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Gait Modification and Optimization using Neural Network-Genetic Algorithm Approach: Application to Knee Rehabilitation

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Abstract

Gait modification strategies play an important role in the overall success of total knee arthroplasty. There are a number of studies based on multi-body dynamic (MBD) analysis that have minimized knee adduction moment to offload knee joint. Reducing the knee adduction moment, without consideration of the actual contact pressure, has its own limitations. Moreover, MBD-based framework that mainly relies on iterative trial-and-error analysis, is fairly time consuming. This study embedded a time-delay neural network (TDNN) in a genetic algorithm (GA) as a cost effective computational framework to minimize contact pressure. Multi-body dynamic and finite element analyses were performed to calculate gait kinematics/kinetics and the resultant contact pressure for a number of experimental gait trials. A TDNN was trained to learn the nonlinear relation between gait parameters (inputs) and contact pressures (output). The trained network was then served as a real-time cost function in a GA-based global optimization to calculate contact pressure associated with each potential gait pattern. Two optimization problems were solved: first, knee flexion angle was bounded within the normal patterns and second, knee flexion angle was allowed to be increased beyond the normal walking. Designed gait patterns were evaluated through multi-body dynamic and finite element analyses.

The TDNN-GA resulted in realistic gait patterns, compared to literature, which could effectively reduce contact pressure at the medial tibiofemoral knee joint. The first optimized gait pattern reduced the knee contact pressure by up to 21% through modifying the adjacent joint kinematics whilst knee flexion was preserved within normal walking. The second optimized gait pattern achieved a more effective pressure reduction (25%) through a slight increase in the knee flexion at the cost of considerable increase in the ankle joint forces. The proposed approach is a cost-effective computational technique that can be used to design a variety of rehabilitation strategies for different joint replacement with multiple objectives.

Keywords: Gait modification, Tibiofemoral knee joint, Time delay neural network, Genetic algorithm, Contact pressure

2

1 **1. Introduction:**

2 Following total knee arthroplasty (TKA), rehabilitation strategies are of significant importance to accelerate 3 patient recovery(Isaac et al., 2005, Klein et al., 2008), reinforce joint functionality(Moffet et al., 2004, Rahmann et 4 al., 2009), decrease gait asymmetry(Zeni Jr et al., 2011), and augment the durability and life time of knee 5 prostheses(Fransen, 2011, Mont et al., 2006). Gait rehabilitations mainly aim to decrease knee joint loading through 6 minor changes in human gait patterns. However, recognizing the synergistic kinematic changes, required for joint 7 offloading, is a challenging task, hence; computational approaches have been used to facilitate the design procedure. 8 To best of our knowledge, most of the current literature on gait modification strategies have been designed through 9 multi-body dynamic (MBD) analysis (Barrios et al., 2010, Barrios and Davis, 2007, Fregly et al., 2009, Hunt et al., 10 2008, Mündermann et al., 2008, Willson et al., 2001, Ackermann and van den Bogert, 2010, Anderson and Pandy, 2001, Fregly et al., 2007). However, iterative "trial-and-error" MBD analysis, that has been performed in such 11 12 studies, is fairly time demanding which limits the applicability and generality of the method. Hence, a cost-effective 13 computational framework that minimizes the computational cost is of particular interest.

14 Besides the computational cost, there are a number of aspects that have not been well addressed by the 15 conventional MBD-based framework. First, MBD-based approach attempts to reduce the peak values of knee 16 adduction moment (KAM) which is not always a reliable measure since decreasing KAM may not necessarily 17 decrease knee joint loading (Walter et al., 2010); and the results of such approach are sensitive to the chosen 18 reference frame (e.g. laboratory, floating reference frames) (Lin et al., 2001, Shull et al., 2012). Second , joint-19 offloading gait patterns are likely to decrease the contact area of articulating surfaces that unfavorably may increase 20 the contact pressure at the knee joint (D'Lima et al., 2008). Therefore, reducing the contact pressure should be 21 concerned as the principal goal of rehabilitation design. Conventional computational frameworks however are 22 inherently unable to consider the contact pressure in the design procedure since the conventional methods require an 23 explicit cost function whilst the relation between gait kinematics and the resultant contact pressure has not been 24 stated explicitly before. Also, predicting the contact pressure requires implementing finite element analysis (FEA) 25 which in turn increases the computational cost (Halloran et al., 2010). A cost-effective surrogate which releases the 26 necessity of iterative FEA is therefore of significant advantage. Third, previous studies could not reach a general 27 consensus about the contribution of knee flexion to the knee joint offloading. Knee flexion is a key synergetic 28 parameter that is often increased within the clinical execution of the rehabilitation patterns (Barrios et al., 2010, 29 Fregly et al., 2007, van den Noort et al., 2013). Several studies concluded that increasing the knee flexion would 30 reduce KAM (Fregly et al., 2009, Fregly, 2008, Fregly et al., 2007), whilst others showed that it has no association 31 with KAM (Creaby et al., 2013) or may even increase contact pressure at the knee bearing surfaces (D'Lima et al.,

