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An approach for improving repeatability and reliability of non-negative matrix factorization for muscle synergy analysis

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ABSTRACT

The aim of this study was to evaluate non-negative matrix factorization (NMF) and concatenated NMF (CNMF) to analyze and reliably extract muscle synergies. NMF and CNMF were used to extract knee joint muscle synergies from surface EMGs collected during a weight bearing, force matching task. Repeatability and between subject similarity were evaluated for each method using intra-class correlation coefficients (ICCs). High repeatability was found for CNMF (>0.99; 0.99–1.0) compared to NMF (>0.26; range 0.26–0.98). Reasonable consistency across subjects was improved using the CNMF over the NMF approach. CNMF was found to be a more reliable approach than NMF and suitable for between subject comparison of muscle synergies.

1. Introduction

The neuromuscular system is highly complex and how the central nervous system coordinates synergistic muscle activation during functional tasks remains unclear. The method of non-negative matrix factorization (NMF) to gain this insight has been increasing in popularity in recent years (Ting and Macpherson, 2004; de Rugy et al., 2013; Kristiansen et al., 2015; Moghadam et al., 2011; Neptune et al., 2009; Torres-Oviedo et al., 2006). NMF is a linear decomposition technique that outputs the optimized basis (synergy) vectors and corresponding weight (coefficient) vectors through minimizing the error between the original signal and the reconstructed data. NMF is a mathematical technique and has been used by a number of studies for simplifying the representation of muscle activities using electromyography (EMG) values obtained during various tasks in animals and humans (Ting and Macpherson, 2004; de Rugy et al., 2013; Kristiansen et al., 2015; Moghadam et al., 2011; Neptune et al., 2009; Torres-Oviedo et al., 2006; Allen and Neptune, 2012; Tresch et al., 2006, 1999; Walter et al., 2014). For example, Torres-Oviedo et al. (2006) were able to account for more than 80% of the total variability in the EMG signals during direction dependent perturbations in cats with only five synergies. Neptune et al. (2009) were successful in optimal control of 2D gait using five synergies. Kristiansen et al. (2015) determined only two synergies were required for bench pressing: one for eccentric phase and one for concentric.

However, as an optimization-based mathematical data decomposition approach, NMF has pitfalls such that its results may not be physiologically relevant. Specifically, NMF might have many local minima (Lee and Seung, 2000) caused by (1) scaling optimal coefficients and synergies by an invertible matrix so that the error still remains the same, (2) swapping of the coefficient/synergy indices (Shourijeh et al., 2014), and (3) non-convergence of the optimization problem, thus leading to unrepeatable results.

In order to address this repeatability issue, Frère and Hug (2012) proposed using paired comparisons for each extracted synergy and generating a number of random permutations of the coefficients. This resulted in 3600 Pearson coefficients. Although their results yielded mean *r*-values >0.71, suggesting the outputs of NMF are repeatable for each subject, the evaluation for the synergies and coefficients were performed separately. Since the variability is split between coefficients and synergies, this method may not be an appropriate representation of the repeatability because the coefficients and synergies are analyzed independently. To our knowledge, no other study has attempted to evaluate the within subject repeatability of NMF.

Another issue arises when trying to use the NMF to evaluate the similarity between subjects in a given group. Frère and Hug (2012) used paired comparisons for their 9 subjects where one subject was arbitrarily set as the reference (control subject). The synergy

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of a second subject was then fixed to the control and coefficient matrix was computed. This method was then repeated to compute the synergy matrix but with the coefficient matrix being fixed. This approach was used by Kristiansen et al. (2015) for bench press movement as well. Similarly, Torres-Oviedo et al. (2006) used paired comparisons to evaluate the consistency of muscle synergies across cats and determined that the synergy output and recruitment patterns were statistically similar, as determined by separate paired comparison of synergies and coefficients. Aside from the tedious process required to evaluate many paired cases, the differences are split between those considered pairs, and also between two variables of coefficients and synergies. Thus, interpretation of the similarity of the NMF outputs may not be valid. NMF is based on subject-by-subject analysis, and it is not encouraged to disassociate synergies and coefficients when evaluating between subject differences (Shourijeh et al., 2014).

Furthermore, due to the local minima issue, NMF outputs require a functional sorting method when comparing different sets of data. Some have tried to reorganize the indices by finding the maximum R^2 between the repeated runs or between subjects (Torres-Oviedo and Ting, 2007). However, it is debatable whether R^2 is an appropriate measure or other quantities, such as intra-class correlation coefficient (ICC), that take the pattern comparison into account only. Regardless of what measure is used for order reorganization, it might not be conclusive as the synergy order switch has occurred along with a numerical local minimum effect, in which case the sorting might be done by a poor R^2 (or ICC) value.

Very recently, Oliveira et al. (2014) studied the influence of concatenating the data of several walking step cycles (trials) on muscle synergy extraction. They showed that data concatenation provided better quality of reconstruction compared to that based on ensemble averaging the data of the gait cycles, but in comparison with single gait cycle analysis, concatenated approach led to less reconstruction quality. However, as they ran NMF on subjects' data separately, they still had the issue of intra-subject similarity assessment mentioned earlier.

