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Towards a realistic biomechanical model of the thumb: the choice of kinematic description may be more critical than the solution method or the variability/uncertainty of musculoskeletal parameters

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Abstract

A biomechanical model of the thumb can help researchers and clinicians understand the clinical problem of how anatomical variability contributes to the variability of outcomes of surgeries to restore thumb function. We lack a realistic biomechanical model of the thumb because of the variability/uncertainty of musculoskeletal parameters, the multiple proposed kinematic descriptions and methods to solve the muscle redundancy problem, and the paucity of data to validate the model with in vivo coordination patterns and force output. We performed a multi-stage validation of a biomechanical computer model against our measurements of maximal static thumbtip force and fine-wire electromyograms (EMG) from 8 thumb muscles in each of five orthogonal directions in key and opposition pinch postures. A low-friction point-contact at the thumbtip ensured that subjects did not produce thumbtip torques during force production. The 3-D, 8-muscle biomechanical thumb model uses a 5-axis kinematic description with orthogonal and intersecting axes of rotation at the carpometacarpal and metacarpophalangeal joints. We represented the 50 musculoskeletal parameters of the model as stochastic variables based on experimental data, and ran Monte Carlo simulations in the "inverse" and "forward" directions for 5000 random instantiations of the model. Two inverse simulations (predicting the distribution of maximal static thumbtip forces and the muscle activations that maximized force) showed that: the model reproduces at most 50% of the 80 EMG distributions recorded (eight muscle excitations in 5 force directions in two postures); and well-directed thumbtip forces of adequate magnitude are predicted only if accompanied by unrealistically large thumbtip torques (0.64 ± 0.28 N m). The forward simulation (which fed the experimental distributions of EMG through random instantiations of the model) resulted in misdirected thumbtip force vectors (within $74.3 \pm 24.5°$ from the desired direction) accompanied by doubly large thumbtip torques (1.32 ± 0.95 N m). Taken together, our results suggest that the variability and uncertainty of musculoskeletal parameters and the choice of solution method are not the likely reason for the unrealistic predictions obtained. Rather, the kinematic description of the thumb we used is not representative of the transformation of net joint torques into thumbtip forces/torques in the human thumb. Future efforts should focus on validating alternative kinematic descriptions of the thumb.

Keywords: Hand; Thumb; Muscle coordination; EMG; Biochemical model; Monte Carlo simulation

Abbreviations: ADD, adductor pollicis muscle; APB, abductor pollicis brevis muscle; APL, abductor pollicis longus muscle; CMC, carpometacarpal; DIO, first dorsal interosseous muscle; EMG, electromyographic recordings; EPB, extensor pollicis brevis muscle; EPL, extensor pollicis longus muscle; FPB, flexor pollicis brevis muscle; FPL, flexor pollicis longus muscle; IP, interphalangeal; LP, linear programming; MP, metacarpophalangeal; OPP, opponens pollicis muscle; SD, standard deviation; PIP, proximal interphalangeal joint; DIP, distal interphalangeal joint; PCSA, physiological cross-sectional area.

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1. Introduction

Impairment of the thumb can severely diminish pinch function and manipulation ability. Surgeries that restore thumb function for pinch grasps should have consistent and predictable outcomes despite anatomical variations across individuals. In practice, improvements in pinch force magnitude and pinch ability vary following surgical treatment of orthopedic (Glickel et al., 1992; Tomaino et al., 1995; Freedman et al., 2000) and neurological (Ramselaar, 1970; McFarlane, 1987; Brandsma and Ottenhoff-De Jonge, 1992; Hentz et al., 1992) conditions of the thumb. Understanding the source of outcome variability can improve the treatment of pinch force deficits.

It is difficult to understand the sources of outcome variability due to the complex mechanics and muscle coordination of the thumb, and anatomical variability. One way to address this clinical question is to create biomechanical computer models to predict how musculoskeletal and kinematic variables affect thumb function. Unfortunately, today there is no validated and realistic model of the thumb that predicts even simple mechanical output, such as maximal static force and the muscle coordination that achieves it. We believe the validity of biomechanical computer models of the thumb remains questionable for four reasons. First, the choice of kinematic description of the thumb remains debatable (Cooney and Chao, 1977; Chao and An, 1978; Giurintano et al., 1995). Second, the predictions of biomechanical models can be sensitive to both the musculoskeletal parameter values (Valero-Cuevas et al., 1998) and the choice of mathematical solution method. Third, there is much uncertainty in published musculoskeletal parameter values for the thumb (e.g., coefficients of variance $>40\%$ are common (Smutz et al., 1998)). And fourth, to our knowledge no biomechanical thumb model has been validated by comparing predictions of both mechanical output and muscle coordination patterns to experimental measurements (i.e., inverse *and* forward validation).

Creating realistic biomechanical models of the thumb requires that we understand the consequences of the choice of musculoskeletal parameters. Three of the four reasons above are associated with the challenge of measuring and assigning musculoskeletal parameters compatible with the kinematic description adopted and representative of the individuals modeled. Most biomechanical models of the digits (Chao et al., 1976; Cooney and Chao, 1977; An et al., 1979, 1985) and the thumb (Cooney and Chao, 1977; Chao and An, 1978; Giurintano et al., 1995) assign average experimental values to each parameter. This approach does not address the potential effects of intersubject variability, which could be a critical factor in predicting surgical outcomes. To explore the biological question of whether including intersubject variability suffices to realistically predict maximal thumbtip forces and their associated coordination patterns, we investigated which factor is most critical (to represent well) in developing a biomechanical model of the thumb: kinematic description, musculoskeletal and kinematic parameters, or solution method. Our results clarify whether future efforts to create realistic models should focus on obtaining more reliable values for musculoskeletal parameters vs. improving kinematic descriptions or solution methods.

