



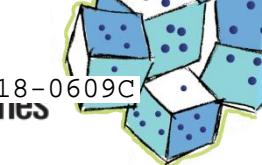
SIAM®

SIAM Invited  
Address,  
JMM18,  
San Diego, CA  
Jan. 11, 2018

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.



Sandia  
National  
Laboratories



# Tensor Decomposition: A Mathematical Tool for Data Analysis

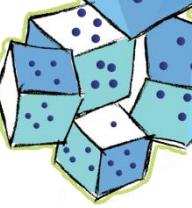
Tamara G. Kolda  
Sandia National Labs, Livermore, CA  
[www.kolda.net](http://www.kolda.net)



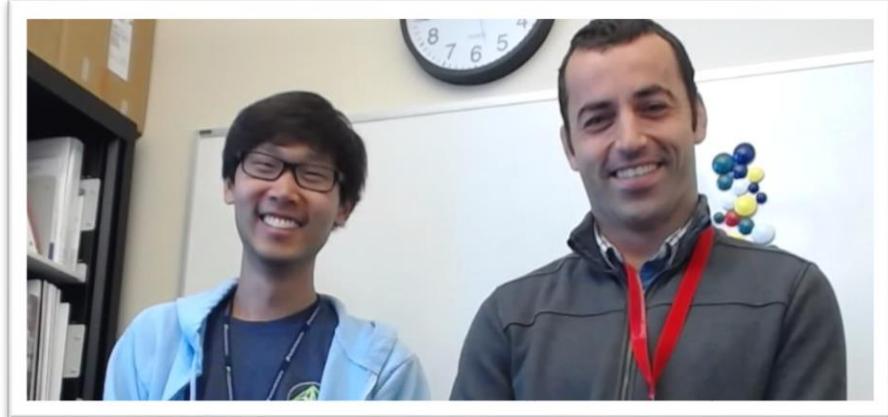
# Collaborators



Sandia  
National  
Laboratories



Grey Ballard (Wake Forrest) &  
Casey Battaglino (Georgia Tech)



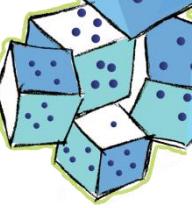
David Hong (Michigan) & Cliff Anderson-Bergman (Sandia)



Jed Duersch (Sandia)

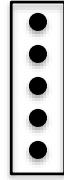


Alex Williams (Stanford)

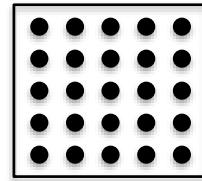


# A Tensor is an $d$ -Way Array

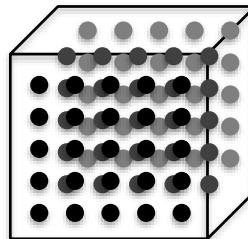
Vector  
 $d = 1$



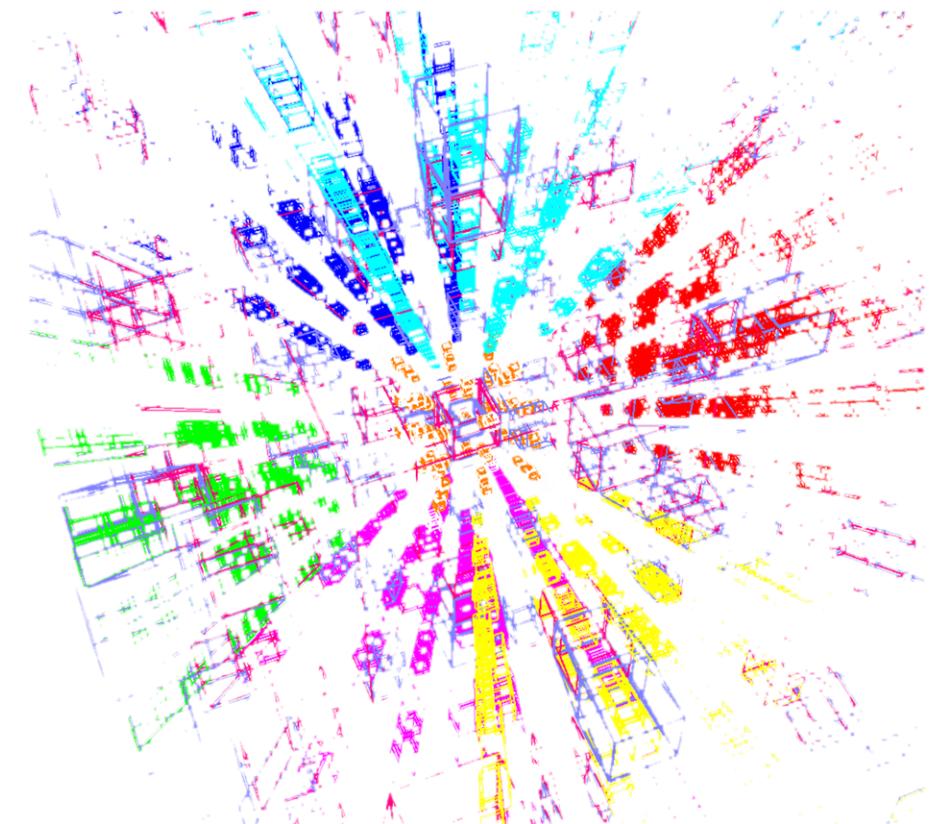
Matrix  
 $d = 2$



3<sup>rd</sup>-order Tensor  
 $d = 3$



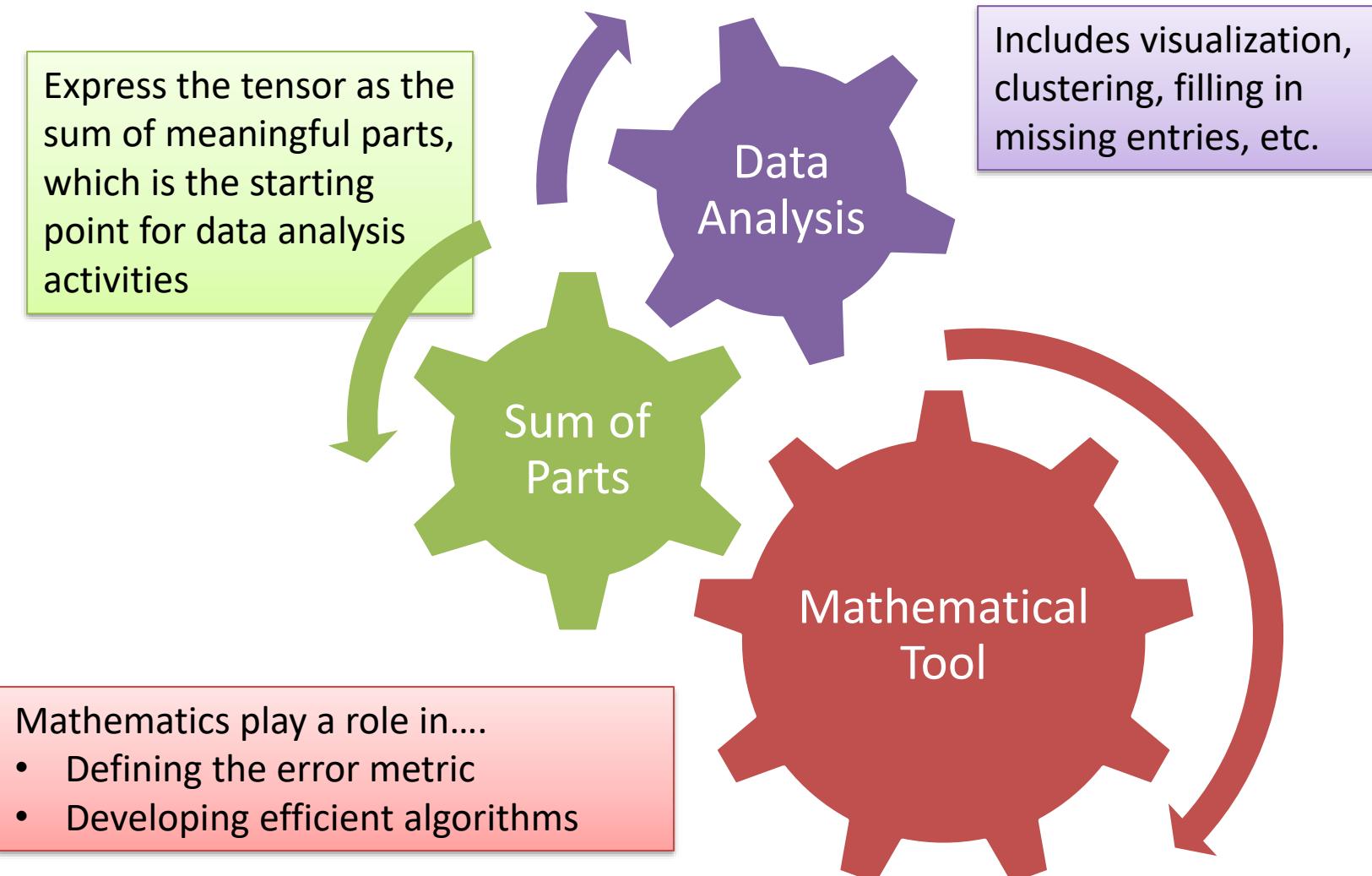
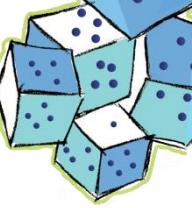
$d^{\text{th}}$ -order Tensor  
 $d > 3$



# Tensor Decomposition: A Mathematical Tool for Data Analysis



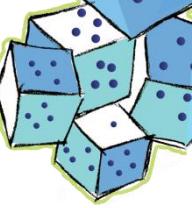
Sandia  
National  
Laboratories



## Related Concepts for Matrices

- Principal component analysis (PCA)
- Singular value decomposition (SVD)
- Independent component analysis (ICA)
- Nonnegative matrix factorization (NMF)
- Sparse matrix factorization
- Matrix completion

# Building Block for Decomposition: Rank-One Tensors = Vector Outer Products



## Matrix Version (2-way)

Given **two vectors**:

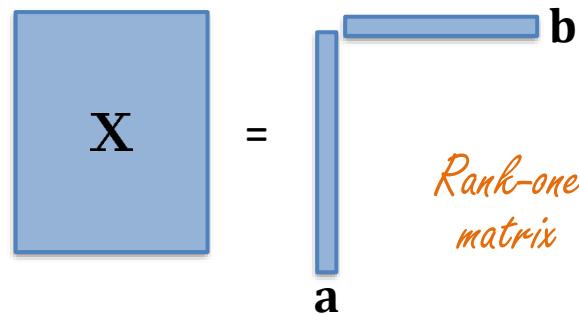
$$\mathbf{a} \in \mathbb{R}^m, \mathbf{b} \in \mathbb{R}^n$$

Their **outer product** is:

$$\mathbf{X} = \mathbf{a} \circ \mathbf{b} \in \mathbb{R}^{m \times n}$$

Each entry is given by:

$$x(i, j) = a(i) b(j)$$



## Tensor Version (3-way)

Given **three vectors**:

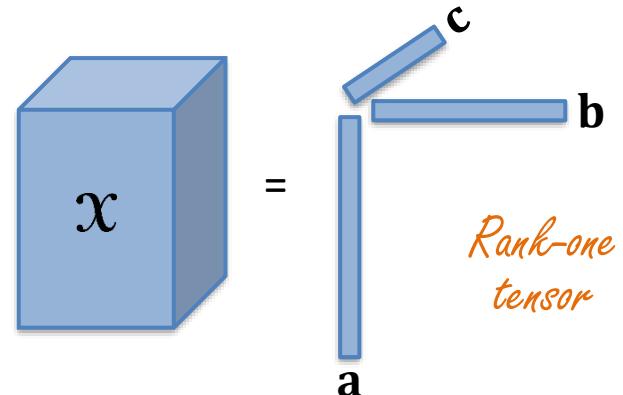
$$\mathbf{a} \in \mathbb{R}^m, \mathbf{b} \in \mathbb{R}^n, \mathbf{c} \in \mathbb{R}^p$$

Their **outer product** is:

$$\mathcal{X} = \mathbf{a} \circ \mathbf{b} \circ \mathbf{c} \in \mathbb{R}^{m \times n \times p}$$

Each entry is given by:

$$x(i, j, k) = a(i) b(j) c(k)$$



## Tensor Version ( $d$ -way)

Given  **$d$  vectors**:

$$\mathbf{a}_k \in \mathbb{R}^{n_k}, \quad k = 1, \dots, d$$

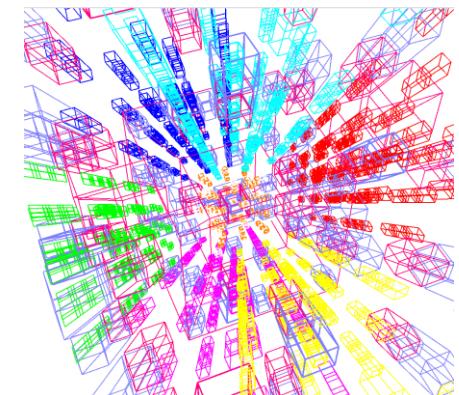
Their **outer product** is:

$$\mathcal{X} = \mathbf{a}_1 \circ \dots \circ \mathbf{a}_d \in \mathbb{R}^{n_1 \times \dots \times n_d}$$

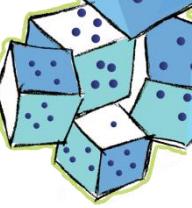
Each entry is given by:

$$x(i_1, \dots, i_d) = a_1(i_1) \dots a_d(i_d)$$

Visualizing gets  
weird...  
But the math is  
still fine!