In order to address the aforementioned issues and determine the efficacy of non-negative matrix factorization in identifying control strategies it may be useful to first explore tasks which are highly repeatable and limit biomechanical variables that make drawing conclusions about the role of the synergy difficult to ascertain. Furthermore, the mathematical method used needs to provide repeatable and consistent results. If this condition is met, between-subject comparison might be investigated and the similarity of activation patterns assessed.

We have developed a weight-bearing ground reaction force (GRF) task which is functional (Flaxman et al., 2012), repeatable (Smith et al., 2012) and highly controlled while still allowing conclusions to be drawn with respect to joint stabilization roles of the knee joint musculature (Flaxman et al., 2012). The purpose of this study is to present and evaluate a concatenated non-negative matrix factorization (CNMF) approach using this dataset (Flaxman et al., 2012) by exploring the repeatability and robustness of matrix factorization under highly controlled conditions. A concatenated matrix will be formed that consists of the EMG signals of all subjects; there will be a corresponding concatenated coefficient matrix that includes the coefficient array of all subjects. An unknown synergy will be kept fixed between all subjects (and/or trials -- if any), which will be determined within the CNMF. We hypothesize that CNMF will be more repeatable and robust than the NMF and its results will therefore facilitate the evaluation of similarity between subjects, as we will be left with only coefficients to be compared. If these conditions are met, this approach would provide a representative synergy matrix outputted from the CNMF that could be used to compare between populations.

2. Methods

2.1. Experimental data

Previously reported data (Flaxman et al., 2012) from eight healthy active males (age 23.9 ± 1.9 yrs.; weight 79.77 ± 9.3 kg; height 1.77 ± 0.05 m; body mass index 25.4 ± 0.06 kg/m^2) were used for analysis. Exclusion criteria included a history of significant lower limb injuries (e.g. ligament rupture), lower limb sprains or fractures within 6 months of participation, or any other physical impairment that may influence knee function. All subjects read and signed an informed consent form. The study was approved by the University of Ottawa Research Ethics Board.

Subjects stood in a staggered stance such that their dominant leg (defined by leg used to kick a ball as far as possible) had joint angle positions of 30° hip flexion, 30° knee flexion, and 10° ankle plantarflexion. The dominant foot was placed in a water-ski boot fixed to a force platform (FP4060-08, Bertec Corp., Columbus, OH) which was used to control a projected image of a cursor by pushing against the force platform with their foot, similar to controlling a computer mouse. The cursor moved upwards/downwards and left/right by generating respective anterior/posterior and medial/lateral GRFs. The size of the cursor was controlled by the amount of body weight exposed to the test leg. Twelve force targets randomly appeared about a circular trajectory in directions spaced by 30°, representing various combinations of medial–lateral–anterior–posterior GRF directions. A successful trial was defined when the subject matched the cursor to a force target for one second; requiring 30% of previously recorded maximal GRF and 50% body weight. Group mean (std) GRF required to reach the anterior, posterior, medial and lateral targets were 0.52 (0.12), 0.45 (0.13), 0.47 (0.14), and 0.43 (0.18) N/kg respectively, levels similar to the magnitude of the GRF shear forces in running initiation (Mademli et al., 2008), and vertical jump landing (McClay et al., 1994). Each target was to be matched three times for a total of 36 trials.

A successful trial triggered data collection of kinematics, GRFs, and surface EMG. Bipolar surface EMG electrodes (SP-E04, DE 2.1, Delsys Inc., Boston, MA) connected to a 16-channel EMG system (DS-B04, Bagnoli-16, Delsys Inc., Boston, MA) were placed over the muscle bellies of the rectus femoris (RF), vastus medialis (VM), vastus lateralis (VL), semitendinosus (ST), biceps femoris (BF), medial gastrocnemius (MG), lateral gastrocnemius (LG), and tensor fascia lata (TFL) of each leg. Electrode placements followed the recommendations by SENIAM (Hermens et al., 2000). Functional tests were also performed during setup to ensure proper placement and check the EMG signal to noise ratio (Hermens et al., 2000). In order to minimize the effect of low frequency artifact while maintaining the broadest myoelectric signal power for our given application (Stegeman and Hermens, 1998; Clancy et al., 2002; Van Boxtel, 2001; De Luca et al., 2010), EMG signals were sampled at 1000 Hz, amplified by a gain of 1000, and band-pass filtered at 20–450 Hz before A/D conversion using a 16-bit board (NI PCI 6229, National Instruments Corp., Austin, TX).

Each subject's EMG was processed to obtain a linear envelope (full wave rectified and low pass filtered with 4th order dual pass Butterworth filter (6 Hz)) for each trial, normalized to previously recorded maximum voluntary isometric contraction, time averaged over the one second of the force match, and ensemble averaged over repetitions for each target location.

