also perform negative work with eccentric contractions, when the speed is practically a negative value. In this regard, the Boltzmann sigmoid functions class has been less investigated, although its parameters have a well-defined physiological interpretation, unlike the polynomial functions.

Therefore, the main purposes of this study were to measure the isokinetic torque of elbow flexors and extensors over the wide range of velocities with isokinetic dynamometer in females and to examine the torque–velocity relationship by means of the fitting problem applied to different function classes, error criteria and presenting of the data points, by using: a) fitting functions – polynomials and Boltzmann sigmoid functions [23], [26], b) error criteria – minimal sum of the squares of the deviations and minimal maximal deviation; c) data points as a cloud (all data points), average, minimum and maximum values and the average of the minimum and maximum values. The third goal was to investigate the model selection problem by classes $M_1, ..., M_k$, which are the sets of polynomials of degree i, $i = 1, ..., k$; by classes M and B, which are the class of all polynomials and the class of Boltzmann sigmoid function correspondingly; and applying selection criterion AIC, BIC, HDC and MMR. The last purpose was to check the best models to predict the torque as a function of velocity, beyond the experimental velocity interval.

2. Materials and methods

2.1. Dynamometric measurements

All testing procedures were approved by South-West University Ethics Committee. Fifteen untrained women (age: 22.0 ± 1.8 years), who gave written informed consent, participated in the study. Their body mass index (BMI), as a ratio of body mass to squared height and lean body mass (LBM), assessed according to the formula of James [24], were calculated. The subjects were tested with isokinetic dynamometer (Biodex, 4 Pro) unilaterally, on the dominant upper limb. The measurements of the elbow flexors and extensors torque, were performed under the following velocities [°/s]: 0, 30, 75, 120, 150 and 210, in a random manner. The peak torque was assessed by three consecutive repetitions, separated by 10-s relaxation and 30-s rest before the next velocity. In order to normalize the values of the torque in percentages, we assessed independently the maximal isometric torque of the elbow flexors and extensors, on separate test day, before isokinetic testing. Maximal voluntary isometric contractions were performed randomly at the following elbow angles (o): 45, 60, 75, 90, 105, 120 and 135. The participants built up either an extension or a flexion torque to maximum within a 3-s period and in each joint position they performed 4 alternatively maximal voluntary contractions – two flexions and two extensions, with 10 s rest intervals between repetitions. The intervals between the joint positions were 60 s. Taking into account the higher value of the torque for each joint position for flexors and extensors, we selected the peak torque between all seven elbow joint positions, for each female participant. This value was set as 100% in the normalization procedure. The values of the anthropometric parameters and the peak torque (in Nm and %), were presented as mean ± SD, obtained by descriptive statistics.

2.2. Data presentation

The independent variable x, which is the velocity, was determined and assumed values $x_1, x_2, ..., x_n$, where n was the number of the velocities. For $x = x_i$, $i = 1,2, ..., n$, (in the course of repeated experiments with different subjects, $S_1, S_2, ..., S_m$), we measured the values $y_{i1}, y_{i2}, ..., y_{im}$ of the dependent variable y, which was the elbow torque for both muscle groups – flexors and extensors. The dependent variable was random and probabilistic by nature. Experimental data in this case is referred to as a point cloud or a 2D cloud of data points because of the way they look in a rectangular coordinate system. The other way of presenting data was commonly used with fitting of such biomechanical relations. In this case, the values of $y_{i1}, y_{i2}, ..., y_{im}$, were being replaced with average, $\bar{y}_i = \frac{1}{m}\sum_{j=1}^{m} y_{ij}$, $i = 1, 2, ..., n$. When presenting the data in this way, as a graphic in the coordinate system, their SD are shown as well. The third way to present the experimental data in the present study was as follows: for each i, $i = 1, 2, ..., n$, for the numbers $y_{i1}, y_{i2}, ..., y_{im}$, we found $y_{i\min}$ and $y_{i\max}$, that was the minimal and maximal number between them. One more method for presentation of the data was applied, in which the values of the $y_{i1}, y_{i2}, ..., y_{im}$, were being replaced with $\frac{y_{i\min} + y_{i\max}}{2}$.

2.3. Classes of fitting functions, fitting criteria and torque–velocity relationships

To analyze the experimental data for torque–velocity relationships of both elbow flexors and extensors of females, we needed to describe them by using the "best" model, based on the assumption that it belonged to some of the classes of models $M_1, ..., M_k$, which correspond to solving purposes 2 and 3, defined in the introduction. This approach comprised the following three steps:

(1) representation of the experimental data in one of the ways described above;
(2) finding the "optimal" model P_i, belonging to class M_i, $i = 1, ..., k$;
(3) comparing the models P_i and finding the "best" model.

Finding the „optimal" models P_i, $i = 1, ..., k$, as members of these classes of models M_i, $i = 1, ..., k$, corresponded to solving the fitting problem for any of the class function M_i, $i = 1, ..., k$. The fitting error criteria used for the optimal fitting of the experimental data points were the minimum residual sum of squares (*RSS*) and the minimum of the maximal absolute residue (*MM*). These criteria are described in Appendix A. Furthermore, we compared the "optimal" models P_i, $i = 1, ..., k$, by model selection criteria. The classes of models $M_1, ..., M_k$ are the sets of polynomials of degree i, $i = 1, ..., k$, where $k = 10$. The experimental data points were also analyzed with a special class of models B, which were Boltzmann sigmoid functions, as a fitting function. Description of the Boltzmann sigmoid functions is presented in Appendix B.

Model selection criteria

In order to compare the „optimal" models Pi form the respective classes, we examined the following optimization criteria, or the, so-called, model selection criteria for finding the "best" model P, by describing the experimentally obtained data in the best way possible: AIC, BIC, MMR and HDC. Detailed description of these criteria is presented in Appendix C.

Prediction

An important objective of this study was to find a model $y = f(x)$, that predicts the response, i.e., the torque of the respective muscle group which is the dependent variable y, while the independent variable is x or the velocity measured in degrees per second. Let $f(x)$ be the "best" fitting model of our experimental torque–velocity relationships of elbow flexors and extensors, for which is known that $x \in [0, 210]$. Furthermore, any calculated value $y = f(x)$, for $x > 210$, we will consider as a predicted value. With this approach, we obtained the graphics of the predicted torque–velocity relationships in the range between 260–350 °/s by optimal polynomials or by optimal Boltzmann sigmoid. Thus, the behavior of $f(x)$ for $x > 210$ °/s, also gives grounds for the assessment of the "best" mathematical model quality.

Softwares

GraphPad Prism (ver. 6) was applied for preparing of the graphs and calculation of the parameters of the models by *RSS* criterion, while for *MM* criterion, the software package was Matlab R2013a. The selection of the best model between the "optimal" models was done by applying the package "Comparing Models" according to [21] and [22].