# Matrix Decomposition: Detecting Low-Rank Structure



*Data*      *Low-Rank Model*

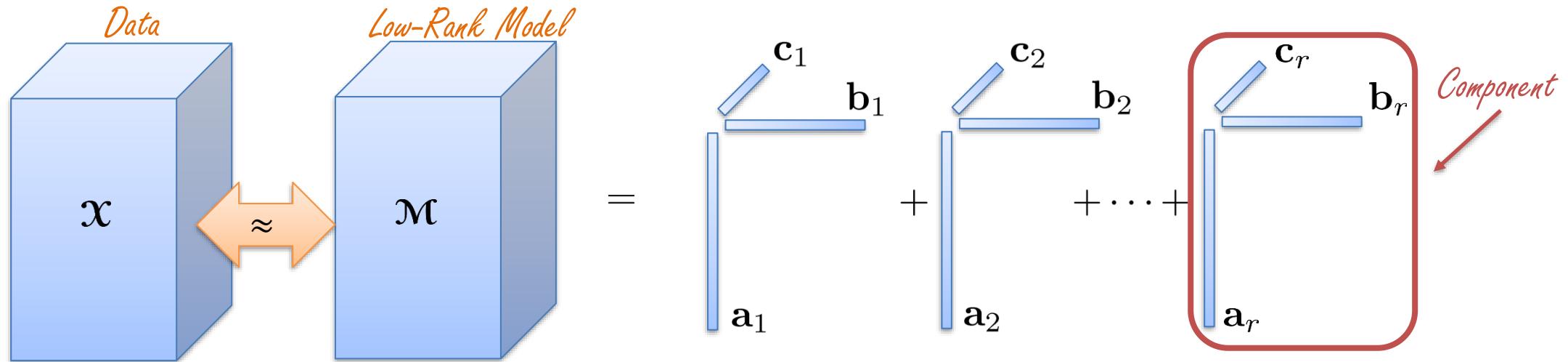
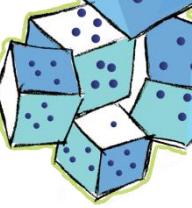
$$\mathbf{X} \approx \mathbf{M} = \mathbf{a}_1 \mathbf{b}_1 + \mathbf{a}_2 \mathbf{b}_2 + \dots + \mathbf{a}_r \mathbf{b}_r$$
$$x(i,j) \approx m(i,j) = a(i,1) b(j,1) + a(i,2) b(j,2) + \dots + a(i,r) b(j,r) = \sum_{\ell=1}^r a(i,\ell) b(j,\ell)$$

*Matrix Notation*  $\Rightarrow \mathbf{X} \approx \mathbf{M} = \sum_{\ell=1}^r \mathbf{a}_\ell \circ \mathbf{b}_\ell = \mathbf{A} \mathbf{B}^T = \llbracket \mathbf{A}, \mathbf{B} \rrbracket$

Sum of Squared Errors (SSE):  $\sum_{ij} (x(i,j) - m(i,j))^2 = \|\mathbf{X} - \mathbf{M}\|_F^2$

Eerily powerful tool for modeling data!  
Google search for “low-rank structure” turns up 5,590,000 results, and Google Scholar yields 127,000 papers!

# CP Tensor Factorization (3-way): Detecting low-rank 3-way structure



$$x(i, j, k) \approx m(i, j, k) = a(i, 1)b(j, 1)c(k, 1) + a(i, 2)b(j, 2)c(k, 2) + \cdots + a(i, r)b(j, r)c(k, r)$$

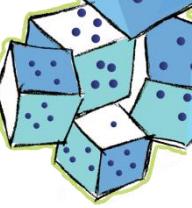
Tensor Notation  $\Rightarrow \mathcal{X} \approx \mathcal{M} = \sum_{\ell=1}^r \mathbf{a}_\ell \circ \mathbf{b}_\ell \circ \mathbf{c}_\ell = [\![\mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$

*Factor Matrices* ↑

Sum of Squared Errors (SSE):  $\sum_{ijk} (x(i, j, k) - m(i, j, k))^2 = \|\mathcal{X} - \mathcal{M}\|^2$

Potentially an *even more* powerful tool for modeling data! But still new. Google search for “low-rank *tensor* structure” turns up only 550,000 results, and Google Scholar yields a mere 14,500 papers.

# CP first invented in 1927



Frank Lauren Hitchcock  
MIT Professor  
(1875–1957)

## THE EXPRESSION OF A TENSOR OR A POLYADIC AS A SUM OF PRODUCTS

By FRANK L. HITCHCOCK

### 1. Addition and Multiplication.

Tensors are *added* by adding corresponding components. The *product* of a covariant tensor  $A_{i_1 \dots i_p}$  of order  $p$  into a covariant tensor  $B_{i_{p+1} \dots i_{p+q}}$  of order  $q$  is defined by writing

$$A_{i_1 \dots i_p} B_{i_{p+1} \dots i_{p+q}} = C_{i_1 \dots i_{p+q}} \quad (1)$$

where the product  $C_{i_1 \dots i_{p+q}}$  is a covariant tensor of order  $p+q$ . When no confusion results indices may be omitted giving

$$\mathbf{AB} = \mathbf{C} \quad (1a)$$

equivalent to the  $n^{p+q}$  equations (1). Boldface type is convenient for indicating that the letters do not denote merely numbers or scalars. Products of contravariant and of mixed tensors may be similarly defined.

A partial statement of the problem to be considered is as follows: to find under what conditions a given tensor can be expressed as a sum of products of assigned form. A more general statement of the problem will be given below.

### 2. Polyadic form of a tensor.

Any covariant tensor  $A_{i_1 \dots i_p}$  can be expressed as the sum of a finite number of tensors each of which is the product of  $p$  covariant vectors,

$$A_{i_1 \dots i_p} = \sum_{j=1}^{j=h} a_{1j}, i_1 a_{2j}, i_2 \dots a_{pj}, i_p \quad (2)$$

where  $a_{1j}, i_1$ , etc., are a set of  $hp$  covariant vectors. When the indices  $i_1 \dots i_p$  can be omitted this may be written

$$\mathbf{A} = \sum_{j=1}^{j=h} \mathbf{a}_{1j} \mathbf{a}_{2j} \dots \mathbf{a}_{pj}. \quad (2a)$$

The right member is now identical in appearance with a Gibbs

F. L. Hitchcock, *The Expression of a Tensor or a Polyadic as a Sum of Products*, Journal of Mathematics and Physics, 1927

### 2. Polyadic form of a tensor.

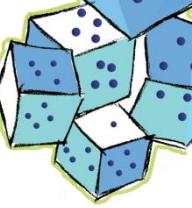
Any covariant tensor  $A_{i_1 \dots i_p}$  can be expressed as the sum of a finite number of tensors each of which is the product of  $p$  covariant vectors,

$$A_{i_1 \dots i_p} = \sum_{j=1}^{j=h} a_{1j}, i_1 a_{2j}, i_2 \dots a_{pj}, i_p \quad (2)$$

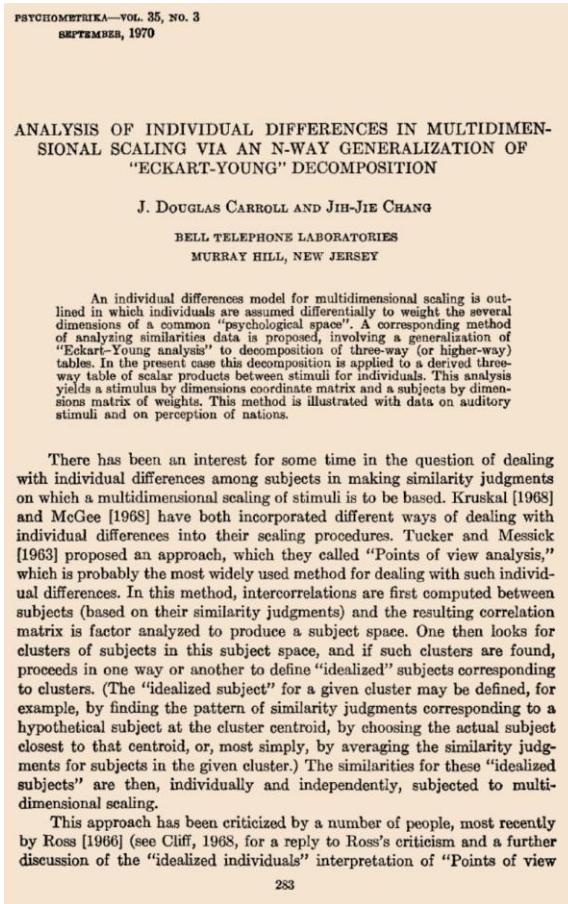
where  $a_{1j}, i_1$ , etc., are a set of  $hp$  covariant vectors. When the indices  $i_1 \dots i_p$  can be omitted this may be written

$$\mathbf{A} = \sum_{j=1}^{j=h} \mathbf{a}_{1j} \mathbf{a}_{2j} \dots \mathbf{a}_{pj}. \quad (2a)$$

# CP Independently Reinvented (twice) in 1970



## CANDECOMP: Canonical Decomposition



J. Douglas Carroll   Jih-Jie Chang  
Bell Labs              Bell Labs  
(1939-2011)        (1927-2007)

## CP: CANDECOMP/PARAFAC

## CP: Canonical Polyadic

Richard A. Harshman  
Univ. Ontario  
(1943-2008)

In 2000, Henk Kiers proposed this *compromise* name

2010: Pierre Comon, Lieven DeLathauwer, and others reverse-engineered CP, revising some of Hitchcock's terminology

## PARAFAC: Parallel Factors

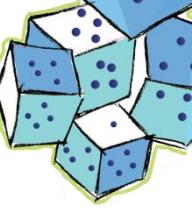
NOTE: This manuscript was originally published in 1970 and is reproduced here to make it more accessible to interested scholars. The original reference is Harshman, R. A. (1970). Foundations of the PARAFAC procedure: Models and conditions for an "exploratory" multimodal factor analysis. *UCLA Working Papers in Phonetics*, 16, 1-84. (University Microfilms, Ann Arbor, Michigan, No. 10,085).

# FOUNDATIONS OF THE PARAFAC PROCEDURE: MODELS AND CONDITIONS FOR AN "EXPLANATORY" MULTIMODAL FACTOR ANALYSIS

by

U C L A  
*Working Papers in Phonetics*  
16  
December, 1970

Many thanks to the following persons for helping me learn about Jih-Jie Chang: Fan Chung, Ron Graham, Shen Lin (husband), May Chang (niece), Lili Bruer (daughter).



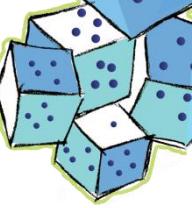
## Example: CP for Mouse Neural Activity

A. H. Williams, T. H. Kim, F. Wang, S. Vyas, S. I. Ryu, K. V. Shenoy, M. Schnitzer, T. G. Kolda, S. Ganguli. **Unsupervised Discovery of Demixed, Low-dimensional Neural Dynamics across Multiple Timescales through Tensor Components Analysis.** bioRxiv, 2017. <https://doi.org/10.1101/211128>

# New Devices Enable Measuring Multiple Neurons Simultaneously



Sandia  
National  
Laboratories

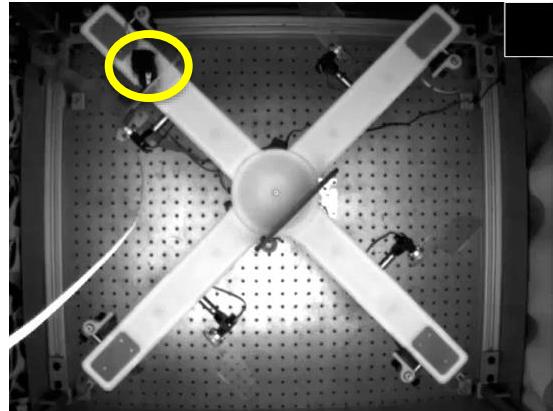


Thanks to Schnitzer Group @ Stanford  
Mark Schnitzer, Fori Wang, Tony Kim

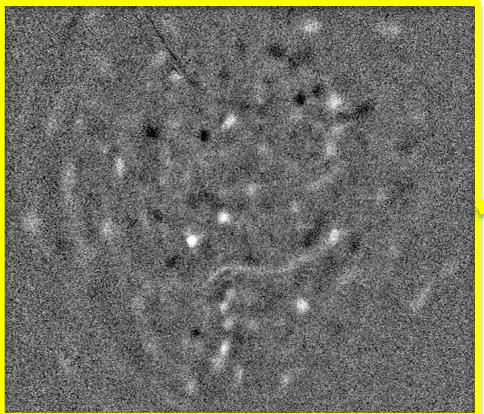
Microscope by  
Inscopix



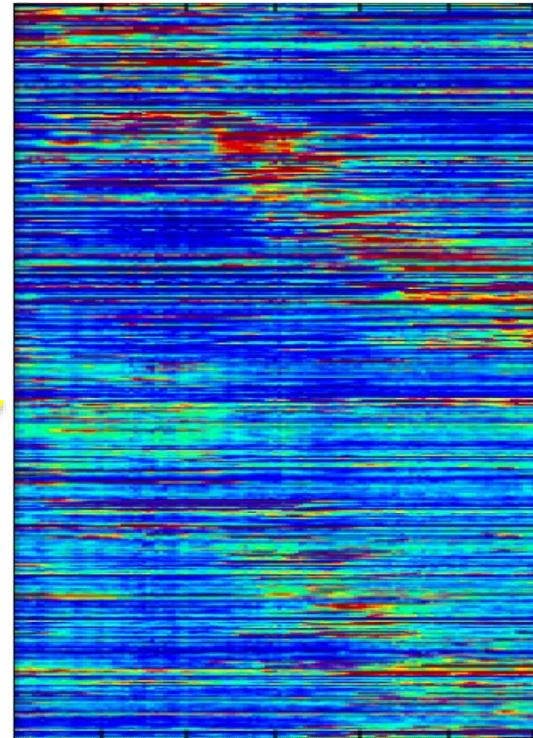
mouse  
in "maze"



neural activity

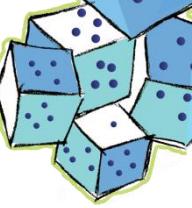


One Trial  
300 neurons  $\times$  120 time bins

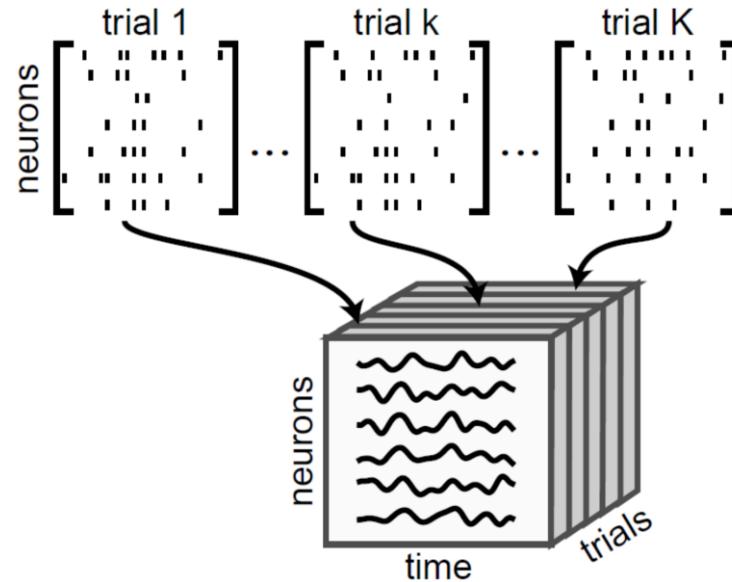


time  $\rightarrow$   
 $\times 600$  trials (over 5 days)