2.2. NMF

For standard NMF analysis (e.g. as in Ting and Macpherson (2004)), a solver builds two matrices such that the error of $A-CS$

is minimized, where A (12×8), C ($12 \times N_s$), and S ($N_s \times 8$) represent the matrices of muscle EMG data, coefficients, and muscle synergies, respectively (number of directions = 12; number of muscles = 8; N_s = number of synergies to be determined). It is assumed that muscle EMG can be reconstructed by more than one synergy. The contribution of a given muscle at a specific direction is the sum of the activations from each synergy multiplied by each synergy's scaling coefficient at that direction. For instance, the reconstructed EMG value of MG at 270° (posterior) must be computed as $\sum_{i=1}^{N_s} C_{270^\circ,i} S_{i,MG}$ where $C_{270^\circ,i}$ (1×1) and $S_{i,MG}$ (1×1) represent the i^{th} coefficient and synergy values at 270° and for MG, respectively where i is the synergy index.

The total variance accounted for (VAF) versus the number of synergies will be studied. VAF for individual participants is defined as

$$\mathrm{VAF} = \left(1 - \frac{\sum_{k=1}^{12}\sum_{j=1}^{8} \varepsilon_{kj}^2}{\sum_{k=1}^{12}\sum_{j=1}^{8} A_{kj}^2}\right) * 100 \quad (1)$$

where ε is the error, i.e., $A-CS$, and the indices k and j designate the rows and the columns of the quantities ε and A.

As NMF is based on trial-by-trial (or subject-by-subject if trials are averaged for each subject) analysis, a sorting post-processing is required, as the synergies and coefficients are inter-versed between trials/subjects. An algorithm used here was inspired from Torres-Oviedo and Ting (2007). Sorting is based on finding maximum R^2 between S and/or C by comparing signals to an arbitrarily chosen reference subject.

2.3. Concatenated NMF (CNMF)

For the CNMF approach, the decomposition vectors along with the original signal data are processed in a concatenated way such that matrix A^c will be 96-by-8, where the number 96 represents 8 subjects multiplied by 12 directions. This CNMF approach has the following objective function:

$$J = \sum_{i=1}^{N_P} \frac{\|A_i^c - C_i^c S\|_F}{\|A_i^c\|_F} \quad (2)$$

where N_P is the number of participants, F represents the Frobenius such that $\|A\|_F$ is the Frobenius norm of a vector that is defined as $\sqrt{tr(AA^{\mathrm{T}})}$. tr represents matrix trace and A^T is the conjugate transpose of matrix A (i.e. the transpose of matrix A as the matrix consists of real numbers only). Note that the coefficients matrix will also be concatenated. The C^c will be 96-by-N_s, whereas the S matrix will remain N_s-by-8. Correspondingly, the concatenated VAF (VAF^c) is defined as:

$$\mathrm{VAF}^c = \left(1 - \frac{\sum_{k=1}^{96}\sum_{j=1}^{8} \varepsilon_{kj}^2}{\sum_{k=1}^{96}\sum_{j=1}^{8} A_{kj}^2}\right) * 100. \quad (3)$$

2.4. Factorization framework

The framework used in this study is shown in Fig. 1. First, random matrices of C and S were attained from *rand* function in MATLAB (MATLAB, 2013). Second, the MATLAB *nnmf* routine used an alternating least squares algorithm to find optimal C and S that satisfy the minimum Frobenius norm of the error $J = \|A - CS\|_F$. The optimal C was then used in a non-negative least squares algorithm (MATLAB *lsqnonneg*) to calculate optimal synergy matrix. Afterwards, the optimal S coming out of *lsqnonneg* was used in an *fmincon* routine with non-negativity bounds to find optimal coefficient matrix. Note that some studies have used only *nnmf* (e.g. Moghadam et al., 2011). A combination of *lsqnonneg* and *fmincon* had been used by Ting and Macpherson (2004). We have added an additional phase in the loop in order to perturb the optimal

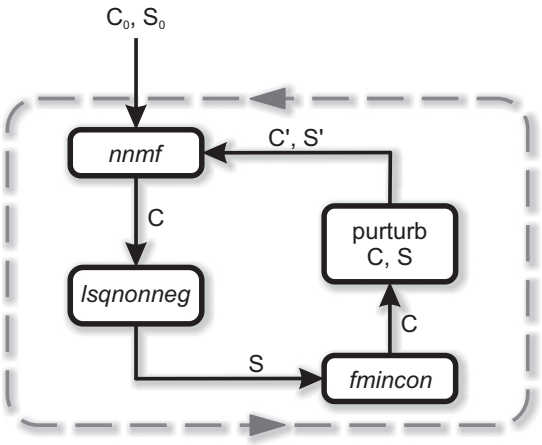

Fig. 1. Framework schematic used for synergy identification: C is the coefficient matrix and S is the muscle synergy array; C_0 and S_0 are the random initial matrices of coefficients and synergies, respectively. *nnmf*, *lsqnonneg*, and *fmincon* are MATLAB routines for non-negative matrix factorization, non-negative least-squares optimization, and constrained gradient-based optimization, respectively.

solution of the series of *nnmf*, *lsqnonneg*, and *fmincon* by adding random values $\tilde{e}_C$ and $\tilde{e}_S$ to C and S, respectively (i.e. $C' = C + \tilde{e}_C$ and $S' = S + \tilde{e}_S$) using MATLAB *rand* function. The whole framework was iterated three times. For the last iteration, the perturbation was not done, and the final solutions of S and C were outputted from *lsqnonneg* and *fmincon*, respectively. Table 1 shows the settings used with these routines.

