A Unifying Framework for the Identification of Motor Primitives

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Abstract

A long-standing hypothesis in neuroscience is that the central nervous system accomplishes complex motor behaviors through the combination of a small number of motor primitives. Many studies in the last couple of decades have identified motor primitives at the kinematic, kinetic, and electromyographic level, thus supporting modularity at different levels of organization in the motor system. However, these studies relied on heterogeneous definitions of motor primitives and on different algorithms for their identification. Standard unsupervised learning algorithms such as principal component analysis, independent component analysis, and non-negative matrix factorization, or more advanced techniques involving the estimation of temporal delays of the relevant mixture components have been applied. This plurality of algorithms has made difficult to compare and interpret results obtained across different studies. Moreover, how the different definitions of motor primitives relate to each other has never been examined systematically. Here we propose a comprehensive framework for the definition of different types of motor primitives and a single algorithm for their identification. By embedding smoothness priors and specific constraints in the underlying generative model, the algorithm can identify many different types of motor primitives. We assessed the identification performance of the algorithm both on simulated data sets, for which the properties of the primitives and of the corresponding combination parameters were known, and on experimental electromyographic and kinematic data sets, collected from human subjects accomplishing goal-oriented and rhythmic motor tasks. The identification accuracy of the new algorithm was typically equal or better than the accuracy of other unsupervised learning algorithms used previously for the identification of the same types of primitives.
Introduction

A fundamental challenge in neuroscience is to understand how the central nervous system (CNS) controls the large number of degrees-of-freedom (DOF) of the musculoskeletal apparatus to perform a wide repertoire of motor tasks and behaviors. A long-standing hypothesis is that the CNS relies on a modular architecture in order to simplify motor control and motor learning [1-3]. Many studies in recent years have indeed shown that kinematic [4-5], kinetic [6-7] and electromyographic (EMG) patterns [8-11] underlying complex movements can be approximated by the combinations of a small number of components, usually referred to as motor primitives or motor synergies. The identification of such components has typically been carried out by applying unsupervised learning algorithms, including principal component analysis (PCA), independent component analysis (ICA) [5, 12-15], non-negative matrix factorization (NMF) [15, 16] or other methods inspired by such algorithms [17]. While these classical methods are based on instantaneous mixture models, that linearly combine a set of basis vectors time-point by time-point, more advanced techniques have also been proposed that involve the estimation of temporal delays between relevant mixture components [15, 18-21]. This multitude of underlying mathematical models complicates the comparison of results from different studies on motor primitives. In addition, even for the same mathematical models often multiple algorithms for the estimation of motor primitives have been proposed, and it is not always clear if their results are comparable. This further complicates the comparison of the results. Finally, how the different definitions of motor primitives relate to each other has never been systematically examined. We propose in this article a new comprehensive framework for the definition of motor primitives and a new algorithm for their identification. We show that many different definitions of spatial, temporal and spatiotemporal primitives given in the literature can be derived from a single generative model that is known as “anechoic mixture” and relies on the combination of components that can be shifted in time. When the delays of all primitives are constrained to be zero, the anechoic model reduces to the instantaneous linear combination model, which underlies the definition of spatial or temporal synergies, usually identified by PCA, ICA or NMF. Similarly, when specific equality and non-negativity constraints are imposed on its parameters, the model can describe spatiotemporal synergies [9, 15]. In addition to this unification of models, we present a new identification algorithm that estimates motor primitives, according to the different definitions, with an accuracy that is equal or even better than the standard techniques that are commonly used for the identifications of these motor primitives. The robustness of this new algorithm results from an integration of smoothness priors and appropriate constraints in the underlying generative model. The new algorithm has been validated by assessing its identification performance both on simulated data sets, for which the properties of the primitives and of the corresponding combination parameters were known, and on experimental EMG and kinematic data sets, collected from human participants accomplishing goal-oriented and rhythmic motor tasks. The new algorithm is publically available, is provided as a toolbox in MATLAB (The Mathworks, Natick, MA) and can be downloaded for free from www.compsens.uni-tuebingen.de. In this way, we aim to provide the field of motor control with a new usable and robust tool for the identification of motor primitives, helping to reduce the inconsistencies and incompatibilities...
between the different generative models.

**Methods**

**Generative models for the description of motor primitives**

We give in this section a brief survey of the definitions of motor primitives and of the corresponding generative models that have been used in the literature for the investigation of the modular organization of motor behavior. The different approaches can be subdivided into different groups, according to the model features that are assumed to be invariant across conditions. In the following, a matrix $X_l$ indicates the data corresponding to a specific trial $l$ ($0 \leq l \leq L$), where $L$ is the total number of trials collected during an experiment. Each row of $X_l$ represents a specific degree of freedom (DOF) of the system under investigation (for instance an angular trajectory associated with a specific joint in the case of kinematic data, or the electrical signals associated with the contraction of a specific muscle in the case of EMG data). Each column of $X_l$ contains the values assumed by the different DOF at a particular point in time. Unless the size of the matrix is explicitly mentioned, from now on $X_l$ will be assumed to have $M$ rows (number of DOF) and $T$ columns (equivalent to the number of time samples in one trial). Signals are supposed to be sampled at constant sampling frequency and to have duration $T_s$. In the following, an individual column that corresponds to the time point $t$ of $X_l$ will also be signified by the column vector $x_l(t)$, so that $X_l = [x_l(1), \ldots, x_l(T)]$. The components of these vectors will be indicated by the variables $x_{ln}(t)$. In the following, we give an overview of different models for motor primitives that have been proposed previously in the literature.

**Spatial primitives**

One classical definition of motor primitive is based on the idea that groups of DOF might show instantaneous covariations, reflecting a coordinated recruitment of multiple muscles or joints. This implies the assumption that the ratios of the signals characterizing the different DOF remain constant over time. This type of movement primitive has been applied in particular in muscle space, where muscle synergies have been defined as weighted groups of muscle activations [3, 10, 22]. Such synergies have also been referred to as “synchronous” synergies, since the different muscles are assumed to be activated synchronously without muscle-specific time delays. Consistent with this definition is the following generative model that, from now on, will be referred to as ‘spatial decomposition’:

$$x_l(t) = \sum_{p=1}^{P} w_p \cdot c_p(t) + \text{residuals}$$

(1)

In this equation the vectors $x_l(t)$ indicate the values of the individual DOF at time point $t$ (assuming discrete time steps, $1 \leq t \leq T$) in trial number $l$. The column vectors $w_p$ define the ‘spatial patterns’ of the muscle synergies, which are assumed to be invariant over trials. The number of primitives is $P$, and the scalars $c_p(t)$ are the time-dependent mixing weights of the primitives. The mixing weights, as well as the residuals, are different in every trial. Processed
EMG data typically consists of time series of non-negative signals, i.e. $x_m^p(t) \geq 0$, for $1 \leq t \leq T$ and $1 \leq m \leq M$. In these models it is typically also assumed that the components of the mixture model (1) (except for the residuals) are non-negative, i.e. $c_{p}^l(t) \geq 0$ and $w_{p,m} \geq 0$ (where the subscript $m$ indicates the $m$-th element of the vector $w_p$).

**Temporal primitives**

An alternative way to characterize motor primitives is based on the idea that they express invariance across time, defined by basic temporal patterns or functions $s_p(t)$ that are combined or superposed in order to reconstruct a set of temporal signals. Temporal components based on this definition have been identified in kinematic [4-5, 18], dynamic [6] and EMG [8, 11-12] space. The underlying generative model (which from now on we will refer to as ‘temporal decomposition’) is mathematically described as:

$$x_m^l(t) = \sum_{p=1}^{P} c_{mp}^l \cdot s_p(t) + \text{residuals}$$  \hspace{1cm} (2)

In this equation $x_m^l(t)$ is the value of the $m$-th DOF at time $t$ in trial number $l$, and the corresponding scalar mixing weights $c_{mp}^l$ change between trials of different types (experimental conditions). The temporal primitives $s_p(t)$, however, are assumed to be invariant over trials. $P$ signifies the total number of temporal primitives. Another more elaborated model of this type has been proposed in [19, 21-23]. This model allows for temporal shifts between the temporal basis functions for different DOF. This can be interpreted as reflecting, for example, delays between the activation of different muscles within the same primitive. Mathematically, this model is characterized by the equations:

$$x_m^l(t) = \sum_{p=1}^{P} c_{mp}^l \cdot s_p(t - \tau_{mp}^l) + \text{residuals}$$  \hspace{1cm} (3)

The time shifts between the basis functions for the different degrees of freedom are captured by the variables $\tau_{mp}^l$. The time delays and linear mixing weights are typically assumed to vary over trials, while it is assumed that the basis functions $s_p(t)$ are invariant, as in model (2). Like for model (1), inequality constraints can be imposed on the mixing weights in models of type (2) and (3), for example to account for the non-negativity of EMG signals.