3. Results

3.1. Anthropometric and peak torque–velocity data

The experimental data (mean ± SD) on age, height, body mass, BMI and LBM were: 1.62 ± 0.06 m, 58.42 ± 10.04 kg, 22.19 ± 3.45 kg/m^2 and 43.93 ± 4.99 kg, respectively, while the coefficients of variation [in %] were as follows: 3.90, 17.90, 15.57 and 11.63. These data show that the group was homogeneous with respect to these anthropometric parameters. The lower coefficient of variation of averages of the normalized torque, compared to the torque in Nm (Table 1), means that data points [in %] were the proper data for modeling of torque–velocity relationships.

Table 1. The peak torque (means ± SD) presented in absolute (Nm) and normalized (%) values

Velocities [°/s]	Peak torque							
	Extensors				Flexors			
	%		Nm		%		Nm	
	$\bar{y}$ ± SD	V [%]	$\bar{y}$ ± SD	V [%]	$\bar{y}$ ± SD	V [%]	$\bar{y}$ ± SD	V [%]
0	100	0	32.2 ± 5.8	17.9	100	0	30.5 ± 6.8	22.3
30	84.1 ± 13.7	16.3	27.2 ± 7.2	26.5	80.5 ± 12.0	14.9	24.8 ± 8.2	33.3
75	71.3 ± 17.2	24.1	22.9 ± 7.2	31.3	72.7 ± 7.5	10.3	22.2 ± 5.9	26.8
120	64.6 ± 15.3	23.7	20.7 ± 6.3	30.2	66.5 ± 8.3	12.5	20.32 ± 5.8	28.7
150	55.6 ± 15.1	27.1	17.9 ± 6.7	37.5	60.9 ± 8.5	13.9	18.7 ± 5.5	29.3
210	48.8 ± 9.9	20.3	15.9 ± 5.7	35.4	58.7 ± 10.0	17.1	17.9 ± 5.3	29.9

3.2. Selection of polynomial functions

It was found that if the polynomial model higher than fourth degree was used, the respective graphs of the torque–velocity relationship would show non-physiological behavior. Therefore, in the case of the relationships studied, the physiological behavior could be expressed in a monotone decrease: if for any x_1 and x_2, $0 < x_1 < x_2$, follows $f(x_1) \geq f(x_2)$. This condition is not complied with polynomials, whose degree is greater than four.

3.3. Comparison of two fitting criteria: *RSS* and *MM*

RSS fitting criterion

The results of finding the optimal solution, using *RSS* criterion (Appendix A) to ensure global minimum, are presented in Table 2. It was established that the values of the parameters of the „optimal" models, reached with *RSS*, in all classes of functions tested, were the same not only in fitting with averages, but also with original point cloud data. This finding could also be proved theoretically (Appendix D). Therefore, using the *RSS* criterion, the optimal polynomials and optimal Boltzmann sigmoid function were the same in both ways of presenting the data (averages or a point cloud data), although the values of minimal *RSS* were different (data not shown).

The meaning of the parameters of a function we model, depends on the nature of the experimental data. In the context of biomechanical data on torque as a function of velocity, it can be said that with regard to polynomials, parameter A concerns the maximum isometric torque. Parameter A in polynomials represents the maximum isometric torque ($f(0) = A$), which is ≈100%, i.e., when the velocity is 0 °/s. Thus, in Table 2, the values of A for flexors ranged between 96.6 (second degree polynomial) and 99.9 (fourth degree polynomial), while in extensors it was between 98.0 and 100. In the optimal Boltzmann model, the parameters have a real meaning as explained in Appendix B, but the results for this model with *RSS* fitting (Table 2) show that due to the positive value of the time constant dx, the lower bound A_2 was 58.04 for flexors and 36.95 for extensors, which predicts the minimum possible percentage of the torque in the joint.

The fitting curves (the graphics of „optimal" models in the plane) of the torque–velocity relationships with the optimal polynomials and Boltzmann optimal function are presented in Fig. 1. It can be seen from this figure that for the two muscle groups only in the second degree polynomial models, the curve character is monotonically decreasing (Fig. 1a), while in the third and fourth degree (Fig. 1b to c) this monotony is disturbed. On the other hand, the behavior of Boltzmann sigmoid function (Appendix B), determined by

Table 2. Values of the parameters of the optimal polynomials and the optimal Boltzmann sigmoid in fitting with the criterion minimum residual sum of squares, using both: averages or a point cloud data of elbow flexors and extensors tested in females

Muscle group	Values of the parameters				Designation of parameters	
	P_2	P_3	P_4	Boltzmann sigmoid model	Polynomial models	Boltzmann sigmoid model
Flexors	96.6	98.6	99.9	500388	A	A_1
Extensors	98.0	99.3	100.0	99086		
Flexors	–0.39	–0.60	–0.98	58.04	B	A_2
Extensors	–0.39	–0.53	–0.78	36.95		
Flexors	1.05E-03	3.67E-03	1.38E-02	–608	C	x_0
Extensors	7.92E-04	2.52E-03	9.05E-03	–962		
Flexors		–8.16E-06	–9.00E-05	64.58	D	dx
Extensors		–5.30E-06	–5.80E-05	130.43		
Flexors			2.00E-07		E	
Extensors			1.29E-07			

Notes: (1) P_2, P_3 and P_4 are second, third and fourth degree polynomial; (2) model equations: Boltzmann sigmoid $y = A_2 + \frac{A_1 - A_2}{1 + \exp^{\frac{(x - x_0)}{dx}}}$, second degree polynomial $y = A + Bx + Cx^2$, third degree polynomial $y = A + Bx + Cx^2 + Dx^3$ and fourth degree polynomial $y = A + Bx + Cx^2 + Dx^3 + Ex^4$.