To evaluate the repeatability of the coefficient and synergy vectors of the non-negative matrix factorization, 5 sets of results were computed for comparison.

NMF might have many local minima; one special case is the following: assume that the objective function is the Frobenius norm of the error, $J^* = \|A - C^*S^*\|_F = \|A - \widehat{C}\widehat{S}\|_F$ with the new local solutions of $\widehat{C} = C^*B^{-1}$ ($\widehat{C} \geqslant 0$), $\widehat{S} = BS^*$ ($\widehat{S} \geqslant 0$) for any invertible matrix B where star sign represents an optimum solution and hat sign designates an alternative solution (Rickard and Cichocki, 2008). One special case of this is when the matrix B is simply a scalar $\{n \in \mathbb{R} : n > 0\}$, then $\widehat{C} = \frac{1}{n}C^*$ and $\widehat{S} = nS^*$. Therefore, for any value of n that belongs to positive real numbers, new C and S will be another local minimum for the problem. Although this is an inevitable series of local minima when using *lsqnonneg* and *fmincon* (e.g. as used in Ting and Macpherson (2004)), the issue is not applicable while using function *nnmf* in MATLAB as it finds optimal C and S such that each row of S has a length of unity, which will therefore remove a set of local minima from consideration.

2.5. Intra-class correlation

To investigate the repeatability and between subject similarity, intra-class correlation coefficients (ICCs) were calculated. Based on McGraw and Wong (1996), two-way mixed models for average

Table 1
Settings of the MATLAB routines used during data analysis as outlined in Fig. 1.

Setting	MATLAB routine		
	nnmf	*lsqnonneg*	*fmincon*
Algorithm	als[a]	active-set	sqp[b]
Function tolerance	1e−6	1e−6	1e−6
Search tolerance	1e−6	1e−6	1e−6
Factorization replicates	30	NA	NA
Constraint tolerance	NA	1e−6	1e−6

[a] Alternating least squares.
[b] Sequential quadratic programming.

measurements with no interactions ($ICC_{(C,k)}$) were used to evaluate the within-target variance of C and S across the 5 repetitions. The similarity between subjects in C and S was also evaluated with $ICC_{(C,k)}$ but with subjects being the measure of repeatability. Based on page 82 of Portney and Watkins (2008), ICC < 0.5, 0.5 < ICC < 0.75, and ICC > 0.75 imply low, moderate, and high correlation, respectively.

3. Results

3.1. Synergy identification using NMF and CNMF

Table 2 shows the individual and concatenated VAF values for the NMF and CNMF approaches: 4 synergies accounted for 95% of the concatenated variance (VAF_c), which is equivalent to mean VAF_i of 97.6%; the corresponding value for NMF is 99.6%.

Figs. 2(a and c) show 4 synergies and respective coefficients of each subject using NMF. Figs. 2(b and d) show 3 synergies and corresponding coefficients of each subject by running NMF. Horizontal axes in coefficient plots show the directions at which the subjects exerted their net planar ground reaction force; 0°, 90°, 180°, and 270° represent lateral, anterior, medial, and posterior directions, respectively. It must be noted that the contribution of a muscle in a direction specific to a synergy group selected is calculated by multiplying the coefficient specific to the direction by synergy of a muscle. For instance, in P1\S1, MG will have a significant contribution at 120° as in P1\C1; the coefficient and synergy values are 0.79 and 0.85, respectively.

Fig. 3(a and c) depict the results of synergies and coefficients of a case with 4 synergy groups using CNMF approach, while Fig. 3(b and d) show similar outputs for a case with 3 synergy groups.

The sorting method for the NMF results may affect the repeatability. For instance, we arbitrarily chose run #1 in our study as the reference once; however, if we changed the reference to run #5, then the minimum ICC increased from 0.26 to 0.64. In contrast, the CNMF does not rely on a reference run. Furthermore, as detailed later, CNMF results were highly repeatable. Therefore, as a post-processing step, results of the NMF in Fig. 2 were sorted by setting CNMF synergy vector as the reference and finding maximum R^2. This was done only for the sake of result presentation and easier comparison between NMF and CNMF outputs.

3.2. Repeatability

NMF: The NMF required the synergies and respective coefficients to be sorted by finding maximum R^2 of S and C between run 1 (as an arbitrary reference) and runs 2–5. There were 160 ($4 * 8 * 5$) values for the ICCs of sorted outputs based on maximum R^2. For synergies, 122/160 cases yielded ICCs > 0.75 indicating high repeatability, 12/160 showed 0.5 < ICCs < 0.75 (moderate repeatability), and the last 26 cases had ICCs < 0.5 (poor repeatability). For coefficients, 101/160 cases yielded ICCs > 0.75 indicating high repeatability, 29/160 showed 0.5 < ICCs < 0.75, and the last 20 cases had 0.26 < ICCs < 0.5.

CNMF: Using the CNMF approach, ICCs were equal to or greater than 0.999 in all 8 subjects for both the coefficients and the synergies, indicating excellent repeatability for both variables.