2. Methods

We measured thumbtip forces and recorded electromyograms (EMG) from individual thumb muscles with methods reported for the forefinger (Valero-Cuevas et al., 1998; Valero-Cuevas, 2000) and thumb (Johanson et al., 2001). Briefly, seven participants (5 female, 2 male, 28.6 ± 6.5 yr) produced maximal voluntary thumbtip force against a smooth, rigidly held 6-axis dynamometer with the distal phalanx of their right-dominant thumb in five orthogonal directions (palmar, distal, lateral, dorsal and medial) defined with respect to the distal phalanx in two thumb postures (key and opposition, Fig. 1). Key posture (Fig. 1 and Table 1) was defined as the thumbtip touching the radial aspect of the forefinger between the DIP and the PIP joints corresponding to the recommended posture for surgical arthrodesis (House, 1985; Hentz et al., 1992). Opposition posture (Fig. 1 and Table 1) is defined with the tip of the thumb in contact with the tip of the forefinger with the joints of the thumb and forefinger in enough flexion and abduction so the two digits formed a ring. These postures placed all joints away from their extremes of range of motion. A custom molded thimble fit snuggly over the distal phalanx and had five 5-mm spherical brass beads embedded on its outer surface in locations corresponding to each force direction. Each bead defined a low-friction point-contact between a polished aluminum plate and the thumbtip requiring participants to produce well-directed force (i.e., within 16° of the perpendicular to the surface) with negligible thumbtip torque, or else the bead would slip and/or rotate (Valero-Cuevas et al., 1998), because a low-friction point-contact cannot transmit torque because of its tendency to slip and roll (Murray et al., 1994). We instructed participants to produce maximal voluntary thumbtip force in three 10-s trials by either ramping to maximal force (ramp trial) or by increasing force in two steps (step trial) (Fig. 2). Visual and auditory feedback motivated the participants to produce their maximal voluntary thumbtip force in each posture. A computer screen displayed either their maximal or their maximal and 50% maximal force output in a stair-step pattern.

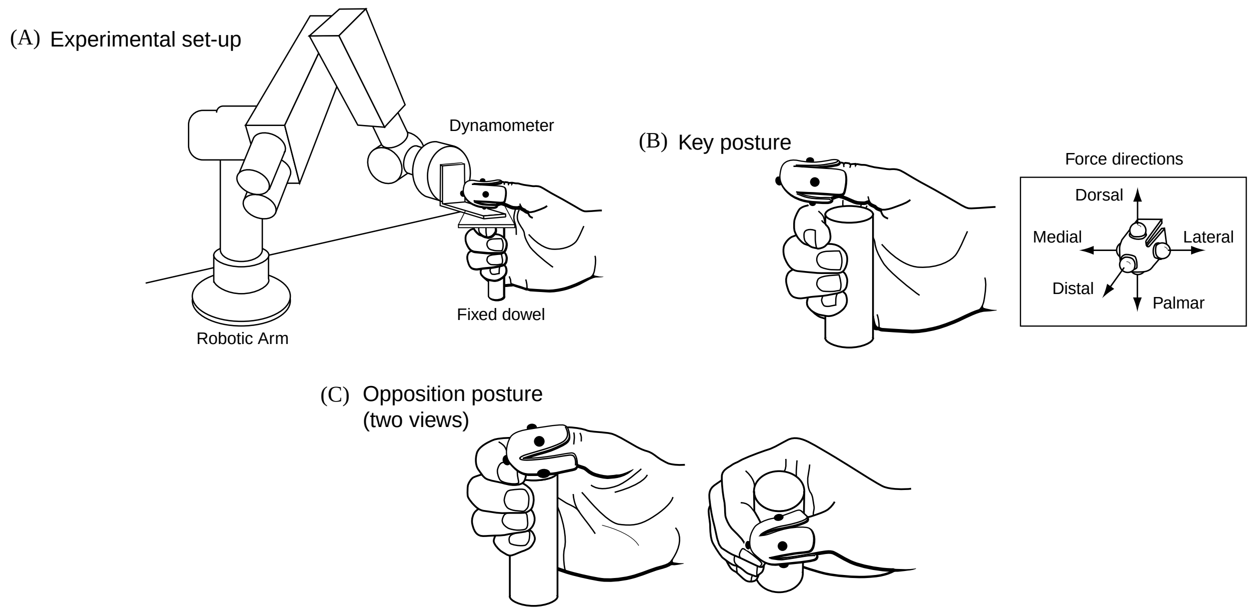

Fig. 1. We used a methodology developed to study forefinger force production (Valero-Cuevas et al., 1998; Valero-Cuevas, 2000), which was recently adapted to study thumb force production (Johanson et al., 2001). (A) Participants were seated with their right dominant arm supported by a trough in elbow flexion and neutral forearm rotation, and wrapped their fingers around a fixed dowel similar to a joystick which placed the wrist in 45° extension, and 0° of ulnar deviation, prevented thumb–forefinger contact and isolated thumb force production. We instructed the participants to maximize isometric thumbtip forces against a dynamometer (6-axis force/torque sensor, Gamma F/T transducer, ATI Industrial Automation, Gardner, NC) mounted on a robotic arm (Stäubli-Unimate Puma 260 programmable robot, Stäubli Corporation, Duncan, SC). The position and orientation of the force plate was pre-programmed for each participant. A computer (PowerMacintosh 7200, Apple Computer, Inc., Cupertino, CA) with data acquisition hardware/software (NB-MIO-16 card and LabView, National Instruments, Austin, TX) collected and stored force data as well as EMG signals processed by BAK model MDA-3 amplifiers. The positioning of the dynamometer was programmed to oppose the thumb in reproducible thumb postures used in key and opposition pinch. Participants wore custom thimbles made of thermoplastic splinting material (MaxD, North Coast Medical, Inc.) with 5 mm brass balls that defined the directions of force production. The few ($<5\%$) cases in which the thimble slipped or rotated were repeated. One-minute rest between trials prevented fatigue (Enoka and Stuart, 1992). Participants had no history of neurological or musculoskeletal hand pathologies or injuries, and read, understood and signed a consent form approved by the Medical Committee for Protection of Human Participants in Research at Stanford University prior to participation. (B) Key posture is defined as the thumbtip touching the radial aspect of the forefinger between the DIP and the PIP joints (Table 1), with the thumb MP and IP joints in moderate flexion, and the CMC joint extended 30° (so that the first metacarpal was extended with respect to the long axis of the radius in the plane of the palm) and aligned with the long axis of the radius in the plane transverse to the palm (neutral abduction) corresponding to the recommended posture for surgical arthrodesis (House, 1985; Hentz et al., 1992). (C) Opposition posture is defined with the tip of the thumb in contact with the tip of the forefinger (requiring pronation of the metacarpal to align the nail-beds) with the joints of the thumb and forefinger in enough flexion and abduction so the two digits formed a ring (Table 1).