32

2008). A systematic investigation is required to enhance our understanding of the contribution of knee flexion to

33 <u>the knee joint offloading</u>.

34 Artificial neural networks (ANN) and genetic algorithm (GA) are two relatively new techniques in the field 35 of biomechanics. Artificial neural network (ANN) can be used as a real-time surrogate model with the ability to 36 learn a nonlinear relationship. Once a set of inputs and corresponding outputs are presented to the network, it will 37 then "learn" the causal interactions between inputs and outputs. Given a new set of inputs, the trained neural network 38 (surrogate model) can generalize the relationship to produce the associated outputs. The ANN surrogate therefore 39 can be of significant advantage especially when the original model necessitates repeating a time-consuming 40 computation. For example, ANN has been widely used as a surrogate of FEA (Campoli et al., 2012, Hambli, 2010, 41 Hambli, 2011, Naito and Torii, 2005, Lu et al., 2013, Simic et al., 2011, Zadpoor et al., 2012). Genetic algorithm is a 42 time-efficient global optimization technique which searches the entire data space to find the best solution(Goldberg, 43 1989). In each iteration, only potential candidates that better optimize the cost function will survive to the next 44 iteration. Thus, regardless of the initial point, the search data space is iteratively modified and GA will rapidly 45 converge to the global optimum solution. This in turn assures the robustness of the method and minimizes the 46 computational effort required to find the best solution. Moreover, GA is capable of dealing with multivariable data 47 space, nonlinear input-output interactions and non-explicit, non-differential cost function.

Therefore, the overall aim of this study was to develop a hybrid framework of time delay neural network (TDNN) and genetic algorithm (GA) to address the aforementioned limitations of the literature. In particular this study aimed to (1) optimize the gait pattern in order to minimize the contact pressure at the knee articulating surfaces and (2) investigate the role of knee flexion in knee joint offloading. The advantage of the proposed approach was also compared over the existing knee rehabilitations in the literature.

- 53 **2.** Materials and methods
- 54

The proposed computational approach was implemented in the following steps:

Step 1) Experimental gait analysis data were obtained from the literature (Section 2.1), and imported into MBD analysis to calculate gait kinematics and kinetics (Section 2.2). Knee flexion angle and three dimensional knee joint loadings were predicted by MBD, and then served as boundary condition and loading profiles for the finite element simulation to calculate contact pressure (Section 2.3). Gait trials were then outlined via a number of kinematic features and the corresponding maximum contact pressure values (CPRESS-max) (Section 2.4). Step 2) A time-delay neural network (TDNN) was trained to learn the nonlinear relationship between kinematic
features as inputs and the corresponding CPRESS-max values as output (Section2.5).

62 Step 3) A genetic algorithm (GA) was implemented to search for the optimum kinematic features (optimization 63 variables) which minimized the CPRESS-max at the knee joint bearing surfaces. In this GA, the trained TDNN was 64 served as a real-time cost function to calculate the objective value (CPRESS-max) (Section 2.6).

65 **2.1. Experimental gait data**

Experimental gait analysis data of a single subject with unilateral TKA (female, height 167 cm, mass 78.4 66 67 kg) was obtained from the literature (https://simtk.org/home/kneeloads; accessed on June 2013). The subject walked 68 with a variety of different gait patterns including normal, medial thrust, trunk sway, walking pole, bouncy, crouch, 69 smooth and fore foot strike. Medial thrust, trunk sway and walking pole were knee rehabilitation strategies, designed 70 to decrease KAM, whilst the remaining gait trials were different walking patterns to cover the span of executable gait 71 for the subject. Compared to normal walking, the subject walked with a slightly decreased pelvis obliquity, slightly 72 increased pelvis axial rotation and leg flexion to implement medial thrust pattern. For trunk sway pattern, the subject 73 walked with an increased lateral leaning of the trunk in the frontal plane over the standing leg. In walking pole, the 74 subject used bilateral poles as walking aids. For each gait pattern, five gait trials were repeated under the same 75 walking condition at a self-selected pace. A total of two complete gait cycles were picked up from each trial, leading 76 to a total of 84 data sets. For further details, see (Fregly et al., 2012). Gait trials were recorded in terms of marker 77 trajectory data (Motion Analysis Corp., Santa Rosa, CA) and ground reaction forces (AMTI Corp., Watertown, MA).