3.3. Between subject ICC

NMF: ICC values for between-subject similarity of the NMF results were 0.67, 0.88, 0.63, and 0.65 for coefficients and 0.79, 0.92, 0.85, and 0.72 for synergy indices 1–4, respectively. The corresponding values for 3 synergies were 0.84, 0.88, and 0.82 for synergy similarity and 0.44, 0.88, and 0.75 for correlation between coefficients.

CNMF: The between-subject ICCs for coefficients using the CNMF were 0.84, 0.89, 0.72, and 0.90 for synergy indices 1–4, respectively. The values for 3 synergies were 0.68, 0.90 and 0.89 for synergy indices 1–3, respectively.

4. Discussion

This study investigated the repeatability and between subject reliability of the NMF method to identify muscle synergies. We also introduced a concatenated approach (CNMF) in order to be more objective in synergy identification. We fixed the synergy vector across subjects, while coefficient vectors were subject-specific. Although the regular NMF approach is fully subject-specific, it is not as repeatable as CNMF. More importantly, for between-subject comparisons, NMF requires a sorting method since the indices of synergies and coefficients change inconsistently among subjects. Although only 4 synergies were required to reconstruct >95% VAF, 3 synergies were believed to provide more distinct synergy groups of muscle EMG contents. We also observed very high ICCs (>0.999) in terms of repeatability when using the CNMF approach.

4.1. Repeatability

Although the repeatability of the majority of NMF synergies and coefficients were considered robust (ICC > 0.75), the lowest ICC values were 0.38 (subject 6, synergy 3) and 0.26 (subject 4, coefficient 2), respectively. Additionally, it is important to note that the variability is divided into two variables (synergies and coefficients), which implies that the overall repeatability of the NMF would be lower and thus less robust.

In addition, the sorting approach used in NMF is sensitive to the chosen reference run although previous studies (Kristiansen et al., 2015; Torres-Oviedo et al., 2006; Frère and Hug, 2012) arbitrarily set a subjects' data/run as the reference. Since the results of the CNMF were highly repeatable (ICCs > 0.999) we could assume them to be unique; we therefore set CNMF synergy results as reference to sort the NMF results. It must be noted that the sorting

Table 2
Variance accounted for of all muscles versus the number of synergies. VAF_i is the individual participant's VAF; and VAF_c is the concatenated VAF. Values are rounded to the first decimal place.

N_s	Individual % VAF (%VAF_i)								Mean (%VAF_i)	%VAF_c
	P1	P2	P3	P4	P5	P6	P7	P8		
NMF										
3	97.3	94.1	99.7	97.7	99.9	94.1	98.0	99.6	97.6	NA
4	99.8	99.2	100.0	99.9	100.0	99.4	99.3	99.7	99.6	NA
5	100.0	99.8	100.0	100.0	100.0	99.7	100.0	100.0	99.9	NA
CNMF										
3	90.4	87.3	90.2	78.2	97.3	86.0	92.1	95.5	89.6	84.6
4	95.6	97.8	99.5	97.1	99.6	96.8	95.9	98.9	97.6	95.0
5	96.7	98.4	99.4	97.2	99.8	97.8	96.8	99.1	98.2	98.1

