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Nonlinear surrogate modeling of tibio-femoral joint interactions

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ABSTRACT

Musculoskeletal modeling can predict muscle forces and the resulting motion and loading during human ambulatory activities. A better understanding of the loading environment on hard and soft tissues can enhance our understanding of ligament injury and prevention, tissue engineering, prosthetic design, osteoporosis, and osteoarthritis. The current state-of-the-art in movement simulation is to use simplified representation of the joints, such as representing the knee as a simple hinge joint. The aim of this study is to produce data-driven surrogate models which effectively capture the complex three-dimensional behavior of tibio-femoral joint interactions and that have the ease of use and computational efficiency required for incorporation in existing neuromusculoskeletal simulations. In order to meet our objective, we explored and compared the performance and sensitivity of nonlinear Hammerstein–Wiener, nonlinear autoregressive, and time delay neural network models under different configurations, individually and in ensembles. These models learned from solutions calculated by a validated multibody model of the knee. Inputs to the surrogate models were positions and orientations of the tibia relative to the femur, and the outputs were resulting forces and torques at the tibia with respect to the femur. Models were mixed using mean (sum) rule, weighted mean, and stacked generalization ensemble methods. It was observed that individually, time delay neural network models performed better than other models with normalized mean square errors between 0.0509 and 0.0889 on test data. Among the ensembles, stacked generalization provided the best results reducing test errors by 13–40%.

1. Introduction

The ability to predict loading on musculoskeletal system tissues during dynamic activity is essential to our understanding of ligament injury and prevention, tissue engineering, prosthetic design, osteoporosis, and osteoarthritis [1–3]. With few exceptions, the forces acting on musculoskeletal tissues cannot be directly measured in vivo. Musculoskeletal modeling and movement simulation can estimate individual muscle forces and provide insight to motor control and joint loading. For example, the forward dynamics method is commonly used in musculoskeletal modeling where the neural command signal provides the model inputs [1,4]. The neural command is sent to muscle models that predict muscle forces that are then applied to the bone. The neural command can come from measured EMG (electromyography), but is often estimated by optimization methods that predict the neural command through iteration. As such, decreasing the computation time per simulation can have a significant effect on overall computation time [5]. Body level musculoskeletal models typically involve simplifications of the joints, muscles, and motor control strategies [6] and the knee is commonly represented as a hinge joint. But, real knees experience translation in the sagittal plane and have significant internal–external and varus–valgus rotation. Prediction of lower limb behavior would be greatly enhanced by a model that incorporated the physiological force–displacement response of the knee. In addition, the artificial constraints of an ideal hinge joint can alter the muscle activation patterns predicted by the forward dynamics and neural command optimization method. The goal of this work is to identify and develop data-driven (black-box) surrogate models that are capable of describing the complex three-dimensional behavior of tibio-femoral joint interactions with a computational efficiency and ease of use necessary for incorporation in existing movement simulation models. Specifically, this methodology will be demonstrated by producing a subject specific nonlinear six-axis displacement–force relationship in a compact format.

To meet the project objective, several nonlinear data-driven models, including mixtures of models (multi-model ensembles), were explored and compared. The solution set for black-box model training consisted of relative motion between the tibia and femur and the forces and torques required to produce this motion for a multibody model of the tibio-femoral joint. This model included representation of the ligaments crossing the joint and deformable

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contacts representing cartilage–cartilage interaction. The menisci were not represented. After training, the inputs to black-box models were the positions and orientations of the proximal tibia relative to the distal femur. The outputs were the resulting reaction forces and torques experienced by the tibia from the motion. The developed tibio-femoral surrogate is analogous to a nonlinear six-axis spring and is meant to be used within a musculoskeletal model of the lower limb that also includes representation of muscles, ground reaction forces, and a hip and ankle.

2. Methods

The datasets required to train the data-driven models were generated using a multibody knee model. First, a computational multibody model was created and validated against experimental measurements obtained from a cadaver knee (Section 2.1). Force–displacement datasets were then generated by multibody model simulations and a series of nonlinear, data-driven models were trained, validated, and tested using this data in order to study different aspects of their performance (Section 2.2). Finally, we compared these computationally efficient surrogate models in order to identify architectures and configurations that are suitable for capturing tibio-femoral dynamics (Section 3).