**Spatiotemporal (time-varying) primitives**

Spatiotemporal (or time-varying) primitives have been proposed as a way to model EMG components that are invariant in both, space and time [9, 15, 24]. Moreover, for each primitive additional temporal delays are admitted, similar to model (3). This results in the following generative model (referred to as ‘spatiotemporal decomposition’), where $x^l(t)$ signifies again the time-dependent column vector of the DOF as function of time:

$$x^l(t) = \sum_{p=1}^{P} c_{lp}^l \cdot w_p(t - \tau_{lp}^l) + \text{residuals}$$  \hspace{1cm} (4)
Again, the mixing weights $c_{lp}$ and the delays $\tau_{lp}$ change between different trial types while the functions $w_p(t)$ are assumed to be invariant, defining the primitives or muscle synergies. The time-varying synergies and the corresponding mixing weights have typically been assumed to be non-negative [15], although also models with unconstrained parameters have been applied to model phasic EMG activity [9].

Space-by-time primitives

Recently, Delis and colleagues [25] proposed a new synergy model for EMG data, which they named ‘space-by-time decomposition’. This model merges the definitions of spatial and temporal components into a new definition of primitives that is given by the following equation:

$$x_l(t) = \sum_{p=1}^{P_{tp}} \sum_{q=1}^{P_{sp}} s(t - \tau_{lpq}) \cdot c_{pq} \cdot w_q + \text{residuals}$$

In this model, $w_q$ and $s_p(t)$ define the trial-independent spatial and temporal components as in models (1) and (2), while the mixing weights $c_{pq}$ and time delays $\tau_{pq}$ are trial-dependent. The constants $P_{tp}$ and $P_{sp}$ indicate the numbers of temporal and spatial components. Since the model was originally designed to account for EMG data, Delis and colleagues assumed all parameters of the model equation (5) to be non-negative (except for the time delays).

Unifying model

All previously discussed models can be derived as special instantiations of a single model, called ‘anechoic mixture model’. This type of model is known from acoustics, where it is applied for modeling of acoustic mixtures in reverberation-free rooms [26-29]. This model assumes typically a set of $R$ recorded acoustic signals $y_r(t)$ that are created by the superposition of $U$ acoustic source functions $f_u(t)$, where time-shifted versions of these source functions are linearly superposed with the mixing weights $a_{ru}$. The time shifts are given by the time delays $\tau_{ru}$. This models the fact that for a reverberation-free room the signals from the acoustic sources arrive receiver with different time delays and attenuated amplitudes, which are dependent on the distances between the acoustic sources and the receivers. The corresponding generative model has the following form (for $1 \leq r \leq R$):

$$y_r(t) = \sum_{u=1}^{U} a_{ru} \cdot f_u(t - \tau_{ru}) + \text{residuals}$$

Equivalence between the unifying model and the other models

By addition of appropriate constraints, the anechoic mixture model (6) can be made equivalent to all previously discussed models for motor primitives. This becomes obvious by the following considerations:

a) Identifying the signals of type $y_r(t)$ with the components of the vectors $x_l(t)$, i.e. $y_r(t) = x_{l(r)m(r)}(t)$ (where the integer functions $l(r)$ and $m(r)$ define a one-to-one mapping between the $m$-th degree of freedom in trial $l$ and the
corresponding signal $y_r(t)$ (with $1 \leq r \leq M \cdot L$), and constraining the time delays $\tau_{ru}$ to be zero, one obtains the model (1). Since in this model the weight vectors $w_p$ are assumed to be invariant over trials, all mixing weights $a_{rp}$ belonging to the same DOF and primitive number $P$ have to be equal and independent of the trial number, so that $a_{rp} = w_{p,m(r)}$, where the function $m(r)$ returns the number of the DOF that belongs to index $r$ independent of the trial number.

The time-dependent mixing coefficients $c^l_p(t)$ of the model (1) correspond to the source functions $f_u$ of the model (6), thus $f_u(t) = c^{l_u}_p(t)$ where here the index $u$ runs over all combinations of the indices $p$ and $l$, thus $1 \leq u \leq U = P \cdot L$ and where the integer functions $l(u)$ and $p(u)$ establish mappings between the number of the source function in model (6) and the time-dependent mixing weights in model (1). Non-negativity constraints can be added for the model parameters $a_{rp}$ and the functions $f_u(t)$, e.g. for the modeling of EMG data.

b) If one identifies the source functions in model (6) with the temporal primitive functions $s_p(t)$, i.e. $f_p(t) = s_p(t)$, $1 \leq p \leq P$ and again constrains the delays $\tau_{ru}$ to be zero, equation (6) becomes equivalent to model (2). In this case, the mixing weights $a_{rp}$ are equated with the mixing coefficients $c^{l_u}_m$ in model (2), where the index $r$ runs over all combinations of $m$ and $l$, formally $a_{rp} = c^{l_u}_{m(r),p}$, with appropriately chosen integer functions $m(r)$ and $l(r)$. Like for model (1), the components of the data vector have to be remapped over DOF and trials according to the relationship $y_r(t) = x^{l(r)}_{m(r)}(t)$. Again, non-negativity constraints can be added for the parameters $a_{rp}$ and to the source functions $f_u$.

c) Dropping the constraints $\tau_{ru} = 0$ in the equivalences described in b), and equating the delays in model (3) according to the relationship $\tau_{rp} = \tau^{l(r)}_{m(r),p}$, makes model (6) equivalent to model (3).

d) Introducing individual sets of basis functions for the different DOF, grouping them into vectors and equating the mixing weights and temporal delays for the components of each vector, transforms model (6) into the model (4). On the level of the time-dependent basis functions, this equivalence can be mathematically described by the equation $f_u(t) = w_{p(m(u)),m(u)}(t)$, where $w_{p,m}$ corresponds to the component of the basis function vector $w_p(t)$ that belongs to the $m$-th DOF, and where the integer functions $m(u)$ and $p(u)$ establish a one-to-one mapping between the indices of the basis functions in the two models and the number of the associated DOF. This assignment is independent of the trial index $l$. The index $r$ in (6) runs over all combinations of DOF and trial numbers, thus $1 \leq r \leq M \cdot L$. The integer functions $m(r)$ and $l(r)$ assign the corresponding trial number and DOF to the index $r$ in the model (6). Thus, the assignment equation for the data vector is again given by $y_r(t) = x^{l(r)}_{m(r)}(t)$ for the $m$-th DOF in the $l$-th trial. The requirement that all mixing weights and temporal delays belonging to the same basis function vector $w_p$ are equal is equivalent to a set of equality constraints, which can be captured by the equation systems $a_{ru} = c^{l(r)}_{p(r)}$ and $\tau_{ru} = \tau^{l(r)}_{p(r)}$. Again, non-negativity constraints can be added, if necessary.

e) In order to establish equivalence with the model (5), the data vectors of the models are mapped onto each other according to the relationship $y_r(t) = x^{l(r)}_{m(r)}(t)$, where again $l(r)$ and $m(r)$ are integer mapping functions that assign the $r$-th element of the data vector of the model (6) to the $m$-th DOF of the data vector $x^l$ for the $l$-th trial in (5) with $1 \leq r \leq M \cdot L$. Model (5) has a total
of $P_q \cdot P_p$ temporal basis functions, where however the functional forms of the basis functions for different indices $q$ (i.e. different spatial components) for the same $p$ (i.e. same temporal component) just differ by time shifts. This is equivalent to an equality constraint for these functions, which can mathematically be characterized in the form $f_u(t) = s_{p(u)}(t)$, with $1 \leq u \leq P_p$ and the index functions $p(u)$ and $q(u)$ that map the index $u$ in the model (6) onto the indices of the temporal and spatial primitive in (5). Since all indices with the same $p(u)$ are mapped onto the same basis function $s_p$ the last equation specifies an equality constraint. With the same integer mapping functions, finally, also the relationship between the mixing weights can be established, which is given by the equation $a_{ru} = \ell_{p(u), q(u)} \cdot w_{q,m}$, where $w_{q,m}$ is the $m$-th element for the vector $w_q$. The last equation specifies a bilinear constraint for the weight parameters of the model (6). Using the same notation, the equivalence between the delays is established by the equation system $\tau_{ru} = \tau_{p(u), q(u)}$. A summary of the established equivalences between the general model (6) and the other models is given in Table 1.