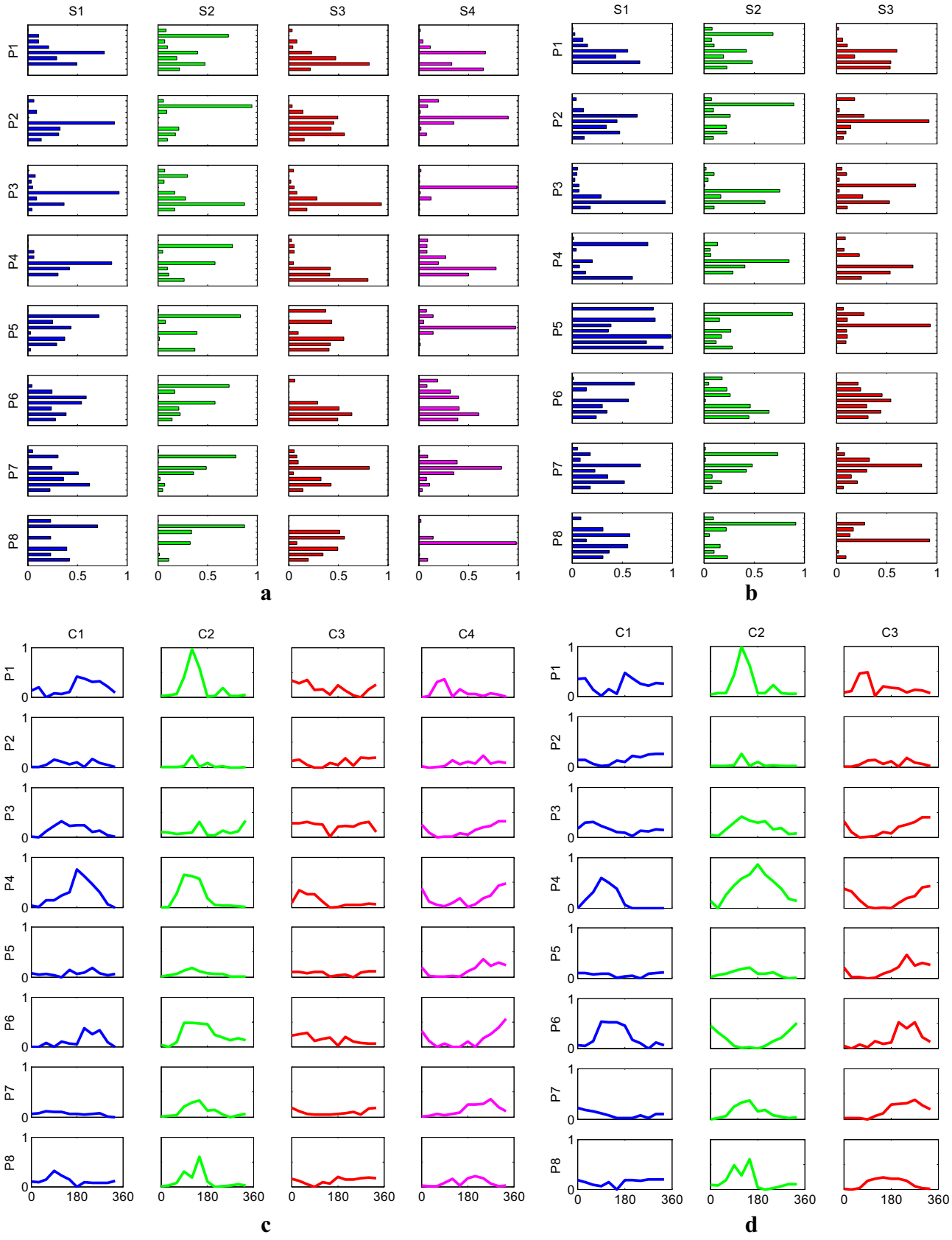

Fig. 2. Individual muscle synergies (a and b) and coefficients (c and d) of 8 subjects with 4 (left column) and 3 (right column) synergies by running NMF. For synergy plots, *y*-axes are the labels for muscles, from bottom to top: RF, VL, VM, BF, ST, LG, MG, and TFL. P stands for participant; the *x*-axis of the coefficient plots shows the direction of the resultant planar ground reaction force: 0°, 90°, 180°, and 270° represent lateral, anterior, medial, and posterior directions, respectively.