Preliminary trials provided the initial targets. For the step force pattern, participants targeted their 50% maximal level, then proceeded to maximal force, and reduced the force to repeat the 50% level of force. For the ramp force pattern, participants increased force monotonically at their chosen speed. We included ramp trials because some subjects could reach higher forces when increasing force at self-selected speed. We randomized the order of thumb postures and force directions within each posture. We simultaneously recorded thumbtip force and EMG using fine-wire electrodes placed in all nine muscles of the thumb (see Fig. 2 for details; Johanson et al., 2001). We excluded the DIO muscle from EMG recordings and the model because others (Brand and Hollister, 1999; Kaufman et al., 1999) and we (Johanson et al., 2001) could only record activity from DIO when both the thumb and forefinger were used to pinch. The DIO was inactive when producing thumb force while relaxing the forefinger. The participants performed three trials: two ramp and one step force pattern. The third trial was always designated as a ramp and the order of the first two trials were randomized for step or ramp. A fourth ramp trial was done without the thimble to insure maximal EMG was recorded without the precariousness of the point-contact for each direction/posture. This additional ramp trial was used only for EMG normalization purposes, and was not used in the force or coordination pattern analysis.

Consistent with biomechanical models of static force production, thumbtip force/torque at a given thumb posture was expressed as a system of linear equations in the activation level of each muscle (Chao and An, 1978; Valero-Cuevas et al., 1998). The model consists of a

Table 1
Musculoskeletal parameters

	Key pinch			Opposition pinch	
	Tendon/Joint	Mean	SD	Mean	SD
Moment arms (mm) (Smutz et al., 1998)					
CMC flexion	FPB	13.50	7.56	12.50	8.50
(flexion +)	ADD	32.00	10.56	26.00	8.50
(extension −)	APB	3.93	3.10	4.20	3.40
	OPP	12.90	3.87	12.80	4.90
	FPL	14.30	4.00	13.60	2.80
	EPB	−13.00	2.47	−14.40	2.20
	EPL	−8.07	2.58	−9.89	3.60
	APL	−7.17	3.44	−7.92	3.00
CMC abduction	FPB	10.50	6.83	6.40	4.90
(abduction +)	ADD	−18.80	15.42	−22.40	13.90
(adduction −)	APB	16.50	6.93	13.20	7.50
	OPP	4.80	4.99	−1.50	4.50
	FPL	0.20	4.90	0.10	2.80
	EPB	3.20	6.69	4.50	2.30
	EPL	−9.50	7.13	−5.70	4.40
	APL	10.50	3.26	7.30	2.70
MP flexion	FPB	5.30	1.59	5.30	1.59
(flexion +)	ADD	4.90	4.12	4.90	4.12
(extension −)	APB	0.70	2.90	0.70	2.90
	FPL	10.90	1.74	10.90	1.74
	EPB	−8.60	0.69	−8.60	0.69
	EPL	−9.30	1.12	−9.30	1.12
MP abduction	FPB	8.70	3.31	7.20	3.30
(abduction +)	ADD	−5.00	4.90	−5.45	5.50
(adduction −)	APB	11.10	4.44	10.00	4.10
	FPL	−0.10	2.40	−1.20	2.10
	EPB	1.40	0.90	1.30	0.90
	EPL	−4.40	1.80	−4.50	1.70
IP flexion	FPL	8.00	1.52	6.60	1.60
(flexion +)	EPL	−5.20	0.52	−4.40	0.40
(extension −)					
Extensor mechanism angles (deg)					
α, projection angle of tendon of ADP's oblique head onto EPL tendon	35.00				
γ, projection angle of tendon of ABPB's medial slip onto EPL tendon	30.00				
θ, medial bifurcation angle of APB	15.00				
β, lateral bifurcation angle of APB	25.00				
PCSA (cm^2) (Lieber et al., 1992; Jacobson et al., 1992; Brand et al., 1981)					
	FPB	0.66	0.20	0.66	0.20
	ADD	4.00	0.80	4.00	0.80
	APB	0.68	0.58	0.68	0.58
	OPP	1.02	0.35	1.02	0.35
	FPL	2.08	0.23	2.08	0.23
	EPB	0.47	0.32	0.47	0.32
	EPL	0.98	0.13	0.98	0.13
	APL	1.93	0.60	1.93	0.60
Bone segment lengths (cm) (measured in participants)					
	Metacarpal	5.29	0.90		
	Prox. phalanx	4.03	0.62		
	Dist. phalanx	3.07	0.31		

Table 1 (*continued*)

	Key pinch			Opposition pinch	
	Tendon/Joint	Mean	SD	Mean	SD
Joint angles (deg) (measured in participants)					
	CMC flexion	−30.00	8.50	−24.00	12.70
	CMC abduction	0.00	0.00	19.00	8.20
	MP flexion	17.00	10.40	24.00	12.90
	MP abduction	0.00	0.00	6.00	2.80
	IP flexion	23.00	11.70	51.00	14.00

Note on model implementation: As was previously described (Valero-Cuevas et al., 1998; Valero-Cuevas, 2000), the isometric force production of each muscle was modeled by scaling its maximal force fo_i by its excitation level e_i ($0 \leqslant e_i \leqslant 1$). Fo_i is calculated by multiplying PCSAs times maximal muscle stress (35.4 N/cm^2; Close, 1972; Brand et al., 1981; Powell et al., 1984; Zajac, 1989). We assumed muscles were at optimal fiber length due to lack of published values, with pennation angles (Jacobson et al., 1992; Lieber et al., 1992; Brand and Hollister, 1999) small enough not to affect Fo_i (i.e., $<10°$; Zajac, 1989). The parameter-based computer model is a matrix equation where a 5×8 matrix embodies the static force production properties of the digit. This matrix includes the nominal Fo_i values (to scale the excitation level of each muscle into muscle force), the moment arm and extensor mechanism values (to calculate the net torque at all joints), and the inverse transpose Jacobian matrix of the three-segment/5-DOF thumb (calculates the thumbtip output produced any net joint torque vector). For each thumb posture, this matrix is a constant non-invertible matrix representing an under constrained system where several coordination patterns can produce a given sub maximal thumbtip force. The linear programming optimization predicted the unique coordination pattern that produces the maximal biomechanically feasible magnitude of thumbtip force in each direction in each posture.