An efficient algorithm for the identification of motor primitives within the unified framework

The solution of anechoic demixing problems is a well-known topic in unsupervised learning, with close relationship to methods such as ICA and blind source separation (cf. e.g. [30-31]). Numerous algorithms have been proposed to solve this problem for the most general case where the functions $f$ are assumed to be elements of relatively general function spaces. For the under-determined case (in which the number of signals/sensors is smaller than the number of sources) well-known algorithms include information maximization approaches [32] and frequency, or time-frequency methods [33-34], such as the DUET algorithm [29]. Other work for the under-determined case is summarized in Ogrady et al. [35], Arberet et al. [36] and Cho and Kuo [37]. The over-determined case (where the signals outnumber the sources) is much more interesting for dimensionality reduction applications, but has been addressed more rarely. Harshman and colleagues [38] developed an alternating least squares (ALS) algorithm for this problem (Shifted Factor Analysis). Their method was later revised and improved by Mørup and colleagues [39], who exploited the Fourier shift theorem and information maximization in the complex domain (SICA, Shifted Independent Component Analysis). More recently, Omior and Giese [19] developed a framework for blind source separation, starting from stochastic time-frequency analysis that exploited the marginal properties of the Wigner-Ville spectrum. The discussed algorithms solve the anechoic demixing problem for the most general case, at the cost that they are computationally expensive. All algorithms for blind source separation require the identification of a large number of parameters. Given model (6), $T \cdot U$ parameters need to be identified to represent all sources $f_u(t)$, and for each trial $l$, $M \cdot U$ weights $a_{ru}$ and $M \cdot U$ delays $\tau_{ru}$. Given a whole data set, this results in a total number of parameters to be identified that is $(T + 2M \cdot L) \cdot U$, where typically $T \gg M, U, L$ (with $T, M, U$ and $L$ indicating the total numbers of time samples, DOF, sources, and trials). For applications in motor control, the relevant signals are subject to additional constraints, which can be exploited for the derivation of more efficient algorithms.
Table 1: Constraints that make the primitive models (1), (2), (3), (4) and (5) equivalent to the general anechoic model (6). See text for details.
Signals in motor control are typically smooth. This allows to reduce considerably the complexity of the anechoic demixing problem and to devise algorithms that are more robust than those developed for general purposes. We present in this section a unifying algorithm for standard anechoic demixing, which can be used for the identification of the parameters associated with the unconstrained model (6). The general version of this algorithm, which from now on we will refer to as FADA (Fourier-based Anechoic Demixing Algorithm), was introduced in a previous study to identify primitives defined according to eq. (3) [18]. Here we describe how this algorithm can be extended by inclusion of additional constraints that make it suitable for the identification of the parameters associated with different models for primitives. The time-courses of signals related to body movements (trajectories as well as EMG traces) often are relatively smooth and thus can be approximated well by anechoic mixtures of smooth signals [18]. This smoothness of the source functions \( f(u) \) can be expressed by appropriate priors that help to stabilize the source separation problem. Smooth temporal sources can be approximated by truncated Fourier expansions. Consequently, each source can be approximated by \( K \) complex Fourier coefficients, where \( K \ll T/2 \). Consequently, the number of parameters to identify drops remarkably to \((K+2M \cdot L) \cdot U\). This decreases substantially the computational costs of the parameter estimation and make it more robust. When the temporal signals \( y_r(t) \) and sources \( f_u(t) \) are assumed to be band-limited they can be approximated by truncated Fourier expansions of the form:

\[
y_r(t) = \sum_{k=-K}^{K} c_{rk} e^{\frac{2\pi i k t}{T_s}}
\]

and

\[
f_u(t - \tau_{ru}) \approx \sum_{k=-K}^{K} \nu_{uk} e^{-ik\tau_{ru}} e^{\frac{2\pi i k t}{T_s}}
\]

where \( c_{rk} \) and \( \nu_{uk} \) are complex constants (\( c_{rk} = |c_{rk}| e^{i\phi_{c_{rk}}} \) and \( \nu_{uk} = |\nu_{uk}| e^{i\phi_{\nu_{uk}}} \)), and where \( i \) is the imaginary unit. The positive integer \( K \) is determined by Shannon’s theorem according to the limit frequency of the signals, and \( T_s \) is the temporal duration of the signal. The source separation algorithm tries to ensure that the source functions \( f_u(t) \) are uncorrelated over the distributions of the approximated signals. This implies \( E\{f_u(t) \cdot f_u'(t')\} = 0 \) for \( u \neq u' \) and any pair \( t \neq t' \). For the corresponding Fourier coefficients this implies \( E\{\nu_{uk} \cdot \nu_{uk'}\} = 0 \) for \( u \neq u' \) and any pair \( k \neq k' \). Combining equation (6), (7) and (8) we obtain by comparison of the terms for the same frequency

\[
c_{rk} = \sum_{u=1}^{U} a_{ru} \cdot \nu_{uk} e^{-ik\tau_{ru}}
\]

From this follows with \( E\{\nu_{uk} \cdot \nu_{uk'}^{*}\} = E\{|\nu_{uk}|^2\} \cdot \delta_{uu'} \) the equation:
The symbol ∗ indicates the conjugate of a complex number. The derivation of this equation replaces the expectations of the Fourier coefficients $c_{rk}$ with their deterministic values and treats the source weights $a_{rk}$ as deterministic trial-specific variables. This can be justified if these mixture weights are estimated separately from the sources in an EM-like procedure. Empirically, however, we obtain reasonable estimates of the model components based on equation (10) also using other methods (see below). Since the signals $f_u(t)$ and $y_r(t)$ are real the corresponding Fourier coefficients fulfill $c_{rk} = c_{r,-k}^*$ and $\nu_{uk} = \nu_{u,-k}^*$. Thus the demixing problem needs to be solved only for parameters with $k \geq 0$.

The previous considerations motivate the following iterative algorithm for the identification of the unknown parameters in model (6). After random initialization of the estimated parameters, the following steps are carried out iteratively until convergence:

1. Compute the absolute values of the coefficients $c_{rk}$ and solve the following equations:

$$|c_{rk}|^2 = \sum_{u=1}^{U} \sum_{u'=1}^{U} a_{ru} a_{ru'} E \{ \nu_{uk} \cdot \nu_{uk}' \} e^{-ik(\tau_{ru} - \tau_{ru'})}$$

$$= \sum_{u=1}^{U} a_{ru}^2 E \{ |\nu_{uk}|^2 \}$$

$$= \sum_{u=1}^{U} |a_{ru}|^2 |\nu_{uk}|^2$$

(10)

2. Initialize for all pairs and iterate the following steps:

(a) Update the phases of the Fourier coefficients of the sources, defined as $\varphi_{\nu_{uk}} = \text{angle}(\nu_{uk}) = \arctan(\text{Im}(\nu_{uk})/\text{Re}(\nu_{uk}))$ by solving the following non-linear least square problem

$$\min_{\Phi} \| C - Z(\Phi) \|_F^2$$

(12)

where $(C)_{rk} = c_{rk}$, $(Z)_{rk} = \sum_{u=1}^{U} a_{ru} e^{-ik\tau_{ru}} |\nu_{uk}| e^{i\varphi_{\nu_{uk}}}$ and indicates the Frobenius norm. (In order to avoid cluttered notation, for the function $Z(.)$ only the arguments with relevance for the optimization are explicitly written).
Keeping the identified source functions \( f_u(t) \) constant, identify for each signal \( y_r(t) \) the weights \( a_{r,u} \) and delays \( \tau_{r,u} \) by minimization of the following cost functions:

\[
\arg \min_{a_r, \tau_r} \| y_r(t) - f(t, \tau_r) a_r \|_F^2 \quad (13)
\]

Optimization with respect to \( a_r \) and \( \tau_r \) is feasible, assuming uncorrelatedness of the functions \( f_u \) and independence of the time delays \([42]\). The column vector \( a_r \) concatenates all weights associated with DOF \( r \), i.e. \( a_r = [a_{r,1}, \ldots, a_{r,U}]' \).

