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Illustration by Chris Brigman

An Overview of Tensor Decompositions for Data Analysis, with Emphasis on Computation and Scalability

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Livermore, CA

Michigan Institute for Data Science (MIDAS) Seminar
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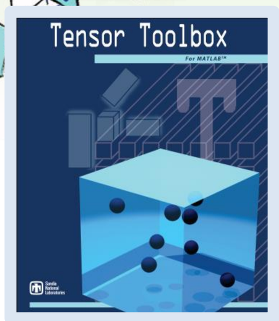
Acknowledgements


Illustration by Chris Brigman

Kolda and Bader, Tensor Decompositions and Applications, *SIAM Review* '09



Tensor Toolbox for MATLAB: Bader, Kolda, Acar, Dunlavy, and others

TUCKERMPI

https://gitlab.com/tensors/TuckerMPI
Klinvex, Austin, Ballard, Kolda

- Evrim Acar (Univ. Copenhagen*)
- **Woody Austin (Univ. Texas Austin*)**
- Brett Bader (Digital Globe*)
- **Grey Ballard (Wake Forest*)**
- Robert Bassett (UC Davis*)
- **Casey Battaglino (GA Tech*)**
- **Eric Chi (NC State Univ.*)**
- Danny Dunlavy (Sandia)
- Sammy Hansen (IBM*)
- Joe Kenny (Sandia)
- **Alicia Klinvex (Sandia)**
- **Hemanth Kolla (Sandia)**
- Jackson Mayo (Sandia)
- Morten Mørup (Denmark Tech. Univ.)
- Todd Plantenga (FireEye*)
- Martin Schatz (Univ. Texas Austin*)
- Teresa Selee (GA Tech Research Inst.*)
- Jimeng Sun (GA Tech)
- **Alex Williams (Stanford*)**

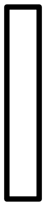
Plus many more former students and colleagues, collaborators for workshops, tutorials, etc.

** = Long-term stint at Sandia*

Intro

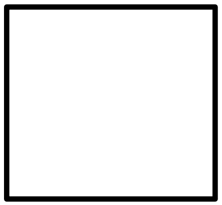
A Tensor is an d-Way Array

Vector
d = 1



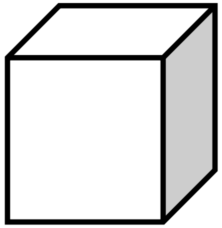
$\mathbf{a}$

Matrix
d = 2



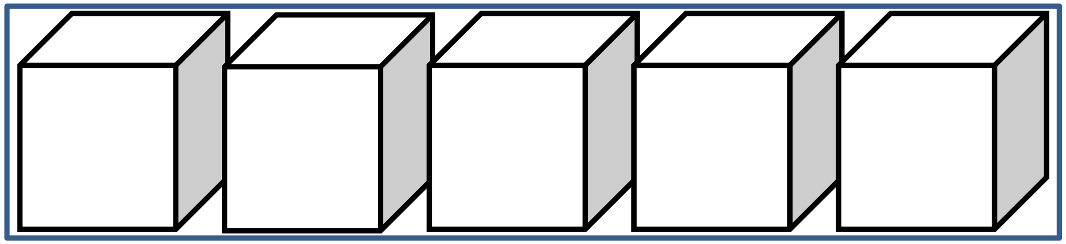
$\mathbf{A}$

3rd-Order Tensor
d = 3



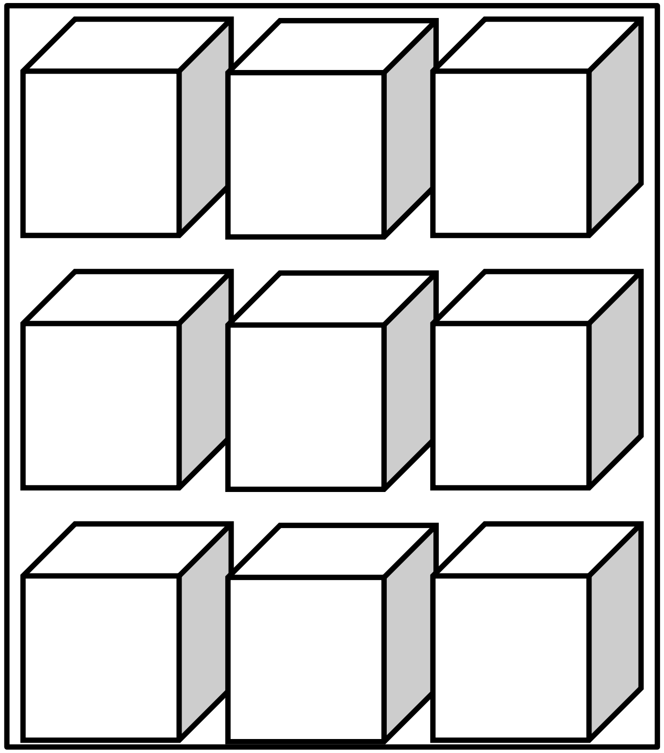
$\mathcal{A}$

4th-Order Tensor
d = 4



$\mathcal{A}$

5th-Order Tensor
d = 5

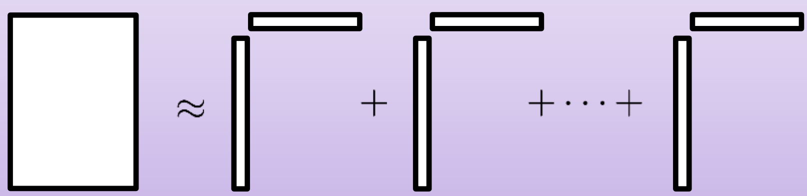


$\mathcal{A}$

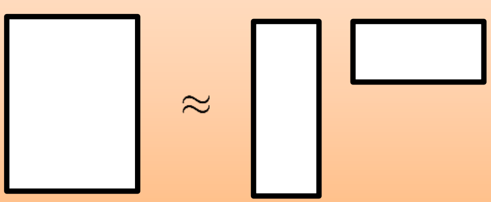
Tensor Decompositions are the New Matrix Decompositions

Singular value decomposition (SVD), eigendecomposition (EVD), nonnegative matrix factorization (NMF), sparse SVD, etc.

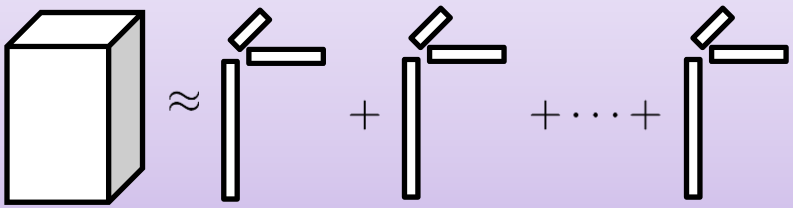
Viewpoint 1: Sum of outer products, useful for interpretation



Viewpoint 2: High-variance subspaces, useful for compression

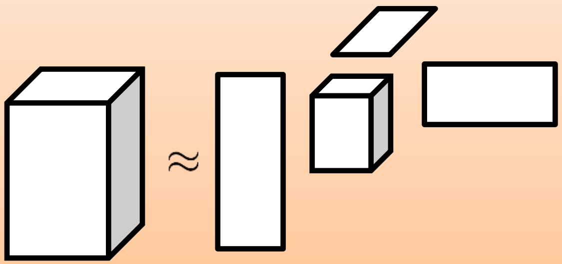


CP Model: Sum of d-way outer products, useful for interpretation



CANDECOMP, PARAFAC, Canonical Polyadic, CP

Tucker Model: Project onto high-variance subspaces to reduce dimensionality

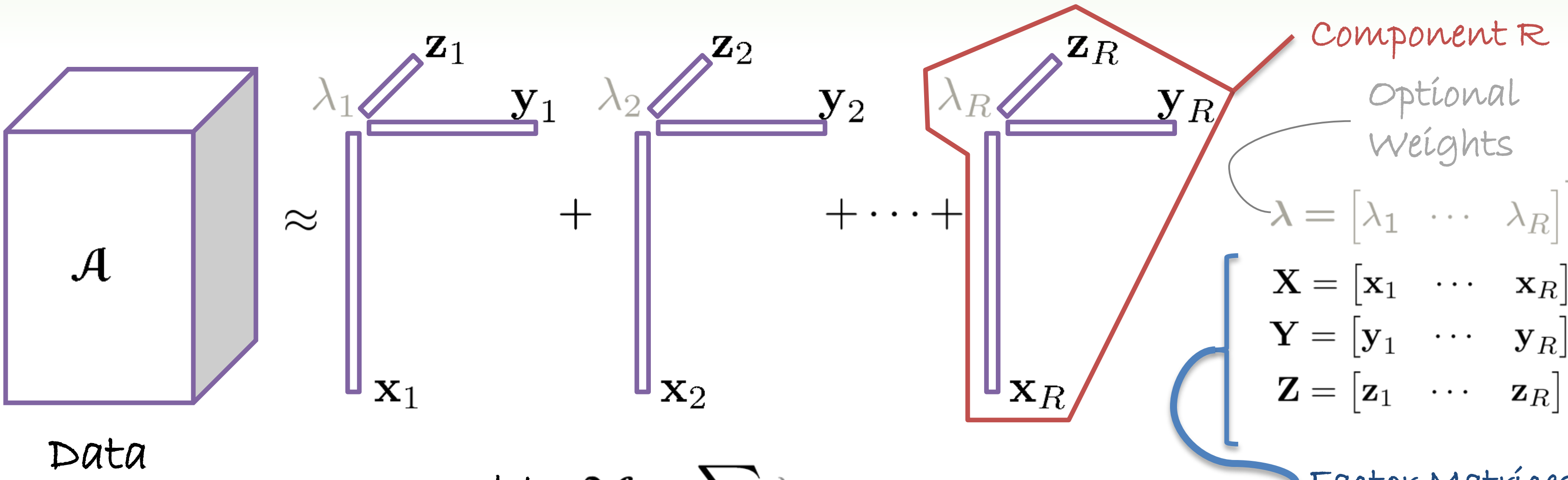


HO-SVD, Best Rank-(R1,R2,…,RN) decomposition

Other models for compression include hierarchical Tucker and tensor train.

CP Tensor Decomposition: Sum of Outer Products

CANDECOMP/PARAFAC or canonical polyadic (CP) Model



Model: $\mathcal{M} = \sum_r \lambda_r \, \mathbf{x}_r \circ \mathbf{y}_r \circ \mathbf{z}_r$

$$\min_{\mathcal{M}} \sum_{ijk} (a_{ijk} - m_{ijk})^2 \quad \text{subject to} \quad m_{ijk} = \sum_r \lambda_r \, x_{ir} \, y_{jr} \, z_{kr}$$

Key references: Hitchcock, 1927; Harshman, 1970; Carroll and Chang, 1970

Motivation

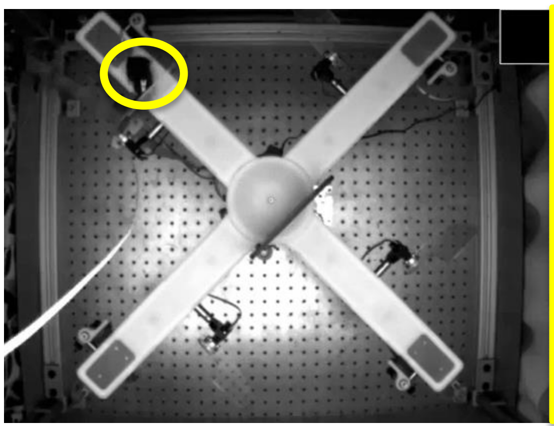
Featuring work of Alex Williams

Motivating Example: Neuron Activity in Learning

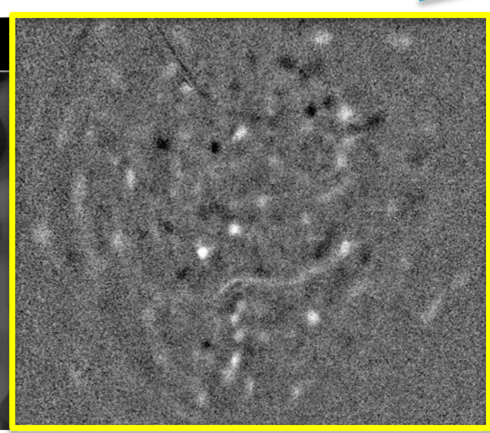
Thanks to Schnitzer Group @ Stanford
Mark Schnitzer, Fori Wang, Tony Kim

Microscope by Inscopix

mouse in “maze”