fixed trapezium, a metacarpal and two phalanges articulated by five pin joints (Fig. 3) actuated by eight independent muscles, plus an extensor mechanism at the MP joint (Fig. 4). The CMC and MP joints have orthogonal and intersecting axes of rotation. The static fingertip force production properties of the thumb are represented by a 5×8 matrix $\mathbf{M}$. $\mathbf{M}$ maps a rank-8 input vector of muscle activation into a rank-5 output vector containing three forces and two torque components. If rigidly coupled to an object, the distal phalanx can impart torques independently of fingertip forces because it has five DOFs (Valero-Cuevas et al., 1998). $\mathbf{M}$ is the concatenation of three matrices ($\mathbf{M} = \mathbf{J}^{-\mathrm{T}}\mathbf{R}\mathbf{F}_0$; Valero-Cuevas et al., 1998; Valero-Cuevas, 2000): the 8×8 $\mathbf{F}_0$ diagonal matrix of maximal muscle force values, which scales the excitation level of each muscle into muscle force; the 5×8 $\mathbf{R}$ moment arm and extensor mechanism interaction matrix, which superimposes the joint torque vector produced by each muscle force to obtain the net joint torque vector; and the 5×5 $\mathbf{J}^{-\mathrm{T}}$ inverse transpose Jacobian matrix corresponding to the chosen kinematic description, which calculates the output force/torque vector produced by the net joint torque vector. The 50 musculoskeletal parameters of the model (Table 1) were either measured by us: in the study participants (3 bone segment lengths and 5 joint angles for key and opposition posture); or in one cadaver thumb (4 angles of the extensor mechanism), or obtained from cadaveric studies: 8 PCSA (Jacobson et al., 1992; Lieber et al., 1992; Brand and Hollister, 1999); and 30 moment arms measured assuming the same kinematic description as our model (Smutz et al., 1998). We measured bone lengths as the distance between the palpable grooves between bones (e.g., metacarpal length was the distance between the CMC and MP grooves). Flexion-extension joint angles were defined between the longitudinal axes of bones, as typically done in the clinic. Total thumb abduction in opposition posture was the angle between the first and second metacarpal bones. This angle was apportioned to the CMC and MP in the ratio of 3:1, consistent with the notion that most thumb abduction occurs at the CMC than at the MP joint (Smutz et al., 1998). All 50 musculoskeletal parameters were described as uniformly distributed pseudo-random variables in a Mathematica® computational package (Wolfram Research, Inc., Champaign, IL) using a G3 Powerbook computer (Apple Computer, Inc., Cupertino, CA) with the bounds set to their mean value ± 1 standard deviation (SD) (Table 1). In no case were these parameter ranges anatomically unrealistic.

We performed three Monte Carlo simulations to predict the distribution of maximal thumbtip forces in the five directions studied in each thumb posture. Each simulation consisted of 5000 iterations (i.e., random instantiations) of the model in each thumb posture. The first two simulations used linear programming (LP) to solve the "inverse" (or muscle redundancy) problem of finding the unique optimal coordination pattern that maximized thumbtip force within 10° of the desired directions for each model instantiation. The objective was to maximize the force vector component in the desired direction while constraining muscle activations to be $\geqslant 0$ and $\leqslant 1$ (see caption to Table 1) (Valero-Cuevas et al., 1998). The directional accuracy constraint was achieved iteratively by progressively adjusting the linear constraints on the components of force perpendicular to the desired direction until their magnitudes were at or below 17% of the magnitude of the component