The vector function \( f_r(t, \tau_r) = [f_1(t - \tau_{r,1}), \ldots, f_U(t - \tau_{r,U})] \) concatenates the functions \( f_u \), shifted by the time delays associated with the \( r \)-th DOF.

The original version of the FADA algorithm was designed to solve the source separation problems without constraints. Additional constraints, such as the non-negativity of the parameters or additional equality constraints for the weights and delays can be easily added, due to the modular structure of the algorithm.

The following sections briefly describe the additional constraints that were introduced in order to implement the identification of the parameters of models (1), (2), (3), (4) and (5).

**Non-negativity of the primitives**

For the case where the primitives \( f_u \) can assume only non-negative values, equation (10) cannot be derived in the way discussed above, and the expression of the non-negativity constraints in the Fourier representation is not straightforward. We decided, instead to estimate the time-dependent values of \( f_u(t) \) directly, taking the inequality constraint \( f_u(t) \geq 0 \) for discretely sampled values of into account. This results in the following algorithm: Starting from random values of the parameters, the following three steps are iterated until convergence:

1. Update of the absolute values of the Fourier coefficients \( |\nu|_uk \) of the primitives \( f_u \), assuming their phases \( \varphi_{nu,k} \) and the mixing weights \( a_{r,u} \) are known, by solving the non-linear constrained optimization problem:

\[
\begin{align*}
\text{minimize} & \quad \| C - Z(N) \|_F^2 \\
\text{subject to} & \quad f_u(N, t) \geq 0, \ u = 1, 2, \ldots U \ \text{and} \ t = 1, \ldots T.
\end{align*}
\quad (14)
\]

In order to avoid cluttered notation, for the functions \( Z(.) \) and \( f_u(.) \) only the arguments with relevance for the optimization are explicitly written.)

The matrix is defined as in (12) and \( (Z)_{rk} = \sum_{u=1}^{U} a_{r,u} e^{-ik\tau_{u,k}} |\nu_{uk}| e^{i\varphi_{nu,k}} \), with \( (N)_{uk} = |\nu_{uk}| \).

2. Assuming the other parameters are fixed, update the phases \( \varphi_{nu,k} \) of the Fourier coefficients of the primitives by solving the non-linear constrained optimization problem

\[
\begin{align*}
\text{minimize} & \quad \| C - Z(\Phi) \|_F^2 \\
\text{subject to} & \quad f_u(\Phi, t) \geq 0, \ u = 1, 2, \ldots U \ \text{and} \ t = 1, \ldots T.
\end{align*}
\quad (15)
\]

Remind that the Fourier coefficients \( \nu_{u0} \) are real so that it is sufficient to regard consider only \( k = 1, \ldots, K \).
3. Update weights and delays as in the unconstrained version of FADA by solving the optimization problem (13).

Non-negativity of the mixing coefficients

Non-negativity of the scaling coefficients $a_{ru}$ of the primitives can be easily imposed in the algorithm. In (13) the scaling coefficients are determined, assuming that primitives and temporal delays are known, solving a least squares problem. The same optimization problem can be solved adding the linear inequality constraints $a_{ru} \geq 0$, $\forall r, u$, resulting in a non-negative least squares problem for the weights $a_{ru}$.

Identification of spatial synergies

The FADA algorithm presented above can be used to identify not only temporal, but also spatial primitives. This can be achieved simply by transposing the data matrix $X$ and constraining all the delays in the algorithm to be equal to 0. In this way indeed, the FADA algorithm identifies a set of invariant spatial (instead of temporal) vectors, interpreting the elements of each vector $x(t)$ as a series of time points. Although there is no theoretical evidence for the existence of any smoothness relation between the values of the different DOF at a given time instant $t$ (so that the smoothness assumptions of FADA on the data are satisfied), it will be shown in the next sections how the algorithm can however still provide identification performance at least as good as those associated with other standard machine learning techniques.

Identification of spatiotemporal synergies

For the identification of spatiotemporal synergies, constraints for the parameters have to be set according to model (4). In a first step, for each DOF $m$ in the data set $P$ source functions $f_p$ are assigned, resulting in a total of $M \cdot P$ independent source functions. The following three steps are then carried out iteratively until convergence:

1. The optimal delays $\tau^l_p$ for each spatiotemporal primitive are found, for each trial $l$, applying a matching pursuit procedure [43-44], consisting of an iterative search for a set of time-shifted primitives that best match the data. For each primitive, the scalar product between the original data and the time-shifted primitive is computed, testing all possible time delays between 0 and $T$-1. The primitive and delay associated with the highest scalar product is then selected and its contribution is subtracted from the data. Then the same procedure is repeated for the remaining primitives on the residual of the data. This search is repeated until all delays have been determined.

2. The combination coefficients $c^l_p$ are updated by minimizing, for each trial $l$, the difference between the original data and the reconstruction, estimated exploiting model (4) and assuming that the source functions $f_u$ and the delays $\tau_{ru}$ are known.
3. Assuming that the weights and the delays are known from the previous steps, the functions $f_u$, which correspond to the components of the spatiotemporal primitives $w_p(t)$ are updated. The Fourier coefficients of the corresponding source function are determined in the same fashion as for the original FADA algorithm without constraints. Non-negativity constraints for the primitives and weights can be imposed in the same way as described above.

**Identification of space-by-time synergies**

We developed a new algorithm for the identification of space-by-time primitives, exploiting the core of FADA algorithm (the mapping onto the Fourier space) for the identification of the temporal primitives associated with the space-by-time factorization. Similar to Delis and colleagues [25], this algorithm was also designed for the processing of EMG-like data and all the parameters in model (5) (with the exception of the delays) are constrained to be non-negative. Given the data matrix $\mathbf{X}$, in the first step of the algorithm $P_{s_p}$ spatial primitives $w_q$ are identified, applying non-negative matrix factorization [41]. Then the FADA algorithm is applied to $\mathbf{X}$ in order to identify $P_{t_p}$ non-negative temporal primitives $s_p(t)$. In the second step of the algorithm, the spatial primitives are kept constant, while temporal primitives, weights and delays are updated. The algorithm consists of the iteration of the two following steps:

1. The Fourier coefficients of the functions $s_p(t)$ are updated as in the constrained FADA algorithm, by minimizing the difference between the Fourier coefficients of the original data and the linear combination of the corresponding Fourier coefficients.

2. Weights and delays are updated minimizing the difference between the original data and the estimates provided by model (5). The optimal delays $\tau_{lqp}$ are found for each trial $l$, following a matching pursuit procedure. Similarly, the weights $c_{lqp}$ are identified, solving for each trial a constrained linear least-squares problem.

To minimize the risk of finding local minima, we always ran the FADA algorithm 10 times on the same data set with different random initial conditions and we considered only the solutions that provided the lowest error in the reconstruction of the original data. To test whether these solutions actually represented points close to the global minimum, we computed the average similarity between the sets of primitives identified at the end of each run of the algorithm (see below for the definition of similarity). Indeed, a high level of similarity between these solutions can be considered as a strong sign that, with very high probability, these solutions are close to the optimal one. In the case, for instance, of an artificial mixture of non-negative temporal components based on model (2), we found that the average similarity between the identified primitives was very high (0.98 on a scale where 1 indicates perfect matching (see equation 16). This high level of similarity allows to rule out the hypothesis that the solutions provided by FADA represent local minima. For the identification of temporal, spatiotemporal or space-by-time primitives, the number of harmonics $K$ was always set according to the following procedure: We computed the average spectrum from all signals within the data and defined $K$ as the closest integer
that approximates the product of the signal duration $T_s$ and the average band-
width $B$ of the data set. This number was always smaller than the limit $K_{max}$
imposed by the Nyquist-Shannon theorem. Differently, in the case of spatial
primitives we always set $K = K_{max}$.