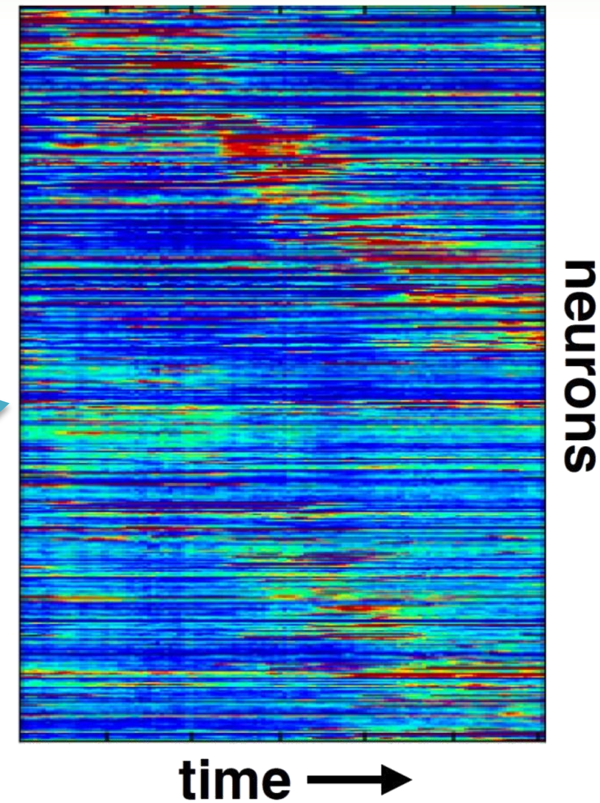
neural activity



One Column of Neuron x Time Matrix

One Trial

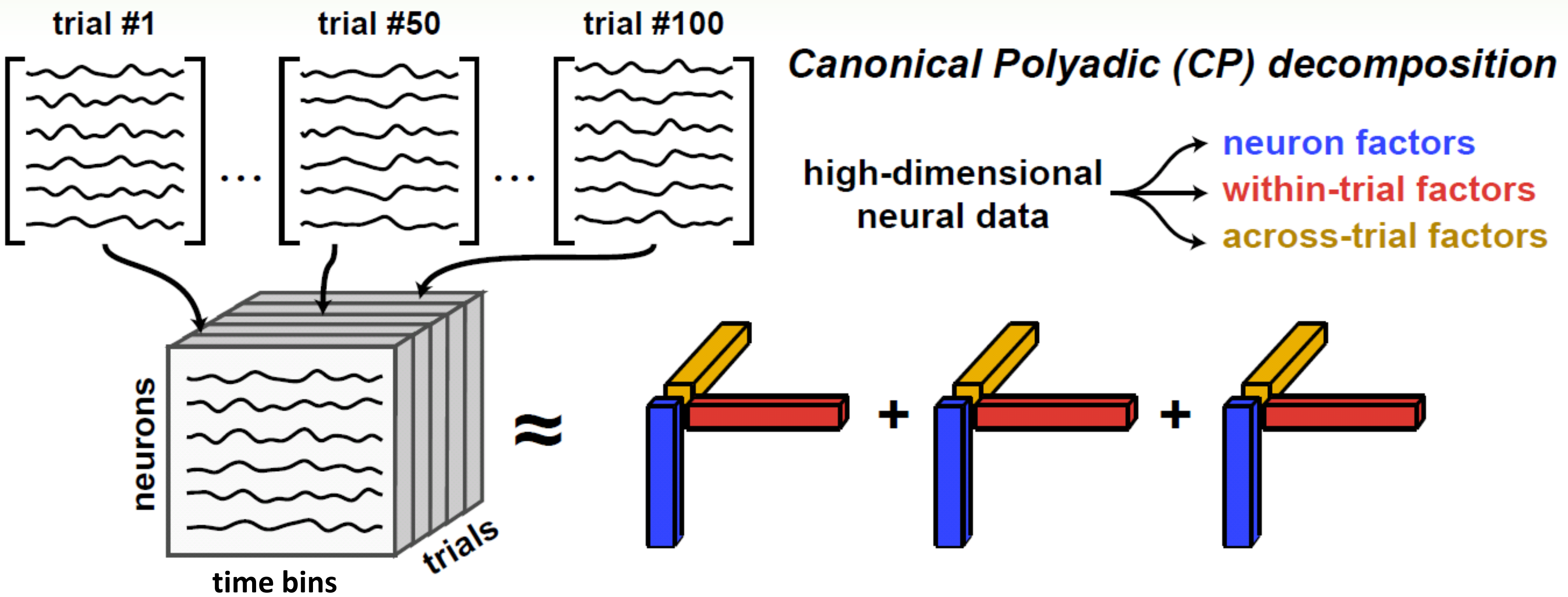
300 neurons × 120 time bins



× 600 trials (over 5 days)

Coming soon: Williams, Wang, Kim, Schnitzer, Ganguli, Kolda, 2016

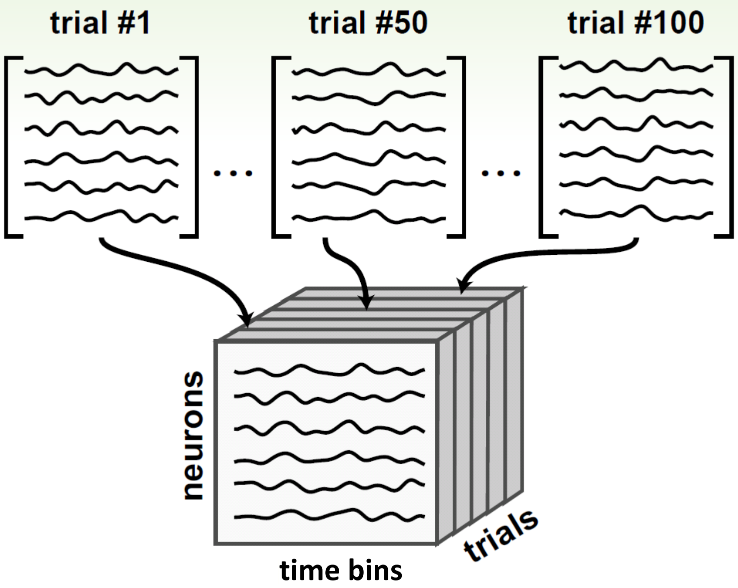
CP for Simultaneous Analysis of Neurons, Time, and Trial

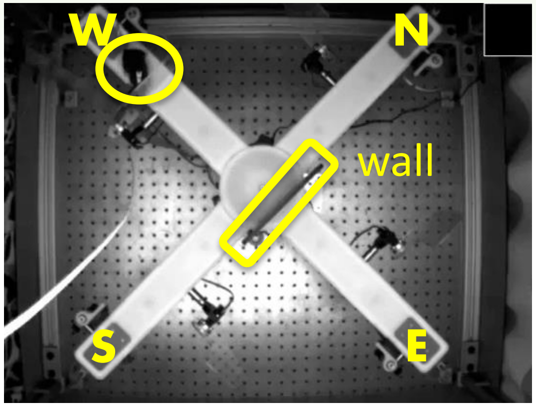


Past work could only look at 2 factors at once: Time x Neuron, Trial x Neuron, etc.

Coming soon: Williams, Wang, Kim, Schnitzer, Ganguli, Kolda, 2016

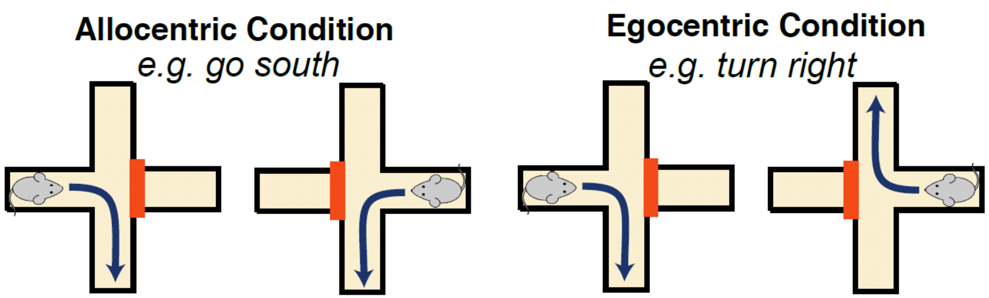
Trials Vary Start Position and Strategies