78 **2.2. Multi-body dynamic**

79 Experimental ground reaction forces and marker trajectories were imported into the three-dimensional multi-80 body dynamic simulation software, AnyBody Modelling System (version 5.2, AnyBody Technology, Aalborg, 81 Denmark). A lower extremity musculoskeletal model was used in AnyBody software based on the University of 82 Twente Lower Extremity Model (TLEM) (Klein Horsman, 2007). This model, available in the AnyBody published 83 repository, had 160 muscle units as well as foot, thigh, patella, shank, trunk and thorax segments. Hip joint was 84 modelled as a spherical joint with three degrees of freedom (DOF): flexion-extension, abduction-adduction and 85 internal-external rotation. Knee joint was modelled as a hinge joint with only one DOF for flexion-extension and 86 universal joint was considered for ankle-subtalar complex. Since the assumptions of the simplified knee joint and 87 rigid multi-bodies were made, the detailed knee implant was not considered in the MBD analysis. Knee flexion angle 88 and three dimensional knee joint loads, aligned in medial-lateral, proximal-distal and anterior-posterior directions, 89 were calculated for each complete gait cycle. A complete gait cycle was defined as the time period from heel strike of

90 one leg to the following heel strike of the same leg(Vaughan et al., 1992). Computations were then normalized to 91 100 samples to represent one complete gait cycle. Knee flexion and three dimensional knee joint loads then served as 92 the boundary condition and load profiles for FEA.

93 **2.3. Finite element method**

94 A typical tibiofemoral knee implant was modelled in the commercial finite element package; 95 ABAQUS/Explicit (version 6.12 Simulia Inc., Providence, RI) using the computer aided design (CAD) of a clinically 96 available fixed bearing knee implant. The knee implant consisted of two main parts; femoral component and tibia 97 insert. Rigid body assumptions were applied to both parts, with a simple linear elastic foundation model defined 98 between the two contacting bodies (Halloran et al., 2005). Tetrahedral (C3D10M) elements were used to mesh the 99 model in ABAOUS. Convergence was tested by decreasing the element size from 8 mm to 0.5 mm in five steps (8, 4, 2, 1, and 0.5 mm). The solution converged on contact pressure ($\leq 5\%$) with over 86000 and 44000 elements 100 101 representing the femoral component and the tibia insert respectively. This was also consistent with the previous 102 mesh convergence studies for similar finite element models (Abdelgaied et al., 2011, Halloran et al., 2005). The 103 physical interaction between femoral component and tibia insert was taken into account as a surface-to-surface 104 contact (femur as the master surface and tibia as the slave surface) through a penalty-based approach with an 105 isotropic friction coefficient of 0.04 (Abdelgaied et al., 2011, Halloran et al., 2005). The tibia insert was constrained 106 in all available DOFs and the femoral component was only allowed for flexion-extension under the three dimensional 107 load which were obtained from MBD analysis. The model calculated the contact pressure at each node for each time 108 increment. An output field was created over all simulation frames to compute the maximum value of the contact 109 pressures (CPRESS_max) over the entire gait cycle. Since the medial compartment experiences the CPRESS-max 110 value (Schipplein and Andriacchi, 1991), this part was considered for the rest of the study (Figure 1a).

111 **2.4. Feature extraction**

During a complete gait cycle, the extent to which a joint can be moved (range of motion) and the corresponding absolute values of motions directly affect the quality of human gait and joint loading. For example, increasing the "maximum" value of hip adduction angle or hip internal rotation would decrease the "peak" values of KAM (Barrios et al., 2010). On the other hand, to design a realistic gait modification strategy, the overall trend of kinematic patterns cannot differ significantly from natural human walking habitudes; otherwise the pattern would not be acceptable and executable by the patient. Thus, only the key features of kinematic waveforms are needed to be modified whilst the overall trends should be preserved consistent. Gait kinematics were therefore outlined through a total of 39 descriptive kinematic features (Table 1 and Figure 1b). These features have been suggested in the literature for a number of studies such as gait analysis (Collins et al., 2009, Gates et al., 2012a, Gates et al., 2012b), gait classification (Armand et al., 2006) , evaluation of joint loading (Simonsen et al., 2010), and joint intercoordination (Wang et al., 2009). Kinematic features (optimization variables) were then allowed to vary within the corresponding ranges of experimental values plus $\pm 20\%$ variations to cover a thorough span of executable movement patterns for the subject. Contact pressure was also characterized by the maximum pressure value occurred over the entire gait cycle (CPRESS-max).