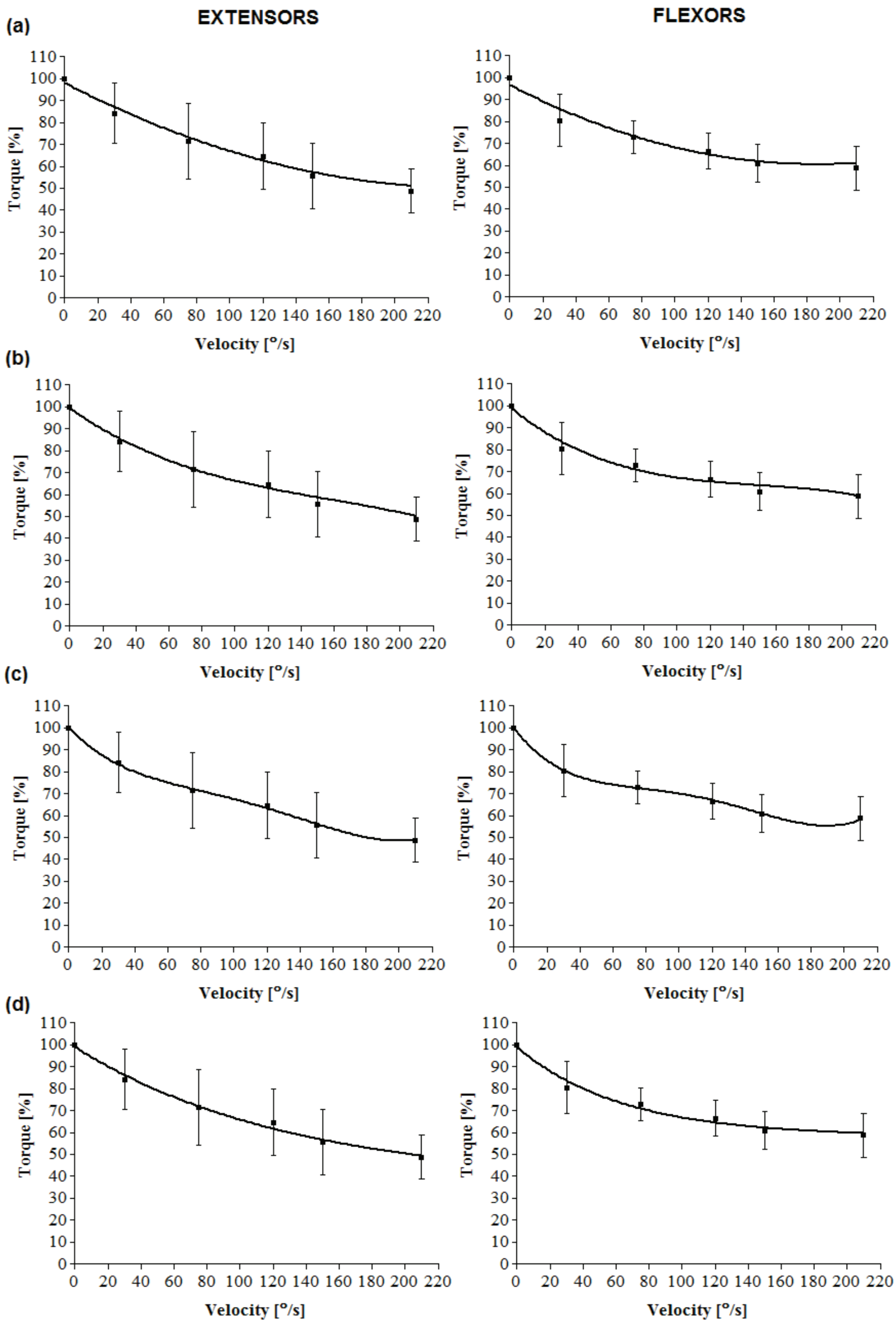

Fig. 1. Curves of the torque–velocity relationships, with fitting criterion residual sum of squares with averages, for elbow extensors and flexors: (a) second degree polynomial, (b) third degree polynomial, (c) fourth degree polynomial and (d) Boltzmann sigmoid

parameters that provide just such monotony, is shown in Fig. 1d. To obtain optimal Boltzmann sigmoidal model, we calculated 4 parameters, two of which were A_1 and A_2; A_2 was the lower or upper bound, while A_1 was the upper or lower bound of the function $f(x)$, respectively. According to the data in Table 2, the parameters found for the optimal function for both muscle groups, corresponded to the case where $A_1 > A_2$, and $dx > 0$. Since the inflection point $x_0 < 0$, we obviously approximated with that section of the curve, which was decreasing and the first derivative was monotone (Fig. 2b). This explained the smooth nature of the torque decrease when increasing the velocity in the two muscle groups, as shown in Fig. 1d.

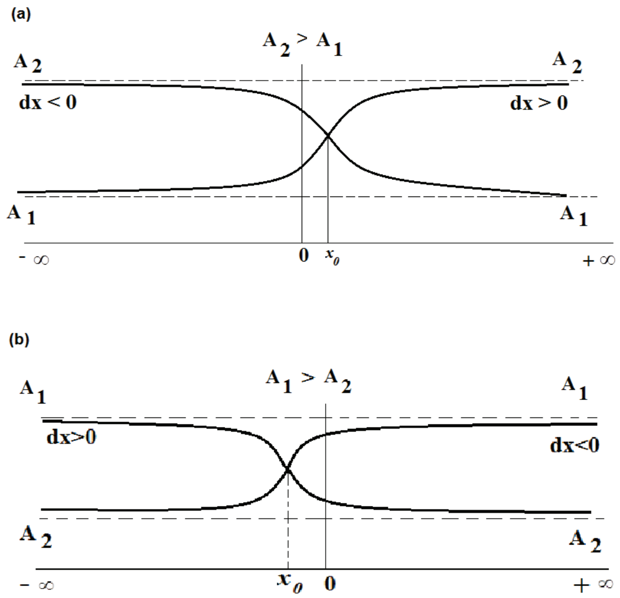

Fig. 2. Changes in upper and lower bound and the sign of the parameter *dx* of the Boltzmann sigmoid function when: $A_2 > A_1$ – (a); and $A_1 > A_2$ – (b)

MM fitting criterion

The criterion *MM* (Appendix A) is proposed for modeling of torque–velocity data for the first time in this paper. This criterion in some sense is better than *RSS*, because it seeks to make the maximal deviation of the fitting function minimal, while *RSS* minimizes the sum of the mean deviations. Moreover, the *RSS* fitting criterion in some cases can lead to unacceptable enlarging of the maximal deviation.

The performance of *MM* criterion for finding the optimal values of the second, third and fourth degree polynomial parameters, and Boltzmann sigmoid function by using a different representation of the input data such as: averages, a point cloud, the averages of the minimum and maximum values in a point cloud, and minimum and maximum values in a point cloud, are presented in Table 3. Together with the optimal parameter values, for each of the classes, the corresponding value of the *MM* criterion or the so-called minimax function are presented. In fact, they are the minimum values of the maximum deviation for the respective optimal fitting models. The data in Table 3 clearly show the significant impact of how experimental data is presented in applying the fitting criterion *MM*, which was not observed under the *RSS* criterion.

Analysis of the different ways of data presentation

This problem concerns finding of optimal models in a specific class of functions. The analysis of the different ways of data presentation, concerning the optimal polynomial models (Table 3), based mainly on the values of parameter *A* and the minimax function, shows that: the best way was using averages, followed by using averages of minimum and maximum value in a point cloud, while presentation of the data with minimum and maximum value in a point cloud or with a point cloud, where not appropriate. This arrangement refers to the two muscle groups (extensors and flexors), excluding the fourth degree polynomial data for the extensors, showing the lowest value of the minimax function (0.60), and the highest values for the maximum isometric torque (99.898).