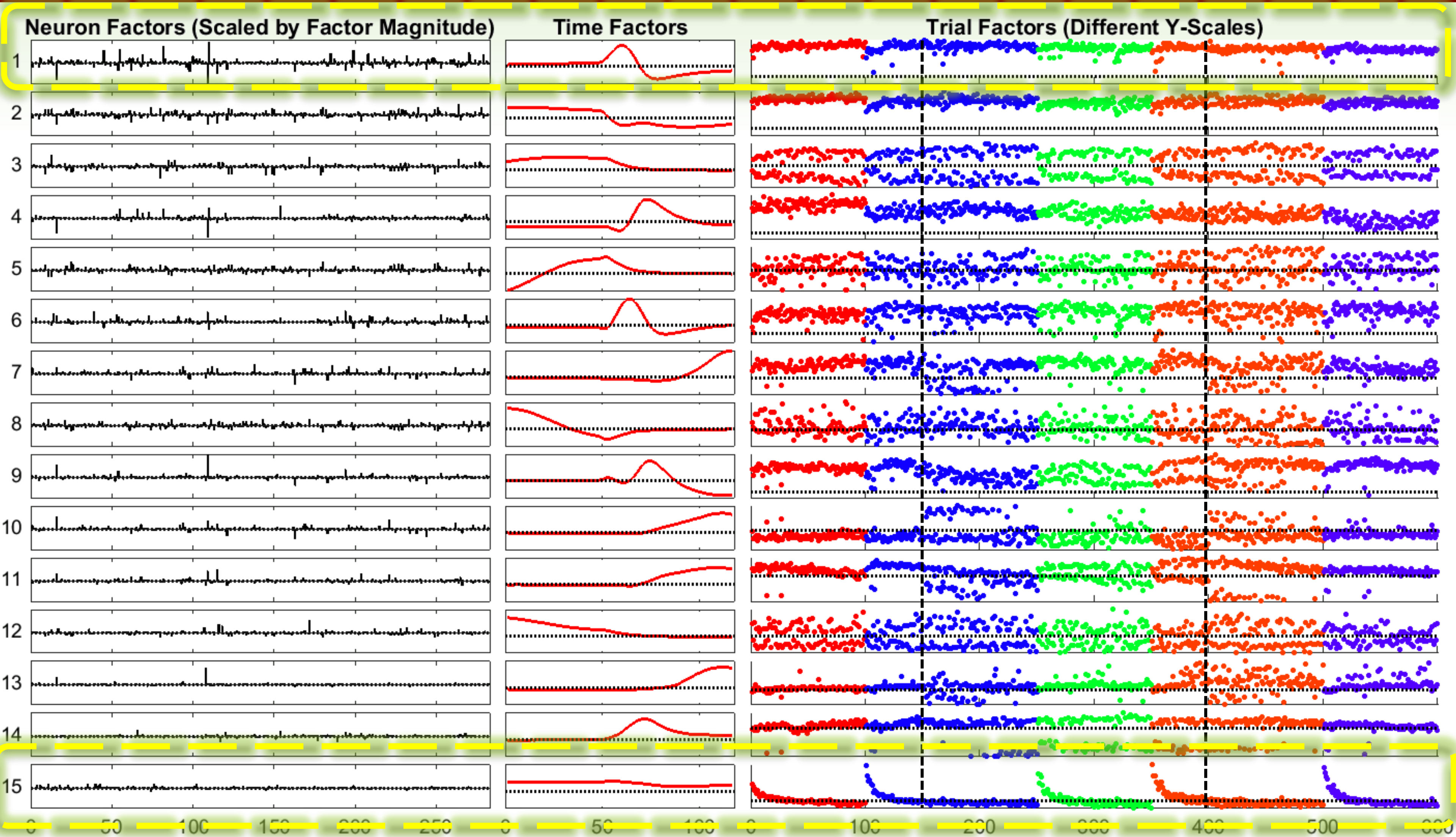
note different patterns on curtains

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

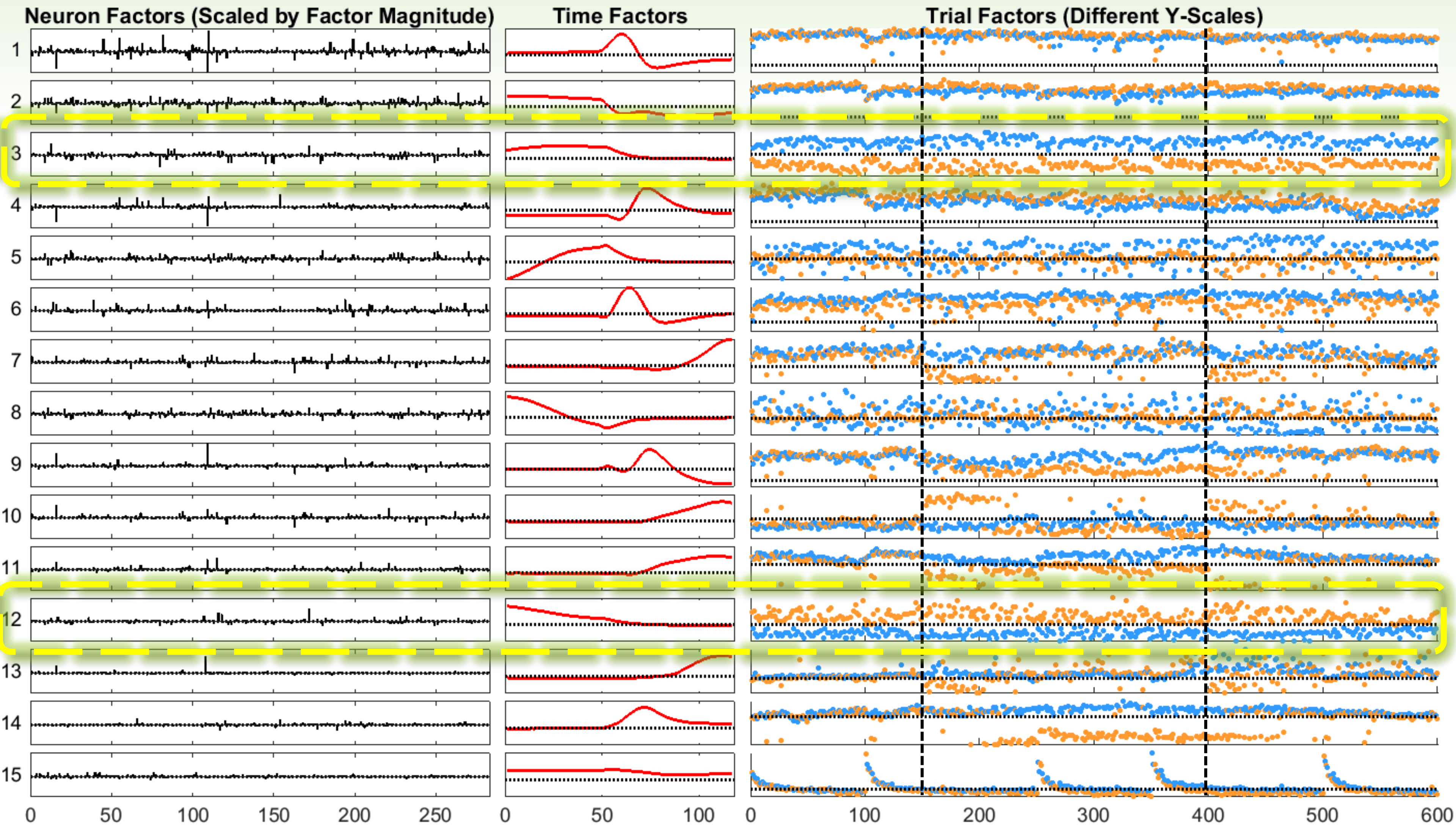


Coming soon: Williams, Wang, Kim, Schnitzer, Ganguli, Kolda, 2016

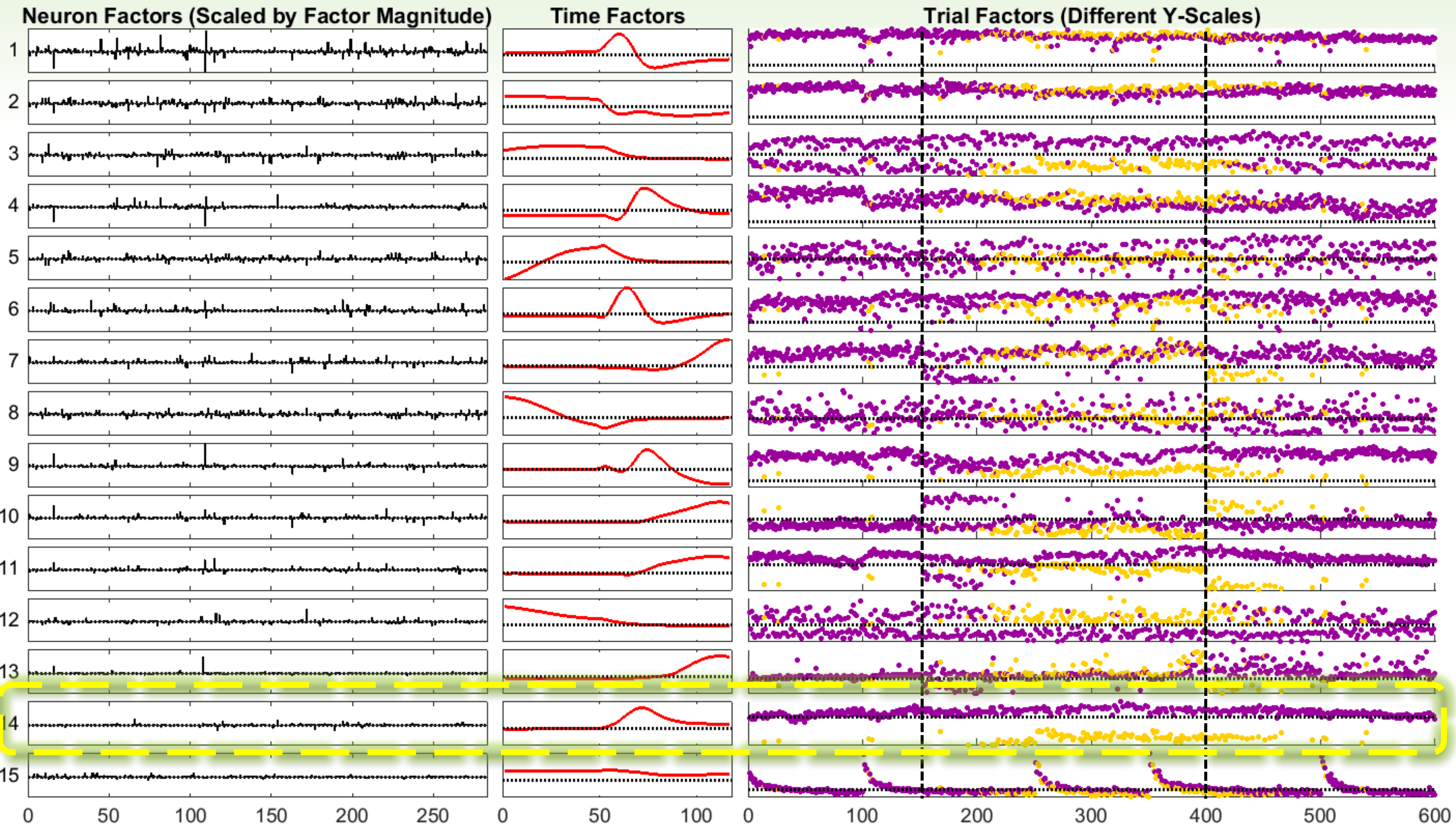
15 Components: Day-Coded (one color per day)



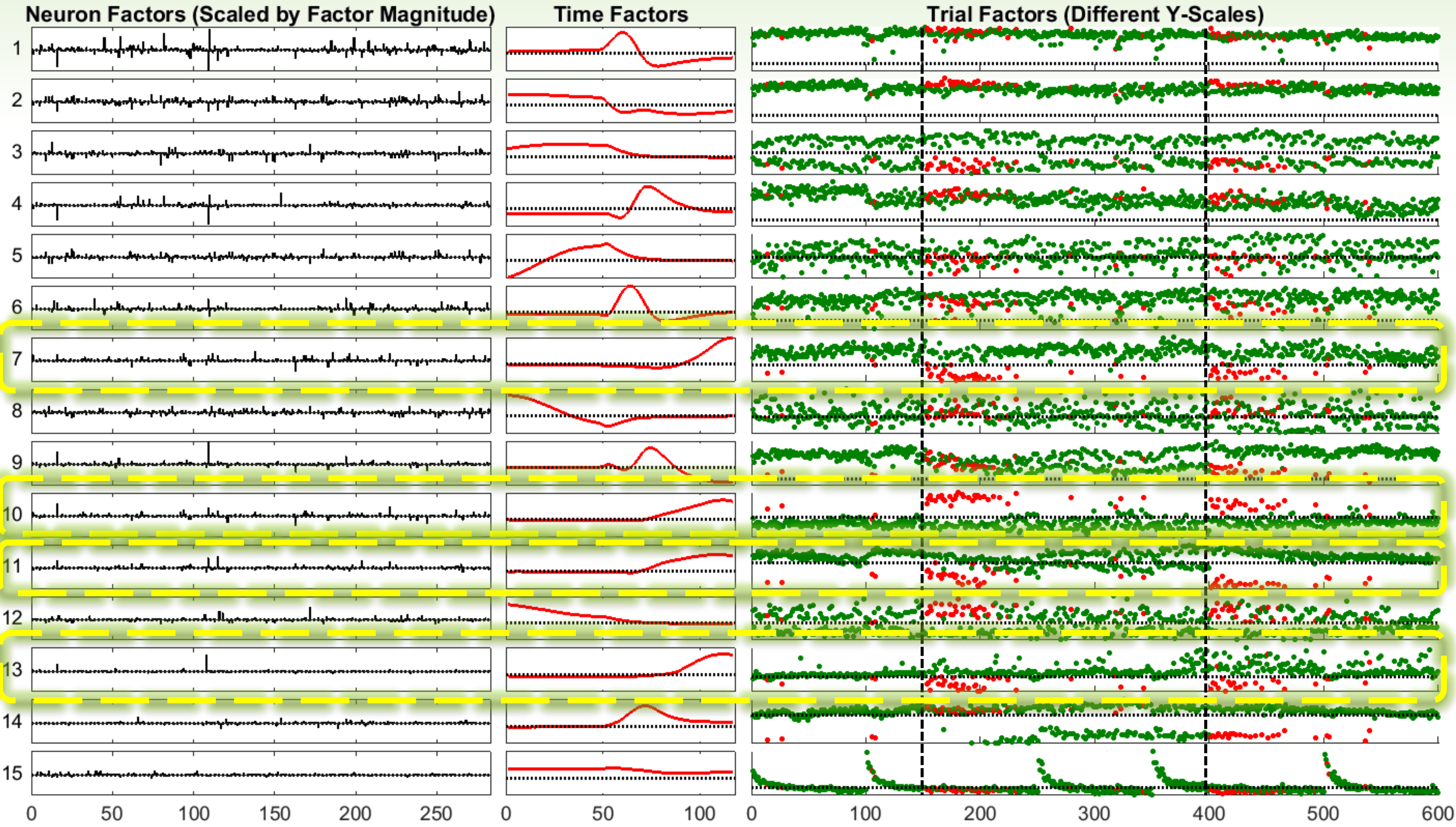
15 Components: Start-Coded (blue = east, orange = west)



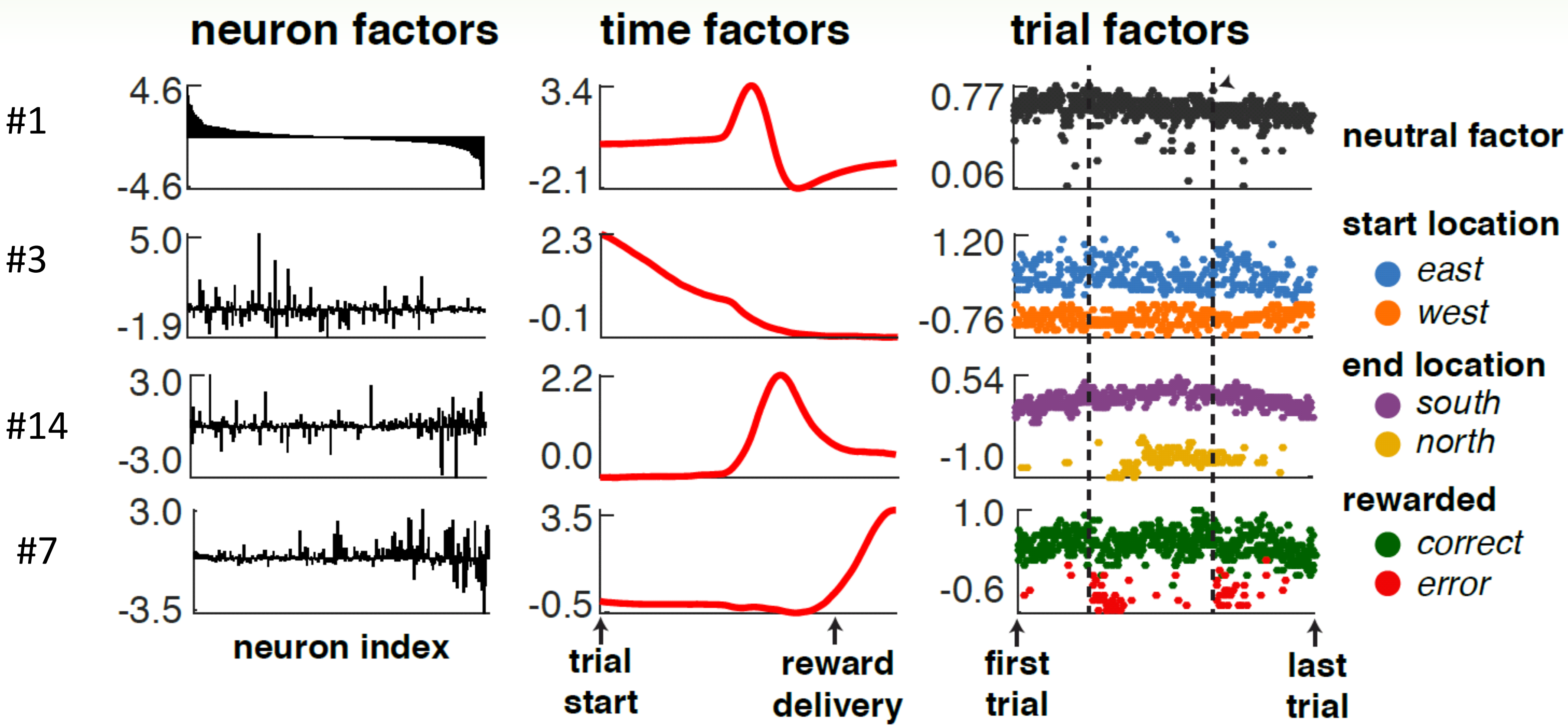
15 Components: End-Coded (purple=south, gold=north)



15 Components: Reward-Coded (green=correct, red=wrong)



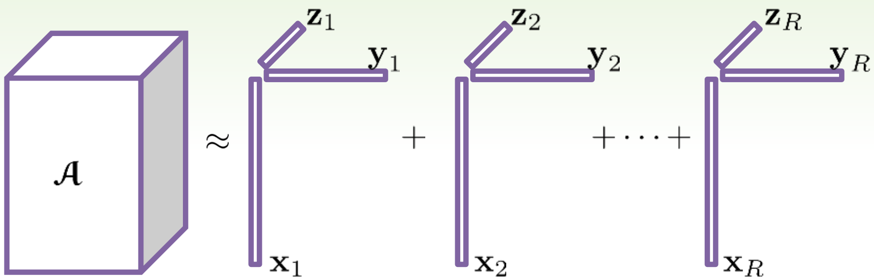
Interpretation of a Subset of 15 Components



Coming soon: Williams, Wang, Kim, Schnitzer, Ganguli, Kolda, 2016

Fitting the CP Decomposition

CP-ALS: Fitting CP Model via Alternating Least Squares



Convex (linear least squares) subproblems can be solved exactly
\+
Structure makes easy inversion

$$f(\mathbf{X},\mathbf{Y},\mathbf{Z}) = \sum_{ijk} \Big(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \Big)^2$$

Repeat until convergence:

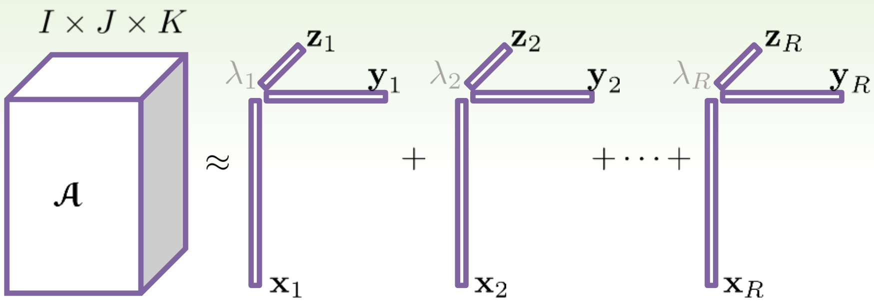
Step 1: $\min_{\mathbf{X}} \sum_{ijk} \Big(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \Big)^2$

Step 2: $\min_{\mathbf{Y}} \sum_{ijk} \Big(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \Big)^2$

Step 3: $\min_{\mathbf{Z}} \sum_{ijk} \Big(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \Big)^2$

Harshman, 1970; Carroll & Chang, 1970

Challenges for Fitting CP Model



variables = $R(I + J + K)$
data points = IJK

Rank = minimal R to exactly reproduce tensor

- **Nonconvex:** Polynomial optimization problem ⇒ *Initialization matters*
- **Permutation and scaling ambiguities:** Can reorder the r's and arbitrarily scale vectors within each component so long as the product of the scaling is 1 ⇒ *May need regularization*
- **Rank unknown:** Determining the "rank" R that yields exact fit is NP-hard (Håstad 1990, Hillar & Lim 2009) ⇒ *No easy solution, need to try many*
- **Low-rank?** Best "low-rank" factorization may not exist (Silva & Lim 2006) ⇒ *Need bounds on components* $\|\lambda_r \mathbf{x}_r \circ \mathbf{y}_r \circ \mathbf{z}_r\| = |\lambda_r| \, \|\mathbf{x}_r\| \, \|\mathbf{y}_r\| \, \|\mathbf{z}_r\|$
- **Not nested:** Best rank-(R-1) factorization may not be part of best rank-R factorization (Kolda 2001) ⇒ *Cannot use greedy algorithm*

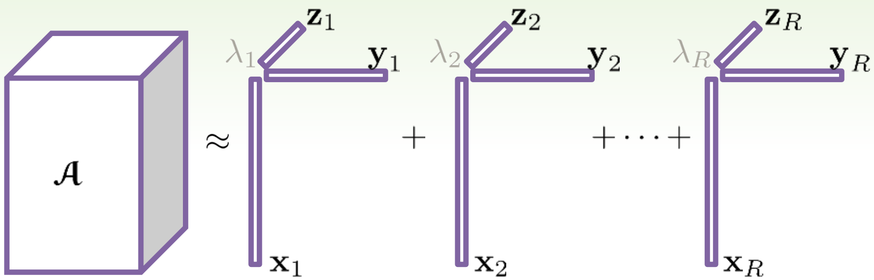
Example 9 x 9 x 9 Tensor of Unknown Rank

- Specific 9 x 9 x 9 tensor factorization problem
- Corresponds to being able to do fast matrix multiplication of two 3x3 matrices
- Rank is between 19 and 23 $\Rightarrow \leq$ 621 variables

$x_{1,1,1} = 1$	$x_{4,2,1} = 1$	$x_{7,3,1} = 1$
$x_{1,4,2} = 1$	$x_{4,5,2} = 1$	$x_{7,6,2} = 1$
$x_{1,7,3} = 1$	$x_{4,8,3} = 1$	$x_{7,9,3} = 1$
$x_{2,1,4} = 1$	$x_{5,2,4} = 1$	$x_{8,3,4} = 1$
$x_{2,4,5} = 1$	$x_{5,5,5} = 1$	$x_{8,6,5} = 1$
$x_{2,7,6} = 1$	$x_{5,8,6} = 1$	$x_{8,9,6} = 1$
$x_{3,1,7} = 1$	$x_{6,2,7} = 1$	$x_{9,3,7} = 1$
$x_{3,4,8} = 1$	$x_{6,5,8} = 1$	$x_{9,6,8} = 1$
$x_{3,7,9} = 1$	$x_{6,8,9} = 1$	$x_{9,9,9} = 1$

Laderman 1976; Bini et al. 1979; Bläser 2003; Benson & Ballard, PPoPP'15

Opportunities for Fitting CP Model



k-rank(**X**) = maximum value k such that *any* k columns of **X** are linearly independent

- Factorization is **essentially unique** (i.e., up to permutation and scaling) under the condition the the sum of the factor matrix k-rank values is $\geq$ 2R + d – 1 (Kruskal 1977)

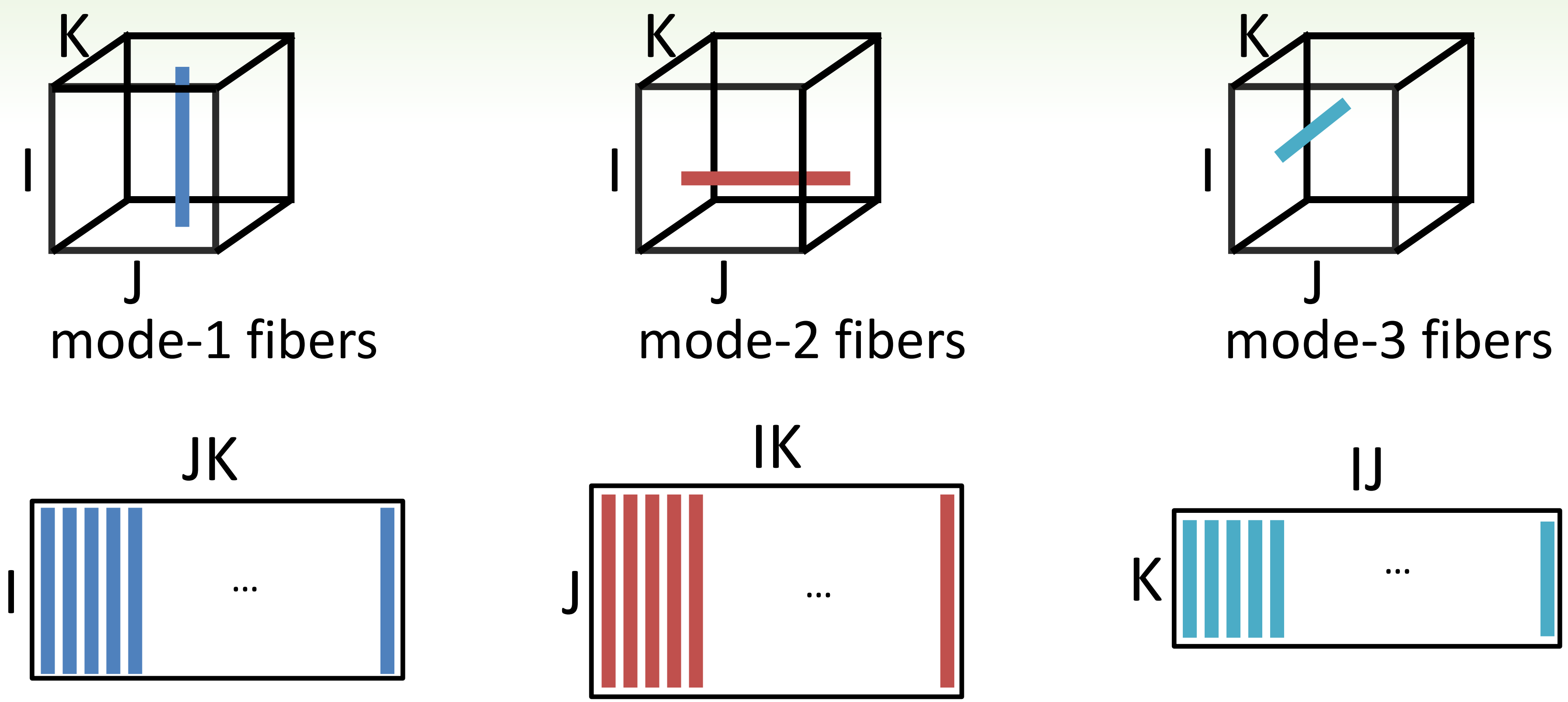
$$\text{k-rank}(\mathbf{X}) + \text{k-rank}(\mathbf{Y}) + \text{k-rank}(\mathbf{Z}) \geq 2R + 2$$

- If $R \ll I,J,K$, then can use **compression** to reduce dimensionality before solving CP model (CANDELINC: Carroll, Pruzansky, and Kruskal 1980)
- Efficient **sparse kernels** exist (Bader & Kolda, SISC 2007)

A Randomized Method for Fitting the CP Decomposition

Featuring work of Casey Battaglino, Grey Ballard

Matricization/Unfolding: Rearranging a Tensor as a Matrix



$\mathbf{X}_{(1)}$ $\mathbf{X}_{(2)}$ $\mathbf{X}_{(3)}$

Mathematically convenient expression, but generally do not want to actually form the unfolded matrix due to the expense of the *data movement*.

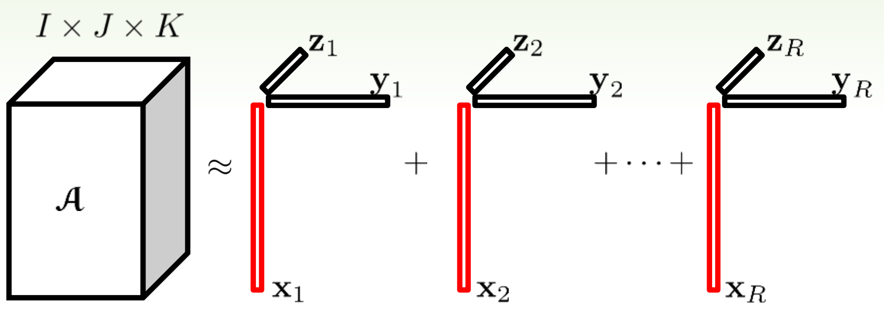
Rewriting CP-ALS Subproblem as Matrix Least Squares

Repeat until convergence:

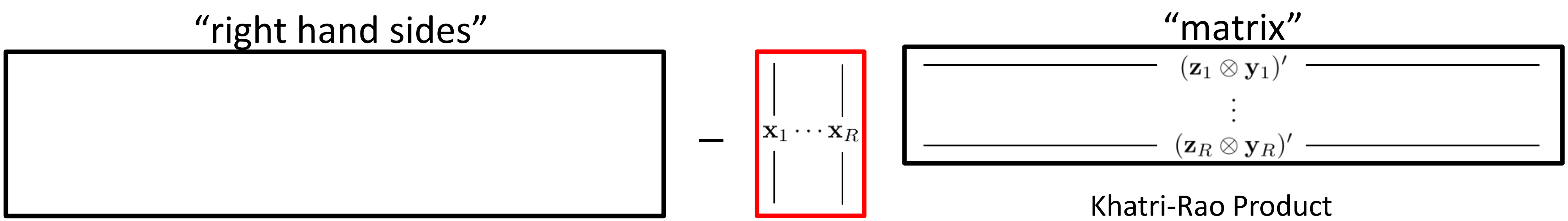
Step 1: $\min_{\mathbf{X}} \sum_{ijk} \Big(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \Big)^2$

Step 2: $\min_{\mathbf{Y}} \sum_{ijk} \Big(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \Big)^2$

Step 3: $\min_{\mathbf{Z}} \sum_{ijk} \Big(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \Big)^2$



Rewrite as matrix least squares problem
(backwards and transposed matrix version!)



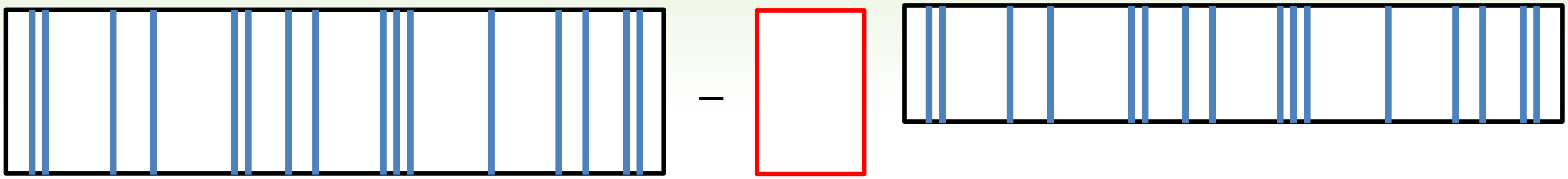
Khatri-Rao Product

$$\| \mathbf{A}_{(1)} - \mathbf{X} (\mathbf{Z} \odot \mathbf{Y})' \|_F^2$$

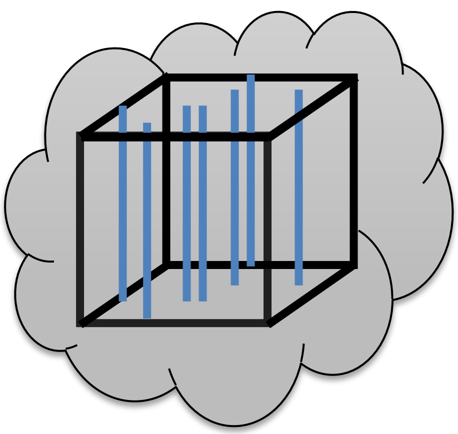
$I \times JK$ $\quad$ $I \times R$ $\quad$ $R \times JK$

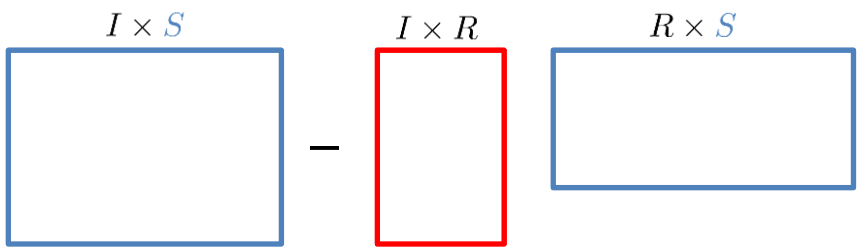
Coming soon: Battaglino, Ballard, Kolda, 2016