126 **2.5. Time-delay neural network**

127 Time delay neural network (TDNN) was implemented to model the highly nonlinear relationship between kinematic features (39 inputs) and CPRESS-max values (one output). The trained network was then embedded in an 128 129 optimization process (GA) as a real-time cost function to calculate the objective values (CPRESS-max). The TDNN 130 architecture consisted of a feed forward neural network in which a tapped delay line was added to the input layer 131 (Figure 2). Similar to other types of neural networks, a number of processor units (neurons) were arranged in a 132 certain configuration (layers). A weighted sum of all inputs was fed into each hidden neuron where an activation function acted on this weighted sum to produce the output of the hidden neuron. All of the hidden neurons were 133 134 activated using "hyperbolic tangent sigmoid" function which linearly scaled its input signal to [-1, 1] interval:

135
$$y_{j}^{m} = \frac{2}{1 + \exp(-2*V_{j}^{m})} - 1 \quad j = 1, 2, \dots, M_{m}$$
(1)

136 Where y_j^{m} is the output of jth hidden neuron located at the mth hidden layer, M_m is the number of hidden neurons 137 at the mth hidden layer, and V_j^m(n) is the weighted sum of the signals from the previous layer which was fed to the jth 138 hidden neuron of mth hidden layer:

139
$$V_{j}^{m} = \sum_{k=1}^{M_{m-1}} (y_{k}^{m-1} * W_{jk}) + b_{j} \quad j = 1, 2, ..., M_{m} , \quad k = 1, 2, ..., M_{m-1}$$
(2)

140 Where W_{jk} is the weight relating the output of kth neuron located at the (m-1)th layer (y_k^{m-1}) to the jth hidden neuron at 141 the mth hidden layer with the bias value of b_j, and M_m and M_{m-1} are the number of neurons at the mth and (m-1)th layers 142 respectively. A weighted sum of all hidden neurons' outputs was also fed into the single output node which was 143 activated by a "pure line" function:

144
$$y_{out} = \sum_{k=1}^{M_m} w_k y_k^m + \overline{y}$$
(3)

145 in which \overline{y} is the output bias.

TDNN was trained using the scaled conjugate gradient algorithm (SCG) (Møller, 1993). The available data 146 147 space, obtained from MBD and FEA, was randomly divided into three main parts: train (70%), validation (15%) and 148 test (15%) subsets. The train and validation subsets were used to train the network whilst the test subset was not 149 included in training. The network prediction error on the validation subset implied how accurate the network has 150 learned the input-output causal relationship (accuracy). On the other hand, the network prediction error on the test 151 subset indicated the extent to which the trained network could generalize this causal relationship for new inputs 152 (generality). Generally speaking, the structure of the FFANN would build a trade-off between "prediction accuracy" 153 and "generality". Whilst increasing the number of hidden neurons/layers would increase the prediction accuracy, using too many neurons would decrease the generality and increase the test error. The number of hidden layers and 154 155 hidden neurons were therefore determined according to the network prediction error for the test and validation subsets. The input delay was also determined by trial and error. 156

157 **2.6. Genetic algorithm**

158

In the present study, gait optimization was stated as follows:

159 Minimize
$$Y : Y=U(X)$$
 $AX \le b$, $X_L \le X \le X_U$ (4)

Where Y is the CPRESS-max, X is the optimization variables (kinematic features), and U is the trained TDNN. Upper 160 161 and lower bounds of the optimization variables (X_L and X_U) were obtained from the experimental gait trials plus \pm 162 20% variations. Matrix A and vector b described the linear inequality constraints in order to control the natural trends 163 of the gait kinematics (Appendix). Genetic algorithm (GA) was used to search for those kinematic features that could 164 minimize CPRESS-max. Kinematic features (optimization variables) were configured as 1*N arrays called individuals (N=39). In each iteration, the GA created a population of individuals and then employed the trained 165 TDNN to calculate the resultant CPRESS-max values associated with potential individuals. Those individuals that 166 led to lower CPRESS-max values were assigned a higher survivorship probability to be selected and make the next 167 168 population. Each individual is indeed a potential solution and each population is a search space of solutions. 169 Accordingly, after passing several iterations, the population (solution search space) evolved toward the optimized 170 individuals.