Other identification algorithms
The FADA algorithm was benchmarked against other unsupervised learning
methods for the extraction of synergies. For data based on the synchronous
unconstrained generative models (1) and (2) we used the fastICA algorithm
[45-46] (function ‘fastica.m’ of the corresponding toolbox). We examined the
performance of fastICA after reducing the dimensionality of the data using
principal component analysis. For the fastICA algorithm we found the level
of similarity between original and identified synergies depended on the num-
ber of principal components and it reached the highest value when the num-
ber of principal components was equal to the number of synergies in the data.
Based on this observation we always set the number of principal components
to the number of identified synergies. Non-negative matrix factorization [34,
41] (NMF) was used to identify the model parameters for synchronous mixture
with non-negative components and mixing weights. We used the Matlab func-
tion “nnmf.m”, implementing the matrix multiplication update rule version of
the algorithm introduced by Lee and Seung [34, 41]. For data relying on model
(3) we used the anechoic demixing algorithm (AnDem) developed by Omlor and
Giese [19] and the shifted ICA algorithm (SICA) by Morup [39] (downloaded
from http://www2.imm.dtu.dk/pubdb/views/publication_details.php?id=5206
[47]). For anechoic demixing with non-negativity constraints we used an ane-
choic NMF algorithm (ANMF) developed by Omlor and Giese [19] and the
shifted NMF (sNMF) by Morup and colleagues [48], who kindly provided us with
the Matlab implementation of the algorithm. To extract time-varying syner-
gies we used the modified NMF algorithm developed by d’Avella and colleagues
[9, 15] (stNMF, standing for spatiotemporal non-negative matrix factorization).
Finally, we compared the performance of the FADA algorithm for the identi-
fication of temporal and spatial primitives from the space-by-time model with
the performance of the sample-based non-negative matrix tri-factorization algo-
rithm (sNM3F) developed by Delis and colleagues [25].

Generation of the simulated data
For the quantitative assessment of algorithm’s performance we simulated kine-
matic and EMG data sets that were compatible with equations (1), (2), (3), (4)
and (5). Each of these data sets approximated coarsely the properties of real
biological signals. Each data set consisted of $M$-dimensional trajectories with
$T$ time steps and $L$ repeated trials. Synthesized EMG signals were constrained
to be non-negative, like real EMG signals after rectification and filtering. All
generative models were based on a set of statistically independent temporal
waveforms. These waveforms (source functions, or synergies) corresponded to
the time-dependent combination coefficients $c^j_p(t)$ in model (1), to the tem-
poral signals $s_p(t)$ in models (2) and (3) and (5), and to the components of
the vector function in model in (4). For the generation of the unconstrained
sources we drew 100 random samples from a normal distribution (Matlab func-
tion “randn.m”) and low-pass filtered with a Butterworth filter with normalized cut-off frequency equal to 0.15 (Matlab functions “butter” and “filtfilt”). This procedure allowed to generate band-limited, smooth sources mimicking the typical properties of real kinematic or kinetic trajectories with a length of \( T = 100 \) time samples. For the generation of EMG-like sources we produced spike trains from a multi-dimensional stochastic renewal process [49], and convolved them with a Gaussian function. The renewal process was a homogeneous Poisson process characterized by random inter-spike intervals drawn from an exponential distribution with mean \( 1/\lambda \), where the rate parameter of the Poisson process was given by \( \lambda = 40 \) Hz. Based on the random inter-spike intervals, spike trains with length \( T = 100 \) were generated. Each spike train was then convolved with a Gaussian filter kernel with a standard deviation of 8 discrete time steps. The generated source signals were used to construct the synergies in the generative models (2), (3), (4) and (5). The weight vectors \( \mathbf{w} \) in (1) and (5) were obtained by drawing \( M \) random samples from a uniform distribution over the interval \([-40, 40]\) for the unconstrained case, and from an exponential distribution with mean 20 for the cases with non-negativity constraints. Examples of generated primitives are shown in Fig 1. For kinematic (unconstrained) data sets based on model (2) and (3) the values of the coefficients \( c_{mp} \) were drawn from a uniform distribution over the interval \([-20, 20]\). For EMG-like data sets based on the models (2), (3), (4) and (5) the scaling coefficients were drawn from exponential distributions with mean 10. For all the models with time delays \( \tau \neq 0 \), the delays were drawn from exponential distributions with mean 10 and rounded to the nearest integer. The time delays sampled from this distribution with values larger than \( T = 100 \) were taken modulo to map them back to the interval \([0, T-1]\). Noisy data was derived by adding signal-dependent noise [50-53] to the generated data. The noise was drawn from a Gaussian distribution with mean 0 and standard deviation \( \sigma = \alpha |x(t)| \), where \( \alpha \) is a scalar and \( x(t) \) is the value of the noiseless data at the time instant \( t \). The slope \( \alpha \) was computed though an iterative procedure. Starting from \( \alpha = 0 \), its value was iteratively increased of a predefined increment until the level of the difference \( 1 - R^2 \) (where the parameter \( R^2 \) describes the level of similarity between two data sets, see below) reached a predefined value. For each noiseless data set, three data sets were generated with \( 1 - R^2 \) levels equal to 0.05, 0.15, 0.25 and 0.35). For each generative model, 20 noiseless data sets were simulated that were consistent with equations (1) to (5), randomly selecting synergies, scaling coefficients and time delays. The number of synergies \( P \) was always set to 4 and the number of simulated DOFs was 10. The number of simulated trials \( L \) was 25. The time duration of each trial was assumed to be \( T_s = 1 \) and the sampling frequency was set to 100 Hz.

**Experimental kinematic and EMG data**

We assessed the identification performance of each algorithm also on actual experimental kinematic and EMG data. The kinematic data set consisted of flexion angle trajectories of the body joints recorded from human actors walking with different emotional styles (neutral, happy and sad). These data were used in previous work on emotional gaits [20, 23, 54]. From this data set, unconstrained temporal primitives were identified with the FADA and the anechoic demixing algorithm. EMG data consisted of previously published recordings [9]
obtained from 16 arm muscles during arm reaching movements. These muscle
activation patterns were used to investigate the production of behaviors through
combination of muscle synergies. The recorded EMG raw signals were digitally
full-wave rectified, low-pass filtered (20 Hz cut-off) and integrated within time
bins of 10 ms. All EMGs signals in the data set were resampled to fit a 75-point
time window (0.75s).

Assessment of algorithm performance
For each algorithm we assessed three different performance measures, quantify-
ing the capability of each algorithm to identify the original movement primitives,
the original activation coefficients and the original delays in comparison to the
parameters used to generate the data. The similarity between original and
extracted primitives was quantified by computing the maximum of the scalar
products between original and identified primitives, taking the maximum over
all possible time delays in cases where model contained temporal shifts. Let
\( p_1(t) \) and \( p_2(t) \) signify the compared primitives or source functions (discretely
sampled in time) and that these signals are normalized so that their norm is
one. The similarity measure is defined by the scalar product of these normal-
ized signals, where one of them is time-shifted with time delay \( \tau \), where this delay
is optimized by maximizing the similarity measure. For models without time
shifts the time delays are constrained to be 0. Mathematically the correlation
measure is given by the equation:

\[
S = \max_{\tau} \sum_{t} p_1(t) \cdot p_2(t - \tau)
\]  

(16)

For the case of time-varying synergies (model 4) the compared signals were
vector-valued. In this case the scalar product of the vectors in (16) was taken
for each (delayed) time step and the signals were normalized ensuring that for
\( \sum_{t} |p_j(t)|^2 = 1 \), for \( j = 1, 2 \). The similarity measure takes values between -1
and 1, where the value 1 corresponds to the situation that both source function
have identical shape (except for maybe a time delay). In order to establish cor-
respondence between the individual primitives of the generative model and the
identified primitives, we first computed the similarity measure \( S \) for all possible
pairings of the primitives and chose then the pairing with the highest similar-
ity score. For this purpose, first the pairing with the highest similarity score
was determined and removed from the original and reconstructed model. Then
this procedure was repeated for the second-best matching pair of the remaining
set of primitives, and so forth. This procedure was iterated until all primitives
had been matched. The similarity between original and identified coefficients
(or time delays) was assessed by computing the correlation coefficients between
activation coefficients (temporal delays) of the matched primitives. These cor-
relation coefficients were then averaged across all matched pairs of primitives.
We also defined a measure of similarity between original and reconstructed data
sets. Since the generated and experimental kinematic or EMG patterns and the
residuals of the reconstruction of the patterns by synergy combinations were
multivariate time-series, a measure of the goodness of the reconstruction (typi-
cally a ratio of two variances) had to be defined. We used the “total variation”
[55], defined as the trace of the covariance matrix of the signals. A multivariate
The statistical distributions of all similarity measures described above for randomized data were assessed for each algorithm and each data set. In order to calculate baseline levels for these similarity measures ($\Sigma_b$), we first randomly generated 20 independent sets of synergies, coefficients, and delays (where appropriate) using the corresponding generative model. The similarities between the identified synergies (activation coefficients or delays) between these randomly generated sets were then computed. The obtained similarities were then averaged over all 20 simulations, resulting in a baseline value $\Sigma_b$ for the corresponding similarity measure. The similarity measures $\Sigma$ resulting from the comparison between the identified and the simulated primitives were then transformed into a normalized similarity measure according to the formula:

$$\Sigma_{norm} = \frac{\Sigma - \Sigma_b}{1 - \Sigma_b}$$

The normalized similarity measure $\Sigma_{norm}$ takes the value one for perfect similarity, and it is zero if the similarity matches the average similarity between two randomly generated data sets.