Randomizing the Matrix Least Squares Subproblem



$$\|\mathbf{A}_{(1)}\mathbf{S} \quad - \quad \mathbf{X} \quad [(\mathbf{Z}\odot\mathbf{Y})'\mathbf{S}]\,\|_F^2$$





Each column in the sample is of the form: (Z(:,k) .* Y(:,j))’

Two “tricks”

1. Never permute elements of tensor A intro $I \times JK$ matrix form
2. Never form full Khatri-Rao product of size $R \times JK$

Coming soon: Battaglino, Ballard, Kolda, 2016

Mixing for Incoherence: One Time & Done

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Need to apply an fast Johnson-Lindenstrauss Transform (FJLT) to $(\mathbf{Z} \odot \boldsymbol{Y})'$ to ensure *incoherence:*

$$\|\mathbf{A}_{(1)}\mathbf{S} - \mathbf{X}(\mathbf{Z} \odot \mathbf{Y})'\mathbf{S}\|_F^2 \Longrightarrow \|\mathbf{A}_{(1)}(\mathbf{DF})\mathbf{S} - \mathbf{X}(\mathbf{Z} \odot \mathbf{Y})'\underbrace{(\mathbf{DF})\mathbf{S}}\|_F^2$$

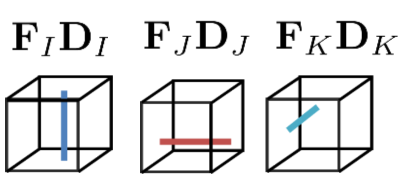
Diagonal Random Sign Flip & FFT

We use a Kronecker product of FJLTs and conjecture it's an FJLT:

$$\|\mathbf{A}_{(1)}(\mathbf{F}_K\mathbf{D}_K \otimes \mathbf{F}_J\mathbf{D}_J)'\mathbf{S} - \mathbf{X}(\mathbf{Z} \odot \mathbf{Y})'(\mathbf{F}_K\mathbf{D}_K \otimes \mathbf{F}_J\mathbf{D}_J)'\mathbf{S}\|_F^2$$

$$\|\mathbf{A}_{(1)}(\mathbf{F}_K\mathbf{D}_K \otimes \mathbf{F}_J\mathbf{D}_J)'\mathbf{S} - \mathbf{X}(\mathbf{F}_K\mathbf{D}_K\mathbf{Z} \odot \mathbf{F}_J\mathbf{D}_J\mathbf{Y})'\mathbf{S}\|_F^2$$

We ultimately transform the tensor <u>one time</u> in all modes and just apply the reverse transform in one mode.



Coming soon: Battaglino, Ballard, Kolda, 2016

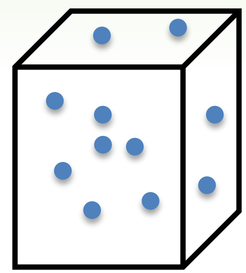
Randomizing the Convergence Check

Repeat until convergence:

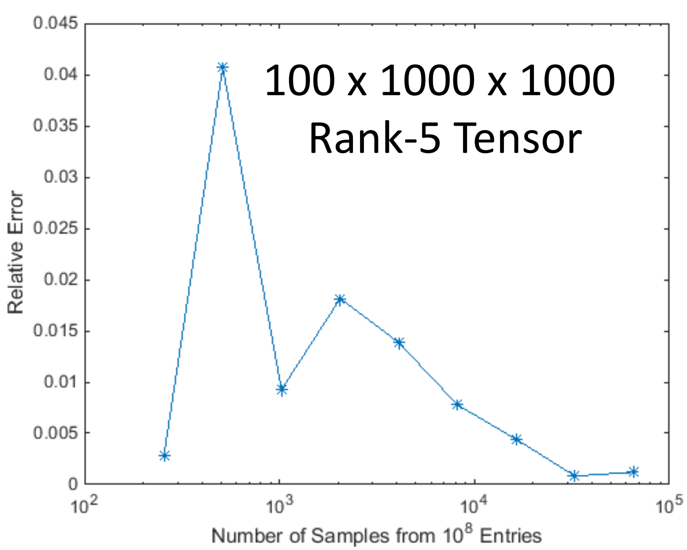
Step 1: $\min_{\mathbf{X}} \sum_{ijk} \left(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \right)^2$

Step 2: $\min_{\mathbf{Y}} \sum_{ijk} \left(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \right)^2$

Step 3: $\min_{\mathbf{Z}} \sum_{ijk} \left(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \right)^2$



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



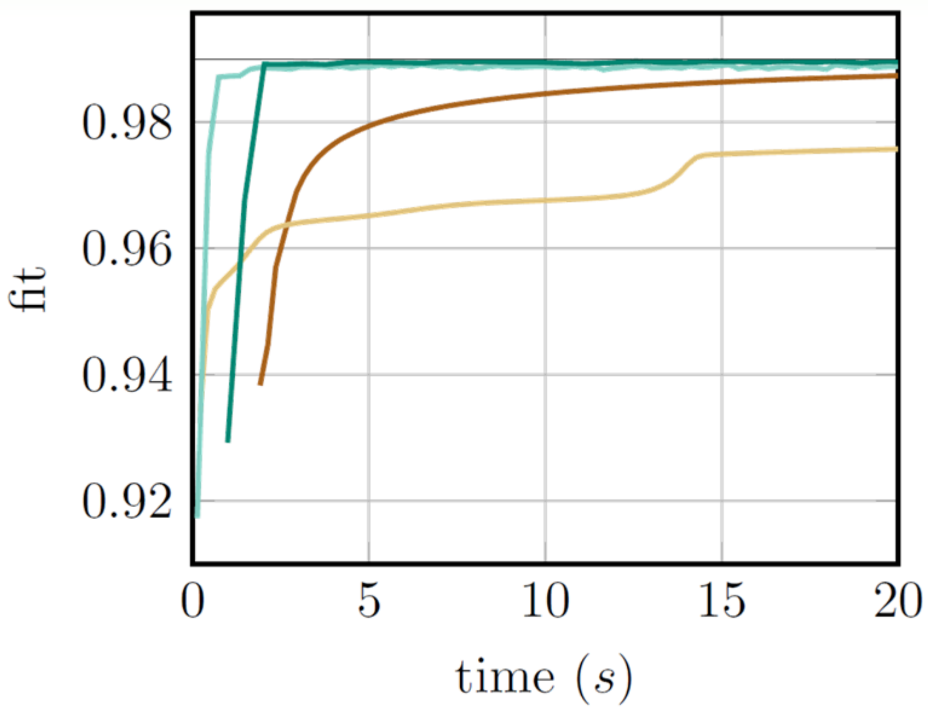
$$f(\mathbf{X},\mathbf{Y},\mathbf{Z}) = \sum_{ijk} \left(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \right)^2$$

$$f(\mathbf{X},\mathbf{Y},\mathbf{Z}) \approx \frac{IJK}{|\Omega|} \sum_{ijk \in \Omega} \left(a_{ijk} - \sum_r x_{ir}\, y_{jr}\, z_{kr} \right)^2$$

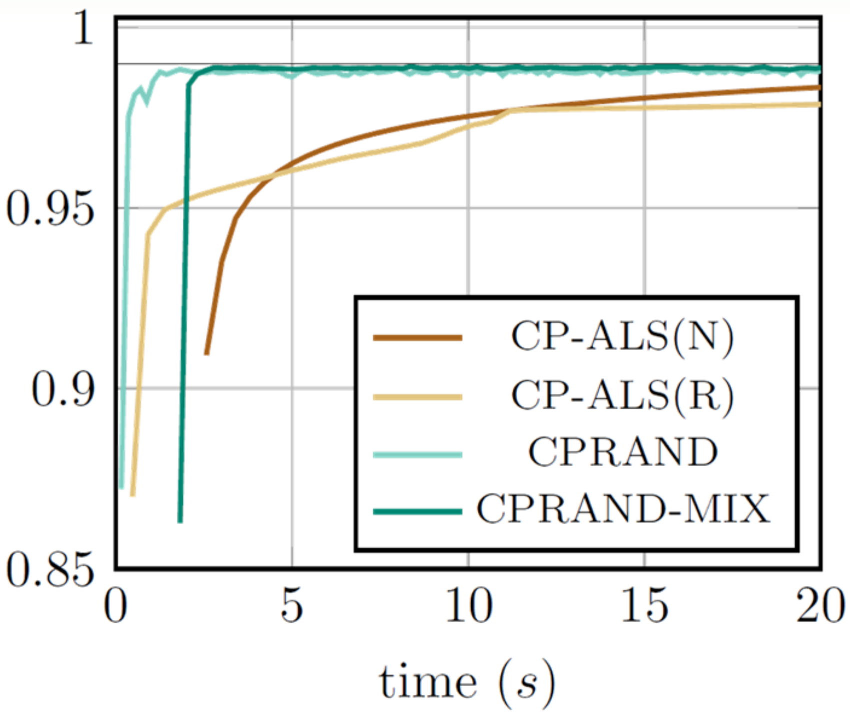
Coming soon: Battaglino, Ballard, Kolda, 2016

CPRAND faster than CP-ALS

Generated Data



(a) Random 300 × 300 × 300 tensor.



(b) Random 80 × 80 × 80 × 80 tensor.

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CPRAND Faster than CP-ALS in Low Noise Conditions

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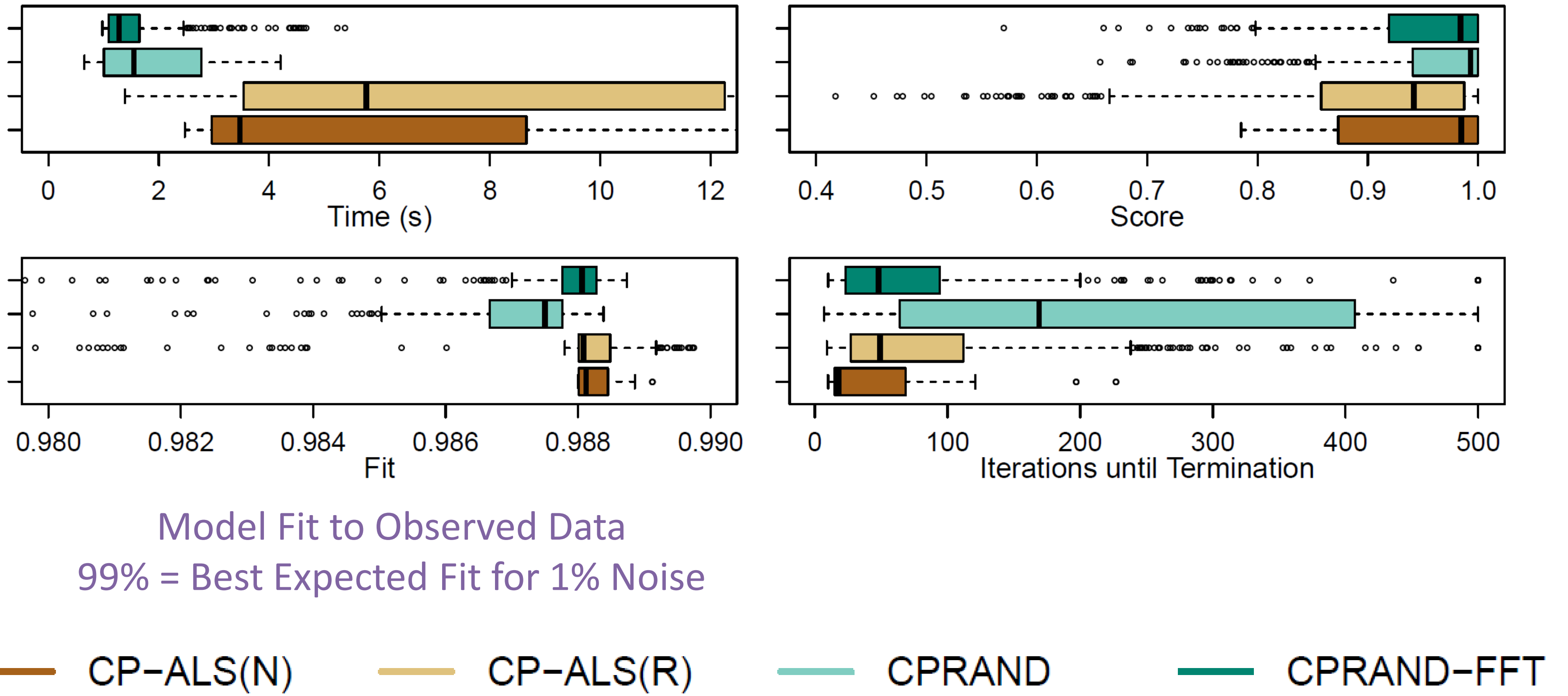
400 x 400 x 400, R = 5, Noise = 1%
200 Tensors, Various Conditions