2.1. Data

A validated six degrees of freedom multibody model of a cadaver knee provided the datasets for surrogate training, validation, and testing. The multibody knee model was created in MD ADAMS (MSC Software Corporation, Santa Ana, CA) using magnetic resonance imaging to create the geometries of the femur, tibia, patella, articular cartilage, and ligaments of a cadaver knee (68-year-old left female knee). A deformable contact law was defined between the cartilage surfaces of the tibia and femur based on Hertzian contact theory and functional cartilage properties [7]. The ligament bundles were represented as nonlinear springs with insertions and zero-strain lengths determined from experimental measurements [8]. The multibody knee model was validated by comparing kinematics to an identically loaded cadaver knee. The knee model was placed in a validated model of a dynamic knee loading machine (Kansas Knee Simulator (KKS), University of Kansas, Lawrence, KS) [9]. The KKS reproduces the net loading and motion of physiological activities, such as walking, using five axes controlled through servo-hydraulic actuators (quadriceps force, vertical force applied at the hip, medial-lateral ankle force, ankle vertical torque, and ankle flexion force) [10]. Experimental measurements collected during testing of the cadaver knee included the forces produced by the servo-hydraulic actuators of the machine and the resulting motion of the femur, tibia, and patella. During simulation, the measured forces were applied to the model of the knee in the KKS and the resulting predicted bone motion was compared to measured bone motion. Once validated, the multibody model of the tibio-femoral joint could be extracted from the knee and KKS model to generate the force–displacement data required for the surrogate training, validation, and testing. This step of creating and validating the multibody model was done for two reasons: (1) reaction forces at the tibio-femoral joint cannot be directly measured experimentally, and (2) the multibody model can easily generate the large amounts of force–displacement data needed for surrogate training. The multibody model of the knee in the KKS was used to generate the motion components of the datasets for surrogate modeling. The simulated motion data extended well beyond the limited motion data measured during experimental testing.

After validation, the model of the cadaver knee in the dynamic knee simulator was used to generate the relative motion between an anatomical coordinate system based on Grood and Suntay [11] which was placed in the tibia (TC) and femur (FC) (Fig. 1). Experimental testing of the cadaver knee in the KKS consisted of a simulated 10 s walk cycle based on ISO specification 1243-1 [12]. The measured forces produced by the actuators of the dynamic knee simulator during experimental testing provided the simulation inputs to the knee and dynamic knee simulator model. The relative motion between the TC and FC was recorded during the simulated walk. Additional motion data was created by repeating the 10 s walk profile and subjecting it to perturbations by applying forces during simulation. The resulting motion data was not meant to encompass the entire envelope of possible tibio-femoral motion, but to provide a continuous and physiologically relevant envelop of motion centered on the ISO walk profile.

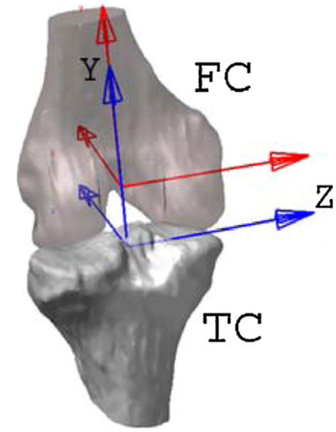

Fig. 1. A posterior view of the knee depicting the locations of tibia (TC) and femur (FC) coordinate systems.

Three different datasets were generated for the purpose of training, validating, and testing our data-driven surrogate models. Five force profiles, $f_i(t)$ $i = 1,2,\ldots,5$, were given as the input to the multibody model; namely 1: hip angle, 2: vertical force, 3: lateral force, 4: vertical torque, and 5: ankle force. They were perturbed to include multiple walking paces. The period of the walk cycle, $T(t)$, was varied by

$$T(t) = 10 + 2.5q\ \sin\left(\frac{2\pi t}{10p}\right) \quad (1)$$

where p and q were set to 190 and 1.75, 175 and 2.0, and 210 and 2.25 for training, validation and testing datasets, respectively.

Forces $f_i(t)$ provided to the model were generated by an nth order Fourier series with $n_{\max}$ being 3 for hip angle, 5 for vertical force, and 4 for remaining force profiles, using a randomized sinusoidal phase angle. The histogram of induced residuals by this method demonstrated an approximately normal distribution.

$$f_i(t) = \sum_{n=1}^{n_{\max}} \left[C_{n,i}\ \cos\left(2\pi n \frac{t}{T(t)} - \varphi_{n,i} - \frac{1}{J_i^2} \cos\left(\frac{2\pi r t}{7}\right)\right)\right] \quad (2)$$

Here, r is a uniformly distributed random number. The modified phase term produced pseudo-random combinations of disturbances over the interval of the datasets, while keeping the inputs to the model near the bounds of the ISO-described force profiles. C_n and φ_n were cosine series' amplitude and phase calculated from the original ISO profile. J_i was equal to 1 for all but $i = 2$, i.e. vertical force. The original profile for this force exhibited sudden fluctuations in time that were poorly approximated using the same J_i and $n_{\max}$ as other profiles. To improve this approximation, the order of the Fourier series $n_{\max}$ was increased to 5 and J_2 was set equal to n to reduce the disturbance factor in each successive term. Additionally, as the knee joint remains in compression during a normal