171 The first population was initialized with random individuals in which features of gait kinematics were 172 randomly chosen due to X_L and X_U . The next populations were created through selected individuals by elitism, crossover and mutation operators of GA (Goldberg, 1989). Table 2 summarizes the setting of the proposed GA in MATLAB (v.2009, Genetic Algorithm toolbox). In the present study, two systematic optimizations were performed: first, knee flexion was bounded to vary within the normal walking. Second, the knee flexion was allowed to vary beyond the normal walking up to the medial thrust pattern. Once the GA converged to the optimum kinematic features, a typical normal gait cycle was adjusted to these optimum features using the curve fitting technique and the optimized gait pattern was reconstructed. Figure 3 shows schematic of the proposed combined TDNN-GA methodology in this study.

180 **3. Results**

181 **3.1. Network training**

182 A four-layer TDNN with four delay units at its input layer, 20 hidden neurons at the first hidden layer and 15 hidden neurons at the second one, was trained using 70% of the generated data base. Then, it was validated and tested 183 184 with the remaining 30%. Figure 4 shows the average performance of the proposed network over 100 training and 185 testing repetitions, each time with a random selection of subsets(Iver and Rhinehart, 1999). According to the results, 186 the TDNN could accurately predict CPRESS-max values for the training, validation and test subsets. Pearson 187 correlation coefficients, between network predictions (Y axis) and real outputs (X axis), were all above p=0.98. Figures 4a, b show that the network learned the nonlinear interaction of kinematics and contact pressure variables 188 189 (p=0.99). Figure 4c shows that the network could predict the CPRESS-max values corresponding to new sets of 190 kinematics which were not included in the training data space (p=0.98).

3.2. Optimization problem

The crossover fraction substantially affects the convergence of GA. Optimization was therefore run for a 192 variety of different values of crossover fraction ranged from 0 to 1 in the step size of 0.05. The crossover fraction of 193 194 0.85 led to the lowest CPRESS-max value (see Figure 5). Thus, this value was adopted for the rest of this study. In 195 the first optimization problem, knee flexion angle was bounded within normal walking. The algorithm was terminated after 75 populations due to stall generation criterion, in which the average change of the objective value 196 (CPRESS-max) was less than 10^{-6} (function tolerance) over 50 populations (stall generations). Figure 6a shows the 197 198 mean and the best CPRESS-max values associated with each population. After successful convergence of the 199 algorithm, TDNN-GA achieved the lowest CPRESS-max value of 25.58 MPa for the best individual of the last 200 population.

201 Using curve fitting technique, a typical normal gait cycle was adjusted to the obtained optimum kinematic 202 features and the optimized gait pattern was reconstructed (Figure 7). The optimized kinematics laid within the 203 experimental gait patterns suggesting that it would be feasible for the subject to execute the optimized pattern. Using 204 multi-body dynamic analysis, the corresponding joint loadings were computed and compared with the span of experimental values (Figure 8). Results show that lower extremity joints (ankle, knee and hip) underwent realistic 205 206 loading conditions i.e. within and with similar pattern to the experimental gait trials. Particularly, hip joint loading 207 was generally low in the anterior-posterior direction. A general reduction at the anterior-posterior component of knee 208 joint loading and significant reduction at its medial-lateral component around 40%-60% of the gait cycle occurred. 209 Moreover, the medial-lateral component of ankle joint loading was significantly decreased accompanied with a reduction at its anterior-posterior component around 40%-60% of the gait cycle. Figure 9 shows the resultant 210 distribution of the maximum contact pressure at the medial tibiofemoral joint over the entire gait cycle. The 211 212 maximum contact pressure was reduced by 21.8% compared to the normal walking, while previously published gait 213 modifications were fairly ineffective to decrease the contact pressure magnitudes.