Total Time to Solution

Similarity Score (1.0 Best): True versus Computed Factors



Model Fit to Observed Data
99% = Best Expected Fit for 1% Noise

Coming soon: Battaglino, Ballard, Kolda, 2016

CPRAND More Robust vs CP-ALS in High Noise Conditions

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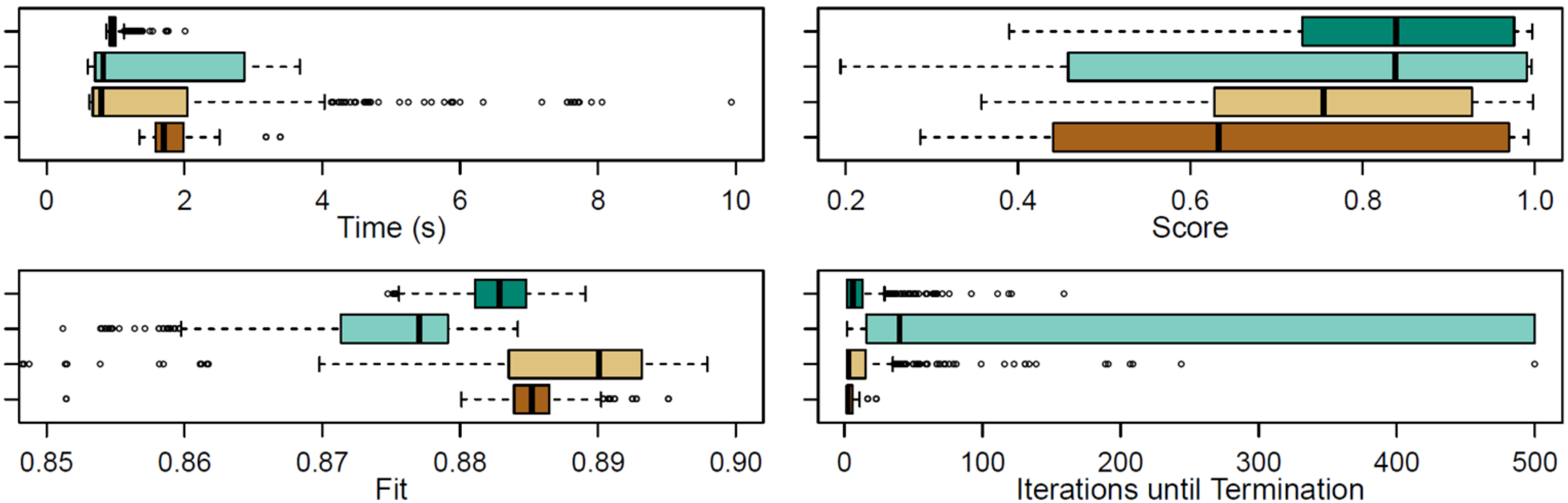
400 x 400 x 400, R = 5, Noise = 10%
200 Tensors, Various Conditions

Total Time to Solution

Similarity Score (1.0 Best): True versus Computed Factors



Model Fit to Observed Data
90% = Best Expected Fit for 10% Noise

CP−ALS(N) CP−ALS(R) CPRAND CPRAND−FFT

Coming soon: Battaglino, Ballard, Kolda, 2016

CPRAND-MIX up to 8X Faster on Coil-20 Video Dataset

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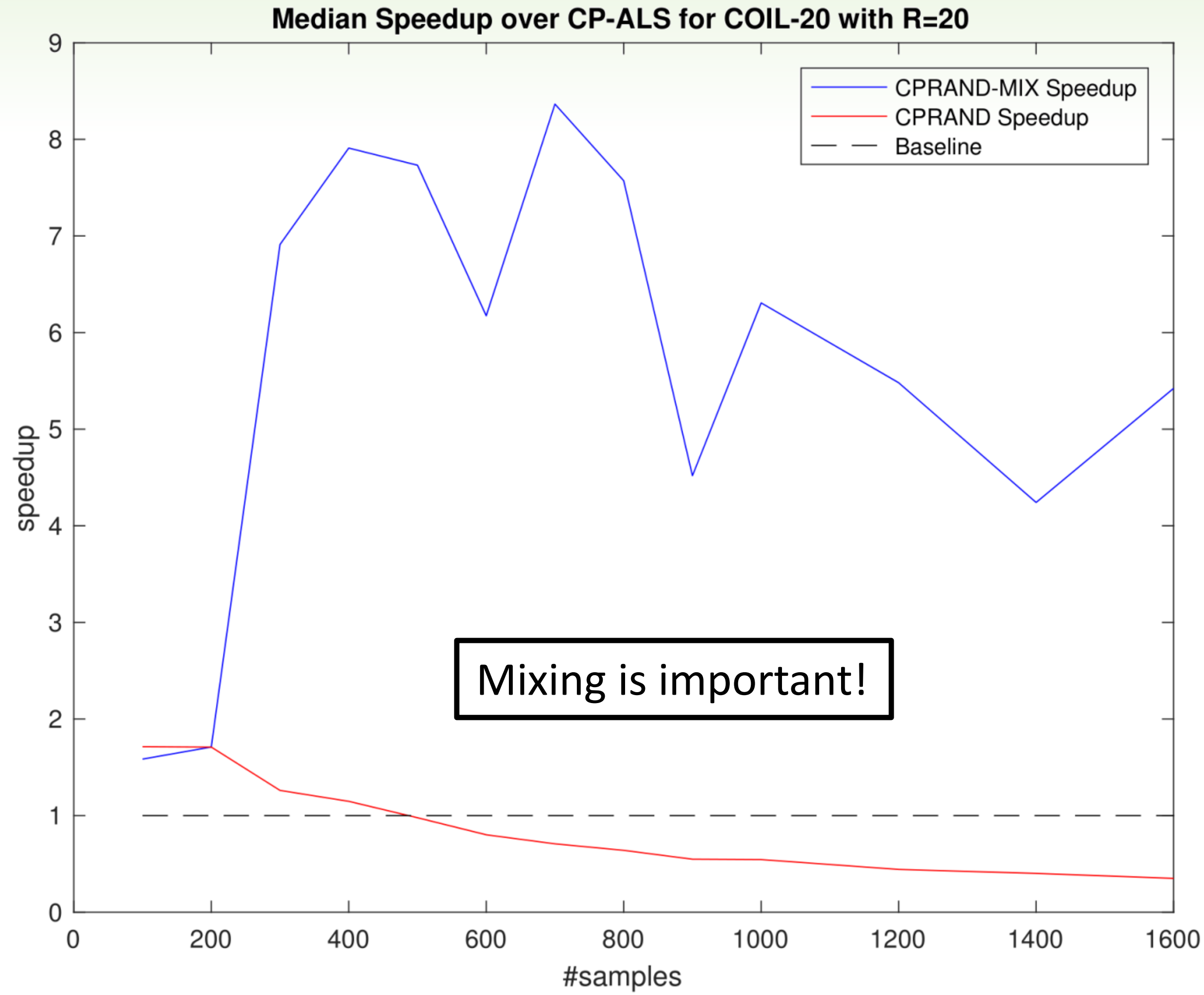
Data: Columbia Object Image Library (COIL)

- 128 x 128 Images
- 3 Colors (RGB)
- 72 Poses per Object
- 100 Objects

We use *20* object classes (COIL-20) to form tensor of size

128 x 128 x 3 x 1440

Glossing over details, but essentially equal fits at termination

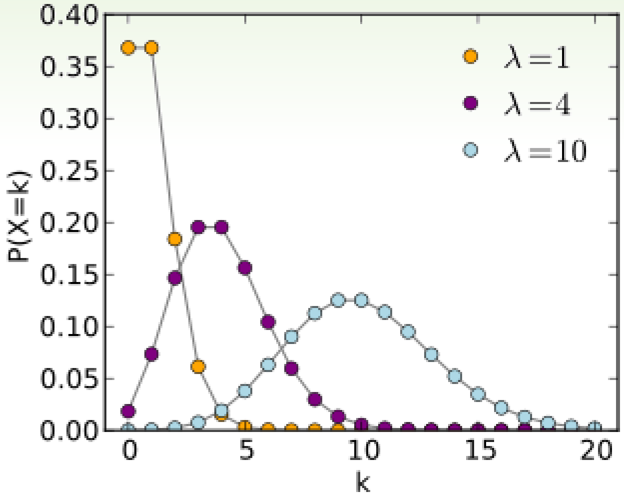


Coming soon: Battaglino, Ballard, Kolda, 2016

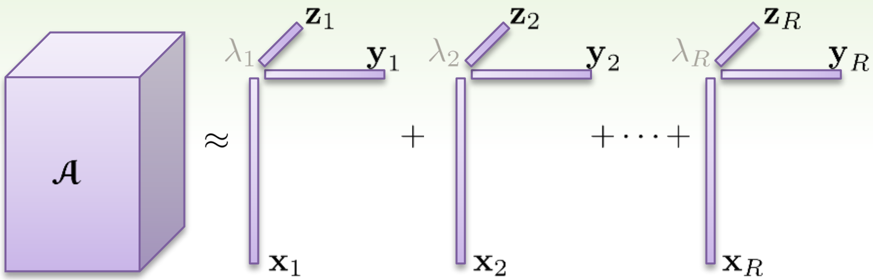
A New Type of CP Decomposition for Count Data

Featuring work of Eric Chi

New "Stable" Approach: Poisson Tensor Factorization (PTF)



$$P(X = x) = \frac{\exp(-\lambda)\lambda^x}{x!}$$



$$m_{ijk} = \sum_r \lambda_r \, x_{ir} \, y_{jr} \, z_{kr}$$

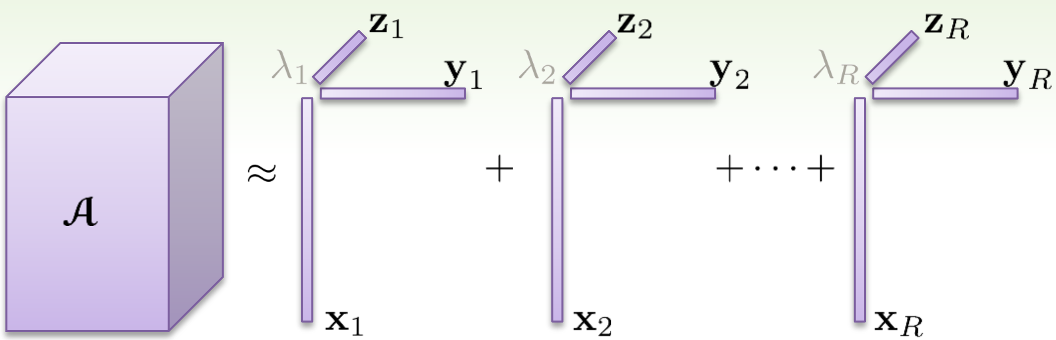
$$a_{ijk} \sim \text{Poisson}(m_{ijk})$$

Maximize this: $$\text{likelihood}(\mathcal{M}) = \prod_{ijk} \frac{\exp(-m_{ijk}) \, m_{ijk}^{a_{ijk}}}{a_{ijk}!}$$

By monotonicity of log, same as maximizing this: $$\text{log-likelihood}(\mathcal{M}) = c - \sum_{ijk} m_{ijk} - a_{ijk} \log(m_{ijk})$$

This objective function is also known as Kullback-Liebler (KL) divergence. The factorization is automatically nonnegative.

Solving the Poisson Regression Problem



$$\mathcal{M} = \sum_r \lambda_r \, \mathbf{x}_r \circ \mathbf{y}_r \circ \mathbf{z}_r$$

$$\boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 & \cdots & \lambda_R \end{bmatrix}^{\mathsf{T}}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_R \end{bmatrix}$$

$$\mathbf{Y} = \begin{bmatrix} \mathbf{y}_1 & \cdots & \mathbf{y}_R \end{bmatrix}$$

$$\mathbf{Z} = \begin{bmatrix} \mathbf{z}_1 & \cdots & \mathbf{z}_R \end{bmatrix}$$

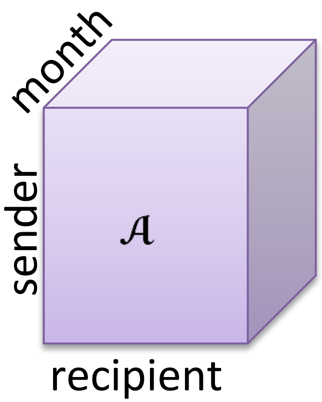
$$\min_{\mathcal{M}} \sum_{ijk} m_{ijk} - a_{ijk} \log m_{ijk} \quad \text{subject to} \quad m_{ijk} = \sum_r \lambda_r \, x_{ir} \, y_{jr} \, z_{kr}$$

- Highly nonconvex problem!
  - Assume R is given
- Alternating Poisson regression
  - Assume (d-1) factor matrices are known and solve for the remaining one
  - Multiplicative updates like Lee & Seung (2000) for NMF, but improved
  - Typically assume data tensor A is sparse and have special methods for this
  - Newton or Quasi-Newton method

Chi & Kolda, SIMAX 2012; Hansen, Plantenga, & Kolda OMS 2015

PTF for Time-Evolving Social Network

Enron email data from FERC investigation.