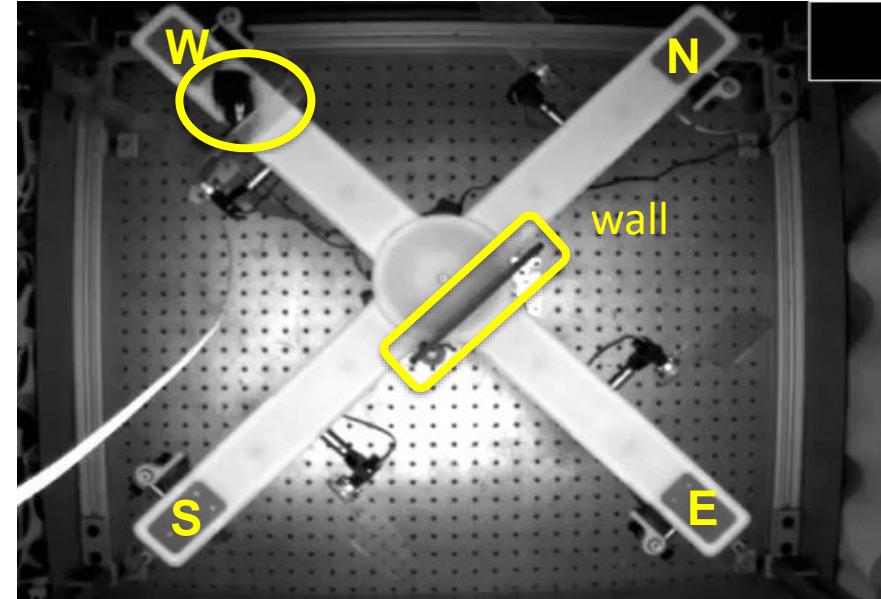
Williams et al., bioRxiv, 2017, DOI:10.1101/211128



# Trials Vary Start Position and Strategies

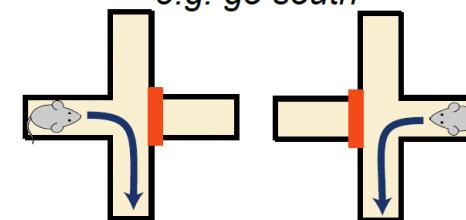


- 600 Trials over 5 Days
- Start West or East
- Conditions Swap Twice
  - ❖ Always Turn South
  - ❖ Always Turn Right
  - ❖ Always Turn South

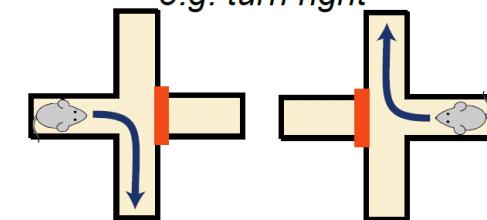


*note different patterns on curtains*

**Allocentric Condition**  
e.g. go south



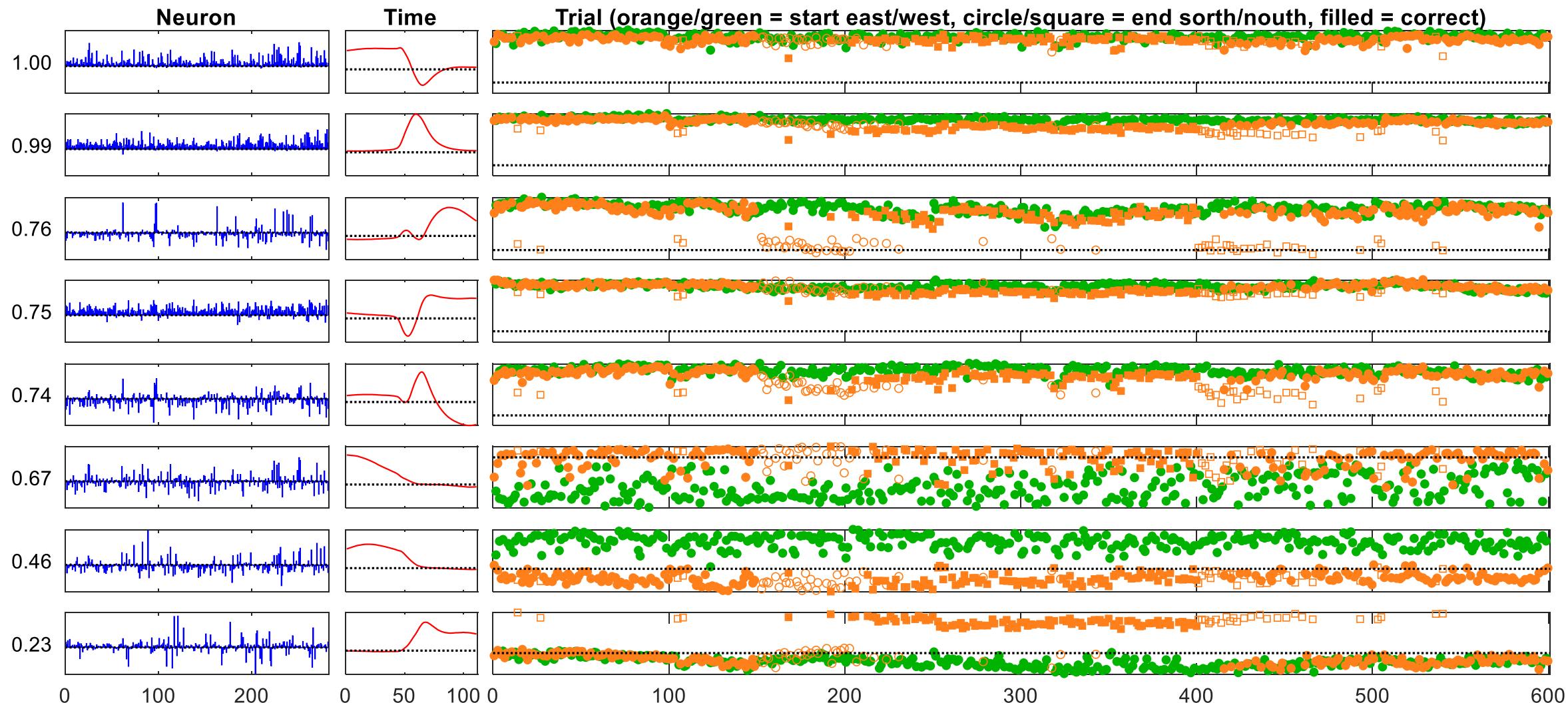
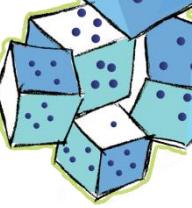
**Egocentric Condition**  
e.g. turn right



# 8-Component CP Decomposition of Mouse Neuron Data



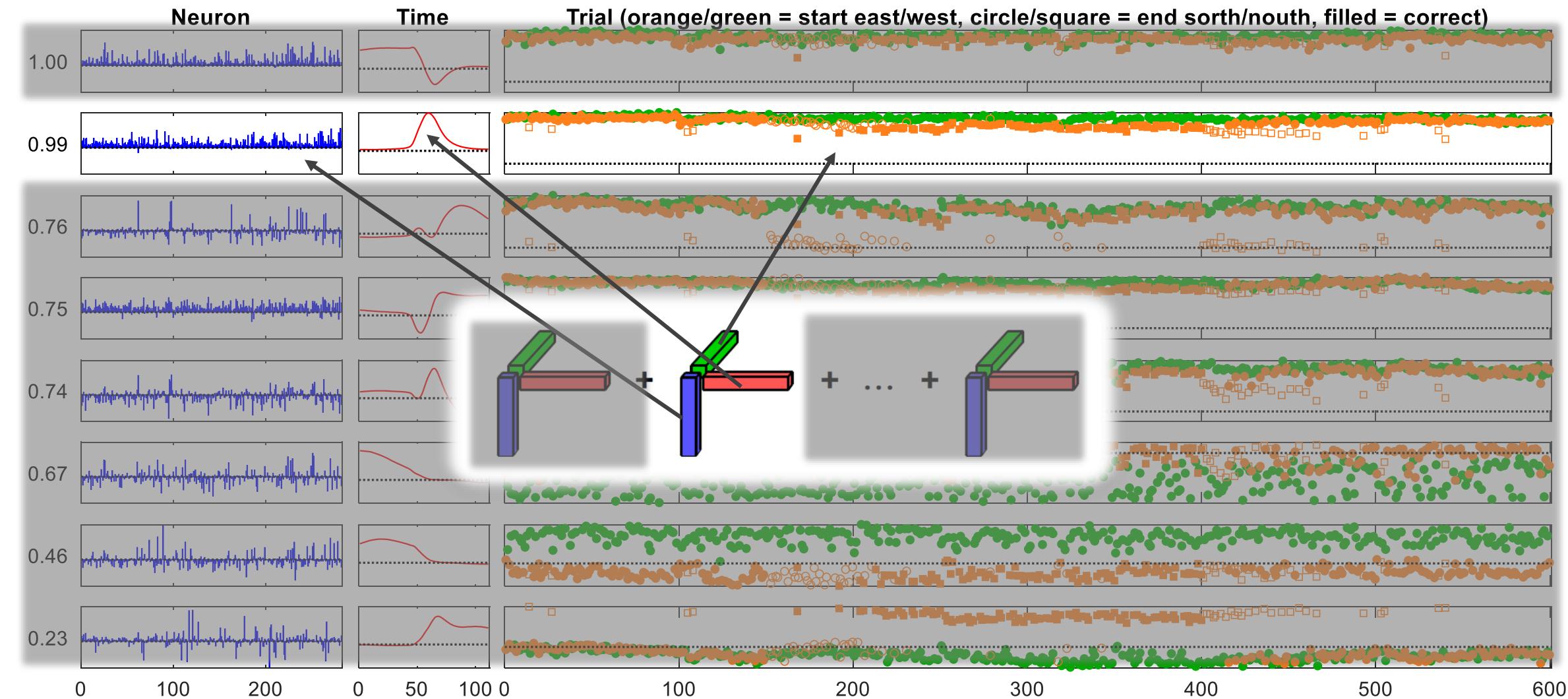
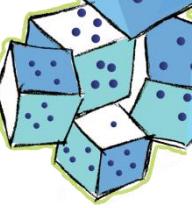
Sandia  
National  
Laboratories



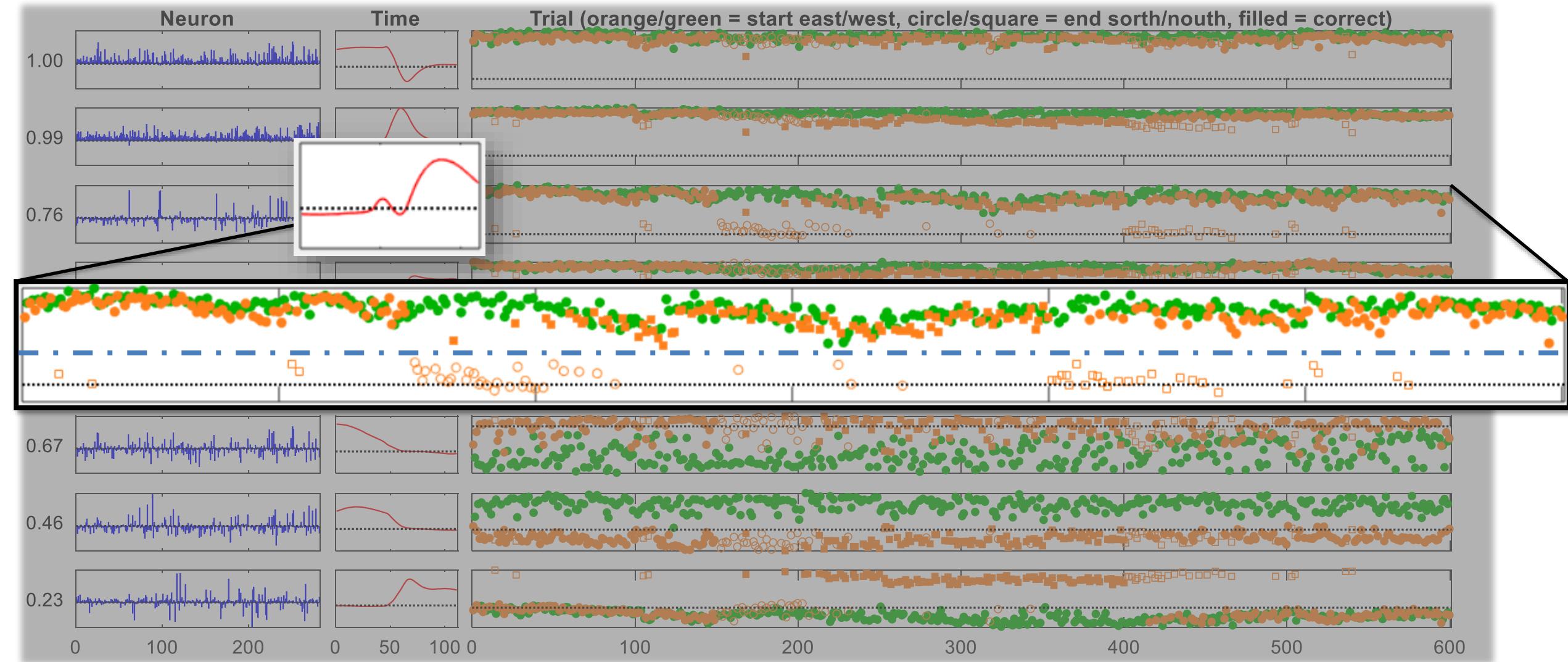
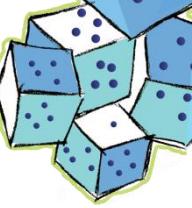
# 8-Component CP Decomposition of Mouse Neuron Data



