Machine Learning for Musculoskeletal Modeling of Upper Extremity

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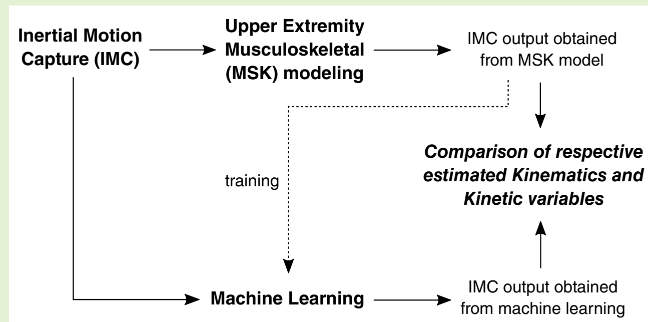
***Abstract*—We propose a novel machine learning (ML) driven methodology to estimate biomechanical variables of interest traditionally obtained from upper-extremity musculoskeletal (MSK) modeling. MSK models facilitate personalized modeling, performing 'what-if' analyses, and potentially enhance clinical decision-making. In certain settings, MSK models are driven by Inertial Motion Capture (IMC) data. IMC systems are portable, user-friendly, relatively affordable, and provide additional biomechanical information. However, MSK models can be computationally expensive, often require extensive data, and can be prohibitively slow in making real-time predictions.**



Our ML method—involving a rigorous hyperparameters search—predicts kinematic and kinetic biomechanical information associated with human upper-extremity movements solely using IMC input data, thereby bypassing MSK models. The scaled cadaver-based MSK model was based on the Dutch Shoulder Model and the spine model implemented in the AnyBody Managed Model Repository. We employ Neural Networks, which are trained on IMC data obtained from five non-disabled subjects in *Subject-exposed (SE)* settings (at least a trial from all subjects is used in training) and *Subject-naive (SN)* settings (no information from test subjects is used in training). We compare the predictions of our ML model with that of an MSK model and find an excellent agreement in SE settings (average *Pearson's* $r = 0.96$, *Normalized RMSE (NRMSE)* $= 0.23$) and strong correspondence in SN settings (average $r = 0.89$, *NRMSE* $= 0.45$). Linear Model performed poorly for SN settings, which motivated a more complex ML model. Our findings suggest that an ML-based approach is highly viable for estimating upper-extremity biomechanical information solely from IMC data.

***Index Terms*—Biomechanical Analysis, Inertial Motion Capture, Linear Models, Machine Learning, Motion Analysis, Musculoskeletal modeling, Neural Networks, Upper Extremity.**

I. Introduction

Computational musculoskeletal (MSK) models have enabled non-invasive estimation of *in vivo* information (e.g., joint and muscle loading) to further improve our understanding of the MSK system [1]–[3]. Several commercial and open-source software like AnyBody™ Modeling System [4], LifeMod [5], OpenSim [6], SIMM [7] offer MSK model construction, simulation, and analysis capabilities. An *inverse dynamics* approach is the most suitable method for estimating *in vivo* information, such as joint and muscle loading, via MSK models due to its robustness and computational efficiency [1], [8]. However, *a priori* knowledge of involved motions is a pre-requisite for inverse dynamics. Experimental motion capture (mocap) information—along with subject-specific scaling data—can be used as inputs to MSK models, or joint angles calculated outside of the MSK modeling framework (e.g., AnyBody™ Modeling System [4] or OpenSim [6]) can be utilized to perform further calculations [6], [9]. However, MSK models are often computationally expensive and require extensive mocap input [1], [10]. Furthermore, commercial MSK modeling software licenses could be prohibitively expensive for users in certain contexts, and some open-source packages might be limiting in terms of applications and/or features. Currently, MSK models are typically laborious and too time-consuming to create, scale, and set up individually. They suffer from computational complexity and implementation difficulties that prohibit the routine use of this technique in clinical settings and limit its use to research environments [1]. Finally, despite the ability to assess *in vivo* information during functional activities, there is little evidence showing the use of MSK modeling as a tool for patient care and clinical decision-

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making [1], [10], [11]. Notably, most clinical applications appraised by Smith et al. [10] deal with the lower extremity, and very few instances correspond to upper extremity. Besides, there are still many barriers to the routine adoption of MSK modeling in a clinical setting.

Compared to clinical gait analysis, motion analyses involving the upper extremity have been limited by numerous issues, e.g., the complexity of movements involved, methodological variability, and a lack of consensus/standardization thereof [12]–[14]. There is a multitude of research and commercial mocap systems available that can help perform upper-extremity motion analyses [13], [15], [16]. These movement tracking systems consistently update spatiotemporal information about human movements in an accurate and reproducible manner. However, each tracking method has its own pros and cons [13], [15]. Amongst these methods, marker-based Optical Motion Capture (OMC) system seems to be particularly suitable for upper-extremity motion analysis, and is widely considered the 'gold standard' for mocap since they are non-invasive, have high accuracy, and do not generally influence task execution [13]. However, OMC systems with passive, retro-reflective markers are limited by marker occlusion, high cost, lengthy setup and post-processing times, as well as being confined to specialized laboratory environment (causing associated limitations due to measurement volume) [16]. On the contrary, an Inertial Motion Capture (IMC) system is relatively portable and cost-effective, user-friendly, and provides full-body measurement capabilities in a 'field condition' but might not be as accurate as OMC data [15], [17]. Nevertheless, this 'field ready' option is desirable in outdoor/real-world applications (e.g., sports, ergonomics) as well as low-resource settings. The Full-body Sensor Network IMC system provides unprecedented ease-of-use, high-quality data (in near-real time), and requires short setup time. The same ease of use translates to setting up the MSK modeling pipeline driven by the IMC data. Compared with OMC data capture, this approach saves time to palpate bony landmarks skillfully for marker placement as well as cumbersome post-processing of markers or lost data.

Inverse-dynamics-based MSK models have traditionally been driven by OMC data [4], [6], although recent studies have demonstrated the utility of IMC data using a Full-body Sensor Network for popular MSK modeling platforms such as AnyBody™ and OpenSim [17]–[21]. Notably, studies have either involved Full-body Sensor Networks [18], [20], [22], [23] or a few inertial measurement units [24], [25]. Using a Full-body Sensor Network allows incorporating assumptions of biomechanical models and applications of sensor fusion algorithms that lead to more accurate kinematics estimation [26]; the disadvantage being, it could limit some applications for real-time and ambulatory use compared to utilizing single/few inertial measurement unit(s). While IMC data are cost-effective to obtain, using the standard MSK model to estimate *in vivo* joint and muscle loading information is computationally expensive. Besides, the development of user-friendly computational tools has been recommended as vital to supporting clinical applications, wherein such tools might combine existing algorithms and MSK models and make them accessible to a broader group of users [1]. It has led to searches for alternative models that are faster and more user-friendly [27]. The use of supervised ML methods in human motion analysis [28], [29], and to bypass an MSK model [30], [31] show that ML methods can augment and sometimes replace standard computational techniques.