214 In the second optimization problem, X_L and X_U were modified and the knee joint flexion was bounded 215 between normal and medial thrust patterns. The GA achieved the convergence value of 24.61 MPa after 77 216 populations (Figure 6b). Reconstructed gait kinematics and the resultant joint loading patterns are presented in 217 Figures 7 and 8 respectively. Results demonstrate that the second optimized gait pattern also laid within the span of 218 executable gait patterns. The second optimized gait modification led to a significant reduction at the three 219 dimensional hip joint loading (anterior-posterior, proximal-distal and medial-lateral) around 0-25% of the gait cycle. 220 This pattern also led to an overall reduction at anterior-posterior component of the knee joint loading. Anteriorposterior and medial-lateral components of the ankle joint loading were substantially low at 0-25% of the gait cycle, 221 222 however ankle joint loading was slightly increased around 40%-60% of the gait cycle. By comparison, the second 223 optimization problem yielded to a more effective gait modification pattern that better reduced the magnitude of the 224 contact pressure by up to 25% (Figure 9).

225 **4. Discussion**

4.1. Hybrid neural network-genetic algorithm

Neural network was employed: first, to model the highly nonlinear relationship between gait kinematics and contact pressure; second, to serve as a real-time cost function that allowed the optimization algorithm to be performed in a reasonable computation time. A recent study by Lu et al. (2013) demonstrated that the dynamic 230 structure of a time delay neural network was preferred for modelling the relation between tibiofemoral cartilage load 231 (input) and von Mises stress (output), compared to the traditional static feed forward neural network. Therefore, this structure was used in this study. Moreover, neural network has been used to calculate joint loading from ground 232 233 reaction forces and gait kinematics (Ardestani et al., 2013, Ardestani et al., 2014) and ground reaction force from gait 234 kinematics (Oh et al., 2013, Ren et al., 2008). In this study, neural network was employed to calculate the contact pressure from gait kinematics. The high correlation that was found between the target values and the network 235 236 predictions for validation and test subsets reassures the reliability of the proposed structure. The TDNN in turn 237 necessitated involving the GA as the optimization technique. In fact, other classical optimization approaches mainly rely on iterative derivation of an explicit cost function however TDNN modelled the problem non-explicitly. 238

4. 2. Current research contribution

There are a number of implications on the gait modification and optimization both in terms of methodology and 240 241 findings. Major limitations of the previous studies were addressed in the present research. First, compared to 242 previous studies in which iterative "trial-and-error" MBD analysis has been used, this study presented a cost-243 effective computational alternative. TDNN provided a real-time cost function for the GA that could rapidly evaluate 244 the contact pressure associated with each potential gait pattern. Moreover, GA is a stochastic direct search method in 245 which the search data space is modified iteratively. This in turn reduced the computational effort required to find the 246 optimized solution. It should be pointed out that although various gait modifications have been developed in 247 association with knee joint offloading, none of them have vet been accepted as a general modification strategy. In 248 fact, due to the large inter-patient variability, reported in gait kinematics and joint loading patterns(Kutzner et al., 249 2010, Taylor et al., 2004), gait rehabilitation strategies should be determined patient specifically. Hence, to design a 250 gait modification strategy, it is crucial that the proposed computational method is cost-effective and easy to recreate.

Second, unlike the previous studies in which KAM reduction has been the principal goal of gait modification, here, contact pressure was adopted as a more accurate criterion for knee joint offloading. This in turn built more confidence in the efficiency of the proposed gait modification. Previous gait modifications were mainly designed to reduce knee joint moment. Although these modification patterns could decrease knee joint loading, none of them could decrease contact pressure at the knee joint bearing surfaces whilst the proposed gait pattern in this study could effectively decrease the contact pressure by up to 25% (see Figure 9).

Third, whilst previous studies have debated on the influence of increasing knee flexion, this study could address the contribution of knee flexion angle to the knee joint offloading in a systematic manner. Two optimizations were performed: first, knee flexion angle was kept within normal patterns to investigate whether it was possible to

decrease knee joint loading through adjacent joints effects. Second, knee flexion was allowed for a non-significant 260 261 increase. Results showed that in the first optimized gait, contact pressure was reduced by up to 21% whilst knee 262 flexion was preserved within normal walking. In the second optimized pattern, a more effective pressure reduction (25%) was achieved with a slight increase in the knee flexion at the cost of considerable increase in the ankle joint 263 forces at 40-60% of the gait cycle. This observation is consistent with previous studies (Fregly et al., 2007) and 264 suggests that perhaps the first optimization pattern in which joint reaction forces were within the experimental range 265 266 might be more physiologically feasible. Allowing the knee flexion angle to be more increased led to higher ankle 267 joint loading and a gradual reduction in the contact area which in turn increased contact pressure.