To examine the qualities of the Boltzmann sigmoid function in the context of the *MM* criterion, we additionally calculated the value of the function at a velocity equal to 0 °/s and obtained a value of $f(0) \approx 100\%$, although the parameter A_2 had very high values. Some example results of these calculations are:

(a) when fitting the data of elbow extensors with the averages or the averages of minimum and maximum values in a point cloud, the values of A_2 are 8610.00 or 26510.92 (Table 3), but $f(0)$ is equal to 98.11 and 96.59, respectively;

(b) in flexors, when fitting with averages or averages of minimum and maximum values in a point cloud, the values for A_2 are 15006.96 or 14368.56, but $f(0) = 96.62$ or 97.80, respectively.

On the other hand, the parameter A_1 gives the asymptotic minimum of Boltzmann sigmoid function, which ensures that for $x > 210$, we cannot obtain value lower than A_1 for $f(x)$ (see Fig. 2b), $dx > 0$). So, the values of A_1 (Table 3) for extensors are between 37 and 53%, while for flexors are between 57 and 59%.

According to the values of parameter A_1 and the minimax function in Boltzmann sigmoid models, the best ways for presentation of data were with averages and with averages of minimum and maximum value in a point cloud.

The graphs of the optimal models obtained with the *MM* criterion with averages (curves are not shown), were visually similar to that with *RSS*, which is also confirmed by the close values of the parameters obtained for the two muscle groups in Table 2 and Table 3.

3.4. Assessment of the best model

The results of applying the AIC, BIC, and HDC criteria for best model selection among the optimal models in the M_2, M_3, M_4 and *B* classes obtained by applying the *RSS* optimality criterion are presented in Table 4, while those obtained by applying the *MM* optimality criterion – in Table 5, where the addition model selection criterion MMR was also used.

Table 3. Values of the parameters of the optimal polynomials and the optimal Boltzmann sigmoid in fitting with the criterion minimum of the maximal absolute residue (*MM*), using: averages, a point cloud, averages of minimal and maximal value in a point cloud and minimal and maximal value in a point cloud

Presentation of data point and minimax function value	Values of the parameters and minimax function				Designation of parameters	
	P_2	P_3	P_4	Boltzmann sigmoid model	Polynomial models	Boltzmann sigmoid model
Extensors						
Averages	97.6	98.1	98.9	37.1	*A*	A_1
	–0.39	–0.46	–0.51	8610	*B*	A_2
	0.0008	0.0018	0.0018	–676	*C*	x_0
		–3.7E-06	–3E-07	–136.8923	*D*	*dx*
			–1E-08		*E*	
Minimax function value	*2.40*	*1.85*	*3.38*	*1.99*		
A point cloud	91.4352	81.0458	76.80	53.1464	*A*	A_1
	–0.3436	–0.0910	–2.3E-05	121.9363	*B*	A_2
	8.60E-04	–0.0008	–0.0009	0.8289	*C*	x_0
		1.9E-06	–6.3E-06	–68.32632	*D*	*dx*
			4E-08		*E*	
Minimax function value	*23.20*	*23.20*	*23.20*	*23.20*		
Averages of minimum and maximum value in a point cloud	95.2890	97.1561	99.8984	51.4272	*A*	A_1
	–0.4497	–0.6581	–1.0844	26510.9157	*B*	A_2
	0.0012	0.0044	0.0156	–473.9043	*C*	x_0
		–1.00E-05	–0.0001	–74.3790	*D*	*dx*
			2E-07		*E*	
Minimax function value	*4.71*	*2.84*	*0.60*	*3.41*		
Minimum and maximum value in a point cloud	91.4352	95.1629	96.4970	53.1464	*A*	A_1
	–0.3436	–0.5428	–0.7263	121.9363	*B*	A_2
	8.60E-04	0.0036	0.0086	0.8289	*C*	x_0
		–1.00E-05	–1.00E-05	–68.2632	*D*	*dx*
			1.00E-07		*E*	
Minimax function value	*23.20*	*23.20*	*23.20*	*23.20*		
Flexors						
Averages	96.2059	97.6782	98.9476	59.7682	*A*	A_1
	–0.4380	–0.6057	–0.8262	15006.9664	*B*	A_2
	0.0013	0.0039	0.0098	–352.3596	*C*	x_0
		–9.00E-06	–5.71E-05	–59.0078	*D*	*dx*
			1.18E-07		*E*	
Minimax function value	*3.79*	*2.32*	*1.05*	*2.20*		
A point cloud	88.9778	82.5945	100.535	58.4044	*A*	A_1
	–0.3391	–0.0424	–1.1292	113.1883	*B*	A_2
	9.90E-04	–0.0021	0.0178	3.3314	*C*	x_0
		8.00E-06	–0.0001	–58.9107	*D*	*dx*
			3.00E-07		*E*	
Minimax function value	*17.40*	*17.40*	*17.40*	*17.40*		
Averages of minimum and maximum value in a point cloud	95.5359	96.6638	100.595	57.35	*A*	A_1
	–0.4164	–0.5428	–1.2625	14368.5631	*B*	A_2
	0.0013	0.0032	0.0230	–417.2373	*C*	x_0
		–7.00E-06	–1.70E-04	–70.7718	*D*	*dx*
			4.00E-07		*E*	
Minimax function value	*4.46*	*3.34*	*4.38*	*3.38*		
Minimum and maximum value in a point cloud	88.9778	98.4102	101.367	58.4044	*A*	A_1
	–0.3391	–0.7860	–1.1682	113.1883	*B*	A_2
	9.90E-04	0.0059	0.0183	3.3314	*C*	x_0
		–1.50E-05	–1.20E-04	–58.9107	*D*	*dx*
			3.00E-07		*E*	
Minimax function value	*17.40*	*17.40*	*17.40*	*17.40*		

Notes: (1) P_2, P_3 and P_4 are second, third and fourth degree polynomial; (2) model equations: Boltzmann sigmoid $y = A_2 + \frac{A_1 - A_2}{1 + \exp\frac{(x - x_0)}{dx}}$, second degree polynomial $y = A + Bx + Cx^2$, third degree polynomial $y = A + Bx + Cx^2 + Dx^3$ and fourth degree polynomial $y = A + Bx + Cx^2 + Dx^3 + Ex^4$.