In biomedical engineering, the use of supervised models, including neural networks (NNs), to bypass computationally expensive optimization problems [11] has become commonplace, e.g., estimating deformable joint contact [32], implant pressure distribution [33], estimating vertical ground reaction forces [24], estimating joint forces [34] and moments [35], and applications in gait analysis [36], [37]. Such ML methods have advantages over MSK models: (i) they are computationally efficient; and (ii) while the initial training of the network takes time, prediction on new data is efficient since it just involves a forward pass through an NN. In addition, advancements in the field of ML can reduce the size of training data required. Moreover, supervised ML methods allow flexibility and can help gain population-level insights [38] (e.g., for product design or ergonomics), in contrast to methods based on independent trials, such as traditional inverse dynamics or static analysis. Also, such models facilitate real-time applications where accuracy and efficiency are a priority.

Numerous other studies have reported the use of ML in the estimation of *in vivo* joint and muscle loading information from either OMC or IMC data [30], [34], [38]–[48]. There is no one-size-fits-all ML architecture; earlier literature relied on simple perceptron and two-layer NN architectures [49]–[51] while convolutional NNs are the predominant paradigm in recent literature. The use of approaches such as Long Short-Term Memory (LSTM) networks that outperform convolutional NN in certain settings [52] has become more prevalent. While ML has proven useful, such techniques require a methodological thoroughness to ensure model reliability and robustness of results, e.g., undertaking a thorough hyperparameters space search, performing cross-validation while reporting results on a held-out test, and comparing with other ML or simpler models, such as generalized linear models.

Literature suggests that ML applications in upper-extremity biomechanical modeling are more limited than those in the lower extremity. This might be because, generally, research on upper-extremity biomechanics has lagged compared to its lower-extremity counterpart [12], [13]. Better modeling of upper-extremity biomechanics is crucial because upper-extremity movements are integral to interacting with the external environment and undertaking a majority of activities of daily living. In addition, there is a growing need to take objective MSK model-based analysis from 'lab to field' [29], [53]–[55], and relatively few studies have been performed involving the human upper extremity. Our work aims to address both these gaps by providing an efficient predictive NN model to replicate the outcome of a computationally expensive MSK model. The rest of the paper is organized as follows. In Section II, we describe our biomechanical dataset, ML methodology, and NN architectures. In Section III, we describe our results. In Section IV, we discuss our ML outcomes and conclude with future directions in Section V.

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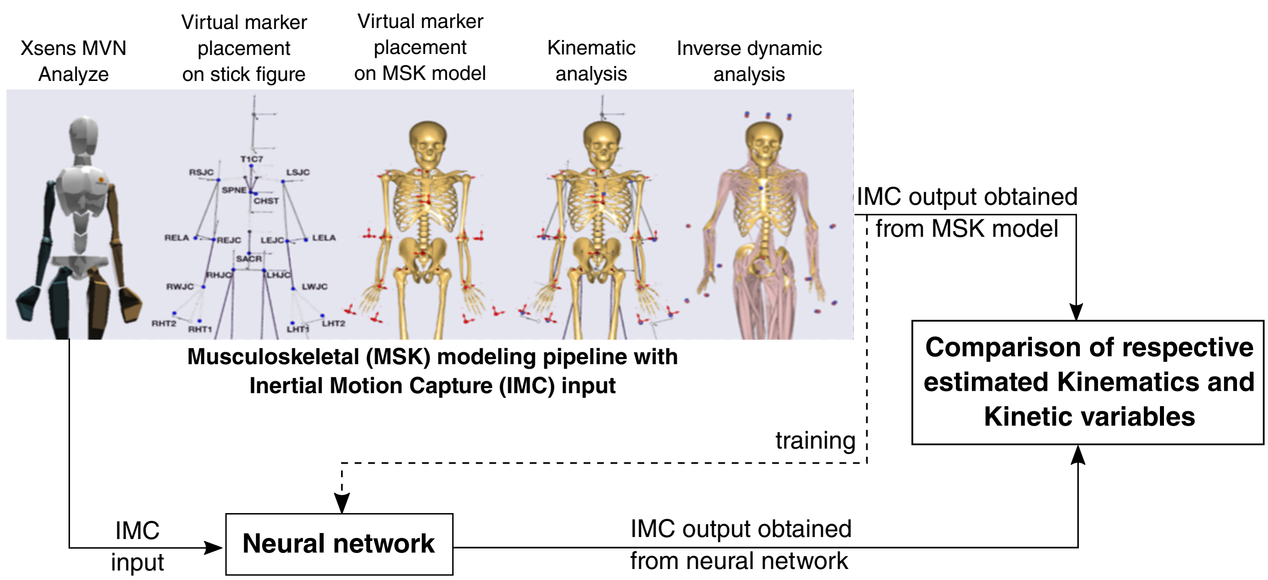

Fig. 1. Pipeline for machine learning for musculoskeletal modeling of upper extremity; image adapted from [18], [19].

II. Materials and Methods

A. Data

The anonymized dataset used here is from an earlier study [19], which was approved by the local Research Ethics Committees (Reference number: 16/SC/0051 and Reference number: 14/LO/1975). In that study, five male, non-disabled adults (Age: 22.80 $\pm$ 0.84 years; Height: 1.75 $\pm$ 0.07 m; Weight: 66.25 $\pm$ 9.72 kg; Body Mass Index: 21.79 $\pm$ 3.49 kg/m^2) had consented to participate.

IMC data capture (sampling frequency: 60 Hz)—for three trials of the Reach-to-Grasp task in the *Forward* direction executed at a self-selected pace—involved a Full-body Xsens MVN Awinda Station with 17 sensors (Xsens Technologies B. V., Enschede, the Netherlands). IMU sensors were placed on the participants' body segments following the recommended protocol from the Xsens MVN User Manual [26]. Besides, IMU setup and calibration also was based on the recommended protocol from the Xsens MVN User Manual [26]. A custom-built apparatus (Supplementary Figure 1) was developed that could be adjusted to suit the anthropometric requirements of different participants and facilitate the execution of the *Reach-to-Grasp* task. The task involved the participant reaching to grasp a 'dumbbell-shaped' object and moving it between various pre-defined points as instructed. The pre-defined *'Front'* point was within 90% of an individual's arm length (i.e., acromion to middle-fingertip length, with the arm hanging down) to minimize the contribution of trunk movement for task execution [56]. Participants performed the task in a seated position on a height-adjustable chair located behind a height-adjustable table with the test apparatus placed on top.

Detailed instructions and a couple of practice sessions were provided for each subject before data collection. First, a calibration sequence was performed for the IMC mocap system, which involved the participants standing in a neutral posture (N-pose) and walking a few steps forward and back to the starting position. This was followed by three trials of the Reach-to-Grasp task with the subject's dominant hand at a self-selected pace. Execution of the task involved moving the hand from the *'Start/End'* position to grasp the 'dumbbell' shaped object from the *'Middle'* block and placing it the *'Front'* block, then without letting go of the object, the hand would follow the same instructions/path in the return phase, and then the hand would return to the *'Start/End'* location. For each trial, the identification of 'start' and 'end' frames (hand leaving and returning at the 'Hand Start/End' position) was performed through a threshold analysis.

The affiliated Xsens MVN Analyze software [57] was used to capture the IMC data and export it in BioVision Hierarchical data (.BVH) file format [26] to be used as inputs for MSK modeling where a stick-figure model was initially reconstructed. Subsequently, scaled cadaver-based upper-extremity MSK modeling was carried out using AnyBody$^{\mathrm{TM}}$ Modeling System (AnyBody$^{\mathrm{TM}}$ Technology A/S, Aalborg, Denmark) with the IMC input mocap data and subject-specific anthropometric scaling dimensions [18], [23]. The *'Inertial MoCap model'* in the AnyBody Managed Model Repository (AMMR) v.2.1.1 was adapted to calculate the kinematic (i.e., Joint Angles) and kinetic (i.e., Joint Reaction Forces, Joint Moments, Muscle Forces, and Muscle Activations) variables of interest. The raw data were filtered using a fourth-order, zero-lag, low-pass Butterworth filter with a cut-off frequency of 6 Hz within the AnyBody$^{\mathrm{TM}}$ Modeling System.