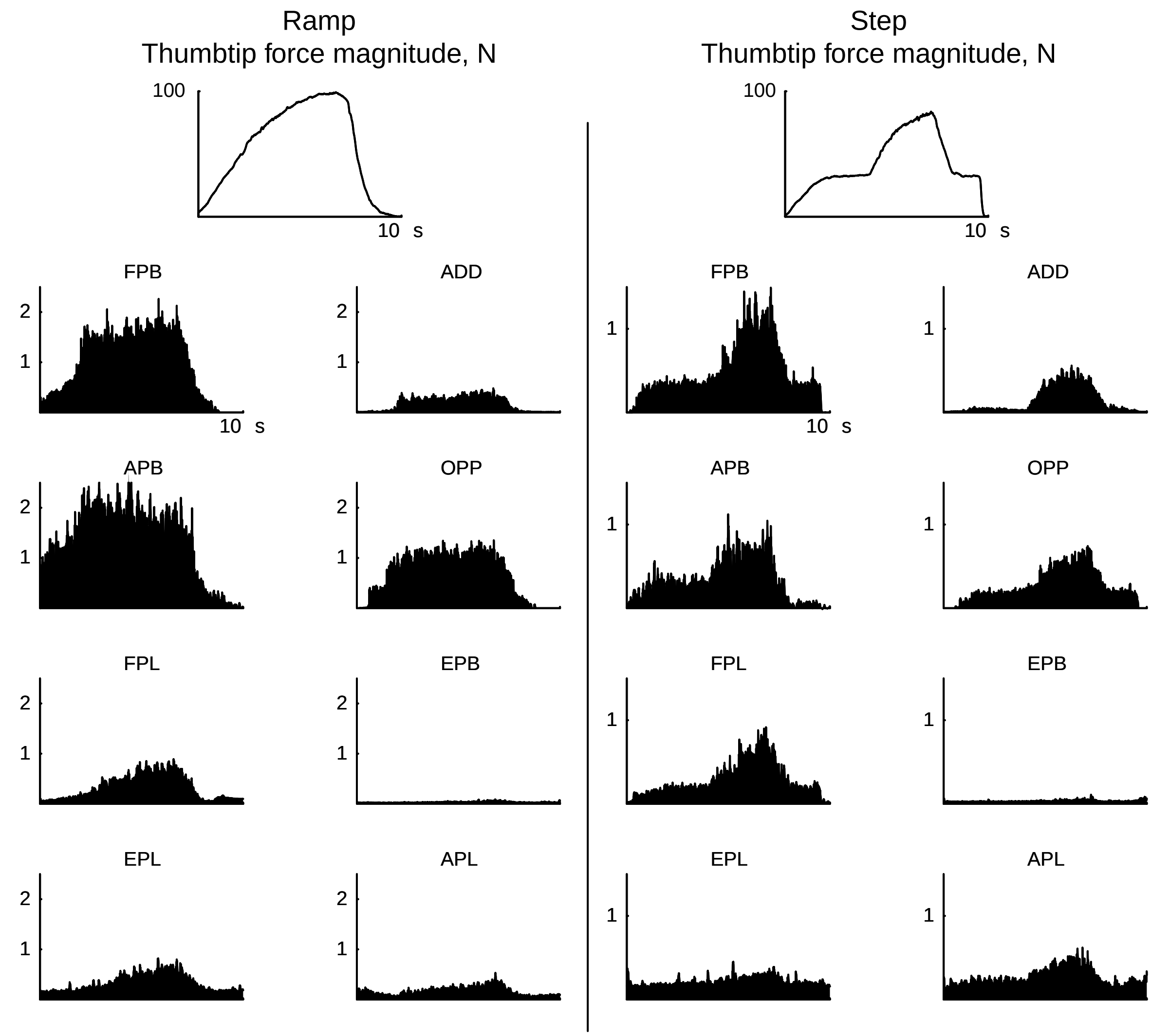

Fig. 2. Representative samples of simultaneous force and EMG recordings for force production in the distal direction in opposition posture for one subject. Participants were instructed to maximize force by ramping to maximal force (ramp trial) and by increasing force in two steps (step trial). In the ramp trials, participants simply increased force at their chosen speed attempting to exceed the 100% target within 10 s. In the step trial, participants targeted their 50% maximum level, proceeded to exceed their previous maximum level, and returned to the 50% level of force. Both ramp and step trials were used because preliminary tests showed individual preference for ramp or step trial to maximize force. For each force direction/thumb posture condition, only the trial with the largest force magnitude was analyzed. Sterile, paired 50 μm wire electrodes with approximately 1 mm recording surface were inserted into flexors pollicis longus (FPL) and brevis (FPB), extensors pollicis longus (EPL) and brevis (EPB), abductors pollicis longus (APL) and brevis (APB), opponens pollicis (OPP), adductor pollicis (ADD) and the first dorsal interosseus (DIO) muscles. Muscle locations were identified by palpation and/or by using monopolar electrodes (Burgar et al., 1997; Johanson et al., 2001). Electrode placement was confirmed using mild electrical stimulation to the target muscle through the wires and by isolated contraction of each muscle. Raw and filtered signals were recorded (band-pass 10–10,000 Hz) and amplified (gain 500–2000). Raw EMG was sampled at 2000 Hz and displayed after each trial to review signals for noise prior to processing. Filtered signals were full-wave rectified and smoothed (50 ms time constant) using custom analog circuits to produce a linear envelope and sampled at 500 Hz. For each participant, the EMG data for each muscle in each trial was that within a 750 ms window centered on peak force as described previously (Valero-Cuevas et al., 1998). EMG data were normalized in each participant for each posture to the highest EMG activity recorded for each muscle within a 750 ms window centered on peak force production in a maximum voluntary contraction in manual muscle testing positions (Kendall and Kendall, 1993) or during thumbtip force production, whichever value was greater. We excluded the DIO muscle from EMG recordings and the model because it adds little to thumb movement and force (Brand and Hollister, 1999; Kaufman et al., 1999), and our EMG recordings have shown activity exclusively with forefinger force production (Johanson et al., 2001).

maximized (equivalent to 10° of misdirection). The first simulation constrained output torque components to $\leqslant 0.05$ N m (a negligible non-zero constraint which is compatible with the experimental conditions). The second simulation did not constrain thumbtip torque. The third Monte Carlo simulation was in the "forward" direction where matrix multiplication calculated the thumbtip output force/torque when EMG was input to the model without applying any constraints. A non-parametric model determined if the predicted activation

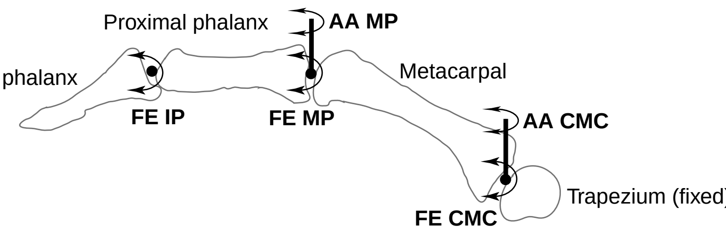

Fig. 3. Kinematic description of the thumb. The kinematics of the thumb were described using 5 hinge-type DOFs with perpendicular and intersecting axes of rotation at the CMC and MP joints, and a single axis of rotation at the IP joint. All flexion-extension axes of rotation were parallel, as were the ad-abduction axes. The radial aspect of a right thumb is shown.