Table 4. The values of model selection criteria: Akaike information criterion (AIC), Bayesian information criterion (BIC) and Hausdorff distance criterion (HDC) with the fitting criterion – minimum residual sum of squares, for elbow extensors and flexors

Muscle group	Presentation of data point	The values of the model selection criteria				Model selection criteria
		Boltzmann sigmoid model	P_2	P_3	P_4	
Flexors	Averages	+∞	60.07	+∞	**<u>–89.09</u>**	AIC
Extensors		+∞	55.77	+∞	**<u>–76.07</u>**	
Flexors	A point cloud	265.91	266.81	266.18	**<u>265.31</u>**	
Extensors		315.20	**<u>313.22</u>**	315.01	316.88	
Flexors	Averages	16.57	19.24	17.08	**<u>–6.34</u>**	BIC
Extensors		14.67	14.94	13.35	**<u>6.72</u>**	
Flexors	A point cloud	275.28	**<u>274.46</u>**	275.54	276.29	
Extensors		324.56	**<u>320.87</u>**	324.37	327.86	
Flexors	Averages	3.17	5.19	3.16	**<u>0.78</u>**	HDC
Extensors		2.92	2.94	2.48	**<u>1.12</u>**	
Flexors	A point cloud	21.33	23.35	23.51	**<u>18.36</u>**	
Extensors		27.43	28.07	26.84	**<u>25.07</u>**	

Note: P_2, P_3 and P_4 are second, third and fourth degree polynomial, respectively. The minimal values of the respective selection criterion, used for determining the optimal model, are bold and underlined.

Table 5. The values of model selection criteria: Akaike information criterion (AIC), Bayesian information criterion (BIC), Hausdorff distance criterion (HDC) and minimum of the smallest maximal absolute residue (MMR), with the fitting criterion – minimum of the maximal absolute residue, for elbow extensors and flexors

Muscle group	Presentation of data point	The values of model selection criteria				Model selection criteria
		Boltzmann sigmoid model	P_2	P_3	P_4	
Flexors	Averages	+∞	61.98	+∞	**<u>–72.50</u>**	AIC
Extensors		+∞	56.03	+∞	**<u>–64.67</u>**	
Flexors	A point cloud	286.24	280.46	299.92	**<u>269.52</u>**	
Extensors		315.20	**<u>313.22</u>**	315.07	316.96	
Flexors	Averages	17.61	21.15	18.30	**<u>10.25</u>**	BIC
Extensors		16.02	**<u>15.20</u>**	15.40	18.18	
Flexors	A point cloud	295.60	288.11	309.28	**<u>280.50</u>**	
Extensors		324.56	**<u>320.87</u>**	324.43	327.96	
Flexors	Averages	2.20	3.79	2.32	**<u>1.05</u>**	HDC and MMR
Extensors		1.99	2.40	**<u>1.85</u>**	3.38	
Flexors	A point cloud	**<u>17.40</u>**	**<u>17.40</u>**	**<u>17.40</u>**	**<u>17.40</u>**	
Extensors		**<u>23.20</u>**	**<u>23.20</u>**	**<u>23.20</u>**	**<u>23.20</u>**	

Note: P_2, P_3 and P_4 are second, third and fourth degree polynomial, respectively. The minimal values of the respective selection criterion, used for determining the optimal model, are bold and underlined.

The data presented in Table 4 show that:

– the HDC criterion always selects the fourth degree polynomial class for optimal;
– AIC and BIC choose a fourth degree polynomial for optimal only when fitting with average values for both flexors and extensors;
– when fitting with a cloud of points, AIC selects as optimal a fourth degree polynomial for flexors and a second degree polynomial for extensors, and BIC selects a second degree polynomial as optimal for both flexors and extensors;
– a fourth degree polynomial is most frequently chosen as optimal among the criteria.

However, according to the equation of the AIC criterion (Appendix C), in order to avoid a division by 0, the number of the experimental points must be greater than 6. Since the number of points in the current experimental data is equal to 6 by fitting with averages, the values of the AIC criteria in Boltzmann sigmoid function and third degree polynomial were +∞. Therefore, the application of the AIC is only possible when the velocities are more than 6.

On the other hand, the data in Table 4 shows that the Boltzmann models are not considered as optimal, according to the criteria used. However, the values of the criteria for the Boltzmann sigmoid functions are very close to those of the optimal models in all ways of presenting data for the two muscle groups. For example, when applying the AIC criterion to a point cloud data in flexors, the value obtained was 263.31 for the fourth best polynomial and 265.91 for the Boltzmann model.

The data obtained according to *MM* fitting criterion in Table 5 show that:

– when fitting with average values, AIC chooses the fourth degree polynomial class as optimal for flexors and extensors, and when fitting with cloud of points, a fourth degree polynomial is optimal for flexors and a second degree polynomial is optimal for extensors;
– BIC selects a fourth degree polynomial as optimal for flexors and a second degree polynomial as op-