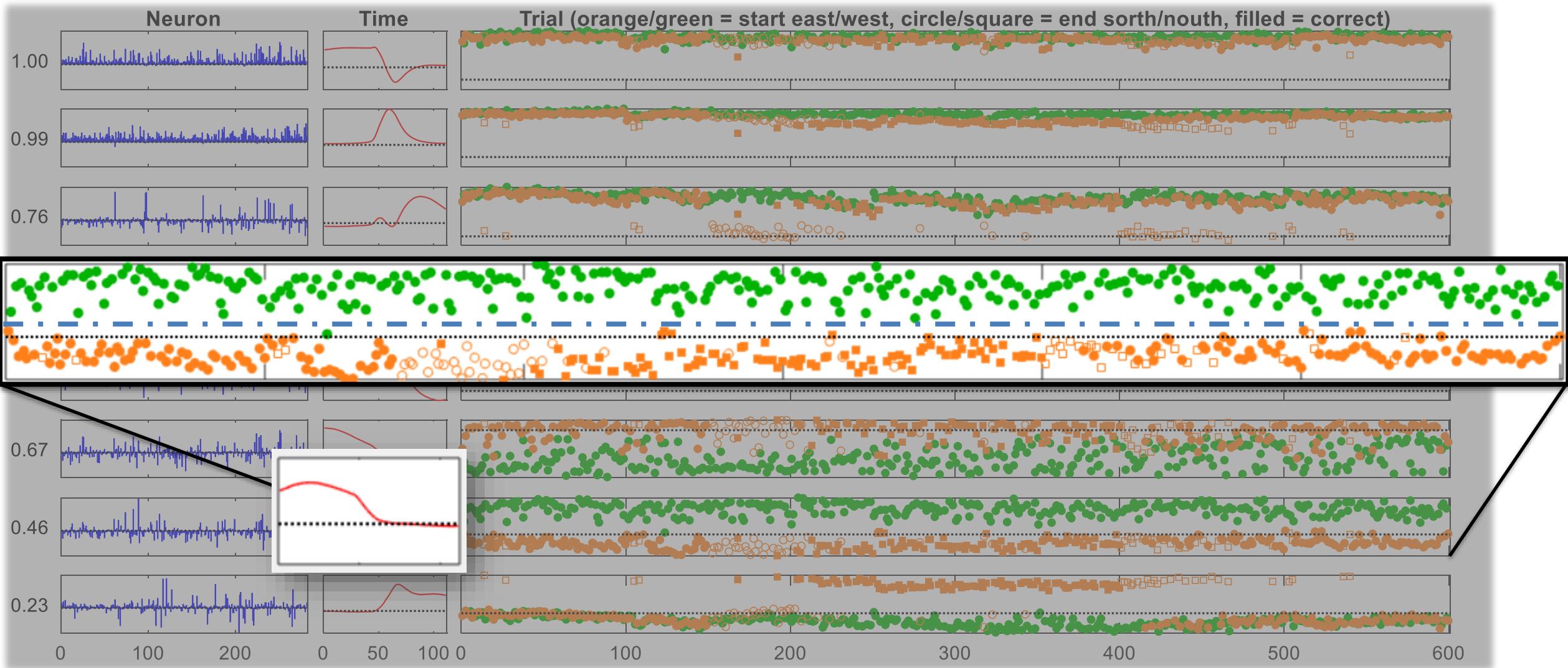
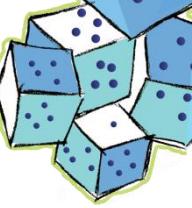
Sandia  
National  
Laboratories



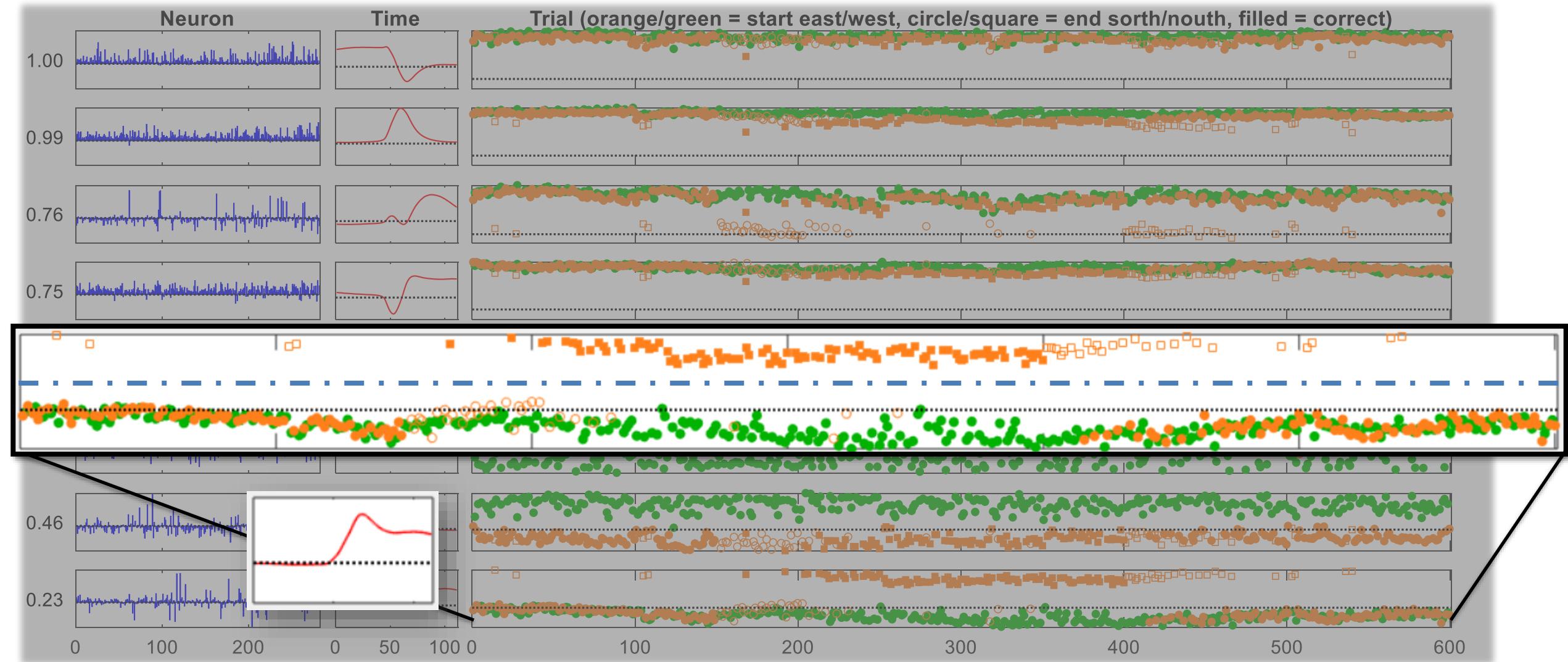
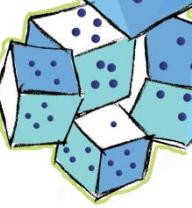
# 8-Component CP Decomposition of Mouse Neuron Data



# 8-Component CP Decomposition of Mouse Neuron Data

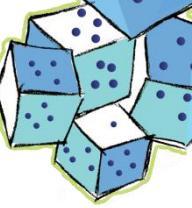


# 8-Component CP Decomposition of Mouse Neuron Data





Sandia  
National  
Laboratories



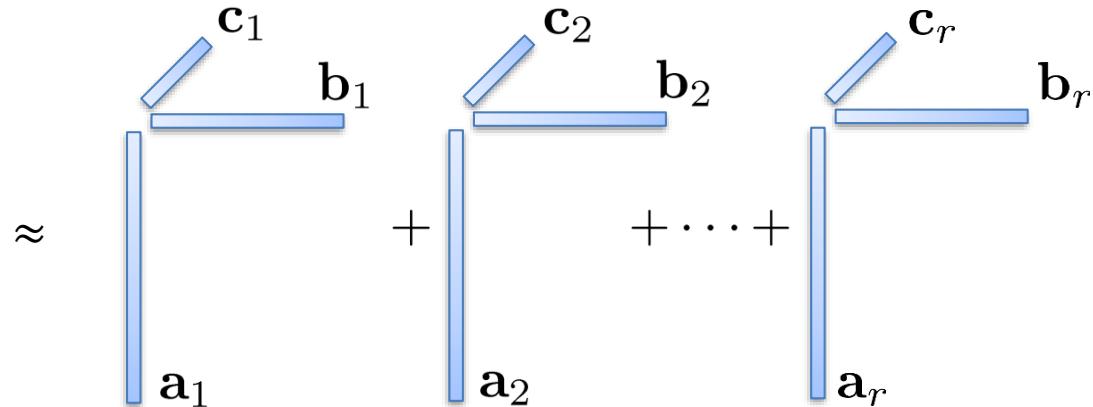
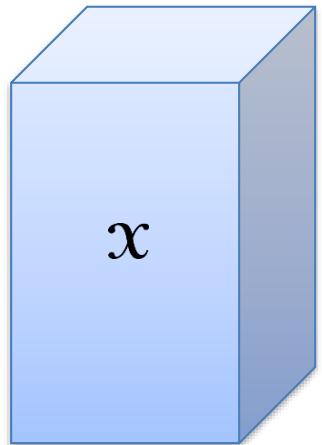
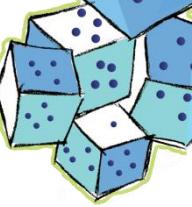
# Randomized Least Squares for CP Decomposition

C. Battaglino, G. Ballard, T. G. Kolda. **A Practical Randomized CP Tensor Decomposition.**  
arXiv:1701.06600, 2017.

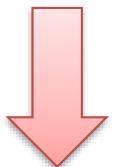
# Fitting CP



Sandia  
National  
Labs

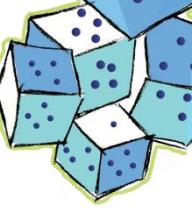


$$\min_{\mathbf{A}, \mathbf{B}, \mathbf{C}} \|\mathcal{X} - \mathcal{M}\|^2 \text{ s.t. } \mathcal{M} = [\mathbf{A}, \mathbf{B}, \mathbf{C}]$$

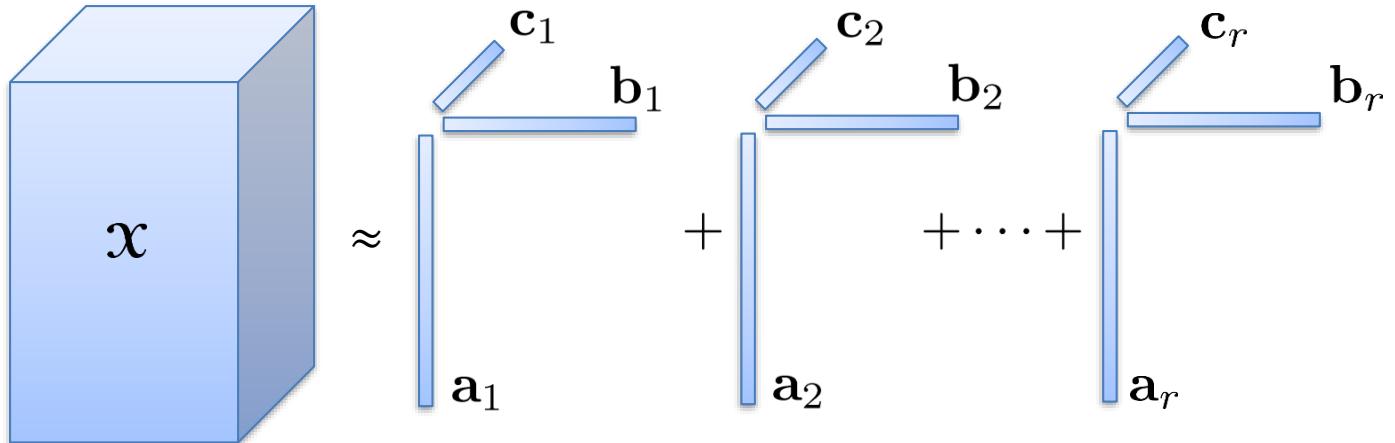


$$\min_{\mathbf{A}, \mathbf{B}, \mathbf{C}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$$

- **Rank ( $r$ ) NP-Hard:** Even best low-rank solution may not exist (Håstad 1990, Silva & Lim 2006, Hillar & Lim 2009)
- **Not nested:** Best rank- $(r-1)$  factorization may not be part of best rank- $r$  factorization (Kolda 2001)
- **Not orthogonal:** Factor matrices are not orthogonal and may even have linearly dependent columns
- **Essentially Unique:** Under modest conditions, CP is unique up to permutation and scaling (Kruskal 1977)



# Fitting CP: Alternating Least Squares



$$\min_{\mathbf{A}, \mathbf{B}, \mathbf{C}} \|\mathcal{X} - \mathcal{M}\|^2 \text{ s.t. } \mathcal{M} = [\mathbf{A}, \mathbf{B}, \mathbf{C}]$$



$$\min_{\mathbf{A}, \mathbf{B}, \mathbf{C}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$$

Repeat until convergence:

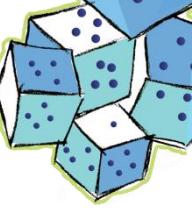
$$\text{Step 1: } \min_{\mathbf{A}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$$

$$\text{Step 2: } \min_{\mathbf{B}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$$

$$\text{Step 3: } \min_{\mathbf{C}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$$

Nonconvex problem with convex subproblems.