The MSK system is assumed to be a rigid body, and only a unilateral (right-handed) upper-extremity body model is considered. The upper extremity is divided into the torso, scapula, clavicle, upper arm, radius, ulna, and hand. Model scaling and segment tracking were performed using markers and anthropometric dimensions per the scaling algorithm by Andersen et al. [58] for the static trial (also called the calibration trial). Tracking for subsequent dynamic trials was performed using an algorithm developed by Andersen et al. [59]. The right-hand MSK model adapted here had 52 degrees of freedom and 135 muscle actuators and was based on an implementation of the Dutch Shoulder Model [60] and the spine model [61]. The 'muscle-tendon' simulation was based on the simple muscle model in AnyBody^{TM} Modeling System, which assumes a constant strength of the muscle regardless of its working conditions [62]. The muscle recruitment problem was solved by the default third-order polynomial criterion [4] as generally, it is a good compromise between different recruitment criteria [62].

Readers interested in any further methodological details are directed elsewhere relevant to the: experimental set-up [23], instructions for task execution [23], calibration [26], sensor placement [26], data capture [19], [23], anthropometric measurements [19], [23], [26], data processing [18], [19], [23], MSK modeling [18], [19], [23], etc. In contrast with an earlier similar study solely involving MSK modeling with OMC input [23], the weight of the grasp object ('dumbbell'; used in the Reach-to-Grasp task) was considered to be a point object with negligible mass in the current MSK output involving the IMC data [19]. Notably, this assumption does not affect objectives of the current study. The IMC data, along with the corresponding MSK model predictions of kinematic and kinetic quantities, were used as data for our ML endeavors.

In human movement analysis, demographic and anthropometric characteristics such as age, height, body weight, and gender have been found to influence the amplitude of the kinematic and kinetic variables. If left uncorrected, individual differences may act as confounding factors [63], [64]. Thus, the kinetic outcome variables were reported per the recommendations by the International Society of Biomechanics on the reporting of intersegmental forces and moments during human motion analysis [64]. Accordingly, the joint reaction force and muscle forces values were normalized to the corresponding subject's body weight, and expressed as a percentage of body weight to facilitate inter-individual comparison [65]. The joint moment values were normalized to the corresponding subject's body weight times height and were expressed as a percentage of body weight times body height. This approach was adopted since the 'body weight times height' normalization method was found to be more effective than the 'body weight' normalization method at reducing gender-based differences [63]. The sign convention for the joint angles was – Flexion (Fl), Forward bending (Fb), Abduction (Ab), Right bending (Rb), Radial deviation (Rd), and Internal rotation (Int) are positive (+ve); Extension (Ex), Backward bending (Bb), Adduction (Ad), Left bending (Rb), Ulnar deviation (Ud), and External rotation (Ext) are negative (-ve).

B. Supervised learning

In the field of MSK modeling, recent studies [30], [34], [41] have shown the utility of using NN architectures in bypassing MSK models. We build upon these works on bypassing MSK modeling platforms to obtain equivalent MSK model outputs solely from IMC data for the human upper extremity (Figure 1). In this article, the IMC data comprises 15 trials (i.e., three trials of Reach-to-Grasp task each obtained from five subjects) with 483 input features [26] while the five IMC-driven MSK outputs considered contain several time-series arrays – ten for joint angles, twelve for joint reaction forces, ten for joint moments, four for muscle forces, and four for muscle activations. We train different ML models for each of the kinematic and kinetic outputs. We apply the following feature transformations before training the model:

1) The time column is normalized between 0 and 1 and represents the fraction of the total time elapsed for the task execution (carried out at a self-selected pace). This captures the temporal aspect of MSK analyses.
2) During MSK modeling, the muscles are discretized into several muscle bundles. In the MSK model outputs, we obtain 21 features corresponding to these bundles for muscle forces and muscle activations for the four muscle groups considered, i.e., a) Pectoralis major (Clavicle part), b) Biceps Brachii, c) Deltoid (Medial), and d) Brachioradialis [23]. The 'maximum envelope' of the tendon forces of selected bundles constituting a particular muscle was identified for analysis. In AnyBody^{TM} Modeling System, muscle activation is a ratio of muscle force to its strength [62]. We reduced muscle forces and activations into the following four groups by taking the maximum envelope of the muscle forces and muscle activations values of the corresponding bundles – a) five features for Pectoralis major (Clavicle part); b) two features for Biceps Brachii; c) six features for Deltoid (Medial); and d) two features for Brachioradialis [23].

Guided by the Occam's Razor principle, we begin our ML analysis by considering linear models first before deploying more complex representations such as NNs. We consider different hyperparameter choices (in initialization, optimizer, batch-size, learning rate, and epochs) for linear models. We found that such linear models perform 'moderately' to 'strongly' (see Subsection II-D) for *subject-exposed* (SE) models and moderately for *subject-naive* (SN) models in terms of Pearson's correlation coefficient (r), while the normalized root mean square error (NRMSE) for such linear models were large, particularly, for SN models (as shown and discussed in Table II as well as Sections III and IV).

Therefore, we concluded that more complex ML models are required. We have used a feed-forward backpropagation architecture of NN (with NRMSE as the cost function) and have used validation accuracy to tune network hyperparameters performing an exhaustive search in the space of choices (144,342 in total) for weight initialization, optimizer, batch-size, epoch, activation function, number of nodes, hidden layers, learning rate, and dropout probability as listed in Table I. We do not use any activation in the final layer of our NN architectures. A typical schematic diagram of NN used in this work is shown in figure 2 which contains I input units, O output units, and N hidden layers each with k neurons.

C. Validation and train-test split

To validate ML models two approaches are commonly used: *subject-exposed* (SE) and *subject-naive* (SN) [30]. In SE setting, the trials of all subjects are pooled together, and a train-test split is performed on the trials such that each subject in the test set has at least one trial in the training set. This approach usually performs better than the SN setting, where a subject is either in training or test data, but not both. While the

Output	Weight initialization	Optimizer	Batch size	Epoch	Activation function	Number of nodes	Hidden layers	Learning rate	Dropout probability
Hyperparameters space explored									
	Xavier normal	Adam	64	50	ReLU	200 to 2000	1, 2, 4,	0.001	0
	Random normal	SGD	256	100	tanh	in steps of 200	6, 8, 10	0.005	0.2
	He normal	RMSProp	1028	200	sigmoid			0.01	0.4
Optimal hyperparameters in Subject-exposed settings									
Joint angles	Xavier normal	Adam	256	200	ReLU	1400	2	0.001	0.0
Joint reaction forces	He normal	Adam	256	50	sigmoid	1400	4	0.001	0.0
Joint moments	Random normal	Adam	64	50	sigmoid	1800	2	0.001	0.2
Muscle forces	Xavier normal	Adam	1028	200	sigmoid	800	4	0.001	0.0
Muscle activations	Xavier normal	Adam	1028	200	ReLU	1200	6	0.001	0.0
Optimal hyperparameters in Subject-naive settings									
Joint angles	Xavier normal	Adam	64	100	ReLU	1200	2	0.001	0.0
Joint reaction forces	Xavier normal	Adam	256	50	ReLU	1400	2	0.001	0.0
Joint moments	Xavier normal	Adam	256	200	sigmoid	800	2	0.001	0.2
Muscle forces	Random normal	Adam	1028	50	sigmoid	1800	2	0.001	0.2
Muscle activations	Random normal	Adam	1028	200	tanh	1400	6	0.001	0.0

TABLE I

HYPERPARAMETERS SPACE EXPLORATION (144,342 COMBINATIONS) FOR THE NEURAL NETWORKS AND OPTIMAL HYPERPARAMETERS FOR VARIOUS OUTPUT CATEGORIES IN SUBJECT-EXPOSED AND SUBJECT-NAIVE SETTINGS.