Data	8540 Email Messages
# Months	28 (Dec'99 – Mar'02)
# Senders/Recipients	108 (>10 messages each)
Links	8500 (3% dense)

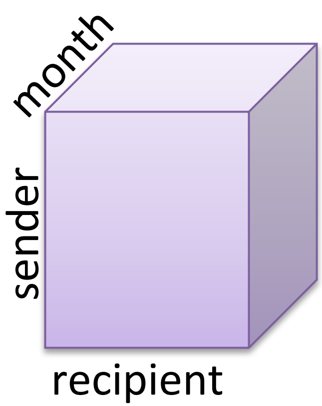
a_{ijk} = # emails from sender i to recipient j in month k

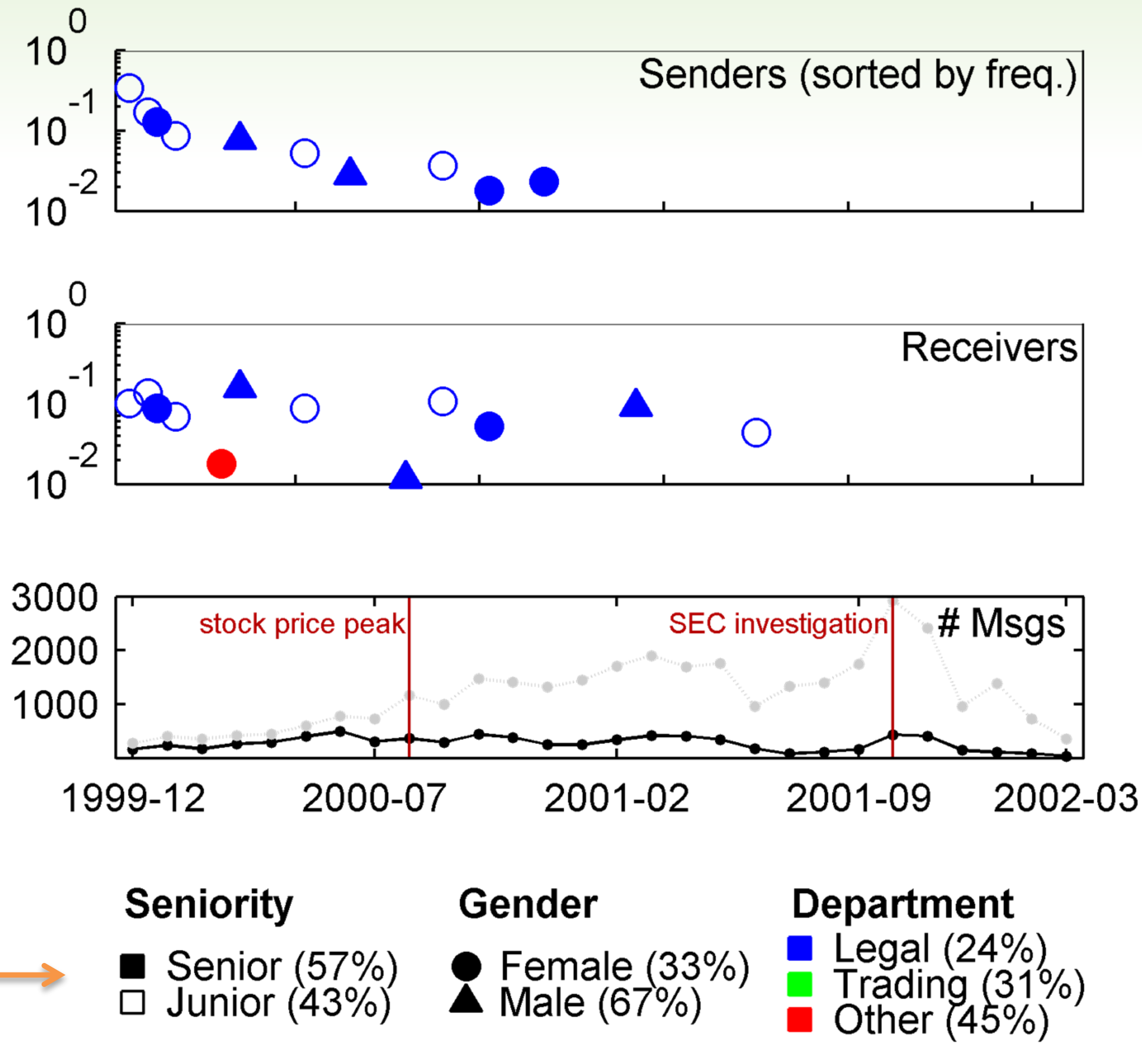
Let's look at some components from a 10-component (R=10) factorization, sorted by size…

Chi & Kolda, On Tensors, Sparsity, and Nonnegative Factorizations, SIMAX 2012

Enron Email Data (Component 1)

Legal Dept;
Mostly Female



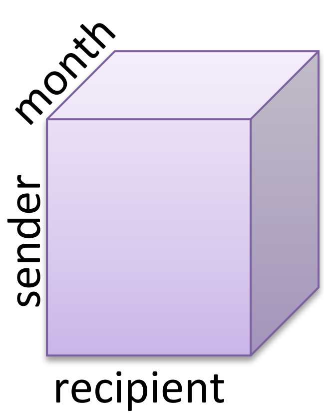


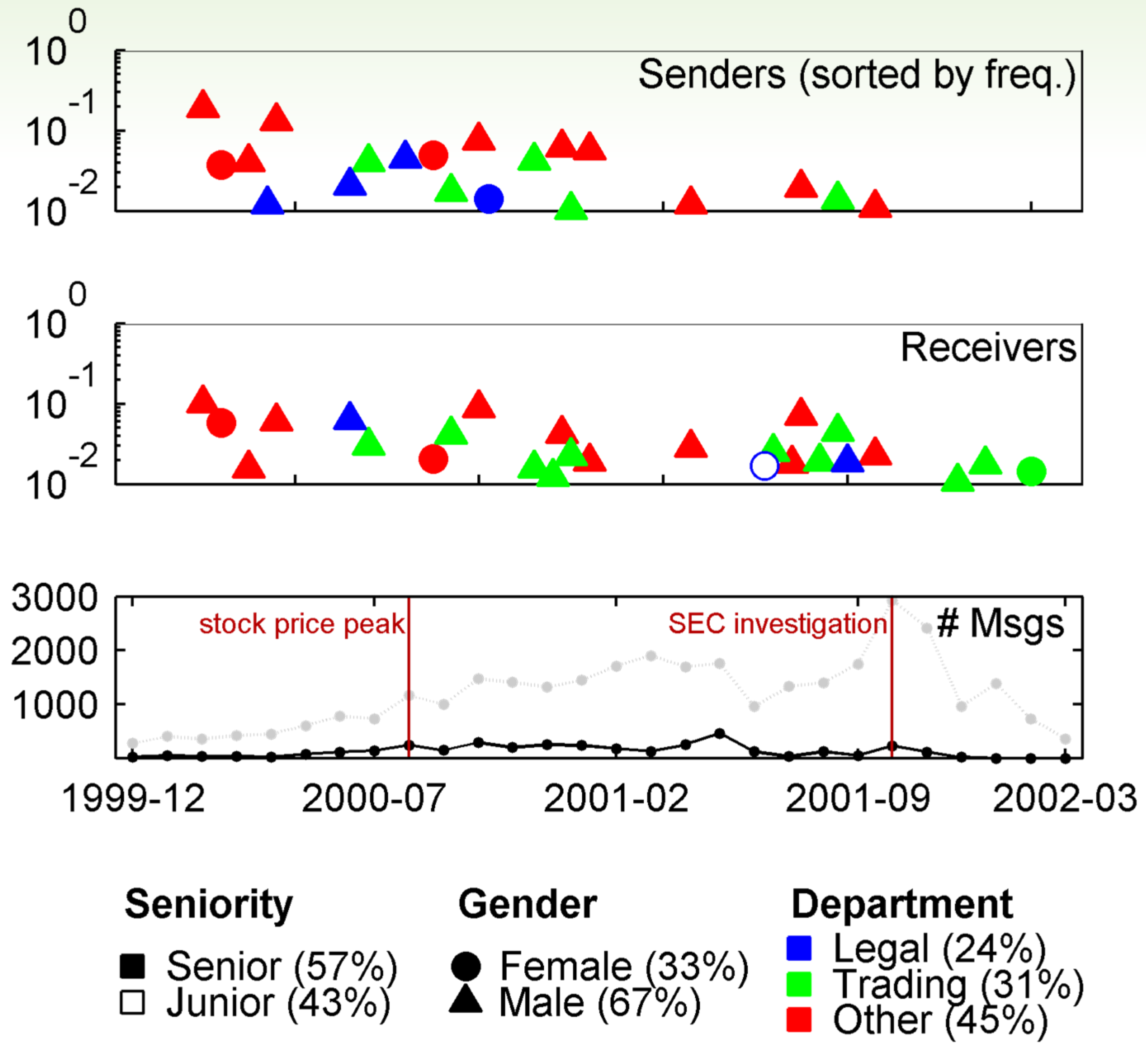
Each person labeled by Zhou et al. (2007)

Chi & Kolda, On Tensors, Sparsity, and Nonnegative Factorizations, SIMAX 2012

Enron Email Data (Component 3)

Senior;
Mostly Male

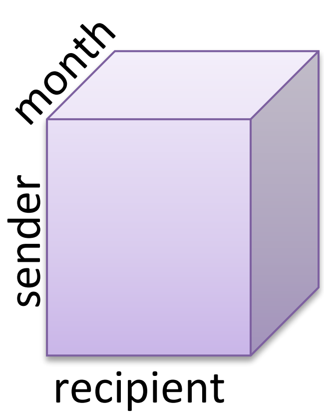


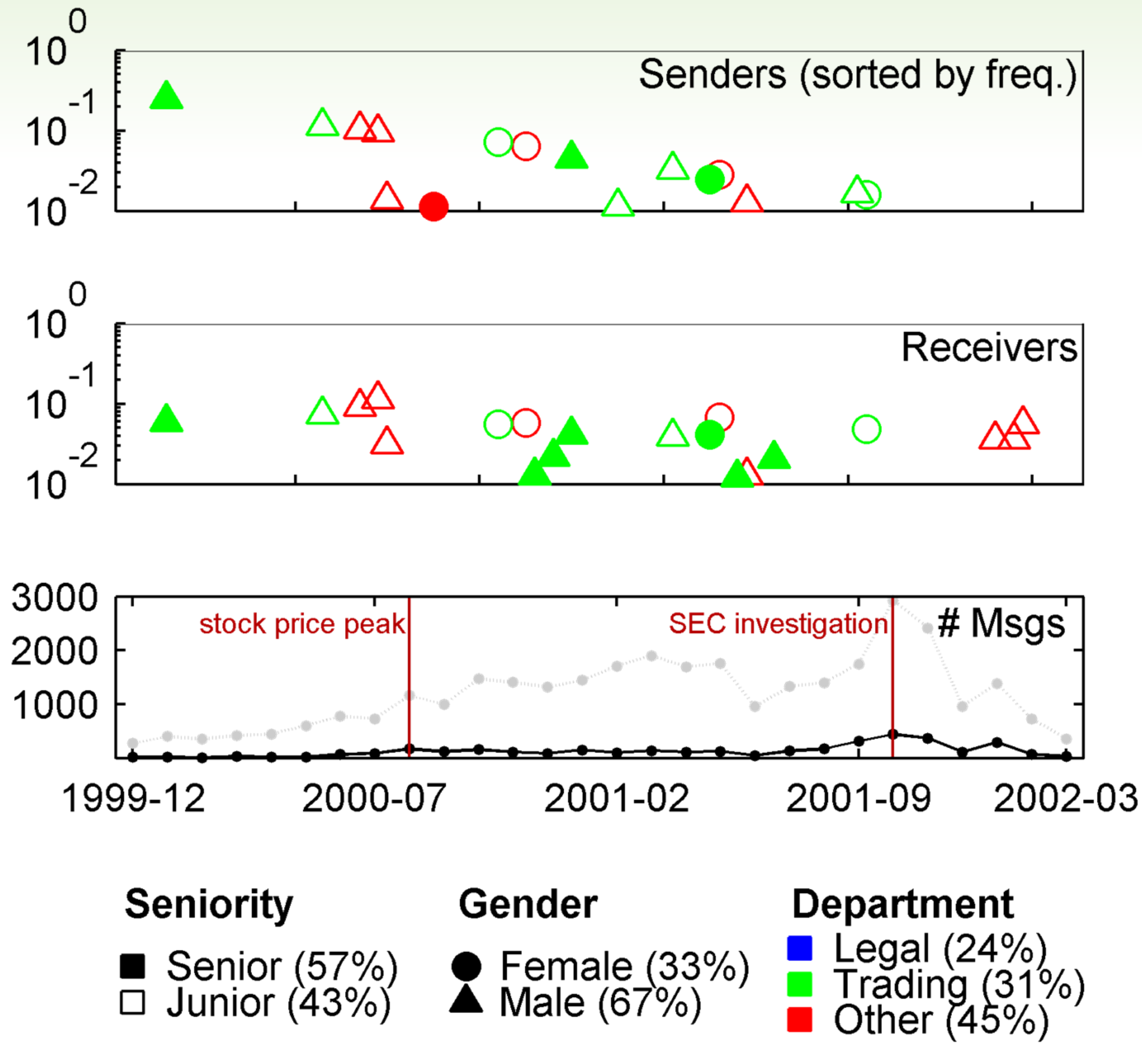


Chi & Kolda, On Tensors, Sparsity, and Nonnegative Factorizations, SIMAX 2012

Enron Email Data (Component 4)