**Statistical analysis**

All tested measures were normally distributed according to a Chi-square goodness-of-fit test. Student’s t-test was used to test whether the reconstructions accuracies and the levels of similarities were statistically different from chance level. Differences between more than two groups were statistically tested by two-way ANOVAs (with Algorithm and Noise Level as factors), where appropriate. Post-hoc analysis was conducted with Tukey-Kramer test, when necessary and appropriate. As level of significance for the rejection of the null hypotheses in this study we chose 5

**Results**

**Comparisons of algorithm performance on simulated data sets**

To assess algorithm performance we simulated ground-truth data sets based on the mixture models described in equations (1), (2), (3), (4) and (5). The aim of our comparison was to show that the FADA algorithm can identify mixture parameters at least as well as other well-known unsupervised learning methods. Fig 2A shows the average performance ($\pm$SD) of the FADA and the fastICA algorithm applied to mixtures of unconstrained synchronous synergies, similar to...
the ones illustrated in Fig 1A. The bar plots indicate the reconstruction accuracy measure $R^2$ and the normalized similarity measures for the extracted synergies $S_{\text{norm}}$, averaged across 20 data sets for five different levels of signal–dependent noise. Asterisks indicate significant differences according to post-hoc testing between average values, obtained with different algorithms for the same level of noise. The figure shows that both algorithms provide a good level of reconstruction accuracy and resulted in an accurate estimation of the original model parameters. Normalized accuracy measures were typically larger than 0.5, and the similarity measures for the recovered primitives and weighting coefficients were always significantly larger than chance level \( t(19) > 9.93, p < 0.001 \). The two-factor ANOVAs revealed a significant main effect for the factor Noise Level for both the reconstruction accuracy and the identification of the primitives (\( F(4,190) \geq 5.08, p < 0.001 \)). We found a significant main effect for the factor Algorithm for all tested parameters (\( F(1,190) \geq 11.92, p < 0.001 \)). The interaction between the two factors was significant for and the similarity of the primitives (\( F(4,190) \geq 5.08, p < 0.001 \)). The post-hoc analysis revealed that, for the same level of noise, the fastICA and FADA algorithm did not provide significantly different identification performance, neither for the identification of the primitives nor for the weighting coefficients \( (p > 0.05) \), although fastICA provided always significantly higher reconstruction accuracy \( (p < 0.05) \).

Similarly to Fig 2A, Fig 2B depicts the identification performance of the algorithms applied to mixtures based on model (1), but synthesized with non-negative parameters. In this case, we compared the FADA algorithm to non-negative matrix factorization (NMF), as the fastICA does not provide a way to constrain parameters to be non-negative. Even in this case both algorithms provided a good fit of the data and very accurate estimates of the original primitives and mixture weights. Not surprisingly, performance of both algorithms degraded with increasing noise, more remarkably than in Fig 2A. ANOVAs indicated a significant main effect of the factor Algorithm on the similarity of the weighting coefficients \( F(1,190) = 23.14, p < 0.001 \). Also the main effect of the factor Noise Level was significant for both, $R^2$ and levels of normalized similarities \( F(4,190) \geq 20.85, p < 0.001 \). The interaction of both factors was significant only for \( F(4,190) = 5.51, p < 0.001 \). The post-hoc analysis showed that only in one case (25% of noise) NMF performed better than the FADA algorithm in terms of the identification of the weight coefficients \( (p=0.74) \). Differently, NMF provided significantly lower reconstruction accuracy \( (p=0.01) \) for the highest level of noise (35%). All average values in Fig 2B were significantly above chance level \( t(19) \geq 6.85, p < 0.001 \).

Fig 3 shows the identification performance of the FADA, fastICA and NMF algorithms applied to synchronous mixtures based on model (2). Fig 3A shows qualitatively that, for the case of unconstrained mixtures, the level of reconstruction accuracy and the level of similarity of the primitives were modulated by the level of noise. In contrast, noise seems to have no significant effect on the estimation of the weighting coefficients. ANOVAs confirmed a significant main effect for the factor Noise level for the accuracy of reconstruction and the similarity of the estimated primitives with the original for the reconstruction accuracy of the data and the estimation of the weights \( F(1,190) \geq 9.67, p < 0.001 \). The interaction between Algorithm and Noise Level was significant only for $R^2$ \( F(4,190) = 5.12, p < 0.001 \). Post-hoc testing revealed that the FADA algorithm performed significantly worse than fastICA in approximating the noisiest data.
Figure 1: Examples of artificial primitives used for the generation of the ground-truth data sets. (A) Unconstrained spatial primitives, associated with model (1). (B) Non-negative spatial primitives, associated with model (1) and (5). (C) Unconstrained temporal components used in models (2) and (3). (D) Non-negative (EMG-like) temporal components associated with model (5). (E) Time-varying non-negative primitives associated with model (4).

sets \((p<0.001)\) and in terms of the identification of the weighting coefficients \((p=0.004)\) for one tested noise level \((15\%)\). For all other cases the identification performance of the FADA and fastICA algorithm did not significantly differ \((p>0.05)\). Fig 3B shows the results of the comparison between the FADA algorithm and NMF applied to non-negative data. The differences in performance between the two methods for the same noise levels were very small. Correspondingly, ANOVAs showed that the factor Algorithm had a significant main effect only for the reconstruction accuracy \(R^2 (F(1,190)=25.99, p<0.001)\), while the factor Noise had significant main effects for all three tested measures \((F(4,190)\geq 17.38 \, p<0.001)\). Post-hoc testing revealed that the FADA algorithm approximated the original data with significantly higher reconstruction accuracy than fastICA, only for the data were corrupted with the two highest levels.
Figure 2: Spatial primitives. Identification performance (mean ± SD) of the Fourier-based anechoic demixing algorithm (FADA), fast independent component analysis (fastICA), and non-negative matrix factorization (NMF) applied to artificial data sets, which are corrupted by different amounts of noise, where data was simulated by combining spatial primitives according to the generative model (1). The number of DOFs in each spatial primitive was set to $M = 10$.

(A) Level of variance explained with the extracted parameters, and similarities between original and identified primitives, and for the corresponding combination coefficients for unconstrained data (see Methods for details). (B) Level of variance accounted for with the extracted parameters, similarities between original and identified spatial primitives, and corresponding combination coefficients for non-negative data.

of noise ($p<0.05$). Taken together, Figs 2 and 3 show that, when applied to data based on synchronous models, FADA was in general able to provide identification performance comparable to those provided by the fastICA and NMF algorithms for the model (2). In terms of identification of the actual parameters, the FADA algorithm had worse performance than the fastICA algorithm only in two single cases concerning the identification of the weights for large noise only for the case of mixtures based on the combination of unconstrained spatial primitives. Interestingly, the variability associated with the similarities between original and identified parameters is higher in Fig. 3A than in Fig 3B. This is most probably due to an increase of regularization in the algorithms introduced by the non-negativity constraints imposed on the model parameters. For the lowest levels of noise (25% and 35%) NMF provided significantly higher reconstruction accuracy ($p<0.05$). All measures in Fig 3 were significantly above chance level ($t(19)\geq8.86, p<0.001$).
Figure 3: Instantaneous mixtures (without delays). Identification performance of the FADA, factICA, and NMF algorithm applied to artificial data sets generated as instantaneous mixtures of temporal synergies, defined by the generative model (2). (A) Level of variance explained by the extracted parameters, source similarities between original and identified primitives, and similarities of corresponding combination coefficients for unconstrained data. (B) Same plot for non-negative data.

Figure 3 continues...