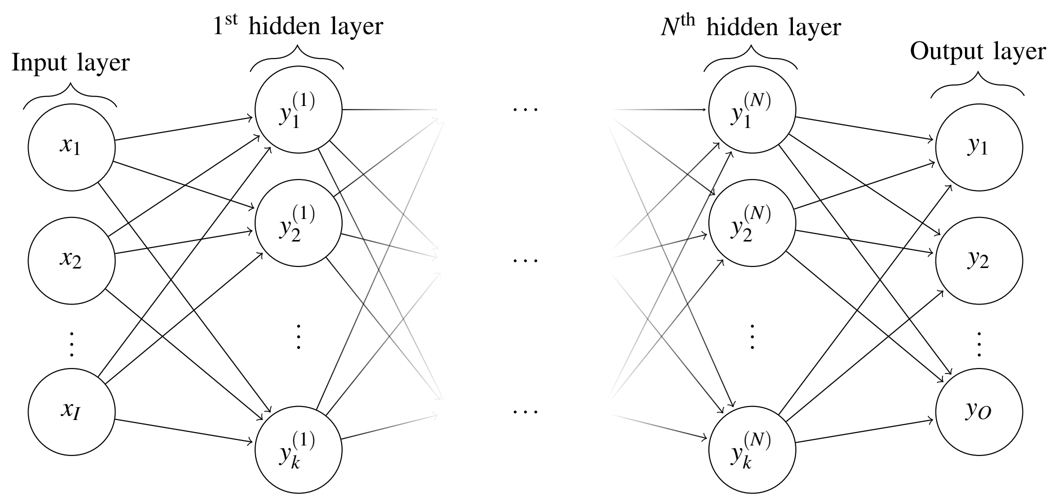

Fig. 2. Typical schematic diagram for a feed-forward backpropagation Neural Network with I input units, O output units, and N hidden layers each containing contains k neurons. The input and output layers are considered as 0^{th} and $(N+1)^{\text{th}}$ layers.

performance is better, SE model has the disadvantage of being a subject-specific model and does not generalize well [34]. In the SE case, for train-test split, we have randomly selected two trials in the test set and the remaining trial in the training set. For hyperparameter tuning, we perform cross-validation by randomly splitting the remaining trials into validation (two trials) and training set (11 trials). While in the SN case, one of the subjects was randomly selected as the test subject and the remaining subjects as the training data. Subsequently, we performed cross-validation, randomly selecting one subject as validation data, while the rest as training data.

D. Error metrics

We use NRMSE as our primary error metric which is defined as RMSE divided by the standard deviation of the variable in the dataset. NRMSE allows the comparison of RMSE for various variables with different scales and units. For NRMSE, the ground truth is the output obtained from MSK modeling driven by the IMC data. Furthermore, we have also provided RMSE values (with units) in supplementary Table 1. Additionally, we also use Pearson's correlation coefficient r between MSK model and linear model or NN-predicted output as a secondary measure with the standard interpretation [66] for r: *weak* ($r \leq 0.35$), *moderate* ($0.35 < r \leq 0.67$), *strong* ($0.67 < r \leq 0.90$), and *excellent* ($r > 0.90$).

III. RESULTS

The average NRMSE and r values for predicting test data using linear models and NNs in both SN and SE settings are listed in Table II. These values are listed for each of the output categories, and an average is taken over all output features in that category). Linear models approximated the underlying function for the MSK model very well in SE settings with average correlation, $r_{\text{avg}} = 0.92$ and $\text{NRMSE}_{\text{avg}} = 0.32$. However, in SN settings, the performance of the linear models are relatively poor with, $r_{\text{avg}} = 0.84$ and $\text{NRMSE}_{\text{avg}} = 2.30$.

The $\text{NRMSE}_{\text{avg}}$ for SN linear models is very large, and for some output features, it is much larger than the range of that feature. This motivated the use of more complex ML models, and therefore, we have employed NNs in this work.

One of the major strengths of this work includes a rigorous search in the hyperparameters space (as listed in Table I) to find the best set of NN hyperparameters using cross-validation. We searched for 144,342 different sets of choices as provided in Table I, along with the best-performing choices for each of the output categories in both SE and SN settings. For each of these sets of choices, we performed cross-validation and selected the best performing set of hyperparameters based on average validation accuracy. Subsequently, the final model was trained for this best performing set of hyperparameters combining training and validation data. For all the output categories, we found that the Adam optimizer performed the best with a learning rate of 0.001 but took a different number of epochs and batch size for training. All the best-performing NNs were deep with 2–6 hidden layers and 800–1800 nodes (not necessarily fully connected). The most successful activation functions in this study were sigmoid and ReLU. We also performed a systematic search (not as large as in the case of NNs) to find the best set of hyperparameters for linear models.

For the best performing NNs, we found a very high degree of correspondence ($r_{\text{avg}} \geq 0.95$, $\text{NRMSE}_{\text{avg}} \leq 0.31$) in NN predictions and MSK outputs in SE settings. For SN settings also, the NN predictions are excellent with an average $r_{\text{avg}} = 0.89$ and $\text{NRMSE}_{\text{avg}} = 0.55$, which is a considerable improvement over linear models (with average $r_{\text{avg}} = 0.84$ and $\text{NRMSE}_{\text{avg}} = 2.30$). However, this is a slight decrease in the performance when compared to SE models. Such SN models are expected to perform worse than SE models but have much better generalizability over new subjects [34].

To better visualize the NN performance for each output category, we have plotted a trial from the test data in Figures 3-7 comparing MSK model output with NN prediction in SN and SE settings. Pearson's correlation r is excellent for each output feature with a slightly better prediction in SE settings than in SN except for Trunk bending features where the NN predictions are very poor (Figure 3). The NRMSEs show similar trends. It should be noted that in Table II, the worst performance of NNs (in terms of correlation between NN prediction and MSK model output) is for joint angles ($r_{\text{avg}} = 0.81$), which is due to poor performance of NN for Trunk bending parameters. All the other joint angle output features show excellent correspondence between MSK model outputs and NN predictions.

A similar comparison for joint reaction forces and joint moments is provided in Figures 4 and 5 which again highlights the potential of NNs to approximate the MSK models for estimating *in vivo* joint and muscle loading. However, not all the output features are predicted with similar accuracy. Moreover, SE models consistently performed better than SN models. For example, in joint reaction force output features, NN predictions for Elbow Proximodistal and Elbow Anteroposterior forces have a poor correlation with the corresponding MSK output. Similarly, in joint moments, Trunk Internal/External rotation parameters have substantially higher NRMSE values for SN model predictions than for SE models. Moreover, the features like Elbow Flexion/Extension moments, which have poor prediction results in both SE and SN settings were not well captured by the ML model.

