Dimensionality reduction of multi-trial neural data by tensor decomposition

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Summary. Decision-making, sensation, and motor behaviors occur within fractions of seconds, while learned memories can require many hours, days, or years to mature. Technologies for long-term monitoring of neural activity enable examination of all these processes in a single experiment. However, exploratory analysis of these data is challenging due their size (thousands of neurons and behavioral trials) and diversity of timescales. Commonly used methods for dimensionality reduction identify low-dimensional features of within trial neural dynamics, but do not model changes in neural activity across trials. We propose to represent multi-trial data as a three-dimensional data array (a third-order tensor) with each entry indicating the activity of a particular neuron at a particular time on a particular trial (Fig 1). Approximating these data with the canonical polyadic (CP) tensor decomposition (reviewed in [**3**]) produces low-dimensional factors that summarize neural correlations, within-trial dynamics, and across-trial changes in dynamics. Applying CP decomposition to simulated multi-trial data precisely identified low-dimensional network inputs that varied across trials, whereas classical methods (PCA and ICA) failed to recover these signals. We then examined two experimental datasets: (a) prefrontal cortical neurons monitored by fluorescence microendoscopy in mice performing a spatial navigation task, and (b) multi-unit extracellular recordings in the premotor and motor cortices of a Rhesus monkey moving a virtual cursor through a brain-machine interface. In both cases, CP decomposition uncovered specific neural sub-populations with interpretable within-trial as well as across trial dynamics, reflecting task structure, strategies, rewards, and BMI perturbations. The CP decomposition is broadly applicable to common experimental designs in systems neuroscience, is simpler to fit and interpret than complex nonlinear models, and is more informative than classical techniques that represent neural data as a matrix.

Additional Detail. CP tensor decomposition is intimately related to PCA.[1] Typically, neuroscientists use PCA to find low-dimensional factor matrices describing neurons ($\mathbf{A} \in \mathbb{R}^{N\times R}$) and within-trial dynamics ($\mathbf{B} \in \mathbb{R}^{T\times R}$), such that neural population activity ($\mathbf{X}_{::k} \in \mathbb{R}^{N\times T}$ for trial k) is estimated by a low-rank matrix, $\widehat{\mathbf{X}}_{::k} = \mathbf{A}\mathbf{B}^T$. Our method extends this concept by adding a third set of low-dimensional factors $\mathbf{C} \in \mathbb{R}^{K\times R}$ that rescale the neuron and time factors on each trial: $\widehat{\mathbf{X}}_{::k} = \mathbf{A}\mathrm{Diag}(\mathbf{c}_{k:})\mathbf{B}^T$. The columns of the factor matrices provide a low-dimensional basis for studying well-studied concepts in systems neuroscience ($\mathbf{a}_{:r}$: functional cell types; $\mathbf{b}_{:r}$: population dynamics; $\mathbf{c}_{:r}$: learning). In addition, CP factors are more amenable to direct interpretation than the factors identified by PCA, demixed PCA [**2**] or Gaussian Process Factor Analysis [**5**], since these methods do not identify a unique set of latent factors. For example, in the case of PCA, an invertible linear transformation $\mathbf{F}$ can produce a new set of factor matrices that yield an equivalent prediction $\mathbf{A}\mathbf{F}\mathbf{F}^{-1}\mathbf{B}^T = \mathbf{A}'\mathbf{B}'^T = \widehat{\mathbf{X}}_{::k}$. The solution to PCA is only unique after imposing that the factor matrices be orthogonal, however there is no reason to believe that latent signals in biological data obey this constraint. In contrast, CP decomposition on higher-order tensors has a unique solution under mild conditions [**3**], which are generically satisfied in experimental scenarios of interest.

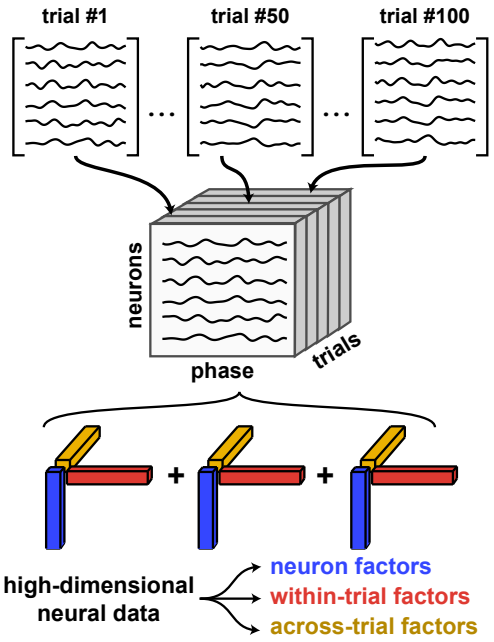

Figure 1: CP Decomposition.

To demonstrate this advantage, we examined simulated data from a linear recurrent network whose inputs changed in magnitude across trials (Fig 2A-B). We compared the results of CP decomposition to performing principal and independent components analysis (PCA and ICA) on the *unfolded* tensor (a $K \times NT$ matrix, see). These classical methods fail to capture across-trial changes in the input signals

[1] In fact, PCA *is* CP decomposition applied to a second-order tensor (i.e. a matrix).

since these dynamics are neither orthogonal nor independent (Fig 2C). In contrast, the across-trial CP factors (columns of **C**) precisely matched the simulation. Theoretical analysis shows that the CP model is well-matched to the multi-trial structure in this synthetic example. This theory only holds for linear networks, but we nevertheless observed similar results (not shown) in a nonlinear model network with nearly chaotic dynamics.