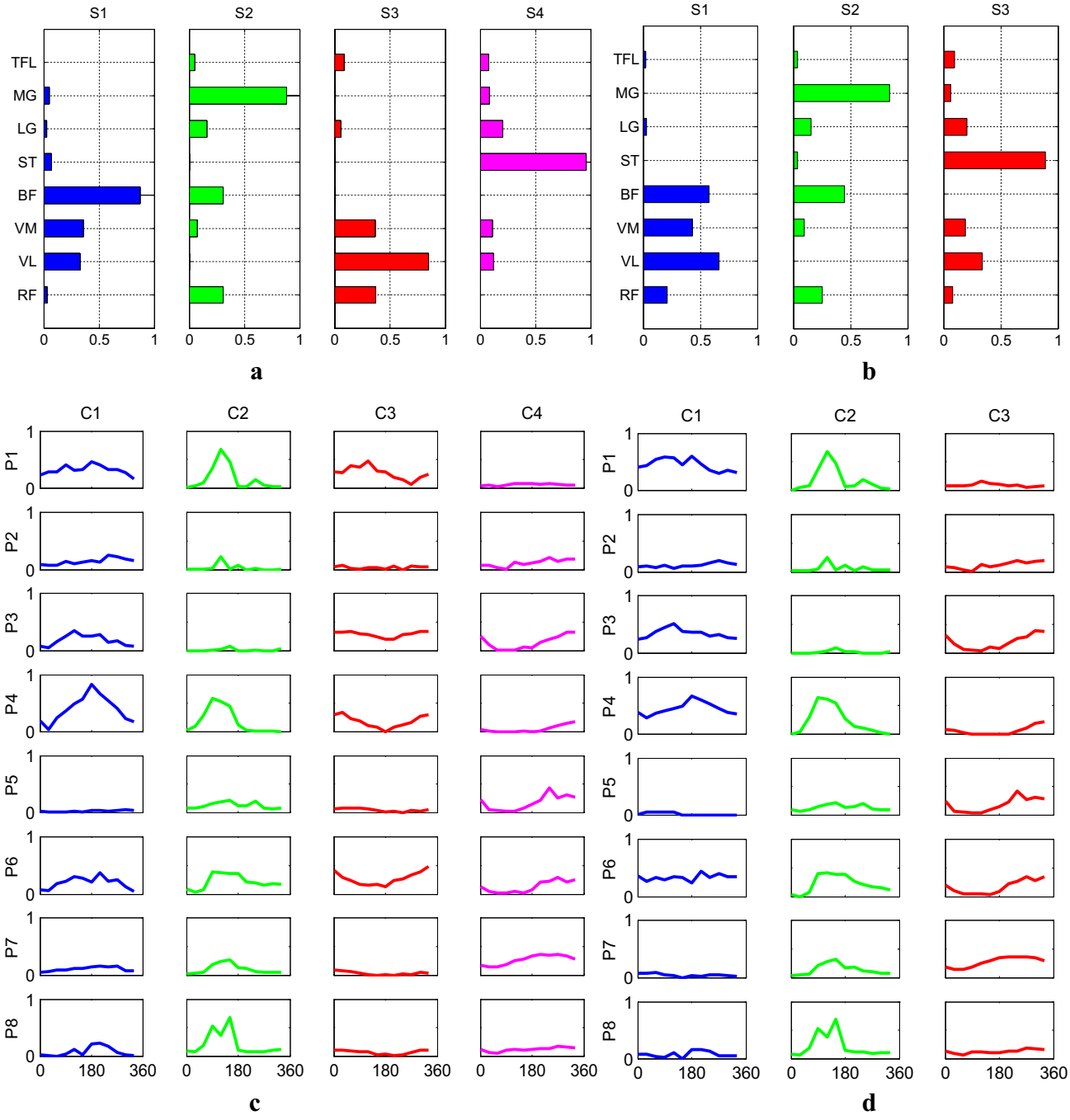

Fig. 3. Optimal synergy (S) and coefficient (C) vectors by running CNMF for a case that (a and c) 4 synergies and (b and d) only 3 synergies are taken into account.

was done post hoc and does not have any effect on the VAF nor quality of reconstruction; furthermore, regardless of the reference data, this approach will provide sorted data but does not imply between-subject similarity. Subject similarity between results might be seen if the original data have insignificant variability between subjects, if the NMF results are repeatable and reliable, and if a valid statistical measure is selected for sorting.

Additionally, sorting for some cases had to be numerically made based on very low ICC or R^2 values (e.g. less than 0.25). Therefore, the sorting approach, as well as being inefficient, is not objective and could significantly affect the results. For example, one might be fairly successful to functionally sort the synergies and coefficients based on either visual or numerical (using R^2; Torres-Oviedo and Ting, 2007) inspection; however, as the NMF approach is prone to get stuck at a different local minimum in different runs, this inspection might lead to unphysiological deductions. In contrast, the aforementioned issues are not present when using CNMF and it can yield near perfect ICCs (0.999+) across all subjects.

One argument could be about the number of datasets one needs to concatenate in order to get repeatable CNMF results. To address this, a test was done in which it was found that by including 5 arbitrarily selected subjects, an ICC of >0.75 was acquired for repeatability of the 5 runs. Of course, this number can change depending on the variability in the data, the number of data points included (12 for each subject in this study), and the convergence of the factorization solver, all of which affect the generalizability of the CNMF approach to data from populations with higher variability, such as pathological subjects' data.

4.2. Between subject ICC

Although the ICC values showed moderate to high correlation between the subjects (ICCs > 0.63 for four synergies), again note that differences of the NMF outputs are split into both variables of C and S, and may be an overestimation of the overall between subjects similarity. Additionally, possible combination of convergence to local minima and synergy index shift may have also occurred, meaning a numerical resorting approach might have been inconclusive.

As stated by Lee and Seung (2000), NMF algorithms are convex in terms of only C or only S matrices, but it is unrealistic to expect an approach to guarantee a global minimum for C and S simultaneously, meaning the problem has most probably several local minima. As such, one major drawback of the subject-by-subject NMF analysis is that there are various local minima available, meaning if an NMF solver is run over a single set of data several times, different results will be acquired. There are different combinations of C and S that can reconstruct the signal with nearly minimum error with the original signal. One special case is 'order switch' of the synergies (Shourijeh et al., 2014). When this occurs, two rows of the coefficients are swapped along with the corresponding columns of the synergies matrix; the objective function will still have the same value, so it is unreasonable to expect the optimizer to find the solution as expected. Although a numerical sorting was performed, for some cases, no obvious distinction could be observed that justified the numerical sorting. This can be due to a local minimum, order switch, an unknown combination of both, or inherent between-subjects data variability. Similar misinterpretations can be made by looking at the synergies. Therefore, between-subject comparisons using NMF might be misleading. To minimize this problem, Torres-Oviedo and Ting (2007) rearranged the synergy and coefficient vectors using R^2; however, this approach can be error-prone in a general case due to the characteristics of the R^2 statistic. Furthermore, the use of an arbitrary reference might be misleading as well since one subject's results might be coming from a local minimum, or even though it is an optimal one, it is not a desired representative of the synergy groups.

To circumvent these issues, the concatenated strategy identifies a single synergy across data sets (subjects and/or trials). By fixing synergies across subjects in the CNMF approach, the search will be limited to finding one concatenated matrix of coefficients and one vector of synergies with the same size compared to that of NMF and the orders of coefficients will not be inter-versed between subjects, i.e., they are automatically organized. Also, the CNMF framework includes 416 optimization variables [C: $8*(12\times4)$, S: 4×8] whereas the NMF approach uses 640 variables, consisting of eight independent runs on eight subject's data, for each of which equals 80 variables (C: 12×4, S: 4×8). As the total number of decision variables (i.e. the dimension of the search space) are reduced by 35%, the number of local minima in CNMF has decreased substantially relative to NMF. These differences will lead to a more robust solution as evidenced by its greater between subject ICC values (0.72–0.90 and 0.68–0.89 for four and three synergies, respectively) compared to NMF (synergies: 0.63–0.88 and 0.82–0.88 for four and three synergies, respectively; coefficients: 0.72–0.92 and 0.44–0.75).