	Linear Model		Neural Network	
Output	r_{avg} Mean (SD)	$\text{NRMSE}_{\text{avg}}$ Mean (SD)	r_{avg} Mean (SD)	$\text{NRMSE}_{\text{avg}}$ Mean (SD)
Subject-exposed				
Joint angles	0.98 (0.02)	0.11 (0.03)	0.96 (0.08)	0.16 (0.14)
Joint reaction forces	0.88 (0.19)	0.32 (0.11)	0.95 (0.05)	0.23 (0.07)
Joint moments	0.93 (0.05)	0.33 (0.14)	0.95 (0.05)	0.31 (0.13)
Muscle forces	0.91 (0.06)	0.40 (0.12)	0.97 (0.02)	0.21 (0.02)
Muscle activations	0.91 (0.06)	0.44 (0.10)	0.97 (0.01)	0.30 (0.04)
Subject-naive				
Joint angles	0.89 (0.15)	2.01 (0.15)	0.81 (0.33)	0.54 (0.40)
Joint reaction forces	0.81 (0.14)	1.72 (1.50)	0.88 (0.13)	0.59 (0.27)
Joint moments	0.84 (0.11)	2.17 (1.62)	0.87 (0.09)	0.84 (0.57)
Muscle forces	0.83 (0.05)	3.94 (1.93)	0.95 (0.02)	0.30 (0.06)
Muscle activations	0.85 (0.04)	1.64 (1.21)	0.94 (0.04)	0.50 (0.05)

TABLE II

AVERAGE PEARSON'S CORRELATION COEFFICIENT AND AVERAGE NRMSE VALUES FOR LINEAR MODEL PREDICTION AND NEURAL NETWORK PREDICTION COMPARED WITH MUSCULOSKELETAL MODEL OUTPUTS. NOTE: THE AVERAGE IS TAKEN OVER ALL OUTPUT FEATURES AND OVER ALL TEST TRIALS (FOR A GIVEN OUTPUT CATEGORY). REFER TO SUPPLEMENTARY TABLE 2 FOR ADDITIONAL INFORMATION.

Furthermore, in Figures 6 and 7, an excellent agreement between NN prediction and MSK output are shown for muscle forces and muscle activations for both SN and SE models. NN predictions are incredibly close to the corresponding MSK output for all the output features, except that in some of the output features, the maximum value of the output predicted by NN is slightly lower than the corresponding MSK output.

Lastly, in the supplementary Table 2, we have provided additional information such as maximum, minimum and interquartile range for r_{avg} and $\text{NRMSE}_{\text{avg}}$. Also, we have tabulated RMSE_{avg} values (with units) for all the output features to provide an absolute error in predicting a given MSK output. However, RMSE must be used with some caution; for instance, RMSE_{avg} of 4.87° for joint angles can not be directly compared with RMSE_{avg} of 0.03 (% Body Weight x Body Height) and thus, must only be used in specific context and scale of that output must be considered.

IV. DISCUSSION

We present an ML approach to estimate the MSK model outputs for human upper extremity exclusively using IMC data. We developed ML models for both subject-exposed (when a subject with trials in the test data has at least one trial in the training data) and subject-naive (when a particular subject is strictly kept in either training or test data) settings. We started with a simpler linear model, which performed well in SE settings. This is notably different from prior work that used linear models to approximate the MSK model for lower extremity [43]. In the SN setting, linear models perform poorly (particularly in terms of NRMSE), which is expected as SN model performance requires higher generalizability. Ruling out linear models allowed us to consider ML approaches, which are extensively used for modeling kinematic and/or

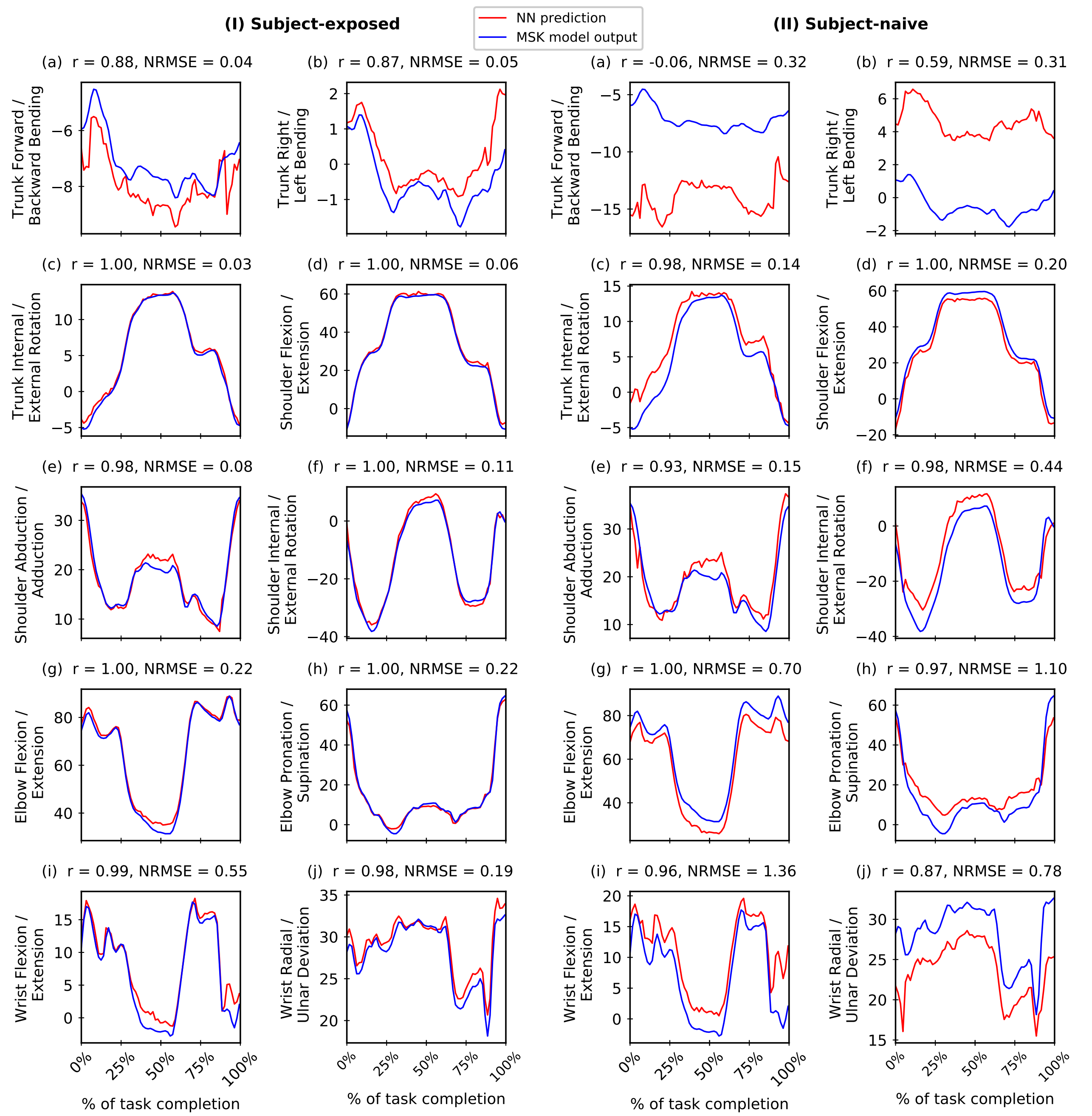

Fig. 3. Neural network (NN) predictions for joint angles (in degrees) versus corresponding musculoskeletal (MSK) model outputs on a test trial.

kinetic variables for the lower extremity but not for the upper extremity. We used a feed-forward backpropagation NN, and unlike previous work [30], [34], performed an exhaustive hyperparameter search that improves the accuracy and reliability of the predictions.