We then examined two multi-trial neural datasets obtained from different species, brain areas, and experimental technologies. First, we used a miniature fluorescence microscope to image the calcium dynamics of hundreds of neurons in the prelimbic cortex of mice navigating a four-armed maze. Mice began each trial in the east or west arms, and were rewarded for either an egocentric (turn-based) or allocentric (place-based) reward contigency (Fig 3A). Mice were able to adapt strategies within 20-30 trials after the reward contigency was perturbed. Applying CP decomposition (Fig 3B) identified neural populations (left column), with particular dynamics (middle column), that were either consistent across trials (top row) or changed with respect to experimental variables (rows 2-4). CP decomposition identified a number of useful features in the dataset in an unsupervised manner. For example, the same neural populations appear to consistently encode error across multiple reward contingency shifts (last row in Fig 3B), and neurons that encode for the start location (second row in Fig 3B) tend to be active at the beginning of the trial suggesting that retrospective coding of position is not a strong signal in this dataset. Our method discovers experimental conditions in an unsupervised fashion (see [**4**] for a tensor-aware, supervised approach to model conditions).

In a second experiment, a Rhesus monkey was trained to make point-to-point reaches to visual targets in a 2D plane with a virtual cursor controlled by their contralateral arm. We recorded approximately 200 units using multi-electrode arrays (Utah arrays, Blackrock Microsystems) implanted in the premotor and motor cortex. We first fit a velocity Kalman filter to decode cursor velocities from firing neural rates, and then perturbed this decoder by rotating the output cursor velocities (a visuomotor rotation) by 30 degrees. Figure 3D shows the results of a rank-3 CP decomposition applied to this dataset. The factors identify neural populations which are preferentially activated by the BMI perturbation.

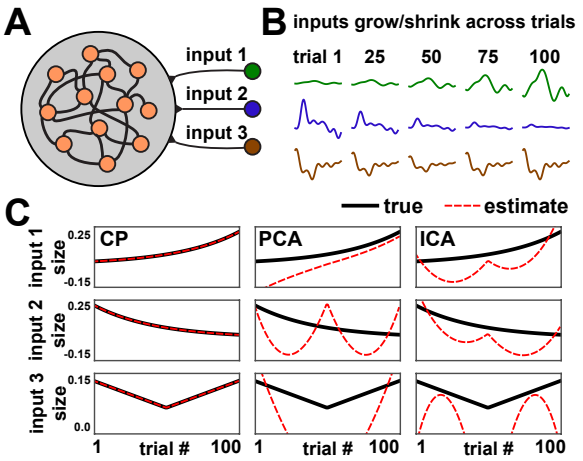

Figure 2: (A-B) Linear network with inputs changing in magnitude across trials. (C) Signal magnitudes estimated by CP decomposition, PCA, and ICA.

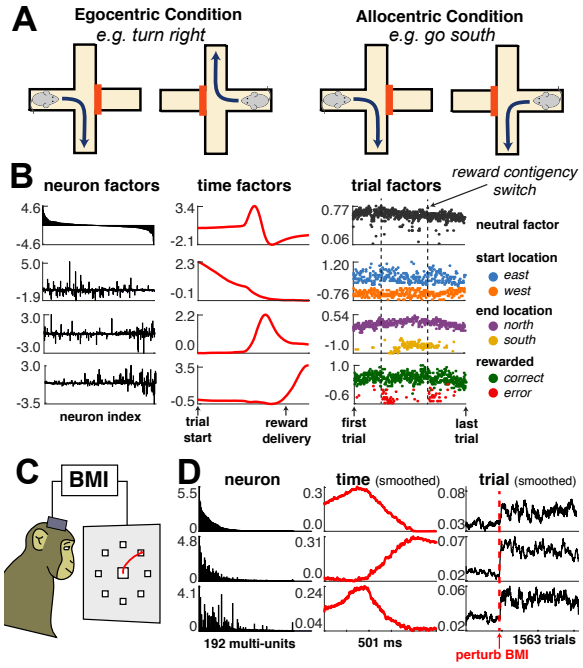

Figure 3: (A) Mice were trained to navigate according to two reward contigencies. (B) 4 sets of CP factors (rows) selected from a rank-15 decomposition of the data. (C) Schematic of center-out BMI task. (D) Rank-3 CP model of the primate BMI task.

Overall, CP decomposition of multi-trial data is widely applicable across model systems, easy to fit using existing open-source tools [**1**], and simple to interpret. Unlike PCA and similar techniques, it explicitly models across-trial changes in dynamics and does not suffer from uniqueness issues.

References. [**1**] Bader, Kolda. *MATLAB Tensor Toolbox Version 2.6*. Available online. Feb. 2015. [**2**] Kobak. *eLife* 5 (Apr. 2016). [**3**] Kolda and Bader. *SIAM Review* 51.3 (2009). [**4**] Seely. *PLoS Comput Biol* 12.11 (Nov. 2016). [**5**] Yu. *J Neurophysiol* 102.1 (2009).