Fig 4 shows a comparison between the identification performance of the FADA algorithm and the alternative methods AnDem, SICA, AnNMF, and sNMF for data generated with model (3) assuming unconstrained (Fig 4A) and non-negative anechoic (Fig 4B) mixtures. In addition to the similarity measures assessed before, we also quantified the similarity between original and identified delays. For the unconstraint case (Fig 4A), FADA performed qualitatively better than both AnDem and SICA. For all levels of noise it provided a higher level of data approximation quality and higher normalized similarities for primitives and weighting coefficients. FADA and AnDem provided comparable performance in the identification of the delays. When comparing FADA and AndDem, ANOVAs revealed a significant main effect of the factor Algorithm on $R^2$ and on the approximation quality for the primitives and the weights ($F(4,190)\geq210.5, p<0.001$). The noise level affected only $R^2$ and the similarity of the primitives ($F(4,190)\geq12.85, p<0.001$). The interaction between noise and the type of algorithm was significant for the estimation of the primitives ($F(4,190)\geq5.85, p<0.001$). Post-hoc analysis revealed that FADA provided significantly higher $R^2$ values, as well as higher similarities of primitives and weighting coefficients ($p<0.05$). Compared to the SICA algorithm, the FADA algorithm showed higher approximation quality of the original data, for almost all levels of noise, and higher similarities between original and identified primitives, weights and delays. ANOVAs confirmed a significant main effect of the factor Algorithm for the estimation of all parameters ($F(4,190)\geq10.57$, $p<0.001$).
p<0.01), while the influence of the factor Noise Level was significant only for $R^2$ and the similarities of the weights ($F(4,190)≥3.85$, p<0.01). Post-hoc testing revealed that the FADA algorithm provided significantly higher $R^2$ values than the SICA algorithm (p<0.001). For the three highest level of noise the FADA algorithm also the estimation of the time delays was more accurate (p<0.001). All measures in Fig 4A were significantly above chance level ($t(19)≥3.23$, p<0.001).

Fig 4B shows the results for the performances of the FADA, AnNMF and sNMF algorithms for data that are derived from non-negative anechoic mixtures. Even in this case the FADA algorithm qualitatively provided, for all levels of noise, higher values of $R^2$ and similarity between original and identified primitives in comparison to the AnNMF algorithm. ANOVAs revealed a significant main effect of the factor Algorithm for $R^2$ and the similarities of primitives and delays with the generative model parameters ($F(4,190)≥6.64$, p<0.05). The ANOVAs revealed also a significant main effect of the factor Noise Level for $R^2$ and all other estimated model parameters ($F(4,190)≥2.69$, p<0.05). The interaction between the Noise level Algorithm was significant only for $R^2$ and the estimation accuracy of the delays ($F(4,190)≥4.29$, p<0.01). The post-hoc testing revealed that the FADA algorithm provided significantly higher $R^2$ values than the AnNMF algorithm (p<0.001), higher similarity of the primitives for noisy data sets (p<0.05) as well as higher similarities between original and identified delays (p<0.05) for three level of noise (0%, 5% and 15%). Comparing the FADA algorithm and sNMF, ANOVAs resulted in a significant main effect of the factor Algorithm for all measures, except for the similarity between original and identified delays ($F(4,190)≥10.34$, p<0.01). The main effect of the factor Noise Level was significant for all parameters ($F(4,190)≥4.41$, p<0.01). The interaction between both factors was significant for $R^2$ and the identification accuracy of the time delays ($F(4,190)≥2.96$, p<0.05). Post-hoc testing showed that the FADA algorithm always resulted in higher reconstruction accuracy and more accurate estimates of the primitives than sNMF (p<0.05), with the only exception of one level of noise (15%). All similarity measures in Fig 4B were significantly above chance level ($t(19)=30.8$, p<0.01), except for the reconstruction accuracy provided by sNMF for the most noisy data sets ($t(19)=0.25$, p=0.80).

Fig 5 shows the ability of then FADA and the stNMF algorithm to identify spatiotemporal synergies and the corresponding weight coefficients and delays from simulated non-negative mixtures, derived from model (4) and mimicking EMG-like features. A significant main effect of the factor Algorithm was found for the reconstruction performance $R^2$ and the accuracies of the estimation of the weighting coefficients and delays ($F(4,190)≥13.34$, p<0.001), but not for the accuracy of the reconstruction of the primitives ($F(4,190)=0.4$, p>0.05). The factor Noise Level had a significant main effect for $R^2$ and the accuracy of the identified parameters ($F(4,190)≥5.15$, p<0.001). The interaction of the factors Noise level and Algorithm was significant for $R^2$ and the accuracy of the estimation of delays ($F(4,190)≥2.84$, p<0.05). Post-hoc testing revealed that the FADA algorithm resulted in significantly higher $R^2$ values than stNMF for all noise levels (p<0.001). Contrasting with this result, the FADA and stNMF algorithm provided indistinguishable identification performance for all parameters (always p>0.05), except for the identification of the delays when data were corrupted with the highest level of noise (p=0.03). For all tested noise levels and algorithms, $R^2$ and the normalized similarities were always significantly above chance level ($t(19)=11.78$, p<0.001).
Figure 4: Mixtures with time delays. Identification performance of the FADA algorithm, the anechoic demixing algorithm by Omlor and Giese (AnDem), anechoic demixing with non-negativity constraints (AnNMF), shifted independent component analysis (SICA) and shifted non-negative matrix factorization (sNMF) algorithm applied to artificial data sets, obtained by combining temporal synergies linearly with time shifts as described by model (3). (A) Level of variance that explained with the extracted parameters, similarities between original and identified primitives, and between corresponding combination coefficients and delays for unconstrained data. (B) Level of variance accounted for, similarities between original and identified primitives, and corresponding combination coefficients and delays for non-negative data.

The identification performance on simulated data based on the space-by-time generative model (5) is summarized in Fig 6. Qualitatively, the FADA
Figure 5: Time-varying primitives. Performance of the FADA algorithm and the identification of time-varying synergies (stNMF) for the learning of the parameters of model (4) from ground-truth data, obtained by combining non-negative spatiotemporal synergies. The top-left panel shows the explained variance of the data for the two algorithms as function of the noise level. In addition, the average similarities between original and identified spatiotemporal primitives (top-right panel) and the similarities of the corresponding weights and delays (bottom-left and bottom-right panels) are shown.

algorithm always provided better data fitting, and more precise identification of the original temporal sources, weights and delays than the sNM3F method. The two methods identified the spatial components with similar levels of accuracy. In the ANOVAs the main effect of the factor Algorithm was significant for all parameters (F(4,190)≥10.72, p<0.001). The factor Noise Level had a significant main effect for $R^2$, as well as on the identification accuracy of weights and delays (F(4,190)≥2.74, p<0.05). A significant interaction of the two factors was found for $R^2$ and for the normalized similarities associated with spatial primitives and weighting coefficients (F(4,190)≥2.46, p<0.05). Post-hoc testing showed that the FADA algorithm always provided significantly better reconstruction of the data for all noisy data sets (p<0.001). Regarding the primitives, the FADA algorithm provided more accurate estimates of the temporal primitives for the most extreme levels of noise (0% and 35%, p<0.01). The algorithms
identified the spatial primitives equally well ($p > 0.05$). The FADA algorithm always outperformed the sNM3F method with respect to the identification of the weighting coefficients and temporal delays ($p < 0.05$). t-tests showed that FADA and sNM3F always provided estimates of the parameters that were better than chance level ($t(19) \geq 3.68, p < 0.01$), with the only exception of the sNM3F estimation of the weighting coefficients identified from data corrupted with 5% of noise ($t(19) = 1.91, p = 0.07$).

Figure 6: Space-by-time primitives. Performance of the FADA algorithm and sampled-based non-negative matrix tri-factorization algorithm (sNM3F) to identify the parameters of model (5) from ground-truth data obtained combining space-by-time synergies. The top-left graph shows the variance explained by the two algorithms as a function of the level of noise. In addition, the average similarities between original and identified primitives, and the similarities of the corresponding weights and delays are shown in the other panels.

Comparisons of algorithm performance on real experimental data

In addition to the validation on synthesized data, we tested the FADA algorithm also using previously published real experimental data sets. In addition, we compared the primitives extracted by the FADA algorithm with those identified with other techniques. The first real experimental data set consists of kinematic joint angle trajectories of the body joints of participants performing emotional walks. Trajectories represented a single gait cycle, resampled with 100 time steps [20, 54]. We tested the FADA algorithm against the anechoic demixing algorithm developed by Omlor and Giese [19]. Fig 7A shows
that for both algorithms the explained variance as a function of the number of primitives. (Such plots were also used in order to determine the number of synergies, similarly to the scree plot in statistics [9].) The number of primitives was identified from the \( R^2 \) curve, determining the point where the slope levels off considerably, forming an “elbow”. For both methods in Fig 7A this point is reached for \( N = 3 \), indicating that three anechoic components are sufficient for a reasonable approximation of the experimental data set. Fig 7B shows also the three primitives extracted by the two algorithms, which explain the largest amount of variance of the data. The sources extracted with the FADA algorithm are almost identical (\( S = 0.96 \)) with those extracted with the other anechoic demixing method.