Training models in both SN and SE settings are infrequently undertaken [28], and this choice has a considerable impact on the accuracy of trained ML models [30], [34], [67]. For instance, in [34], the authors found that NN predictions for joint reaction forces remarkably worsen in SN settings than SE settings for both r ($r_{\mathrm{SE}} = 0.89-0.98$ reduced to $r_{\mathrm{SN}} = 0.45-0.85$) and NRMSE ($\mathrm{NRMSE}_{\mathrm{SE}} = 0.67-2.35$ reduced to $\mathrm{NRMSE}_{\mathrm{SN}} = 1.6-5.39$). Similar observations were made in [30], [67]. However, both SN and SE settings have several advantages of their own. SE models, which suffer from reduced generalizability for new subjects, are useful when we require accurate, reliable predictions for a single subject, which can be observed over time. By including one or more trials of the subject in the training data, highly accurate predictions for future trials can be computed efficiently, which is useful in situations requiring real-time prediction, such as sports or outdoor situations. Conversely, SN models are effective when we require accurate predictions for a new (unrelated) subject. Even though predictions for a few output features might be poor (e.g., large NRMSE), such models are excellent for pattern analysis on a large ensemble of new subjects.

In this work, both models (SE and SN) have high predictive power $r_{\mathrm{avg}} = 0.96$ and $\mathrm{NRMSE}_{\mathrm{avg}} = 0.24$ for SE models, which decrease to $r_{\mathrm{avg}} = 0.89$ and $\mathrm{NRMSE}_{\mathrm{avg}} = 0.55$ for SN models. The poor performance of SN mod-

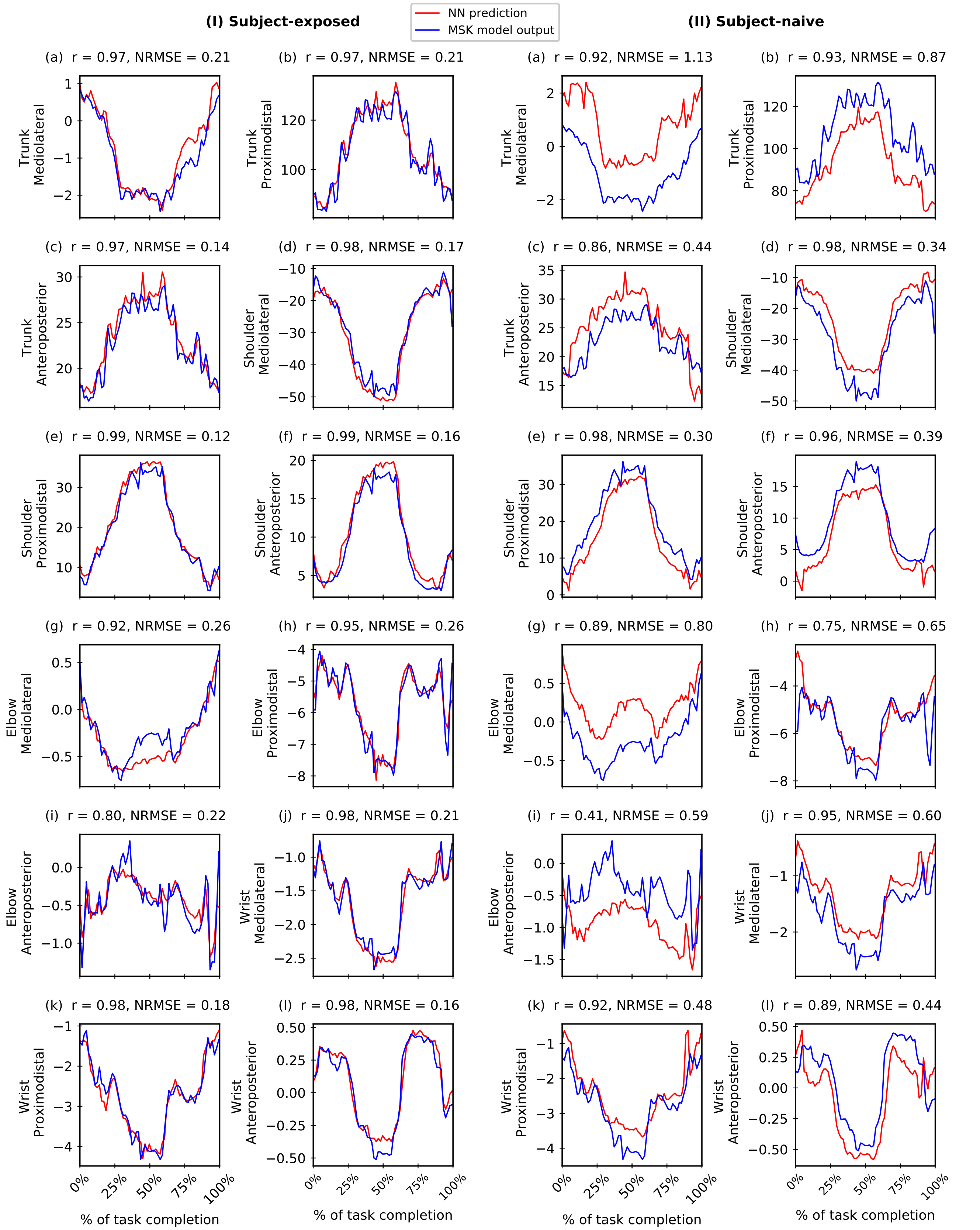

Fig. 4. Neural network (NN) predictions for joint reaction forces (% Body Weight) versus corresponding musculoskeletal (MSK) model outputs on a test trial.