# Solving the Least Squares Problem



$$\min_{\mathbf{A}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} \mathbf{a}_{i\ell} b_{j\ell} c_{k\ell} \right)^2 \quad \longrightarrow \quad \min_{\mathbf{A}} \|\mathbf{X}_{(1)} - \mathbf{A}(\mathbf{C} \odot \mathbf{B})'\|_F^2$$

“right hand sides”

$$\mathbf{X}_{(1)}$$

Matrix Unfolding

3-way case

$$n \times n^2$$

$d$ -way case

$$n \times n^{d-1}$$



$\mathbf{A}$

“matrix”

$$\begin{array}{c} \hline & (\mathbf{c}_1 \otimes \mathbf{b}_1)' & \hline \\ \vdots & \vdots & \vdots \\ \hline & (\mathbf{c}_r \otimes \mathbf{b}_r)' & \hline \end{array}$$

Khatri-Rao Product

$$(\mathbf{C} \odot \mathbf{B})'$$

$$n \times r$$

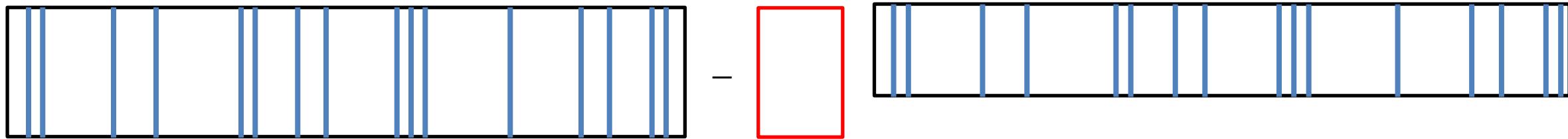
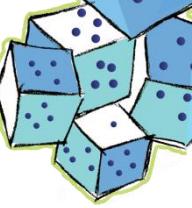
$$n \times r$$

$$r \times n^2$$

$$r \times n^{d-1}$$

Short & Very Wide Matrix

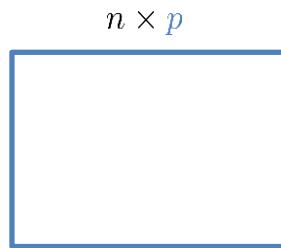
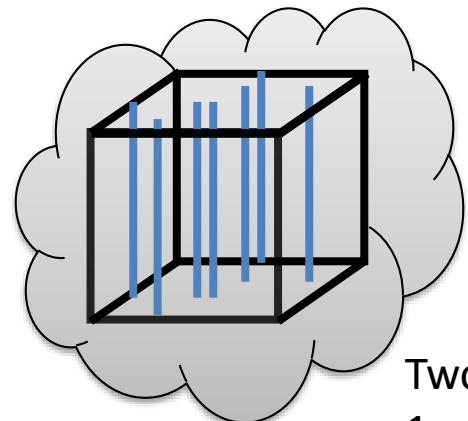
# CPRAND: Randomized Matrix Least Squares Subproblem



$\|\mathbf{X}_{(1)} \mathbf{S}$

$- \mathbf{A}$

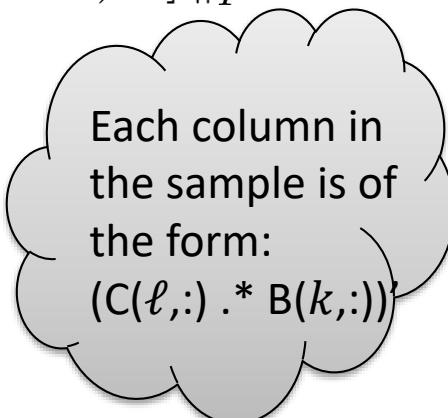
$[(\mathbf{C} \odot \mathbf{B})' \mathbf{S}] \parallel_F^2$



$n \times p$

$- \mathbf{A}$

$r \times p$



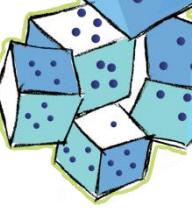
Each column in the sample is of the form:  
 $(\mathbf{C}(\ell,:) \cdot^* \mathbf{B}(k,:))'$

Two “tricks”

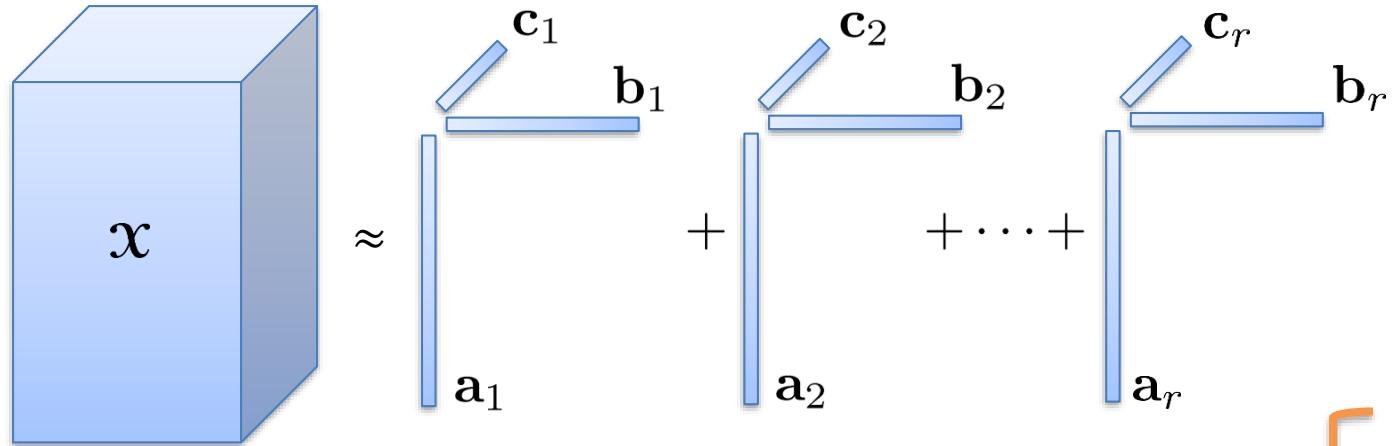
1. Never permute elements of tensor  $\mathbf{X}$  into  $n \times n^2$  matrix form
2. Never form full Khatri-Rao product of size  $r \times n^2$

**CPRAND-MIX:** Apply fast Johnson-Lindenstrauss Transform to mix the data in each direction to ensure “incoherence” – introduces some preprocessing cost

Battaglino, Ballard, Kolda, *A Practical Randomized CP Tensor Decomposition*, Jan 2017, arXiv:1701.06600



# Convergence Check Become the Bottleneck!



Very fast with  
matrix sketching

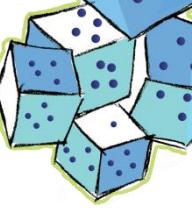
Repeat until convergence:

Step 1:  $\min_{\mathbf{A}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$

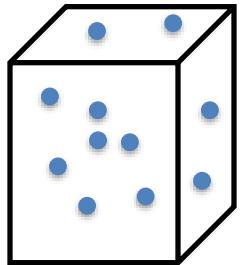
Step 2:  $\min_{\mathbf{B}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$

Step 3:  $\min_{\mathbf{C}} \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$

# Randomizing the Convergence Check



$$F(\mathbf{A}, \mathbf{B}, \mathbf{C}) = \sum_{ijk} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$$

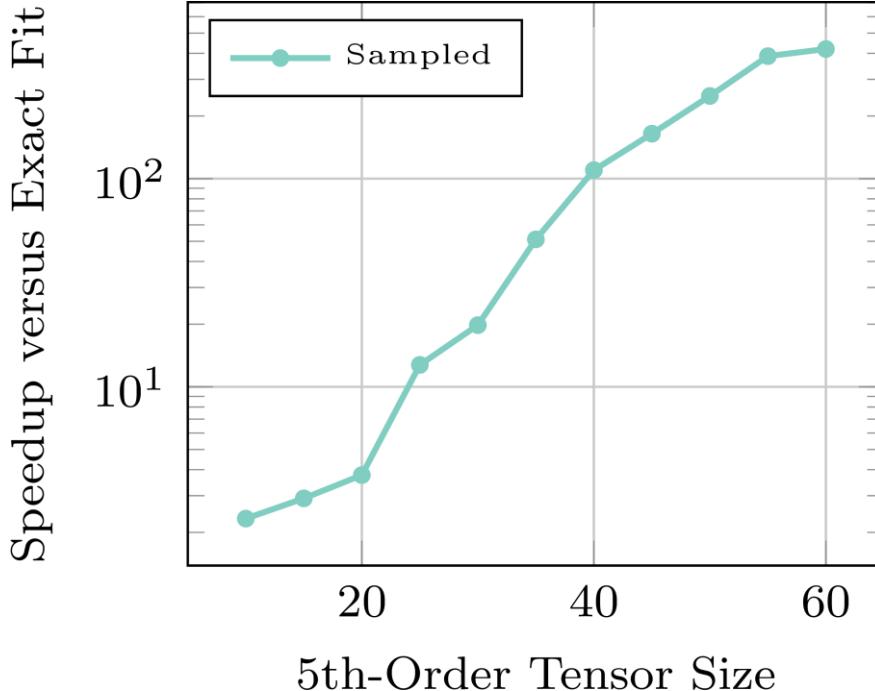


Estimate convergence of  
function values using small  
random subset of elements  
in function evaluation  
(use Chernoff-Hoeffding to  
bound accuracy)

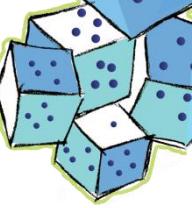
$$\hat{F}(\mathbf{A}, \mathbf{B}, \mathbf{C}) = \omega \sum_{ijk \in \Omega} \left( x_{ijk} - \sum_{\ell} a_{i\ell} b_{j\ell} c_{k\ell} \right)^2$$

16000 samples < 1% of full data

$$\frac{|F - \hat{F}|}{|F|} < 10^{-3}$$

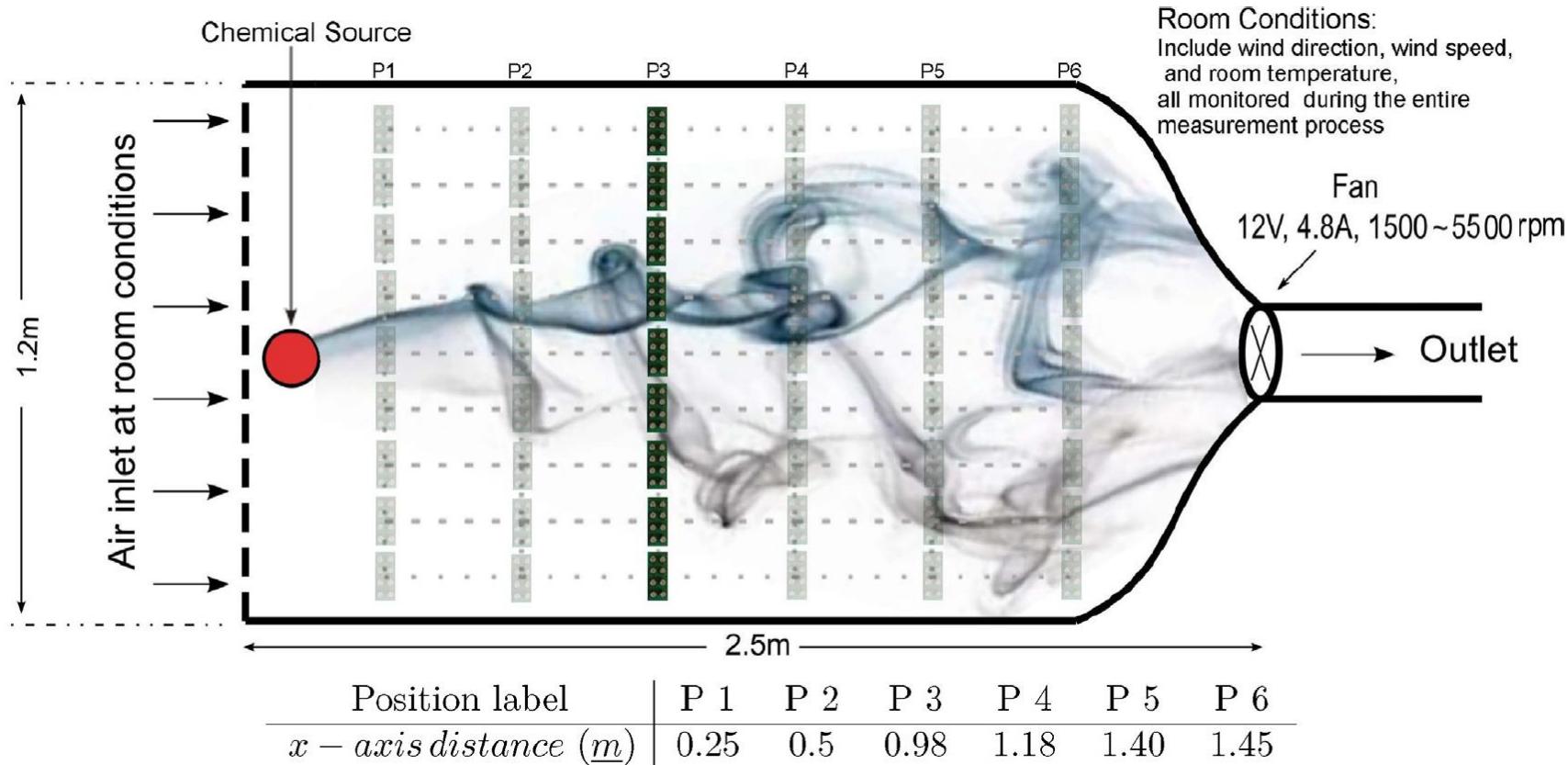


Battaglino, Ballard, & Kolda 2017



# Application to Hazardous Gas Dataset

71 Sensors  $\times$  5000 Timepoints  $\times$  5 Temperatures  $\times$  140 Experiments  $\approx$  2 GB

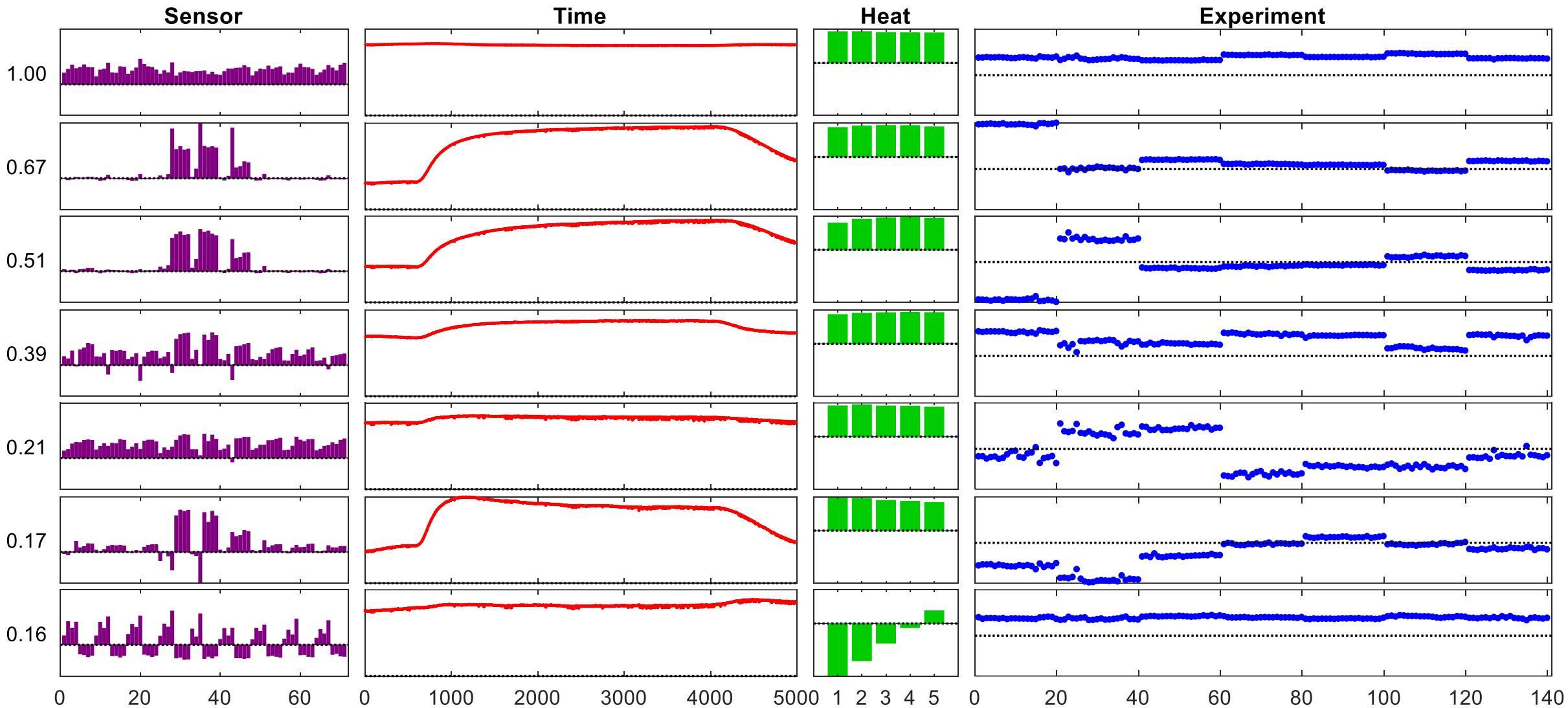
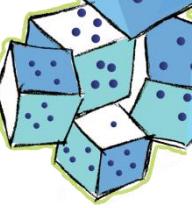