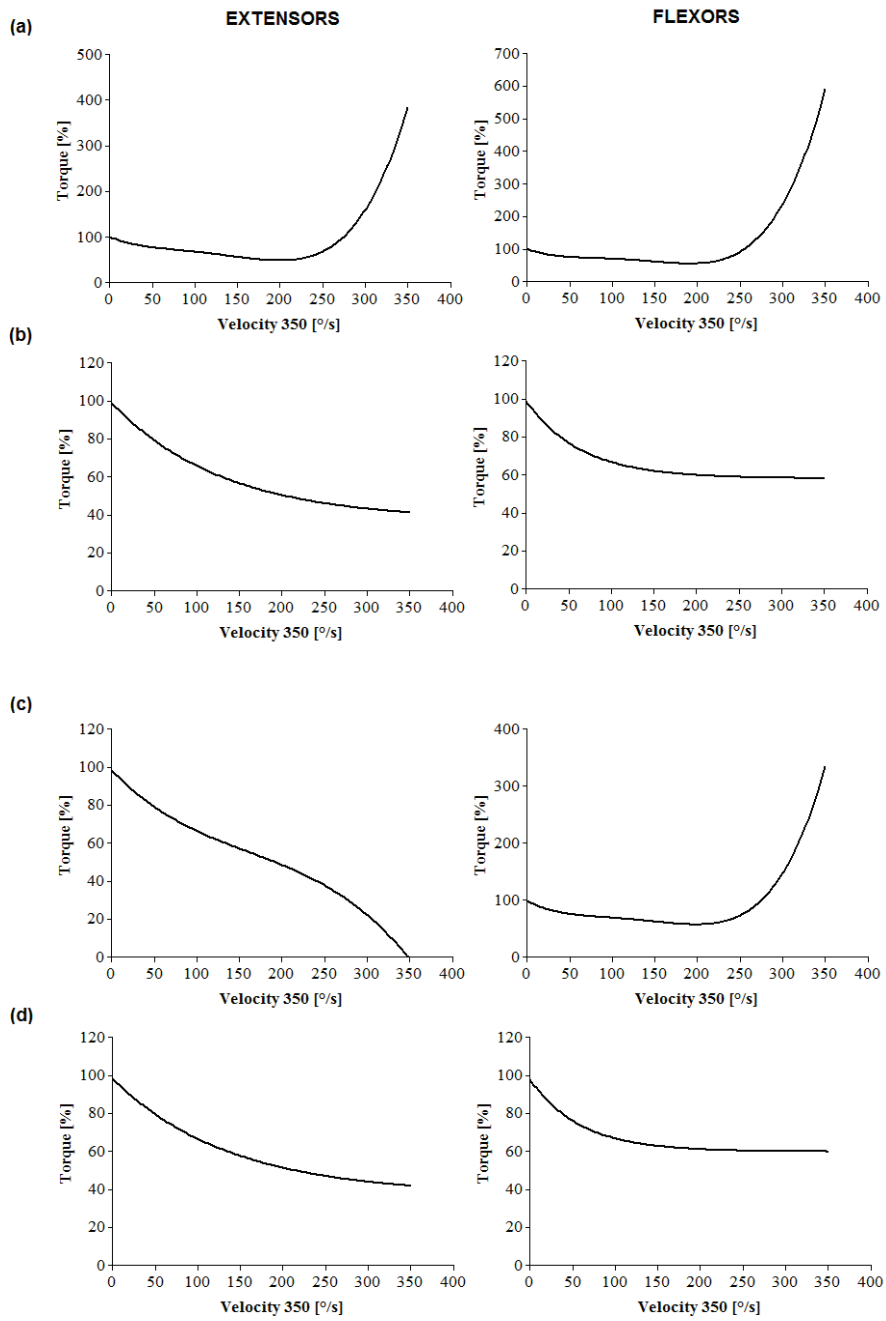

Fig. 3. Predictive torque–velocity curves of the optimal models with averages, using two fitting criteria: residual sum of squares, fourth degree polynomial (a) and Boltzmann sigmoidal function (b) for both, extensores and flexors;
– minimum of the maximal absolute residue, third degree polynomial for extensors, but fourth degree polynomial for flexors (c) and Boltzmann sigmoidal function (d) for both, extensores and flexors

timal for extensors, regardless of whether the fitting is with average values or cloud of points.

The MMR and HDC criteria lead to absolutely identical results – when fitting with average values, they choose a fourth degree polynomial as optimal for flexors and a third degree polynomial as optimal for extensors. When fitting with a cloud of points, these two criteria give the same evaluation for all models, for both flexors and extensors. Data presented in Table 5 show that the model most frequently chosen as optimal for flexors is a fourth degree polynomial, while for extensors it is a second and a third degree polynomial.

Considerations on the relation between the number of measured velocities (number of experiment points) in modeling with averages and calculation of AIC criterion, using fitting criterion *MM* were the same as for *RSS*. This explains the appearance of the values $+\infty$ in Table 5. On the other hand, similarly to the results with *RSS* fitting criterion, the Boltzmann models fitted with *MM* were also not considered as optimal and again were very close to them. For example, in the case of averages, the values of MMR and HDC for the optimal third degree polynomial were 1.85, while for the Boltzmann models were 1.99.

3.5. Prediction of the elbow torque beyond the experimental velocity interval

In Figure 3 the graphs of the best models are presented, using both fitting criteria, *RSS* and *MM*. The best model applying *RSS* fitting criterion is the optimal polynomial of fourth degree, while the best model applying *MM* criterion is the optimal polynomial of third degree for extensors and fourth degree for flexors. But it should be noted that the best polynomial models concern the experimental data points in the range of 0–210 °/s. The graphs in all best models in this velocity range are close to the physiological behavior, while those beyond the experimental velocity interval (210–350 °/s), reveal non-physiological character. Therefore, these, although best polynomial models, cannot be used to predict the values of the torque. However, in both cases (with *RSS* and *MM* criteria in Fig. 3) Boltzmann sigmoid function has more physiological behavior and this is due to the values obtained for parameter A_1 and A_2. This illustrates the validity of all stated considerations for the rationality of its parameters, and the behavior of its graph, represented by a fitting curve, including those beyond the experimental velocity interval.

4. Discussion

In this study the anthropometric parameters of the females investigated were assessed, before mathematical modeling, because they are an important landmark in comparative analysis and interpretation of the strength characteristics of skeletal muscles [27]. The results obtained suggest that the detected changes in the magnitude of the torque depending on the velocity, should not be attributed to differences in anthropometric parameters, but rather to the strength profile of the flexors and extensor in the elbow joint. This fact naturally makes it interesting to find an explicit model (function) describing the torque–velocity relationship.

The following trends can be distinguished from the literature data for modeling the force-velocity or torque–velocity relationship, which represent the fundamental property of the contractile system: It was considered that the strength assessments have largely focused on the curvilinear functions, first identified by Hill's equation [16], until 1995 [15], [19]. Higher-grade polynomials were considered to be good torque–velocity relationship models from 1995 to 2009 [4], [8], [11]. Various logistic functions have been used in the torque–velocity modeling since 2010 [12], [20]. This interest in non-linear models in recent years is one of the reasons for this development, which analyzes and compares polynomials and Boltzmann sigmoid functions as models of torque–velocity relations.

The AIC, BIC, and HDC criteria are quantitative criteria for finding of the best model among the optimal models in the given classes. The obtained numerical results show that polynomials from varying degrees are the best models. The numerical results also show that the meanings of the criteria for the optimal Boltzmann models are close to the meanings of the criteria for the best models. This leads us to compare the best models and the optimal Boltzmann models in how they model the physiological behavior, and predict it beyond the experimental velocity interval. Analyzing the curves of the best models and the optimal Boltzmann models, at least visually, demonstrates that if we apply these two "criteria" – the meanings of AIC, BIC and HDC, and the curves behavior outside the experimental velocity interval, in some cases, it is natural to use Boltzmann sigmoid functions as models of torque–velocity relationship. Although polynomials are convenient for fitting experimental data, they have some significant disadvantages as models of such relationships. The results of the present study show that polynomials, as torque–

velocity models, are inappropriate because: – only coefficient A has a physiological interpretation; it is the maximum torque in velocity equal to 0 °/s, while the others are difficult to interpret, and because the graphs of the optimal polynomials in almost all cases, including those beyond the experimental velocity interval (in prediction), have no physiological behavior. Experimental evidence of non-physiological behavior of polynomials in 2D and 3D modeling of this relation were also presented by other authors [20].

In this article, we tried to avoid the disadvantages of the polynomials by using Boltzmann sigmoid functions for fitting. The application of logistic and Boltzmann type functions have been also applied by other authors [14], [17]. Modeling of experimental data with Boltzmann sigmoid function was also applied because the function parameters have physiological interpretation and display its asymptotic behavior, moreover, if under certain parameters the value of the function at $x = 0$ is calculated (i.e., when the velocity is equal to zero), and the resulting value is equal or close to the experimental average value of the maximal peak–torque during isometric contraction of a muscle group, it is a reliable physiological feedback for fitting and for a model. It is also applied because it can serve as a reference for applying different fitting criteria, as in the case of *RSS* and *MM*. Parameters of this function have reliable physiological explanation and can act as a corrective when studying the possibilities of the polynomials to predict such kind of relationships, even when applying the criteria for comparing of the "optimal" models.