Overall, hip adduction, ankle flexion, subtalar eversion, pelvis posterior rotation and pelvis medial-lateral rotation were increased during the stance phase for both optimized gait patterns (see Figure 7). However it should be noted that the exact amount of kinematic changes, compared to normal gait, was not reported in this study since specific gait rehabilitation, designed for a particular subject, may not be equally applicable for other patients. Therefore, the quantitative amount of kinematic variations, compared to normal gait, was not focused in this study.

4.3. Limitations

There were several limitations in this study: (1) there was a lack of clinical investigation on the estimated 274 kinematics. Nevertheless, from a technical point of view, the predicted kinematic waveforms are expected to be 275 feasible since the TDNN was trained based on executable walking patterns. Once the network learns this dynamic, it 276 277 uses this dynamic as the acting function to respond to new sets of inputs. Therefore, it is unlikely that it would generate highly aberrant kinematics. Regardless, further investigations are required to test whether the predicted 278 279 kinematics is feasible to implement for compensatory or unexpected effects on the other joints or the contra-lateral limb; (2) rigid body constraints were applied to both the femoral and tibia components. Halloran et al.(2005) showed 280 that rigid body analysis of the tibiofemoral knee implant can calculate contact pressure in an acceptable consistence 281 with a full deformable model whilst rigid body analysis would be much more time-efficient. Therefore, in order to 282 produce the training data base, required to train the neural network, rigid body constraints were applied. This was 283 consistent with the present multi-body dynamic analysis in which no detailed modelling on the knee implant was 284 included; (3) a typical knee implant was adopted in the present study. Although this implant has been widely used in 285 literature (Clayton et al., 2006, Dalury et al., 2008, Ranawat et al., 2004, Willing and Kim, 2011), its dimensions 286 287 were different from the original knee prosthesis by which the subject was implanted. In fact, the subject was implanted with a custom-made sensor-based prosthesis which was specifically produced to measure in vivo knee 288 joint loading(Fregly et al., 2012). Accordingly, in this study, a typical commercial knee implant was preferred to test 289

the

290 <u>efficiency of the proposed knee rehabilitation patterns. Nevertheless, the proposed methodology should be equally</u> 291 applicable to other implant geometries and (4) the knee joint was modelled with only one DOF (flexion-extension). 292 Although six DOFs are possible for the knee joint, the dominant movement of the knee joint takes place in the 293 sagittal plane and knee joint has been mostly simplified as a hinge joint, especially for the knee rehabilitation design 294 purposes (Ackermann and van den Bogert, 2010, Anderson and Pandy, 2001, Fregly et al., 2007).

295 **5. Conclusion**

296 A time-delay neural network was embedded in a genetic algorithm to predict a gait pattern that would minimize the contact pressure at the knee joint bearing surfaces. The proposed algorithm suggested an optimum gait 297 298 pattern in which hip adduction, ankle flexion, subtalar eversion, pelvis posterior rotation and pelvis medial-lateral 299 rotation were slightly increased during the stance phase. Compared to the available gait rehabilitations, the proposed 300 gait pattern could decrease the knee contact pressure by up to 25%. Compared to the conventional MBD-based 301 framework in gait rehabilitation design, the present methodology facilitated a more practical and reliable design 302 procedure at a lower computational cost :(1) instead of using knee adduction moment, contact pressure was 303 considered as a more accurate criterion which led to a more efficient gait modification, (2) using the time-delay 304 neural network, the proposed computational framework was considerably faster and time-efficient. The 305 computational framework therefore can be easily repeated for any given subject. Moreover, (3) the conflicting effect of the knee flexion was addressed through two systematic optimization frameworks: (i) knee joint may be offloaded 306 307 without any changes in the knee flexion angle (ii) a slight increase in the knee flexion angle might better reduce 308 contact pressure but at the cost of ankle joint over loading and (iii) large increase in the knee flexion angle reduced 309 the contact area and yielded to an increase in the contact pressure.

Various future direction from this study can be considered: (1) on the methodological level, more rigorous tribological metrics (e.g. wear), constraints (e.g. energy expenditure) or gait balance requirements can be included into the computational framework to enhance the predications; (2) on the validation level, further clinical studies are required to validate the finding of such studies; (3) on a wider application level, the proposed methodology in this study has wider implications in design and development of rehabilitation protocols for broader numbers of subjects and other joints such as hip and ankle.