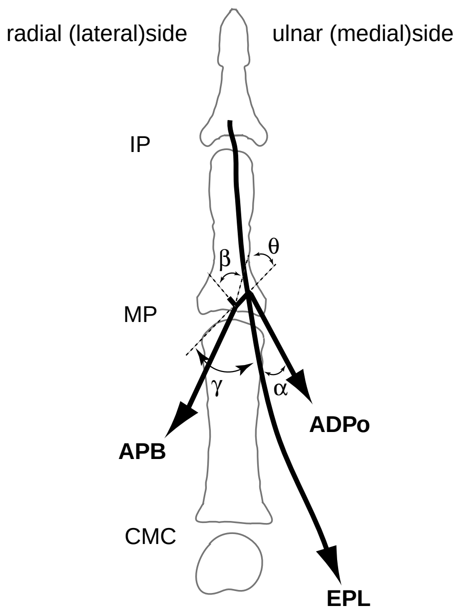

Fig. 4. Extensor mechanism on dorsal aspect of right thumb. Arrows represent the muscles involved, and the angles among them (see Table 1) The extensor mechanism model was based on thumb anatomy (Kendall and Kendall, 1993), cadaver dissections, and personal communications with a hand surgeon (Hentz and Chase, 1999). For a given set of angles, tendon forces are combined as if the mechanism were a flat, floating net (Valero-Cuevas et al., 1998).

range for each muscle was compatible with EMG in each test condition. We required that $\geqslant 50\%$ of EMG data lay within the predicted central 50th percentile. Due to the small number of EMG values, we were conservative to avoid type I errors by requiring that all EMG data lay within the predicted central 90th percentile (Sokal and Rohlf, 1995).

3. Results

The number of valid instantiations in each posture was sufficient for convergence of thumbtip force magnitudes. The mean and coefficient of variance ($100 * \mathrm{SD}/\mathrm{mean}$) of all thumbtip force magnitudes were within 2% of the final mean and coefficient of variance, respectively, for the last 10% of valid instantiations (Table 2) (Fishman, 1996). An instantiation was considered valid if it resulted in non-zero thumbtip forces in all five directions, and the Euclidean magnitude of the palmar, dorsal, lateral and medial forces normalized by the distal force were within the range seen experimentally.

The first inverse simulation produced unrealistically low thumbtip force magnitudes in both postures. The model consistently underestimated the magnitude of maximal thumbtip force by a mean ratio of 4.1 ± 2.9 (Fig. 5, Tables 2 and 3). The predicted distribution of activation levels were compatible with EMG measurements in 40 out of 80 muscle activations studied ($8 \times 5 \times 2$: eight muscle excitations in each of 5 force directions in each of two postures; Fig. 6). Activity in $\geqslant 5$ muscles was compatible with EMG in only three force directions (palmar, distal and ulnar directions for key posture). All inverse simulations produced thumbtip forces directed within 10° of the desired direction because of the constraints imposed.

The second inverse simulation (unconstrained thumbtip torque) predicted higher thumbtip force magnitudes than the first simulation, but still predicted unrealistic coordination patterns for all directions in both postures. The ratio of measured to predicted thumbtip force magnitudes 1.96 ± 1.28. The predicted distribution of activation level was statistically compatible with EMG measurements in 29 out of 80 muscle activations studied. Predicted muscle activity was compatible with EMG in 5 out of 8 muscles only for the medial force direction in opposition posture. The average magnitude of the thumbtip torque was $0.64 \pm 0.28\,\mathrm{N\,m}$, which is an unrealistic amount because the thimble worn by the participants precluded the production of thumbtip torque.

The third simulation (forward method) predicted thumbtip force magnitudes comparable to the second simulation, but the thumbtip force vectors were misdirected and accompanied by unrealistically high thumbtip torques. The ratio of measured to predicted thumbtip force magnitudes was 2.32 ± 1.82. On average, thumbtip force vectors were deviated $74.3 \pm 24.5^\circ$ from the desired direction, and the accompanying average thumbtip torque was $1.32 \pm 0.95\,\mathrm{N\,m}$ (Table 2).

Table 2
Results summary

		Modeling approach		
Methods	Type	Inverse	Inverse	Forward
	Technique	Linear programming	Linear programming	Matrix multiplication
	Goal	Maximize thumbtip force	Maximize thumbtip force	Calculate thumbtip force
	Stochastic variables	Musculoskeletal parameters	Musculoskeletal parameters	Musculoskeletal parameters and EMG inputs
	Constraints	Force direction and fingertip torques	Force direction only	—
Predictions	Min. valid sols. per posture	1620	2250	2460
	Convergence	Within 2%	Within 2%	Within 2%
	Fingertip force magnitude	Unrealistically low	OK	OK
	Force direction	OK	OK	Very misdirected
	Fingertip torques	OK	Unrealistically high	Unrealistically high
	Coordination patterns	Unrealistic	Unrealistic	—
Possible model flaw	Kinematic model	Yes	Yes	Yes
	Solution method	Yes	Yes	No
	PCSA	Yes	No	No

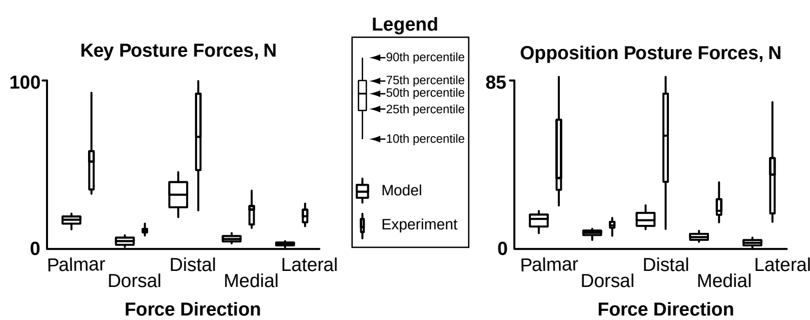

Fig. 5. Comparison of maximal thumbtip force distributions in each direction for both postures. The maximal voluntary thumbtip forces measured in the participants are shown in the narrow gray box plots. The maximal predicted thumbtip forces from the valid solutions from the first inverse Monte Carlo simulation are shown in the wide white box plots. Note that the predicted maximal thumbtip forces were lower than the thumbtip forces measured in the subjects.

4. Discussion

This study evaluated the validity of a 5-axis, 8-muscle biomechanical computer model of the thumb by comparing the predicted ranges of maximal static force production and muscle activity to experimental measurements of maximal voluntary thumbtip force and EMG. We will argue that, when taken together (Table 2), our results suggest that the musculoskeletal parameters and solution methods are sound; but the chosen kinematic description may not represent the transformation of net joint torques into thumbtip forces/torques in the anatomical thumb. We do not argue that the model's predictions would become entirely realistic if we used an alternative, perfectly realistic kinematic model. Rather, we conclude that, in this particular model of the thumb, the kinematic description appears to be the dominant factor in preventing realistic predictions of isometric force production and the coordination patterns that achieve them.