The optimal models obtained on the relationship studied with Boltzmann sigmoids, as well as the additional calculations with the obtained parameters, prove that according to the physiological interpretation of the parameter A_1 as an asymptotic minimum of the sigmoid, the maximum decrease of the torque at velocity equal to or higher than 210 °/s is about 40 to 60% at the two muscle groups of the elbow joint. This range of torque decrease, which is a consequence of mathematical modeling with Boltzmann sigmoid function, is very similar to the one found in our previous studies on elbow flexors and extensors in untrained males [18] and is also in accordance with the literature data for elbow flexors [13] and plantar flexors [10].

In the article we use four ways of experimental data presentation, and the aim is to decrease the quantity of experimental information without losing of fitting optimality. This problem concerns finding of optimal models in a specific class of functions. The comparative study of the different methods of presentation of the experimental data showed that the choice of a particular variant is an important point in choosing the "optimal" model or models, as well as in selecting the best model. According to the results obtained, it is advisable to find the optimal models by averages of a comparative analysis of the four different ways of presenting the data. If the representation of the data covers fewer numbers, as it is the case with most proposed variants, with the exception of a cloud of points, the probability of an error is smaller, and when input data covers fewer numbers and engages less computer memory, data entry errors significantly decrease.

When examining an optimal data fitting problem, it is important to add that the introduction of proper constraints on the parameters of fitting functions may change the behavior of their graphs. In the case of torque–velocity relation, when the fitting function decreases, the constraint when the first derivative is negative and growing and converges to zero, serves as an example for a meaningful constraint and could be considered a formal definition of physiological behavior.

Usually, in optimization packages, the algorithms for finding the optimal solution are of gradient type and there is not always a guarantee that we have found the global minimum. That is why we solve the fitting problem many times, by starting the gradient method with points which are far or very close to the solution found at the beginning. If the application of this procedure leads us in the solution initially found, then it can be argued with a high probability that the solution found (in respective case of the parameters of the polynomials or Boltzmann sigmoid function) is the global minimum [21].

5. Conclusions

The main results obtained in the present study on the fitting problem of torque–velocity relationships are:

– two new ways of presenting the experimental data (averages of minimum and maximum value in a point cloud and minimum and maximum value in a point cloud) were introduced and used for comparison with the already existing ones, averages and point cloud,
– a new fitting criterion, *MM*, was suggested for assessment of the torque–velocity experimental data,
– new criteria MMR and HDC for model selection were introduced, that is to determine the best model among the optimal models of model classes,

– it was shown that the way for presentation of the experimental data influences the results of optimal fitting,
– Boltzmann sigmoid functions of a special type were applied for the first time for detailed comparative investigation with polynomials in the modeling of torque–velocity relationship,
– it was shown and experimentally proven that if the optimal model criterion *RSS* is applied by data presentation with averages or with a point cloud, the optimal polynomial model is the same,
– a detailed study was conducted for modeling the torque–velocity relationship by combining two fitting criteria with four optimization criteria for model selection and four ways of presenting the experimental data.

The results obtained show that the model selection criteria should be carefully applied because they give quantitative, numerical estimates of the best models without assessing the physiological behavior of their respective curves.

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Appendix A

Let experimental data be given in the form (x_i, y_i), $i = 1, ..., n$. Let us also assume that the optimal fitting function belongs to some class of functions M depending on s parameters $a = (a_1, ..., a_s)$, i.e. $f(x, a_1, ..., a_s)$.

RSS criterion is defined as follows:

$$F_1(a) = \sum_{i=1}^{n} (y_i - f(x_i, a_1, ..., a_s))^2 .$$

The problem is to find such $a^* = (a_1^*, ..., a_s^*)$ that minimizes $F_1(a)$.

MM criterion is defined as follows:

$$F_2(a) = \max_i | y_i - f(x_i, a_1, ..., a_s) | .$$

The problem is to find such $a^* = (a_1^*, ..., a_s^*)$ that minimizes $F_2(a)$. At the same time the function F_1 and F_2 are called error functions.

Appendix B

In general, logistic functions or logistic curves have an S-shape form and are named sigmoidal curves. The Boltzmann functions are special type sigmoid functions and many authors use them by the same name [23], [26]:

$$y = A_2 + \frac{A_1 - A_2}{1 + \exp^{\frac{(x - x_0)}{dx}}} ,$$

depends on 4 parameters, where: A_2 is the lower or upper bound, A_1 is the upper or lower bound of the function $f(x)$, respectively; x_0 is the x-axis of the so-called inflection point of the respective graph and the value of the function $f(x)$ in this point is $f(x_0) = \frac{A_1 + A_2}{2}$; and dx, as a change in time constant (time), is a parameter that determines the behavior of the function $f(x)$ when $x \to \infty$ or $x \to -\infty$, depending on whether it has a positive or negative value.

There are the following 2 cases, concerning A_1 and A_2: $A_2 > A_1$, and $A_1 > A_2$, which graphs are presented in Fig. 2.

(1) Let us consider the case $A_2 > A_1$ (Fig. 2a). When $dx > 0$:

$$\lim_{x \to +\infty} f(x) = A_2 \text{, i.e., } A_2 \text{ is the upper bound;}$$

and

$$\lim_{x \to -\infty} f(x) = A_1 \text{, i.e., } A_1 \text{ is the lower bound.}$$

In the case of increasing function, the first derivative of $f(x)$ increases before the inflection point $\left(x_0 ; \frac{A_1 + A_2}{2} \right)$, in the interval $(-\infty; x_0)$; and it decreases in the interval $(x_0; +\infty)$. In both cases it is positive. When $dx < 0$, $\lim_{x \to -\infty} f(x) = A_2$, i.e., A_2 is the upper bound, and $\lim_{x \to +\infty} f(x) = A_1$, i.e., A_1 is the lower bound.

In the case of decreasing function, the first derivative of $f(x)$ increases before the inflection point $\left(x_0 ; \frac{A_1 + A_2}{2} \right)$ in the interval $(-\infty; x_0)$, and it decreases in the interval $(x_0; +\infty)$. In both cases it is negative.

(2) Let us analyse the second case, where $A_1 > A_2$ (Fig. 2b).