316 **Conflict of interest statement**

317 The authors have no conflict of interests to be declared.

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Table 1

Table 1 Description of gait kinematic features

Joint	Kinematic feature	Description	
Hip	H1	Hip flexion at initial contact	
Hip	H2	Maximum hip extension at stance	
Hip	Н3	Maximum hip flexion at swing phase	
Hip	H4	Hip abduction at initial contact	
Hip	Н5	Maximum hip adduction at midstance phase	
Hip	H6	Maximum hip adduction at stance phase	
Hip	H7	Hip external rotation at initial contact	
Hip	H8	Maximum hip internal rotation at swing phase	
Knee	KI	Knee flexion at initial contact	
Knee	K2	Maximum knee flexion at stance	
Knee	K3	Maximum knee extension at stance	
Knee	K4	Maximum knee flexion at swing phase	
Ankle	A1	Ankle flexion at initial contact	
Ankle	A2	Maximum ankle dorsiflexion at midstance	
Ankle	A3	Maximum ankle dorsiflexion at stance	
Ankle	A4	Maximum ankle plantar flexion at swing phase	
a 1 - 1			
Subtalar	S1	Subtalar inversion at initial contact	
Subtalar	S 2	Maximum subtalar eversion at stance	
Subtalar	S3	Maximum subtalar inversion at stance	
Subtalar	S4	Maximum subtalar eversion at swing	
Pelvis	PP1	Maximum posterior tilt of pelvis	
Pelvis	PP2	Maximum anterior tilt of the pelvis	
Pelvis	PP3	Maximum lateral obliquity of the pelvis	
Pelvis	PP4	Maximum medial obliquity of the pelvis	
Pelvis	PP5	Pelvis vertical position at initial contact	
Pelvis	PP6	Maximum pelvis upward position at stance	
Pelvis	PP7	Maximum pelvis downward position at stance	
Pelvis	PP8	Maximum pelvis upward position at swing	
D-1- '	DD 1	Delais anticipated and the state	
reivis	rK1	Pervis anterior rotation at initial contact	
Pelvis	PK2	viaximum peivis posterior rotation at stance	
Pelvis	PK3	Maximum pervise posterior rotation at swing	
Pelvis	PK4	Pelvis medial rotation at initial contact	
Pelvis	PR5	Maximum pelvis lateral rotation at stance	
Pelvis	PR6	Maximum pelvis medial rotation at stance	
Pelvis	PR7	Maximum pelvis lateral rotation at swing	
Pelvis	PR8	Pelvis axial rotation at initial contact	
Pelvis	PR9	Maximum pelvis axial rotation to the left at stance	
Pelvis	PR10	Minimum pelvis axial rotation to the right at stance	
Pelvis	PR11	Maximum pelvis axial rotation to the left at swing	

Table 2

Table 2 Genetic algorithm settings in MATLAB	
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Genetic algorithm parameter	Value
Population size	50
Scaling function	Rank
Selection function	Tournament
Elite count	2
Crossover fraction	0.85
Crossover function	Single point
Mutation function	Adaptive feasible
Maximum number of generations	100



(b)

Figure 1 (a) Experimental gait measurements were imported into multi-body dynamics analysis to calculate joint kinematics/kinetics which were then used by finite element analysis to calculate contact pressure (b) Joint angles were parameterized by extremum features (red circles). Due to the periodicity of the gait, joint angle values at the end of the gait cycle (gray points) were equal to the initial values at 0% of the gait cycle except for pelvis anterior-posterior position.



Figure 2 A schematic diagram of a four-layer TDNN used in this study. The network calculated the maximum values of contact pressure (output) based on gait features (inputs).



Figure 3 The flowchart of the proposed TDNN-GA.



Figure 4 Network predictions versus actual CPRESS-max values for (a) train (b) validation and (c) test subsets.



Figure 5 Mean and standard deviation of the optimized CPRESS-max for different values of crossover fraction in the GA process.





Figure 6 Convergence of the GA for (a) the first optimization problem in which the knee flexion angle was bounded to normal patterns,(b) the second optimization problem in which the knee flexion angle was allowed to increase beyond normal pattern. "fitness" refers to the calculated value of CPRESS-max for each individual.



Figure 7 Kinematics of the first optimized gait pattern (black line) and the second optimized pattern (pink line) laid within the extent of experimental gait trials (gray span). Those kinematics that underwent considerable changes have been marked by



Figure 8 Resultant joint contact forces of the first optimized gait pattern (black line) and the second optimized pattern (pink line) laid within the extent of experimental gait trials (gray span).



Figure 9 The resultant maximum values of contact pressures for the optimized gait patterns versus contact pressures obtained from normal gait and other previously published gait modifications.

Supplementary Material Click here to download Supplementary Material: Appendix.docx