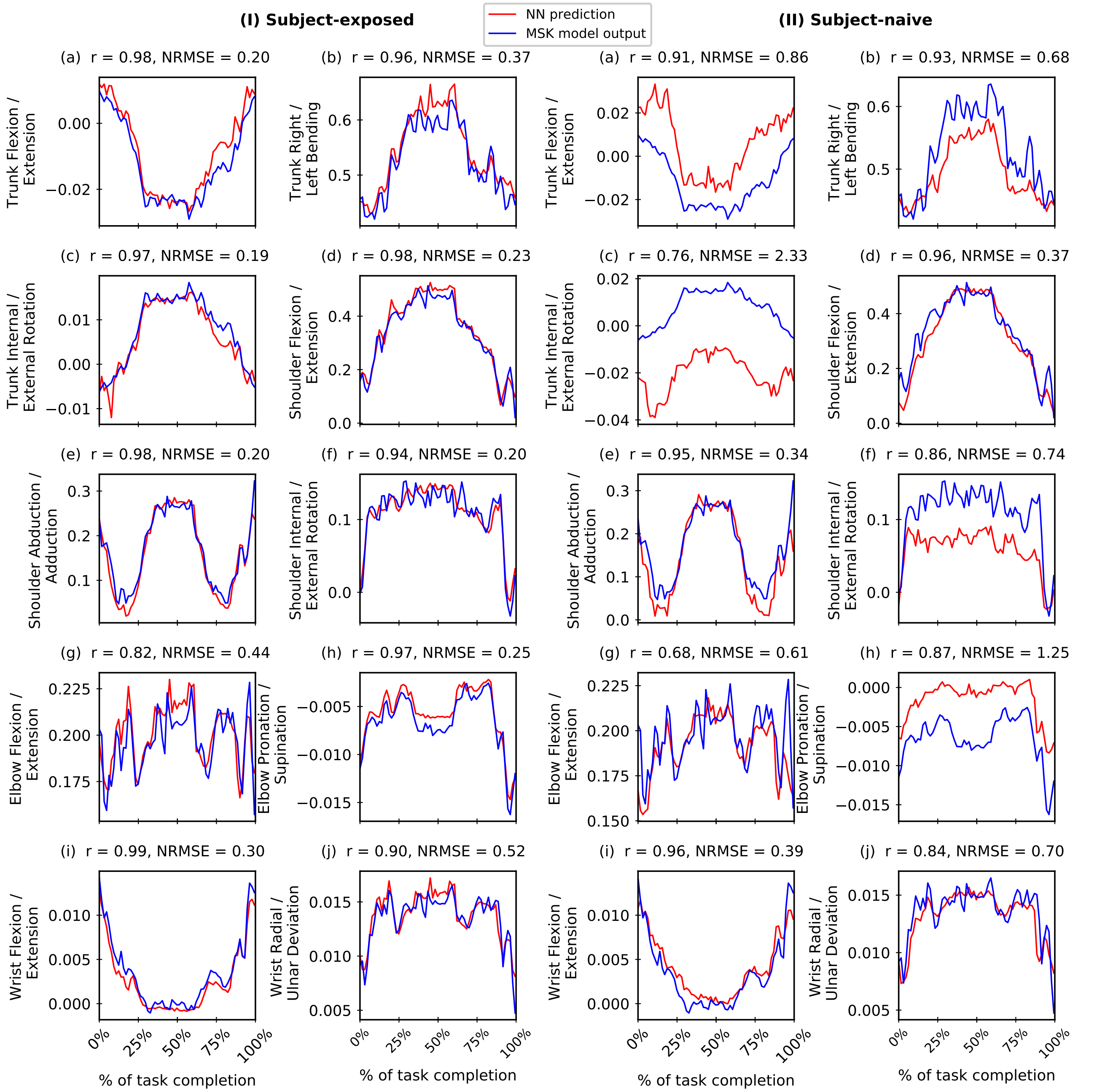

Fig. 5. Neural network (NN) prediction for joint moments (% Body Weight x Body Height) versus corresponding musculoskeletal (MSK) model outputs on a test trial.

els is limited to only a few features of joint angles (e.g., Trunk Bending (Forward/Backward and Left/Right)), joint reaction forces (e.g., Elbow Anteroposterior) and joint moment features (e.g., Trunk Internal/External Rotation and Elbow Flexion/Extension). This poor performance could be caused by the low joint range of motion incurred during the Reach-to-Grasp task. For instance, the range of motion for trunk bending (both Forward/Backward and Left/Right) is less than 5°, which is notably less than the variations ($20^\circ - 60^\circ$) in other joints. In such low ranges of motion, noise can have dominating effects that impede ML training and leads to poorer predictions for new subjects. Moreover, some of the output features might have subject-specific dependence, negatively affecting generalizability for new subjects. Such issues are more critical in the case of limited training data, which is often the case in this field [28]. Synthetic data generation using physics-based biomechanics models [42], [44] can be a solution, though limited by various modeling approximations and domain-specific assumptions. We hope to consider such data augmentations in the future.

The experiments were performed in a laboratory setting; hence, the measured performance may not be ecologically valid as the laboratory setting can seldom replicate each subject's experience in a real-world setting. The ML model in this work is trained for a particular constrained/cyclical/goal-oriented Reach-to-Grasp task, which is essential and frequent in daily life activities [23]. In an earlier lower-extremity study [30], NNs were shown to generalize well for new subjects

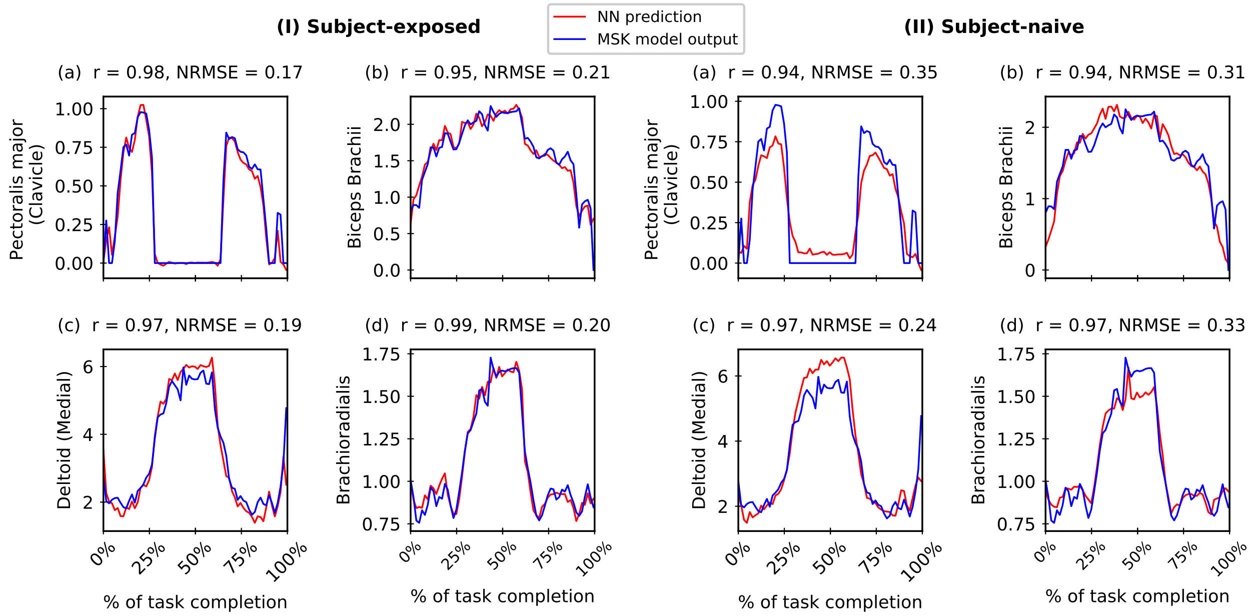

Fig. 6. Neural network (NN) predictions for muscle forces (% Body Weight) versus corresponding musculoskeletal (MSK) model outputs for a test trial.