The second data set comprises EMG signals assessed during point-to-point arm reaching movements, recording from 16 different muscles [9]. We used the FADA and the stNMF algorithm to extract time-varying synergies. The most-left panel in Fig 8A shows the curve obtained with the FADA algorithm. In this case, both methods identify \( N = 4 \) as levelling-off point of the \( R^2 \) curves. The other panels in the figure show the five time-varying synergies that were identified by the FADA algorithm. Fig 8B shows the results obtained applying the stNMF algorithm. Similarly to the results obtained for the FADA algorithm, the curve levels off for \( N = 4 \). The synergies of Fig 8B matched closely those in Fig 8A according to their (not normalized) level of similarity. Average similarity across the four pairs of synergies was \( S = 0.97 \pm 0.01 \), indicating that, also on real EMG data, the identification performance of the FADA algorithm was comparable to the one of the time-varying synergies algorithm.

Discussion In this article, we have developed a new mathematical framework that unifies, for the first time, many different definitions of motor primitives. We have described how the different kinds of primitives can be derived from a more general mixture model, which is known as anechoic mixture, by addition of appropriate constraints. Starting from this mathematical framework, we have implemented a new efficient unsupervised learning algorithm for the identification of motor primitives that achieves an identification performance typically at least as good as the other standard methods used to study modularity in human motor control. Such framework simplifies the comparisons between the results from different studies using different generative models for the definition of motor primitives. In addition, our general and robust algorithm (Fourier Anechoic Demixing Algorithm, FADA) allows to extract motor primitives according to specific generative models as special cases. To promote wide adoption of the algorithm by researchers in motor control and neurophysiology, we provide a downloadable implementation as a MATAB toolbox. Our quantitative validation indicated that this new algorithm performs typically equal or better than the established methods for the extraction of primitives using different underlying mathematical models. In the following, we discuss in detail some computational aspects associated with the FADA algorithm and the other unsupervised learning techniques compared with this algorithm. Moreover, taking a broader perspective, we discuss to what extent the different definitions of motor primitives can be really linked to a single model.

Computational considerations regarding the FADA and other unsupervised learning algorithms As in previous studies [56-60], we compared FADA with other unsupervised learning techniques and assessed identification performance on both ground-truth and experimental data sets. Differently from all the
Figure 7: Kinematic primitives extracted from experimental data. (A) Explained variance as function of the number of extracted synergies. The blue curve refers to the FADA algorithm and the red one to the AnDem algorithm. (B) Temporal synergies identified by the two algorithms applied to kinematic data collected from human participants executing emotional walks.

Other techniques, which are based on a single generative model and sets of constraints for the corresponding parameters (e.g. statistical independence or non-negativity), the FADA algorithm allows to test different types of constraints
Figure 8: EMG primitives extracted from experimental data. Spatiotemporal synergies extracted with the FADA (A) and the stNMF algorithm (B) applied to muscle activations collected during point-to-point arm reaching movements. Synergies are grouped according to their similarity. Most left panels show the explained variance as function of the number of extracted synergies for both algorithms. The dependence of this measure on the number of extracted synergies is consistent with previously reported data, indicating that five synergies are sufficient to account for the significant part of the variability in the data.

within the same class of generative models. In this way the proposed algorithm provides a unifying framework for the extraction of motor primitives. A key element of the FADA algorithm is the mapping onto a finite Fourier basis. This mapping reduces remarkably the number of identified parameters in comparison with more general anechoic demixing methods [19, 39], but at the cost that only band-limited data can be adequately modelled. For almost all data in motor control (including at least kinematic or electromyographic data) the informative part of the frequency spectrum typically never exceeds 100Hz after appropriate processing. The reduction of the dimensionality of the parameter space results in a more reliable and robust estimation of the primitives (even in presence of substantial levels of noise) and in a lower probability of getting stuck in local minima during the optimization. Consequently, the FADA algorithm performed better than other methods for the identification of anechoic primitives (Fig 4) and of temporal components associated with space-by-time decompositions (Fig 6). The only case where it showed lower performance was the comparison with the fastICA algorithm for the identification of unconstrained spatial primitives using generative model (1) (Fig 2). In this case, due to the structure of the data matrix, the data was not smooth along the dimension that is smoothed by the FADA algorithm. In this case the inherent smoothness prior might thus have reduced approximation quality. In spite of this problem, the reconstruc-
tion accuracy of the FADA algorithms was high also in this case and so were the similarity scores for the reconstructed sources and weight matrices. For all models including temporal delays the FADA algorithm outperformed the other algorithms in terms of approximation quality, potentially due the reduced number of estimated parameters. For the anechoic unconstrained model (Figs 4), all tested algorithms achieve relatively low values of similarities between original and identified weighting coefficients and temporal delays, while (with the exception of Fig 6) the similarity is significantly above chance level. Opposed to the other tested algorithms in [25, 39, 48] we allowed for large delays and did not restrict the tested delays to a small interval. A more detailed investigation, which is beyond the scope of this paper, shows that the low reconstruction accuracy is caused by ambiguities in the estimation of delays and source functions, especially for sources with higher fundamental frequencies. For real data the FADA algorithm provided estimates for the primitives that were consistent with those obtained with other traditional techniques. Also the estimated numbers of primitives for a good approximation of the data matched between the FADA and other established algorithms (cf. Figs 7 and 8). In addition, the functional forms of the estimated primitives were very similar for the FADA and stNMF algorithms. Despite its good identification performances and flexibility, the FADA algorithm also suffers from a number of limitations. In situations where the frequency spectrum of the real sources is not band-limited the truncated Fourier approximation can decrease the identification performance, as likely in the case of synchronous mixtures with few time samples (see Fig 2). Moreover, the identification of the parameters presently is realized by a gradient descent procedure. There exist faster optimization methods that could be integrated in the future. For the simulations carried out for this study the cross-correlation procedure for the identification of the delays was implemented using entirely Matlab built-in functions. Due to the modular architecture of FADA algorithm, it should be easy to replace different steps by more speed-optimized implementations and optimization methods. In this study we focused on the design of a highly flexible rather than of a speed-optimized algorithm.

Different definitions of motor primitives and the problem of model selection
The central mathematical contribution of this article is that we derived how different models of motor primitives relate mathematically to each other and how they can be derived from the anechoic mixture model (6) by addition of appropriate constraints. This raises the question how for a given data set the most appropriate model structure can be found. As solutions for this model selection problem classical criteria, such as the Akaike or the Bayesian Information criterion (BIC) can be applied [61-62]. Alternatively, one can also use Bayesian model selection. For this purpose, all tested models are embedded in a joint model space, and one marginalizes the prediction error (evidence) using an uninformative prior distribution over all possible model architectures [63]. This procedure typically finds automatically a good balance between the goodness-of-fit and simplicity of the model. An implementation of this idea for automatic model selection has been proposed in [63], where the resulting non-Gaussian distributions were approximated using a Laplace approximation in order to obtain an analytically tractable selection criterion that allows to compare different demixing models, including ones with time delays. The same type of procedure also allows to make inferences about the most suitable smoothness priors for a given data set.
Conclusion

Inspired by the idea of Bernstein [64], experimental investigations in the last couple of decades have put forward the hypothesis that the CNS might simplify the control of movement by relying on a modular organization of control [1, 2]. The modules (primitives) underlying such a control architecture have been defined in multiple ways [65], and by applying a variety of unsupervised learning algorithms to kinematic, dynamic and EMG data sets (see for instance [56]). This heterogeneity of approaches makes the comparison of results across different studies very difficult. We have developed a unifying mathematical framework for the identification of motor primitives that links these approaches, and we have implemented a unifying identification algorithm (FADA) that implements many different methods as special cases as a free Matlab toolbox (FADA) that is available online. We demonstrated that the FADA algorithm typically shows identification performance that is competitive with other classical unsupervised learning techniques. In some cases, it even outperforms these techniques for data from motor control, especially in presence of noise. We hope that the new Matlab toolbox will help to establish more solid links between different definitions of motor primitives, helping neuroscientists with the comparison between different theoretical models and their data.

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