The choice of individual musculoskeletal parameter values is not the likely reason for the underestimation of thumbtip force or discrepancies in coordination patterns. Monte Carlo simulations explicitly calculate the sensitivity of model predictions to parameter variability and uncertainty, and mitigate the limitations associated with adopting average or subject-specific musculoskeletal parameters (Fishman, 1996). Because all simulations converged, running additional iterations (i.e., different parameter values) would not change the distribution of the thumbtip forces reported here.

Table 3
Measured thumbtip force magnitudes and predicted magnitudes for first Monte Carlo simulation (N)

Direction	Key posture			Opposition posture		
		Mean	SD		Mean	SD
Dorsal	Experiment	11.0	2.2	Experiment	11.5	2.7
	Model	4.7	2.6	Model	7.7	2.1
ratio Exp:Model		2.3			1.5	
Palmar	Experiment	51.9	20.4	Experiment	47.8	27.2
	Model	16.9	3.7	Model	14.1	4.1
ratio Exp:Model		3.1			3.4	
Distal	Experiment	65.0	27.9	Experiment	56.0	34.1
	Model	32.6	10.3	Model	15.1	4.8
ratio Exp:Model		2.0			3.7	
Medial	Experiment	21.3	7.8	Experiment	20.7	6.9
	Model	6.2	2.4	Model	6.1	2.2
ratio Exp:Model		3.4			3.4	
Lateral	Experiment	19.5	4.8	Experiment	36.6	21.5
	Model	3.0	1.4	Model	3.1	1.9
ratio Exp:Model		6.6			11.7	
Mean Exp:Model		3.5			4.7	

The underestimation of thumbtip force and discrepancies in coordination patterns in the first inverse simulation could result from inappropriate PCSA values, solution method, and/or kinematic description (Table 2). PCSA values set the baseline strength of the model, and affect the prediction of coordination patterns by specifying relative muscle strengths. Because PCSAs are generally measured from specimens belonging to older individuals, they likely underestimate the thumb strength of the young participants we studied. This may explain some "weakness" in biomechanical models (Valero-Cuevas et al., 1998), but it is unlikely that it would explain force under-prediction of a factor of 4, or the discrepancies of the predicted coordination patterns. PCSA values may, nevertheless, be adequate because the other simulations produced higher thumbtip forces. As argued previously (Valero-Cuevas et al., 1998), we do not feel justified in increasing the value for maximal muscle stress from $35.4\,\mathrm{N/cm^2}$ because this is already the larger of the two generally accepted (Close, 1972; Brand et al., 1981; Powell et al., 1984; Zajac, 1989) (the other being $22.5\,\mathrm{N/cm^2}$). For recent detailed reviews supporting this range of values see (Zajac, 1989; Lieber, 1992; Brown et al., 1998).

The kinematic description specifies the transformation of net joint torques into thumbtip forces/torques (Yoshikawa, 1990). Thus, an inappropriate kinematic description could contribute to both the underestimation of thumbtip force and discrepancies in coordination patterns of the first simulation. Removing the constraints on the thumbtip torque in the second simulation doubled the magnitude of the thumbtip forces and produced unrealistically large thumbtip torques suggesting that the model is not inherently weak. Agreement between measured to predicted force magnitudes (i.e., a ratio of 1) is already within ± 0.75 SD of the mean ratios for the last two simulations, and can be further improved by doubling PCSA values—a reasonable adjustment compatible with weakness in older adults (Mathiowetz et al., 1985).

All Monte Carlo simulations have the limitation that assuming parameter independence can broaden the predicted distributions. This increases the likelihood of false-positive matches with the experimental data because we were, in fact, simulating a wider variety of thumbs than are likely to exist in reality. Additional limitations include: The moment arms of Smutz et al. (1998), and the ranges we used (based on their reported standard deviations), should not be taken as definitive as they note their data do differ at times from other reports of muscle moment arms. We assumed the extensor mechanism apportions tendon tensions by acting as a floating net (as in Valero-Cuevas et al., 1998) were unaffected by thumb posture. We also approximated the fan-shaped ADD muscle as a single line of action. Variability in the experimental muscle coordination patterns was most likely due to the force–EMG relationship that can change with different muscles, force magnitude, muscle fiber type (Lawrence and De Luca, 1983; Basmajian and De Luca, 1985) and excitation history (Burke et al., 1976; Zajac and Young, 1980; Bigland-Ritchie et al., 1983). Although EMG artifacts and possible cross-talk cumulatively can increase signal variability, cross-talk from wire