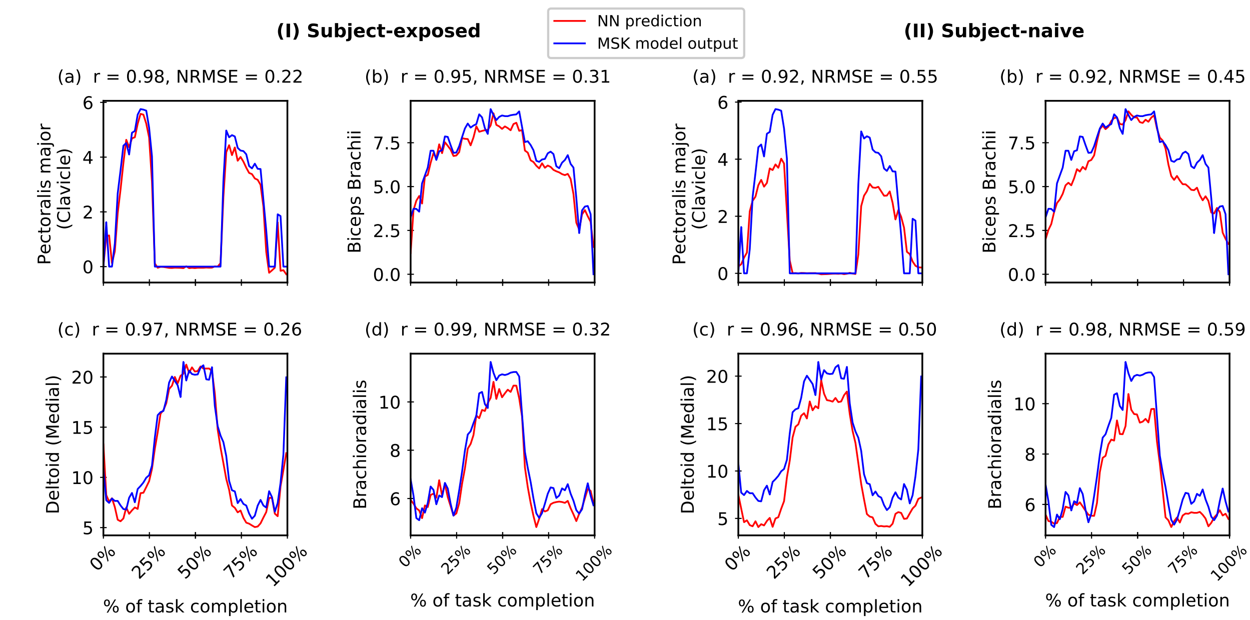

Fig. 7. Neural network (NN) predictions for muscle activations (%) versus corresponding musculoskeletal (MSK) model outputs for a test trial.

of different age and body morphology that can often lead to different gait patterns. However, upper-extremity movements (compared to lower-extremity movements) necessitate a larger degree of freedom in motion [12], [13], which questions how applicable are ML models (obtained in this study) for (a) "what-if" scenarios such as the same constrained Reach-to-Grasp task is performed but with an object of different shape, size, and/or weight, and (b) other activities of daily living involving the upper extremity. For "what-if" scenarios, we believe that the currently-trained ML model should give reasonable predictions for at least the tasks which do not differ too much from those used in the training data.

The ML methodology presented here can easily be adapted for stereotypical constrained/cyclical/goal-oriented tasks. In the literature, few such studies (both in upper and lower extremities) have been done in which a model is generalizable over different tasks. For instance, de Vries *et al.* [68] trained NN for solely predicting shoulder joint reaction forces on several pre-defined upper extremity movements while holding objects with different known masses. The authors found that the large variability in the tasks performed leads to poor NN approximations and their results suggested task-specific models should be designed over general models and question the reliability of such NN for new tasks. However, the NN trained in the same study by de Vries *et al.* is a simple shallow NN model with one hidden layer and merely 20 neurons. For a 'multitask' ML model, a deep NN that can capture the underlying non-linearity of the MSK function as well as diverse and extensive training data for various upper-extremity activities are required. Such 'multitask' models will be considered in future work.

Traditional MSK models are laborious, computationally expensive, and time-consuming [1]. Some recent approaches such as actual Inverse Kinematics, Inverse Dynamics, and Static Optimization can process data in real-time. However, it should be noted that these real-time predictions are made with a compromise on accuracy by making assumptions to simplify the MSK models. For instance, inverse dynamics with static optimization to resolve muscle forces frequently ignore tendon compliance and enable estimation of muscle forces and joint loads. However, tendon compliance becomes crucial when the research question depends on the interaction between muscle and tendon during a motion or when elastic storage of energy in a tendon is a known or likely contributor to the motion of interest (e.g., high-force motions like running) [69]. Further, recent work in predictive simulation has shown that muscle-tendon dynamics are required to achieve human-like motion [70], [71]. Moreover, these simplified models are solved numerically only for a few steps to make it real-time. It has been shown in the previous work that when solved offline (not real-time predictions), the accuracy of these simplified models improve [72]–[74]. Thus, Inverse Kinematics, Inverse Dynamics, and Static Optimization are limited in several aspects and cannot be generalized for complex and various movements due to underlying assumptions, often movement-specific. In contrast, NN/ML models capture MSK functions without making such assumptions. Even though different models might be required for various tasks, NN/ML models are highly accurate models that can be easily trained for any additional task. Unfortunately, the results from these studies [72]–[75] are not readily comparable with our work. In future, we hope to understand the trade-off between speed and accuracy, if any, of (near) real-time MSK models vis-á-vis ML-driven models such as those that appear in our work.

For training and testing the ML model, the ground truth was obtained using the MSK model, and thus, the ML model's prediction accuracy is limited by underlying modeling assumptions and inaccuracies. MSK model verification & validation remains a vital topic of ongoing research [1], [69], [76], [77]. Consequently, further improvements to MSK model verification & validation could lead to more accurate kinematic and kinetic estimates and thereby help make better ML model-based predictions.

Another avenue for future research is undertaking methodological variations on the NN approach, such as comparing various NN frameworks and assessing their suitability for different tasks [52], as well as using alternative prediction paradigms such as Gaussian Processes (which have been used in MSK models for robotics [78], [79] and ergonomics [80]) that are better at modeling uncertainty. We also aim to use more extensive and diverse training datasets for a more accurate and generalizable model.

V. Conclusion

Following ML best practices in this work, we have developed ML models that can provide highly accurate estimates of upper-extremity kinematic and kinetic parameters solely from Full-body Sensor Network IMC system measurements. Such models can act as viable alternatives to the MSK modeling process, the latter often being traditionally computationally more expensive. To our knowledge, this is one of the first ML approaches that comprehensively estimate kinematic (e.g., joint angles) and kinetic variables (e.g., joint and muscle loading) for human upper-extremity movements. Moreover, this is among the few studies in this field that performs a rigorous search in hyperparameters space to find the best ML model for each output feature. The efficiency and accuracy of the ML models make it viable as an accessible and affordable solution, especially in resource-poor settings, for taking motion analysis and MSK modeling beyond the lab. Further work will address questions such as the viability of ML models when considering a combination of IMC and OMC data-driven MSK models, and the performance of different classes of ML models for upper-extremity biomechanical modeling.

Data Availability

The datasets presented in this article are not readily available due to ethical and privacy reasons. The Python codes for NN implementation and data analysis as well as the test data are available on https://github.com/rahul2512/MSK_ML_codes.

Author Contributions

VHN and CM conceived the project. VHN conceptualized the biomechanical methodology, and developed the anonymized dataset. CM conceptualized the ML methodology. RS, AD, RC, CM, and VHN contributed to data processing and development of the ML models. RS developed the ML methodology and implemented the codes for ML and analysis with contributions from CM and AD. RS, AD, CM, and VHN contributed in the analysis and writing of final results. All authors contributed to drafting, review, and editing. All authors have read and agreed to the final version of the manuscript.

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