4.3. 4 or 3 synergies

Visual inspection of coefficients in Fig. 3c of synergies 3 and 4 (C3 and C4) shows the curves in C3 and C4 peak similarly at the beginning and at the end of the direction range. Although their coefficients are fairly similar, their synergies look distinct; i.e., S3 has high weightings of VM, VL, and RF, while S4 has high weightings of ST. This means that the extracted C vectors, although leading to a very high VAF, are not visually distinct. As a test, we reduced the number of synergies to 3 where we observed that synergies one and two changed minimally (ICCs 0.89 and 0.99) while the new synergy 3 is mostly a combination of the old synergies 3 and 4. Interestingly, the coefficients are nearly the same (ICCs > 0.86, 0.94, 0.97 for respective C1, C2, and C3 of three-synergy case versus C4 of four-synergy). In the authors' opinions, the coefficient outputs of the three-synergy case are more distinct than those of the four-synergy case. Despite the VAF decrease, it is still high enough to imply a good quality of reconstruction of the original data (VAF = 89.6) although it is against some literature-defined criteria, e.g. VAF > 0.9 (Oliveira et al., 2014) or VAF > 0.95 (Ting and Macpherson, 2004). It should be noted that in case 3 synergies are selected, the repeatability ICCs are still >0.99. Therefore, the proposed approach is remarkably repeatable regardless of the number of synergies finally selected, which depends on the preferred value for the total VAF and/or the desired yet physiologically meaningful distinction between synergy/coefficient groups.

It might be argued that by concatenating data across subjects, synergy analysis is necessarily constraining consistency between subjects, leading to lower individual VAF. However, even though the synergies are fixed, CNMF leaves the coefficient free to fluctuate, preserving subject specificity. Individual mean VAF only decreases 2.7% (from 97.6% to 95%; Table 2) resulting in nearly perfect subject specific reconstruction. Although CNMF fixes synergies across subject/trials, it was utilized as a representation technique that can evaluate grouping and temporal contents of muscle EMGs. It must be noted that NMF is a mathematical representation approach and although studies have used it for muscle synergy analysis, there is no factual evidence that synergy and coefficient vectors are physiologically representative of CNS control. That said, if the approach is to be used to help interpret physiological events, the first step is applying a technique that is repeatable and robust, and our technique is a step in this direction.

In this study, data from young healthy active adults were used, which we deemed physiologically reasonable to be concatenated since previous work showed high between subject reliability of the data used (Flaxman et al., 2012) and we can conclude our approach improved the repeatability and robustness of the factorization. However, like with NMF, the repeatability and robustness also depends on variability in the dataset, number of data points included, and convergence of the factorization solver. The generalizability of our method must therefore be taken in the context of the above factors. Future users of our approach must consider how their testing conditions might affect the solver and interpret their results within this context. Furthermore, a number of options exist for comparing between conditions and/or groups and will depend on the research question. For example, in an intervention study synergies can be fixed based on a precondition and then used to reconstruct post-intervention, leaving the coefficients to vary and act as the dependent variable. Conversely, two groups can be analyzed separately (healthy vs injured) and using the healthy as the 'gold standard' statistical testing of both the synergy and coefficient vectors can be made.

Finally, regarding the proposed optimization framework in Fig. 1, we ran a test using only *nnmf* to evaluate the effect of other phases. Running only *nnmf* on the proposed CNMF made less than 2% of change on the ICCs compared to the case that the whole framework was applied. Therefore to simplify and to speed up the process, others might prefer to remove the *lsqnonneg, fmincon* and perturbation phases.

5. Conclusions

A novel way of using the NMF approach was detailed for running analysis on muscle EMGs. To increase robustness, the CNMF

approach keeps synergies fixed across subjects while a concatenated coefficient matrix is composed of individual subject coefficient arrays. Additionally, CNMF circumvents the subjective and unreliable sorting step required by the classic NMF. Combined, these results support our hypotheses that CNMF is more repeatable and robust than traditional NMF and a more appropriate tool for evaluating similarity between subjects and differences across groups.

As applications of muscle synergies are growing in rehabilitation and motor control research every day, the CNMF approach will be helpful for deductions on muscle synergies and EMGs from different subjects and populations in different movements.

This study tested the CNMF for extracting muscle synergies in a static weight-bearing task. Although CNMF, like NMF, is a representation technique from the mathematics standpoint and can be applied on any dataset; as a future extension of this research, one study can be to verify this technique in dynamic movements that are cyclic and have been undergone synergy analysis before, such as walking, running, and squatting and investigate physiological relevance of the outputs.

Conflict of interest

The authors hereby declare to have no conflict of interest.

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