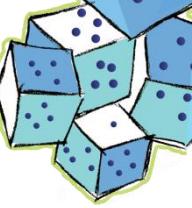
CP-ALS:  
65 seconds

CP-ALS-RAND:  
27 seconds

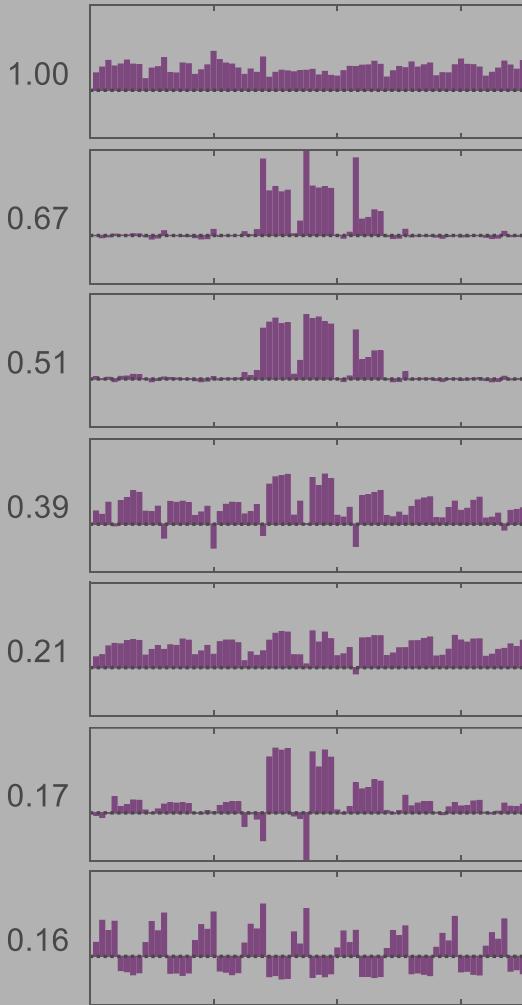
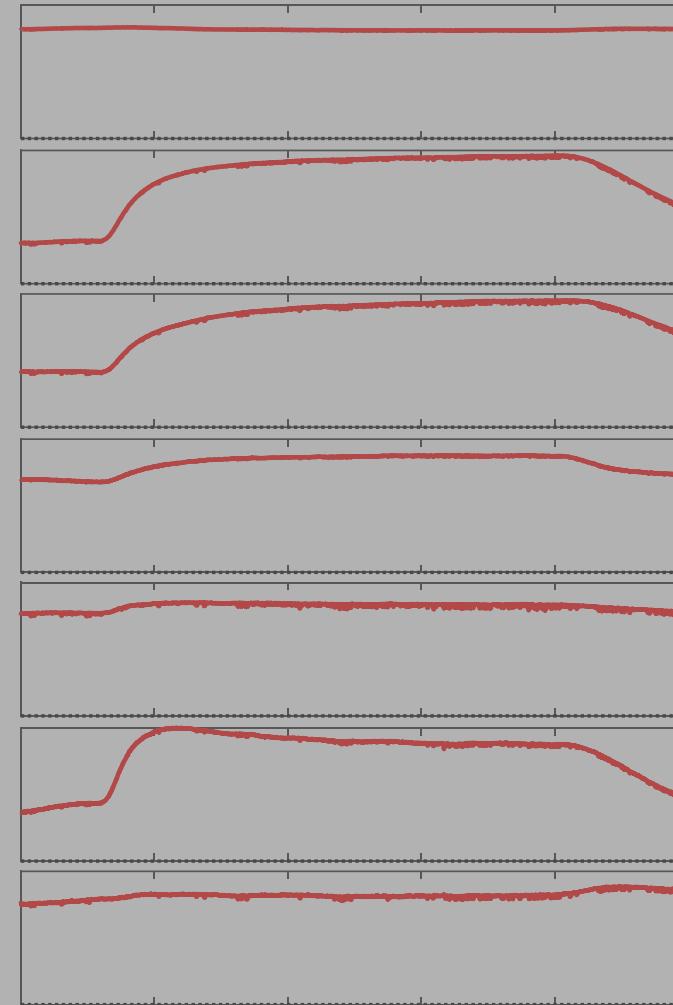
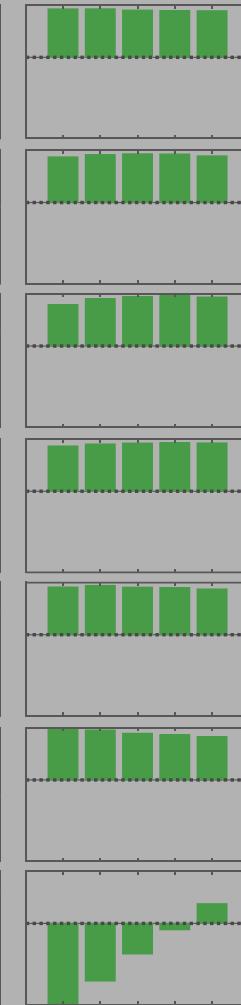
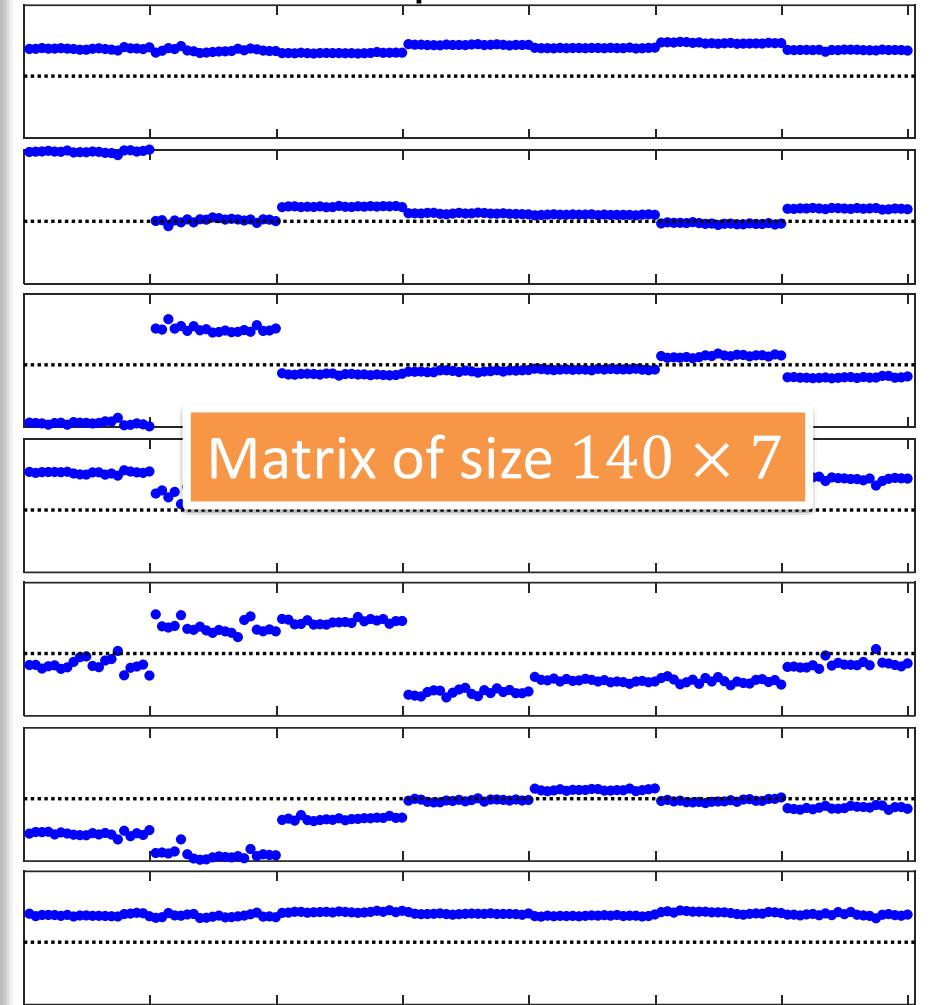
A. Vergara, J. Fonollosa, J. Mahiques, M. Trincavelli, N. Rulkov and R. Huerta, *On the performance of gas sensor arrays in open sampling systems using Inhibitory Support Vector Machines*, Sensors and Actuators B: Chemical, 2013, [doi:10.1016/j.snb.2013.05.027](https://doi.org/10.1016/j.snb.2013.05.027)

# Factors from Gas Dataset

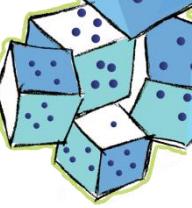




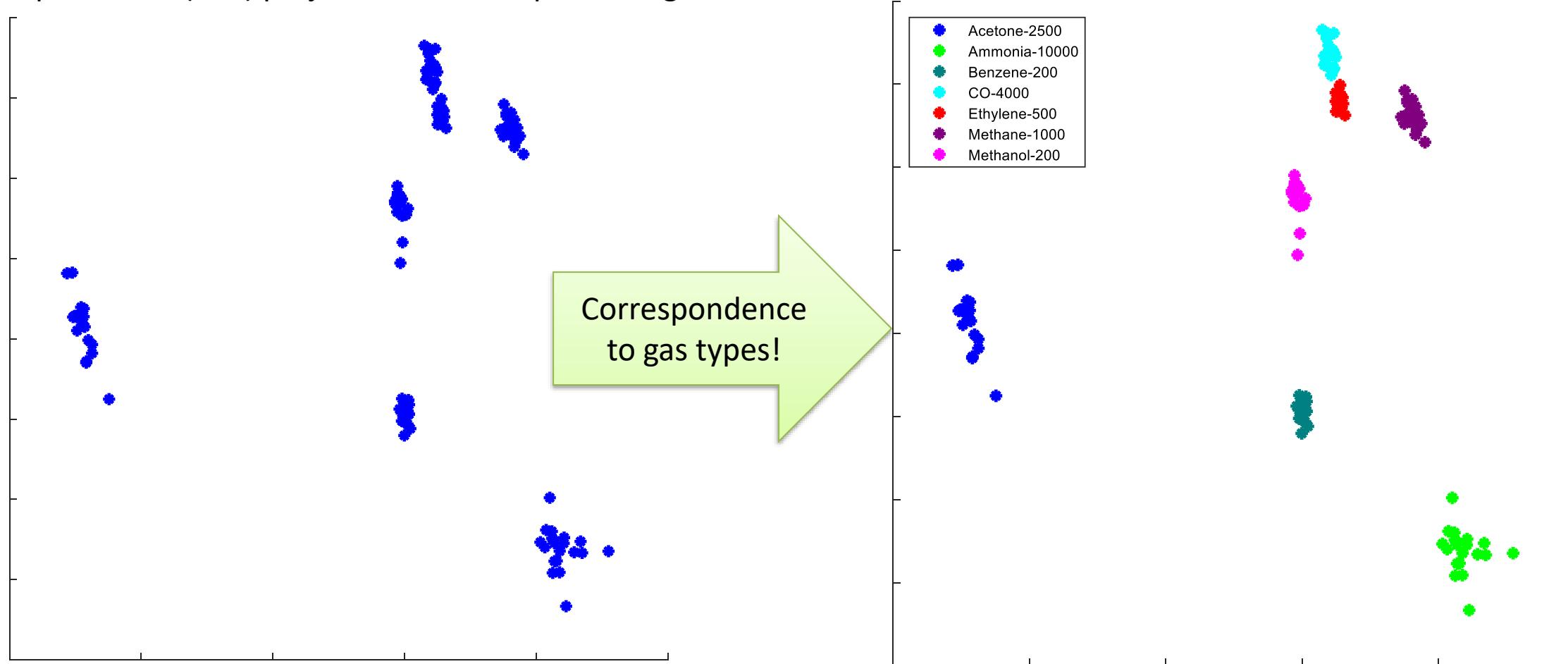
# Factors from Gas Dataset

**Sensor**

**Time**

**Heat**

**Experiment**


# Viz of Experiment Factor Matrix Using PCA Projection

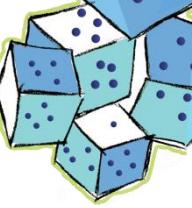


Experiments (140) projected onto 2D space using PCA



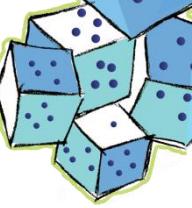


Sandia  
National  
Laboratories

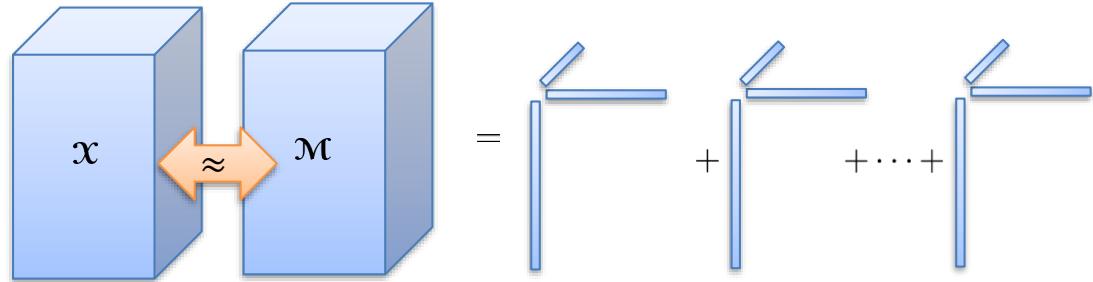


# Generalized CP Decomposition

Cliff Anderson-Bergman, J. Duersch, D. Hong, T. G. Kolda, **Generalized Canonical Polyadic Tensor Decomposition**, 2018 (coming soon)