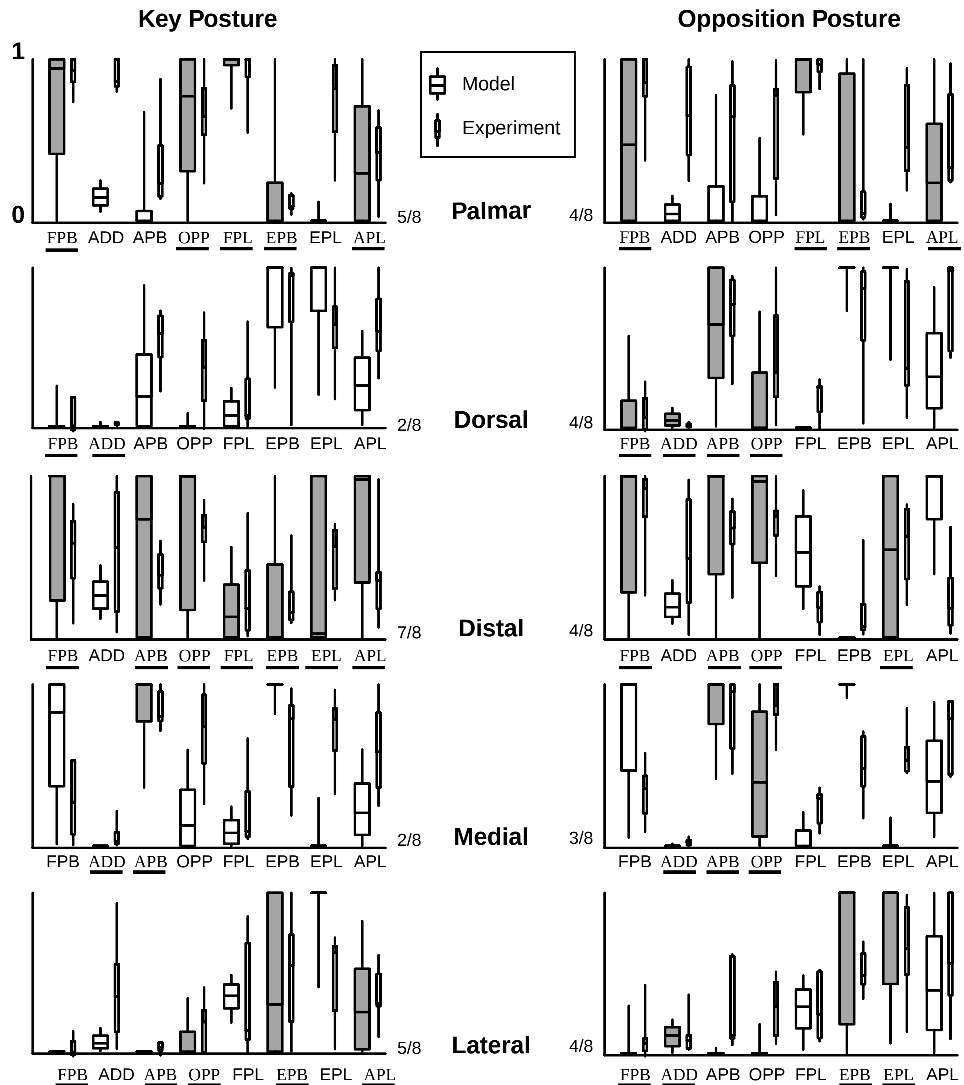

Fig. 6. Comparison of distributions of activation levels during maximal thumbtip force production in each direction for both postures. The normalized EMG during maximal voluntary thumbtip forces measured in the participants is shown in the narrow gray box plots. The maximal predicted thumbtip forces from the valid solutions from the first inverse Monte Carlo simulation are shown in the wide white box plots. The fraction next to each force direction indicates the number of muscles for which the predicted distribution includes the measured EMG, and the matching muscles have their labels in bold. We used a non-parametric statistical test to determine if the predicted activation range for each muscle was compatible with EMG for each force direction at each posture. To accept compatibility with 90% confidence, we required that ⩾50% of EMG data lay within the central 50th percentile of the predicted distribution, and all EMG data lay within the central 90th percentile.

electrodes has been reported to be insignificant at around 2% of their maximal value (Solomonow et al., 1994). To control for intersubject variability, all of the EMG signals were normalized within each posture since joint position has been shown to have an effect on EMG magnitude (Onishi et al., 2002). Regarding the advantages and limitations of LP, this optimization method predicts the maximal possible output of linear systems because it finds the system's boundary of performance (Chvátal, 1983). The coordination patterns predicted by LP reflect the mechanical consequences of the model and state the muscular interactions necessary to maximize well-directed thumbtip forces. If anything, LP tends to overestimate thumbtip force because we assumed independence of muscle activations and placed no constraints on muscle activation other than the production of well-directed thumbtip force. Reformulating the optimization to include possible, but not currently known, muscle synergies could only weaken the model further. Similarly, alternative non-linear cost functions or optimization methods would affect the coordination patterns predicted, but could not improve upon the force magnitudes found here. The limitations of LP to predict realistic coordination patterns are related to conjectures from EMG studies that thumb muscle may at times act to stabilize joints via co-contraction instead of contributing to output force (Chao et al., 1989). In contrast, LP assumes all muscle activity optimally contributes to the output force. Even if subjects did co-contract to stabilize joints, this would not imply the system is not linearizable or solvable with LP. Rather, it would mean the thumb has additional DOFs, such as sliding at the incongruous CMC joint, whose control may depend on joint configuration and active/passive loading—much like the knee. If such DOFs were present, kinematic descriptions using fixed hinge-type joints would be inappropriate to describe the interactions among joint contact geometry, passive structures, muscle forces and thumbtip forces/torques. Non-linearities in the transmission of tendon tension are also possible.

The third (forward) and last simulation suggests that LP was not responsible for the model's underestimation of thumbtip force and the discrepancies in coordination patterns. The results of the forward simulation again suggested that PCSA values are likely appropriate because the model was able to produce thumbtip forces within a factor of 2 of the experimental values. Moreover, both the direction of thumbtip forces and the magnitude of the thumbtip torques were unrealistic (Tables 2 and 3). These results, together with the first two simulations, strongly suggest the adopted kinematic description does not accurately represent the transformation of muscle forces to thumbtip output in the human thumb. All available kinematic descriptions of the thumb idealize articulations as invariant hinge-type joints (Cooney and Chao, 1977; Chao and An, 1978; Giurintano et al., 1995), but it is conceivable that in vivo muscle forces affect thumb kinematics and that more elaborate descriptions may be necessary to replicate the biomechanical complexity of articulations.

In light of our results, future efforts to create realistic biomechanical computer models of the thumb should explore alternative kinematic descriptions. In this study we used a straightforward 5-DOF kinematic description in the spirit of Occam's Razor, and because experimental moment arm data compatible with this description exist (Smutz et al., 1998). An inverse model of the thumb using a more elaborate 5-DOF description with non-orthogonal and non-intersecting axes (Giurintano et al., 1995) found coordination patterns for palmar force in the key posture that were less compatible than our predictions. In our model, 5/8 muscles agreed with our EMG data vs. 2/8 muscles in theirs. However, it is unclear how the choice of optimization method, musculoskeletal parameters, and/or kinematic description in their model affected their results. The lack of DIO in our model is immaterial to this comparison because DIO was inactive in their prediction. Future work should explore how the number, location, orientation and type of DOFs affect the biomechanical predictions of mechanical output and the muscle coordination that achieves it in the presence of parameter variability.

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