When $dx > 0$, the function is decreasing and then:

$$\lim_{x \to +\infty} f(x) = A_2 \text{, i.e., } A_2 \text{ is the lower bound,}$$

while

$$\lim_{x \to -\infty} f(x) = A_1 \text{, i.e., } A_1 \text{ is the upper bound.}$$

But, when $dx < 0$, the function is increasing and then:

$$\lim_{x \to -\infty} f(x) = A_2 \text{, i.e., } A_2 \text{ is the lower bound,}$$

while

$$\lim_{x \to +\infty} f(x) = A_1 \text{, i.e., } A_1 \text{ is the upper bound.}$$

In the context of the torque–velocity modeling in biomechanics, only the cases when $dx < 0$ if $A_2 > A_1$ and $dx > 0$ if $A_1 > A_2$ should be taken into account.

Appendix C

Model selection using AIC: For any of the "optimal" models Pi, we calculate AIC_i, for a small sample:

$$AIC_i = n\ln\left(\frac{RSS_i}{n}\right) + 2k_i + \frac{2k_i(k_i+1)}{n-k_i-1}, \quad n \neq k_i + 1,$$

where: RSS_i – the residual sum of squares; n – the number of observations; and k_i – the number of the parameters of the model plus one (because RSS_i is a parameter that is also calculated). The "best" model P is defined to be the model P_{i_0}, where i_0 is the index, such that $AIC = AIC_{i_0} = \min_i AIC_i$.

The AIC is used as the standard measure for ranking and model selection. The lower the AIC, the better the fit to the data and the higher the ranking the model gets. The formula presented corrects the AIC for small number of observations, which is commonly used in medico-biological investigations.

Model selection using BIC: For any of the "optimal" models P_i, we calculate BIC_i:

$$BIC_i = n + \ln\left(\frac{RSS_i}{n}\right) + k_i \ln(n),$$

with the same meaning of RSS_i, n and k, above. The "best" model P is defined to be the model P_{i_0}, where i_0 is the index, such that $BIC = BIC_{i_0} = \min_i BIC_i$.

Model selection using MMR criterion: This criterion can be applied only in the cases when „optimal" P_1, ..., P_k are found by using the maximal absolute deviation as an error function. For any of the "optimal" models P_i we calculate MMR_i, according to the following equation:

$$MMR_i = \max_j |y_j - P_i(x_j, a_i)|,$$

where: (y_j, x_j), $j = 1, \ldots, n$, are experimental data points, $a_i = (a_0, \ldots, a_i)$ are the coefficients of P_i, $i = 1, \ldots, k$. The "best" model P is defined to be the model P_{i_0}, where i_0 is the index such that $MMR = MMR_{i_0} = \min_i MMR_i$.

Model selection using HDC: The Hausdorff distance $H(A, B)$, between two non-empty sets $A = \{a_1, \ldots, a_n\}$ and $B = \{b_1, \ldots, b_m\}$ in a metric space is defined as follows:

$$H(A,B) = \max(h(A,B), h(B,A))$$

where:

$$h(A,B) = \max_{a\in A} \min_{b\in B} \|a-b\|,$$

$$h(B,A) = \max_{b\in B} \min_{a\in A} \|b-a\|,$$

and $\|\bullet\|$ is Euclidean norm $\|x\| = \sqrt{\Sigma x_i^2}$. The function $h(A, B)$ is called the directed Hausdorff distance from A to B.

We use the Hausdorff distance H to define a criterion HDC, in r to compare point sets A and B_i, for $i = 1, \ldots, k$, defined as follows:

$A = \{a_1, \ldots, a_n\}$, where $a_j = (x_j y_j)$, $j = 1, \ldots, n.$

(experimental data);

and the sets B_i:

$$B_i = \{b_{i1}, \ldots, b_{in}\},$$

where

$b_{ij} = (x_j, P_i(x_j))$; $i = 1, \ldots, k; j = 1, \ldots, k$, P_i, $i = 1, \ldots, k$, "optimal" models. The "best" model P is defined to be the model P_{i_0}, where i_0 is such index, that

$$HDC = H(A, B_{i_0}) = \min_i H(A, B_i).$$

Appendix D

Here is the proof that the parameters $a^* = (a_1^*, \ldots, a_s^*)$ for the optimal fitting with an error function $F_1(a)$ (Appendix A) with average values and a cloud of points are the same. The error function and the minimization problems are defined as follows for both cases:

$$F_1(a) = \sum_{i=1}^{n} (\bar{y}_i - f(x_i, a_1, \ldots, a_s))^2 \to \min$$

and

$$\widetilde{F}_1(a) = \sum_{i=1}^{n} \sum_{j=1}^{k_i} (y_{ji} - f(x_i, a_1, \ldots, a_s))^2 \to \min,$$

where $a = (a_1, \ldots, a_s)$

The necessary conditions a^* to minimize $F_1(a)$ and $\widetilde{F}_1(a)$ are:

$$\frac{\partial F_1(a)}{\partial a_m} = 0, \; m = 1, \ldots, s \; \text{ for average values}$$

and

$$\frac{\partial \widetilde{F}_1(a)}{\partial\, a_m} = 0,\ \ m = 1, ..., s \ \text{ for cloud of points.}$$

After rearranging the systems we have:

$$\sum_{i=1}^{n} \overline{y}_i \frac{\partial f}{\partial a_m} - \sum_{i=1}^{n} f(x_i, a_1, ..., a_s) \frac{\partial f}{\partial a_m} = 0,\ \ m = 1, ..., s\,,$$

$$\sum_{i=1}^{n}\sum_{j=1}^{k_i} y_{ji} \frac{\partial f}{\partial a_m} - \sum_{i=1}^{n}\sum_{j=1}^{k_i} f(x_i, a_1, ..., a_s) \frac{\partial f}{\partial a_m} = 0,$$

$$m = 1, ..., s.$$

Having in mind that

$$\overline{y}_i = \frac{1}{k_i}\sum_{j=1}^{k_i} y_{ji} \ \text{ or } \sum_{j=1}^{k_i} y_{ji} = k_i \overline{y}_i,\ \ i = 1, ..., n$$

it follows

$$\sum_{i=1}^{n} k_i \overline{y}_i \frac{\partial f}{\partial a_m} - \sum_{i=1}^{n} k_i f(x_i, a_1, ..., a_s) \frac{\partial f}{\partial a_m} =$$

$$\sum_{i=1}^{n} k_i (\overline{y} - f(x_i, a)) \frac{\partial f}{\partial a_m}.$$

In the case $k_i = k$, $i = 1, ..., n$,

$$\frac{\partial F_1(a)}{\partial a_m} \equiv \frac{\partial \widetilde{F}_1(a)}{\partial a_m},\ \ m = 1, ..., s$$

and if the fitting function $f(x, a_1, ..., a_s)$ has “good” properties, the same a^* minimizes both error functions $F_1(a)$ and $\widetilde{F}_1(a)$.