# Generalizing the Goodness-of-Fit Criteria



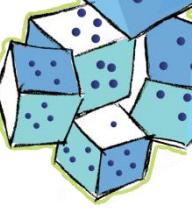
$$\mathcal{X} \approx \mathcal{M} = \sum_{j=1}^r \mathbf{a}_j \circ \mathbf{b}_j \circ \mathbf{c}_j = [\![\mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$$

$$\min_{\mathbf{A}, \mathbf{B}, \mathbf{C}} \sum_{ijk} (x_{ijk} - m_{ijk})^2 \text{ s.t. } \mathcal{M} = [\![\mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$$

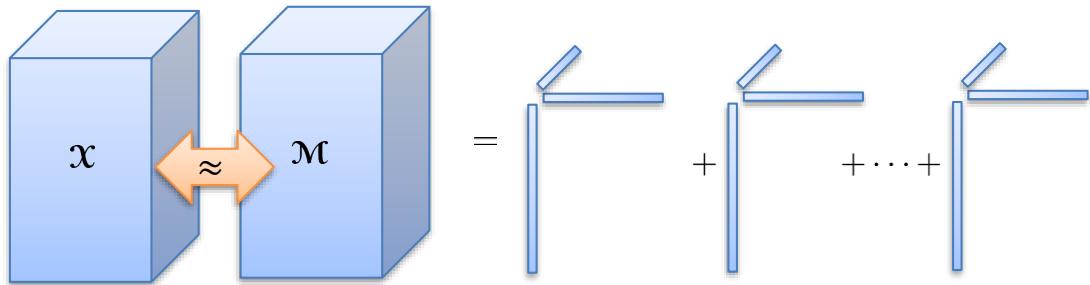
$$F(\mathbf{A}, \mathbf{B}, \mathbf{C}) = \sum_{ijk} (x_{ijk} - m_{ijk})^2$$



$$F(\mathbf{A}, \mathbf{B}, \mathbf{C}) = \sum_{ijk} f(x_{ijk}, m_{ijk})$$



# “Standard” CP via Maximum Likelihood



Typically: Consider data to be low-rank plus “white noise”

$$x_{ijk} = m_{ijk} + \epsilon_{ijk}, \quad \epsilon_{ijk} \sim \mathcal{N}(0, \sigma)$$

Equivalently, **Gaussian** with mean  $m_{ijk}$

$$x_{ijk} \sim \mathcal{N}(m_{ijk}, \sigma)$$

Gaussian Probability Density Function (PDF)

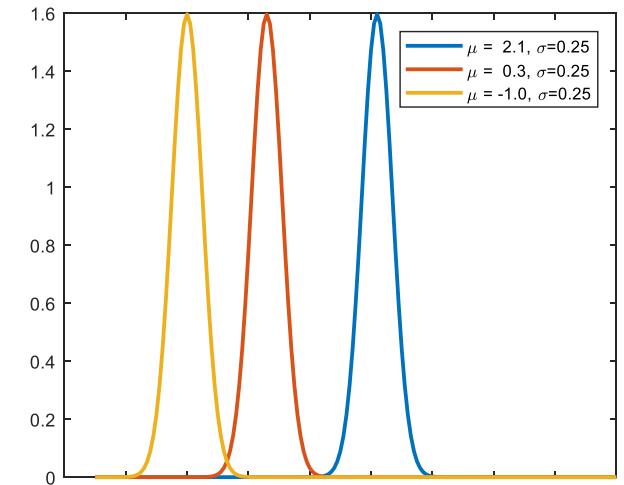
$$\frac{e^{-(x-\mu)^2/2\sigma^2}}{\sqrt{2\pi\sigma^2}}$$

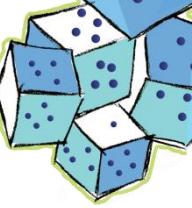
Minimize **negative log likelihood** with  $\mu_{ijk} = m_{ijk}$  and  $\sigma$  constant for all entries:

$$-\log(\mathcal{L}(\mathcal{M})) = \sum_{ijk} \frac{(x_{ijk} - m_{ijk})^2}{\sigma^2} + 1/2 \ln 2\pi\sigma^2$$

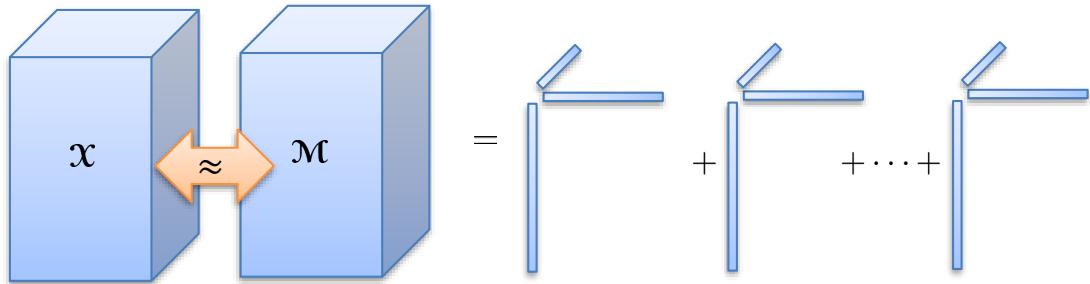
$$\min F(\mathcal{M}) = \sum_{ijk} (x_{ijk} - m_{ijk})^2$$

Probability Distribution Function:  
Normal-distributed with constant  $\sigma$





# “Rayleigh CP” with Linear Link



What if the data is nonnegative ( $x_{ijk} \geq 0$ )?

Assume data is Rayleigh-distributed.

$$x_{ijk} \sim \text{Rayleigh}(m_{ijk})$$

Requires  $m_{ijk} \geq 0$

Rayleigh Probability Density Function (PDF)

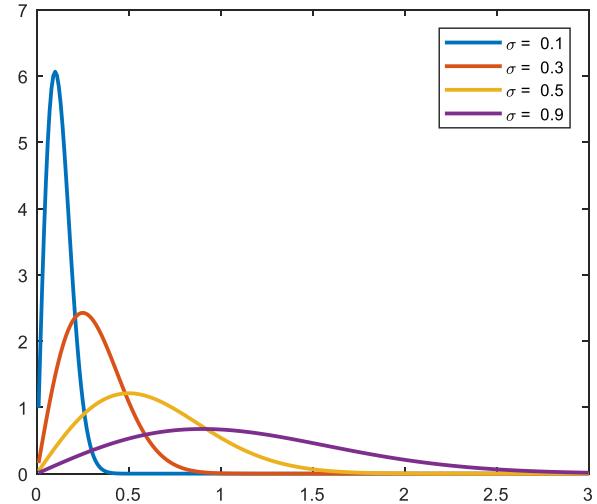
$$\frac{x}{\sigma^2} e^{-x^2/(2\sigma^2)}$$

Minimize **negative log likelihood** with  $\sigma_{ijk} = m_{ijk}$ :

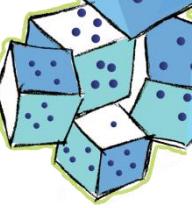
$$-\log(\mathcal{L}(\mathcal{M})) = \sum_{ijk} -\log \sigma_{ijk} + 2 \log m_{ijk} + \frac{x_{ijk}^2}{2m_{ijk}^2}$$

$$\min F(\mathcal{M}) = \sum_{ijk} 2 \log m_{ijk} + \frac{x_{ijk}^2}{2m_{ijk}^2}$$

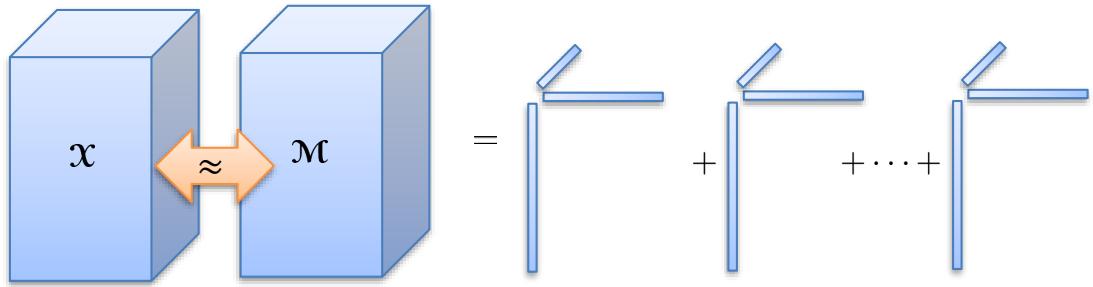
Probability Distribution Function:  
Rayleigh-distributed



$$\mathbb{E}(x_{ijk}) = m_{ijk} \sqrt{\frac{\pi}{2}}$$



# “Boolean CP” with Odds Link



What if data is binary ( $x_{ijk} \in \{0,1\}$ )?

$m_{ijk}$  = odds ratio of  $x_{ijk} = 1$ .

$x_{ijk} \sim \text{Bernoulli}(m_{ijk}/(1 + m_{ijk}))$

$$\mathbb{E}(x_{ijk}) = \frac{m_{ijk}}{1 + m_{ijk}}$$

Requires  $m_{ijk} \geq 0$



Random Coin Flip: Probability versus Odds

$p \in [0,1]$  : probability of 1  
 $r \geq 0$  : odds ratio of 1

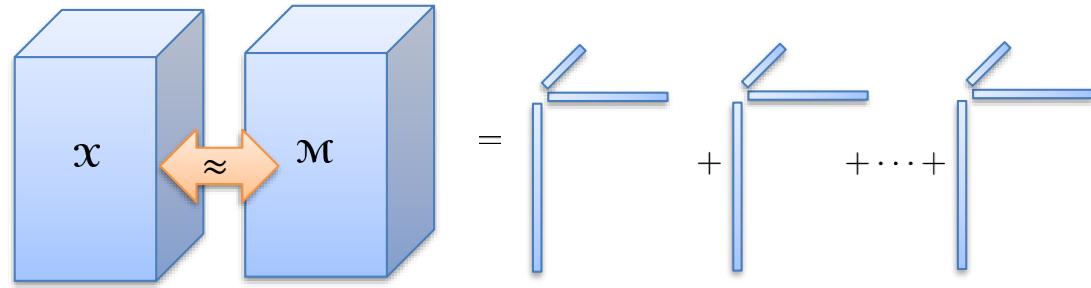
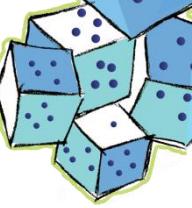
$$r = \frac{p}{1 - p} \Leftrightarrow p = \frac{r}{1 + r}$$

Probability Mass  
Distribution (PMF)

$$p^x(1 - p)^{1-x} \Leftrightarrow \left(\frac{r}{1+r}\right)^x \left(\frac{1}{1+r}\right)^{1-x}$$

$$\min F(\mathcal{M}) = \sum_{ijk} \log(m_{ijk} + 1) - x_{ijk} \log m_{ijk}$$

# Generalized CP



$$\min_{\mathbf{A}, \mathbf{B}, \mathbf{C}} \sum_{ijk \in \Omega} f(x_{ijk}, m_{ijk}) \quad \text{s.t. } \mathbf{M} = [\![\mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$$

Standard ( $x, m \in \mathbb{R}$ ):  $f(x, m) = (x - m)^2$

Rayleigh ( $x, m \in \mathbb{R}_+$ ):  $f(x, m) = 2 \log(m) + x^2/(2m^2)$

Boolean-Odds ( $x \in [0,1]$ ,  $m \in \mathbb{R}_+$ ):  $f(x, m) = \log(m + 1) - x \log(m)$

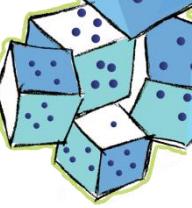
Poisson ( $x \in \mathbb{N}$ ,  $m \in \mathbb{R}_+$ ):  $f(x, m) = m - x \log(m)$

Similar ideas have been proposed in matrix world,

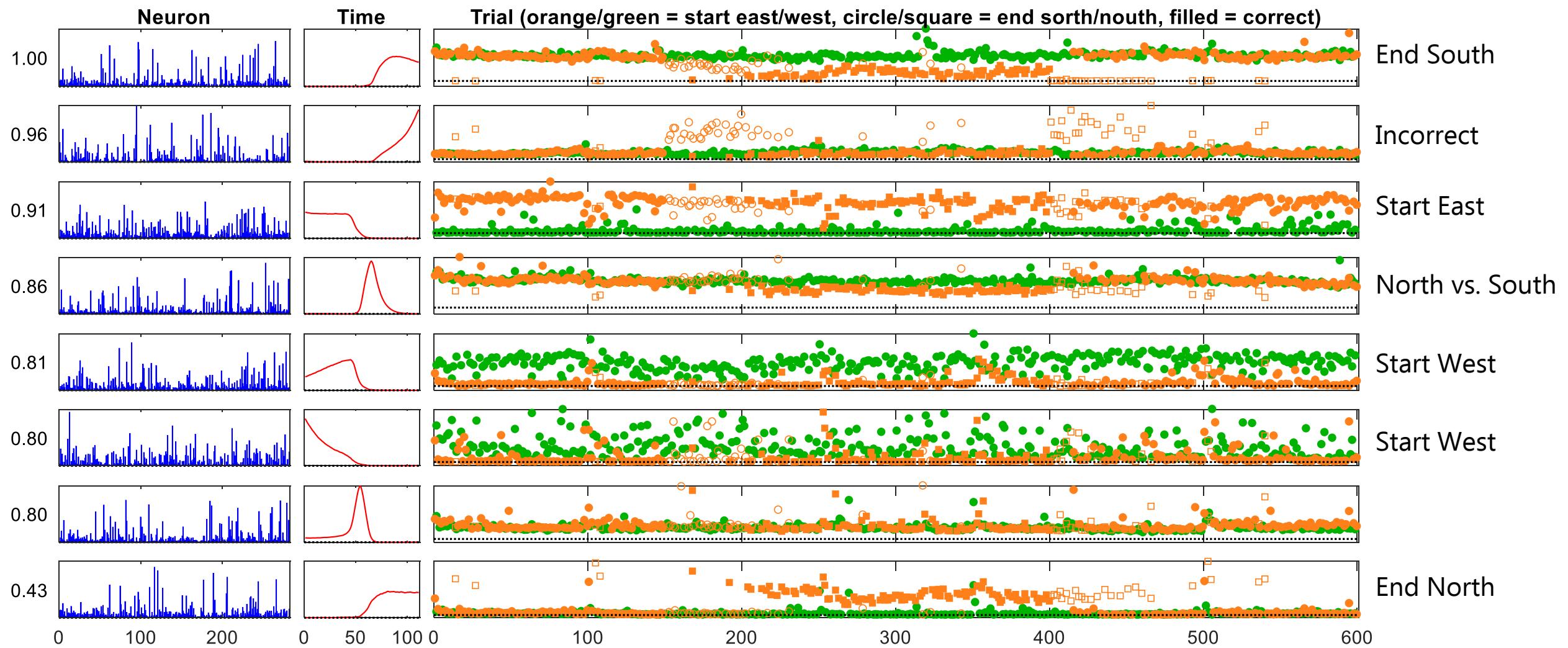
e.g., Collins, Dasgupta, Schapire 2002

## Algorithm Notes

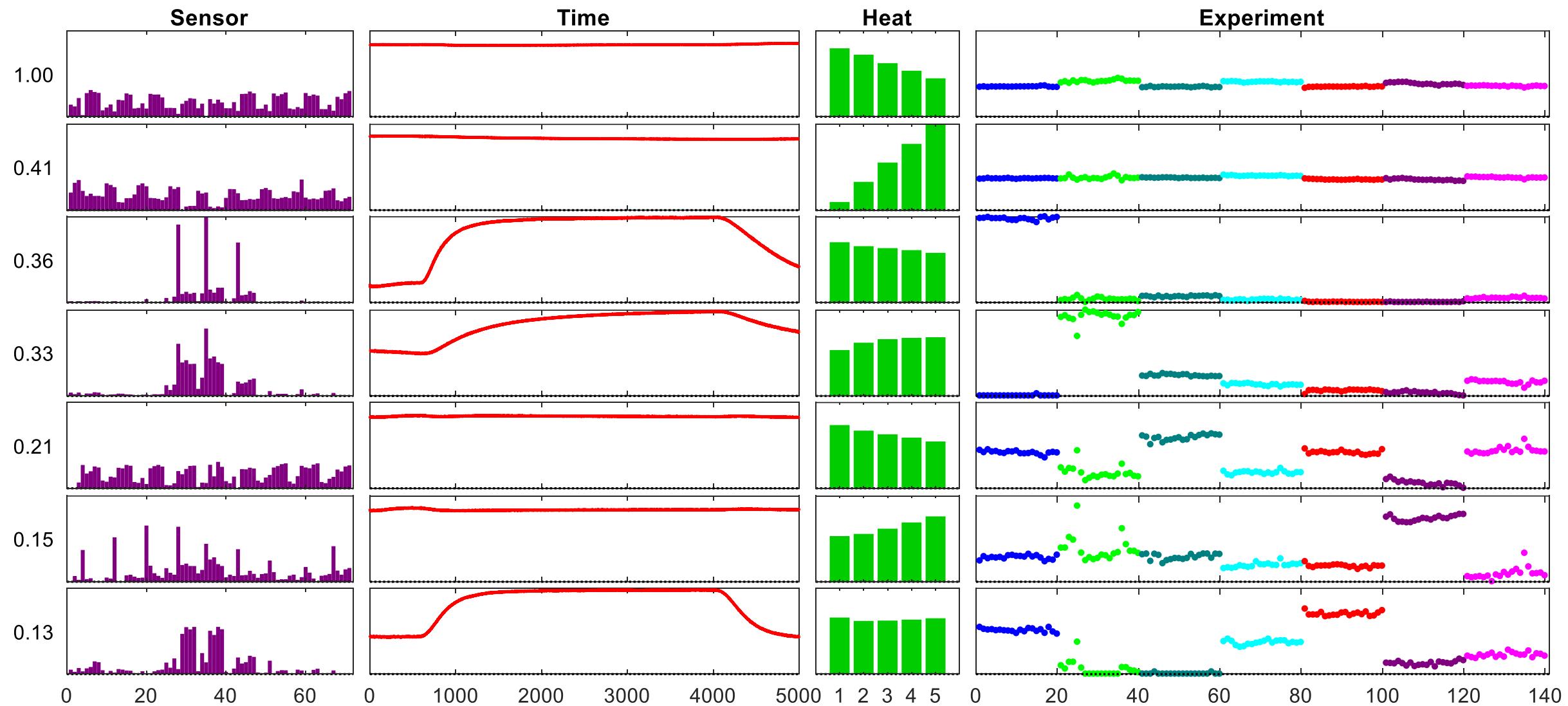
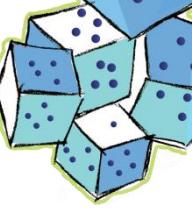
- Can be solved via alternating or all-at-once optimization
  - ✓ Fewer knobs to tweak for all-at-once
  - ✓ Prefer all-at-once if any data is missing
- Gradient has an elegant form
  - ✓ Involves “MTTKRP”
- Missing data is handled by omitting from the sum in the objective function
  - ✓ Introduces sparsity into the gradient computation
- Large-scale problems require stochastic approach
  - ✓ Stratification needed for sparse problems

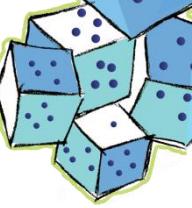


# Mouse Data using Rayleigh (Nonneg)



# Gas Data Using Rayleigh





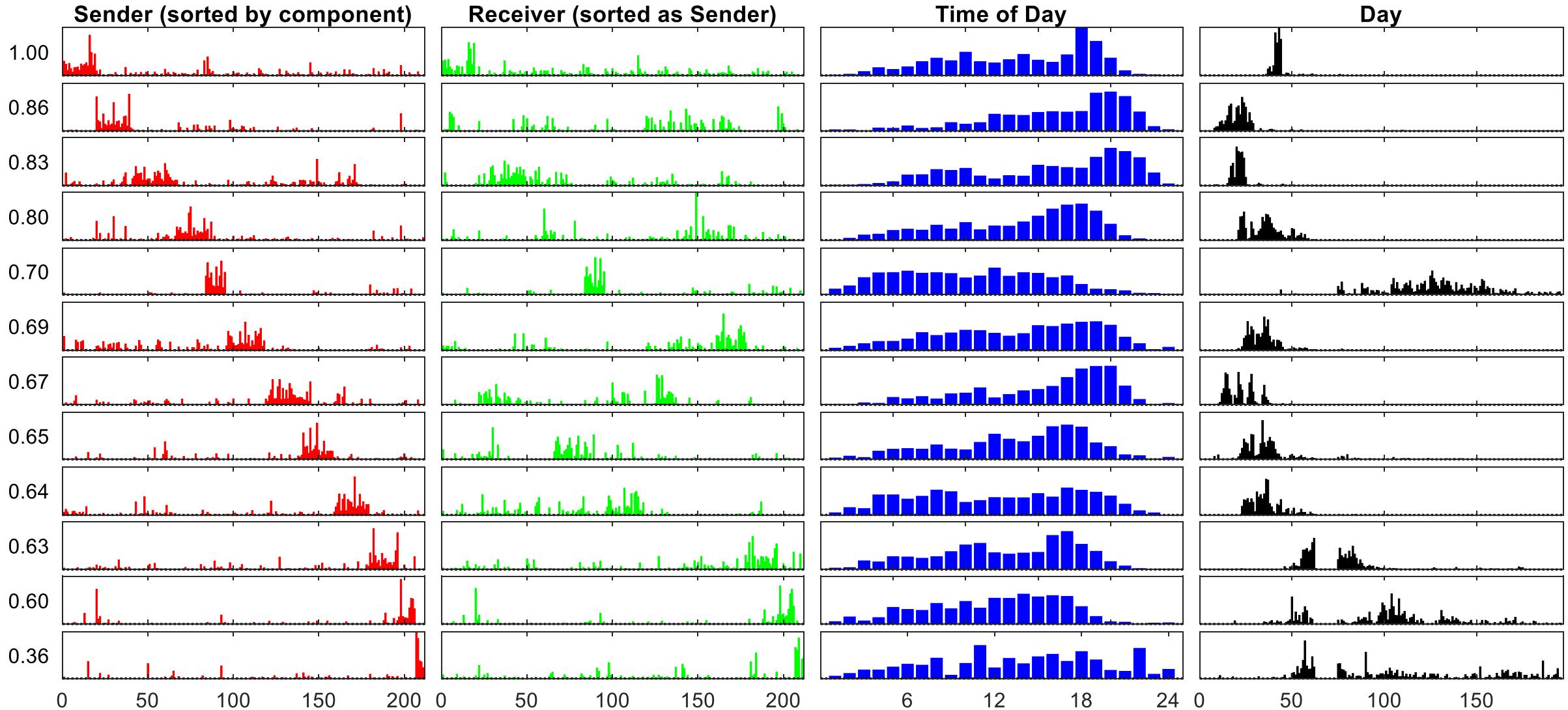
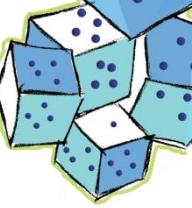
# A Sparse Binary Dataset

- UC Irvine Chat Network
  - 4-way binary tensor
    - Sender (211)
    - Receiver (211)
    - Hour of Day (24)
    - Day (196)
  - 14,849 nonzeros (very sparse)
- Goodness-of-fit (Boolean-odds):
 
$$f(x, m) = \log(m + 1) - x \log m$$
- Use GCP to compute rank-12 decomposition



Opsahl, T., Panzarasa, P., 2009. Clustering in weighted networks. *Social Networks* 31 (2), 155-163, doi: 10.1016/j.socnet.2009.02.002

# Binary Chat Data using Boolean CP





## SIAM Journal on Mathematics of Data Science

- New journal, launching in Spring 2018

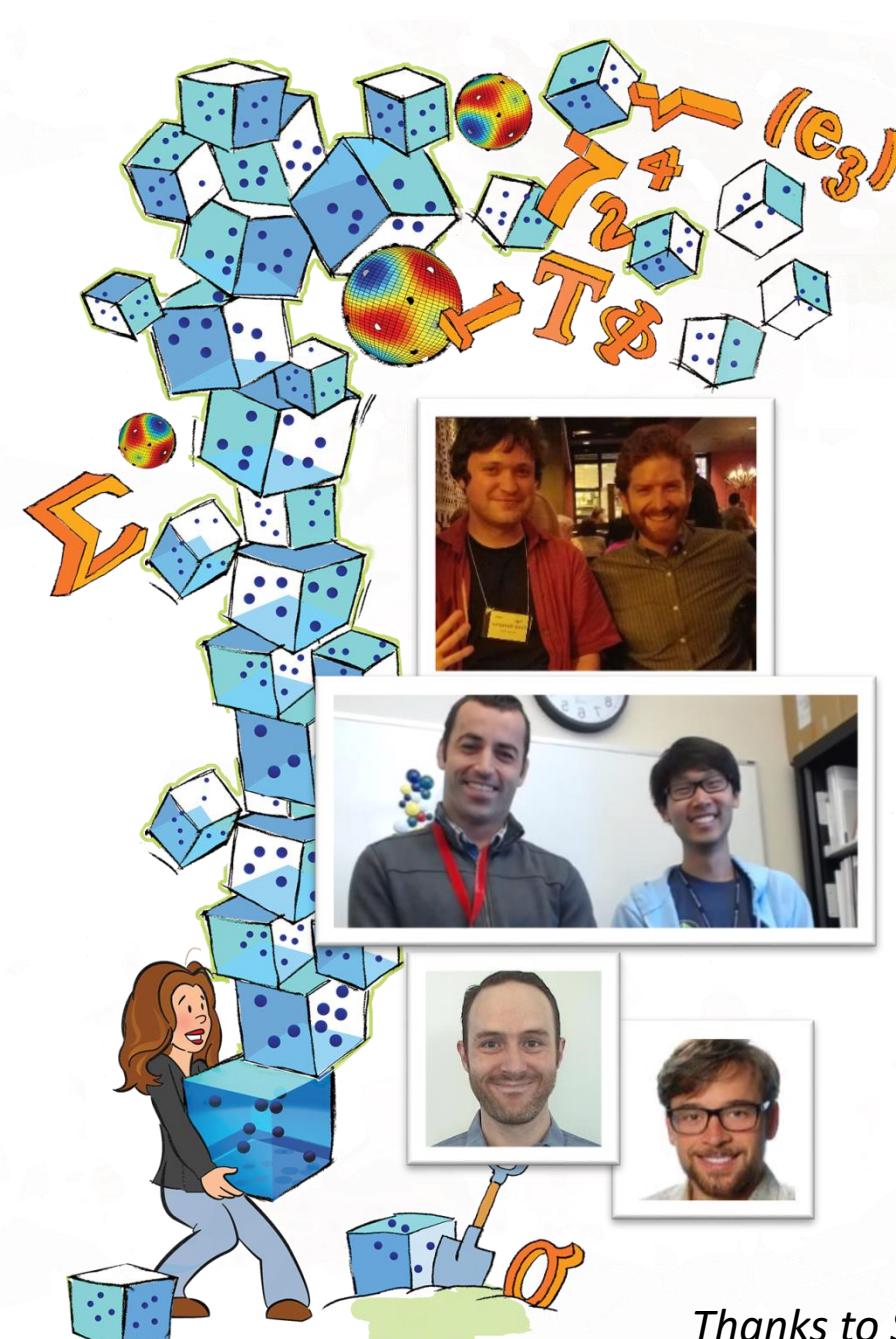
### Focus

- Role of applied mathematics in data science, as complemented and intertwined with other key areas: statistics, computer science, network science, signal processing, etc.

Editor in chief: Tamara G. Kolda, Sandia

### Section editors

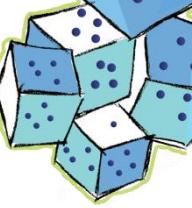
- Alfred Hero, Michigan
- Michel Jordan, Berkeley
- Robert Nowak, Wisconsin
- Joel Tropp, CalTech



# CP Tensor Decomposition & Data Analysis



Sandia  
National  
Laboratories



- CP Tensor Decomposition is a key tool for data analysis
  - Latent factor analysis
  - Dimensionality reduction
- Randomized methods enable scaling
  - Initial evidence for increased robustness in global optimization
  - Many, many algorithm and implementation details
- Flexible data type via Generalized CP
  - Nonnegative, Boolean, Poisson data
- *Many open math problems remain!*
- Links
  - Tensor Toolbox for MATLAB: [www.tensortoolbox.org](http://www.tensortoolbox.org)
  - Parallel CP and GCP implementations: <https://gitlab.com/tensors/genten>
  - My web page: [www.kolda.net](http://www.kolda.net)

*Thanks to SIAM for the invitation to speak and to YOU, the audience, for your attention!*