Not Legal

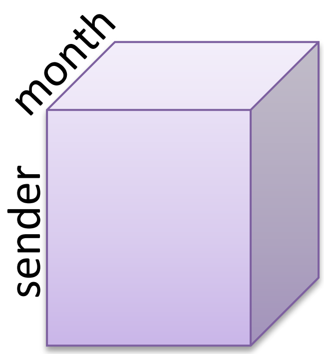


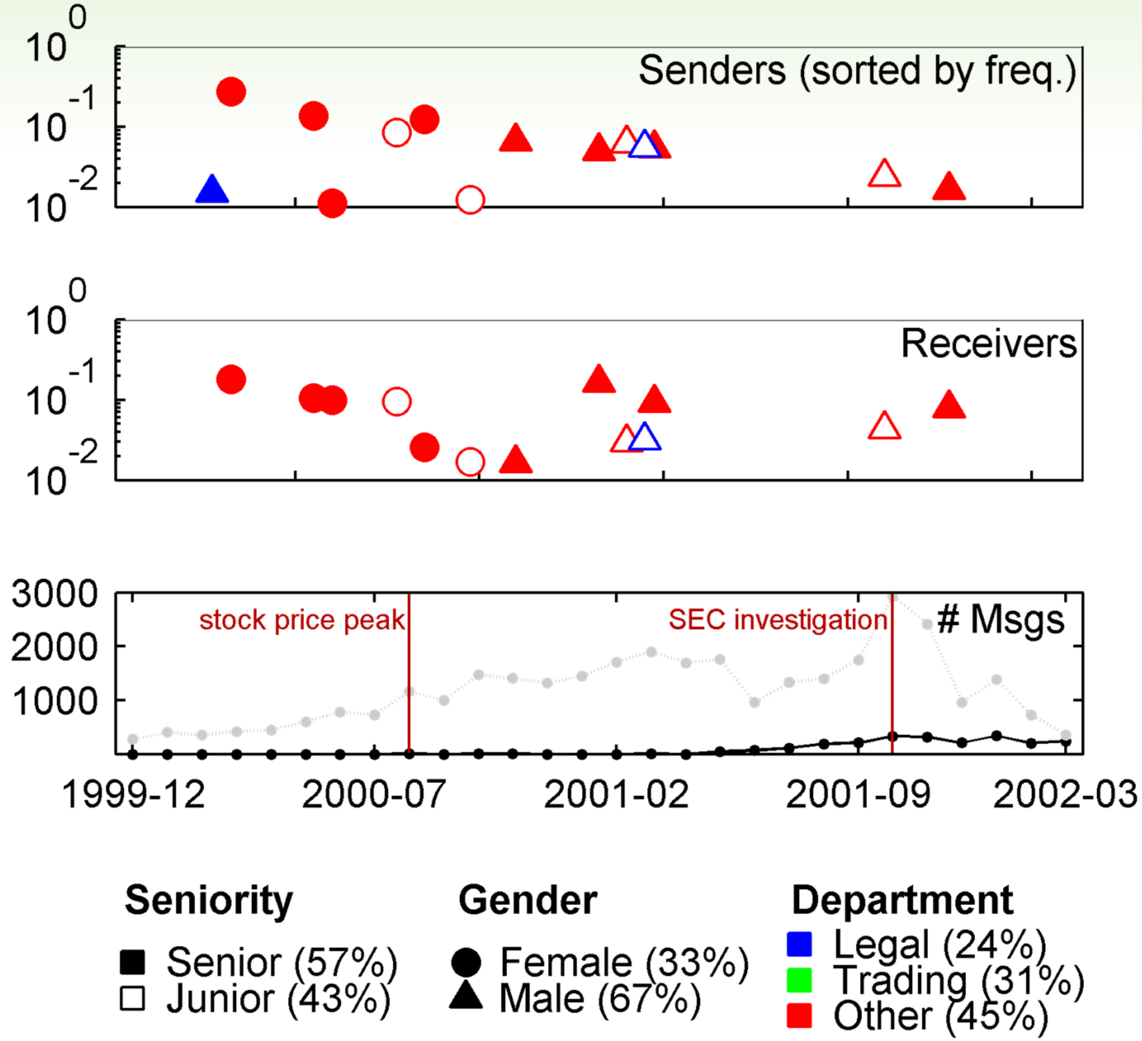


Chi & Kolda, On Tensors, Sparsity, and Nonnegative Factorizations, SIMAX 2012

Enron Email Data (Component 5)

Other;
Mostly Female



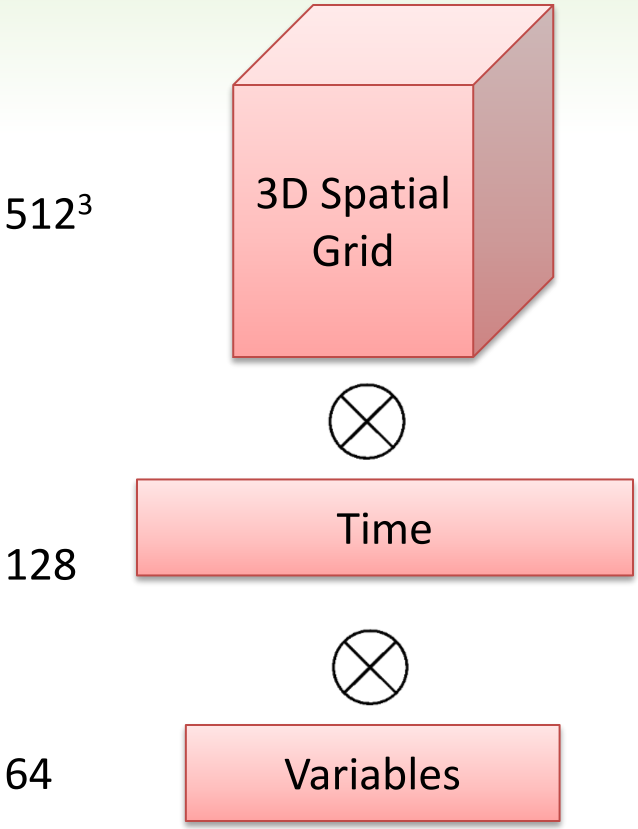


Chi & Kolda, On Tensors, Sparsity, and Nonnegative Factorizations, SIMAX 2012

Parallel Tucker Decomposition for Data Compression

Featuring work of Woody Austin, Grey Ballard, Alicia Klinvex, Hemanth Kollda

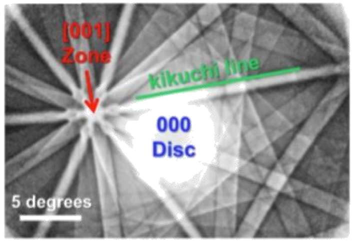
DOE Advanced Simulations and Experiments Deluged by Data

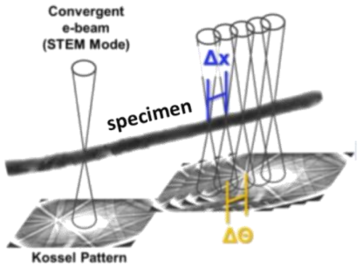


2^{40} elements

8TB (double precision)

- Combustion simulations
  - S3D used direct numerical simulation
  - Gold standard for comparisons, but…
  - Single experiment produces terabytes of data
  - Storage limits spatial, temporal resolutions
  - Difficult to analyze or transfer data
- Electron microscopy
  - New technology produces 1-D spectra and 2-D diffraction patterns *at each pixel*
  - Single experiment produces terabytes of data
  - Usually 10-100 experiments per
  - Limited hardware utilization due to storage limits

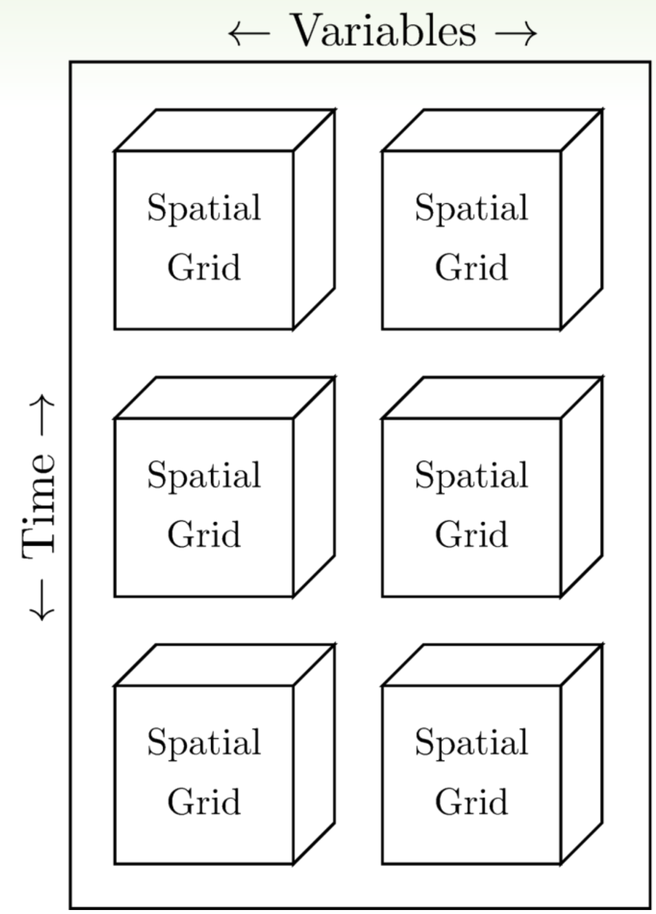




- Other applications
  - Telemetry
  - Cosmology Simulations (with LBL)
  - Climate Modeling (with ORNL)

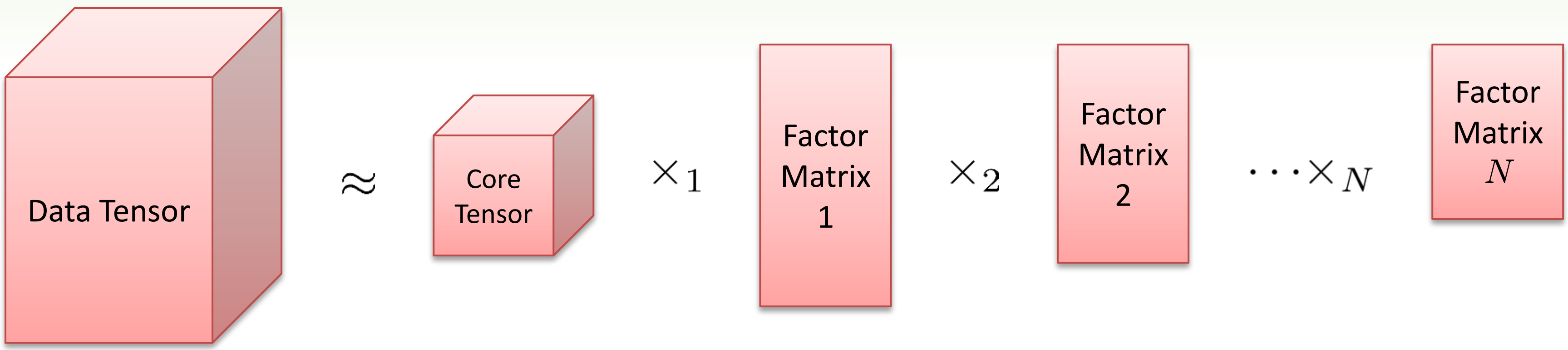
Goal: Reduce Storage Bottleneck via Multiway Compression

- Typical compression methods includes
  - Bzip
  - Wavelets
  - Interpolation
- Standard methods generally ignore multidimensional structure
  - Most science data sets have natural multidimensional structure
- Propose to use multiway compression
  - Always as good as and generally exceeds compression of lossy two-way methods
  - Initial experiments show 90-99% reductions
- Many scientific data sets have natural multiway (N-way) structure
  - 3-D spatial grid
  - Temporal data
  - Multiple measurements
- Parallel compression required to handle large data sets!



Reduction based on Tucker Tensor Decomposition

$$\mathcal{X} \approx \mathcal{G} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \cdots \times_N \mathbf{U}^{(N)}$$



$I_1 \times I_2 \times \cdots \times I_N$ $\quad R_1 \times R_2 \times \cdots \times R_N$ $\quad I_1 \times R_1$ $\quad I_2 \times R_2$ $\quad I_N \times R_N$

Storage: $\prod_{n=1}^{N} I_n$

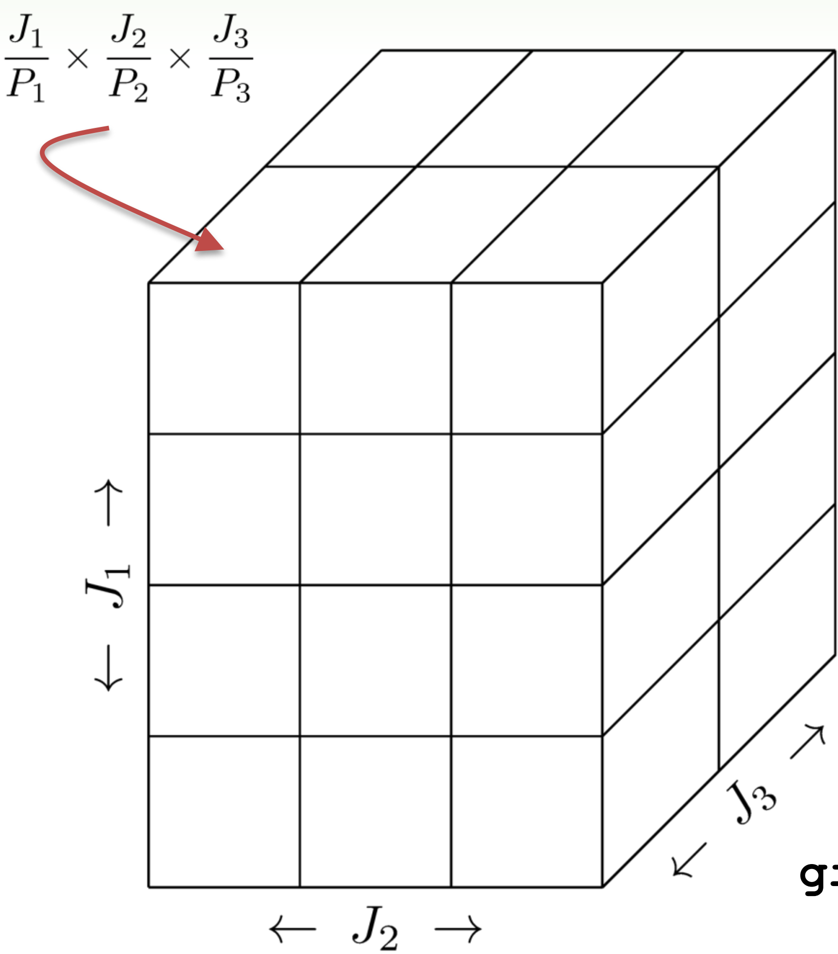
Storage: $\prod_{n=1}^{N} R_n + \sum_{n=1}^{N} R_n I_n$

<u>History</u>:

- Hitchcock (1927) – Mathematical definition
- Tucker (1966) – Algorithms and applications for 3-way data
- Kapteyn, Neudecker, Wansbeek (1986) – Algorithms for N-way data
- Vannieuwenhoven, Vandebril, and Meerbergen (2012) – Sequentially-truncated algorithm

New Contribution: Parallel Tucker Decomposition

Processor Grid: $P_1 \times P_2 \times P_3$



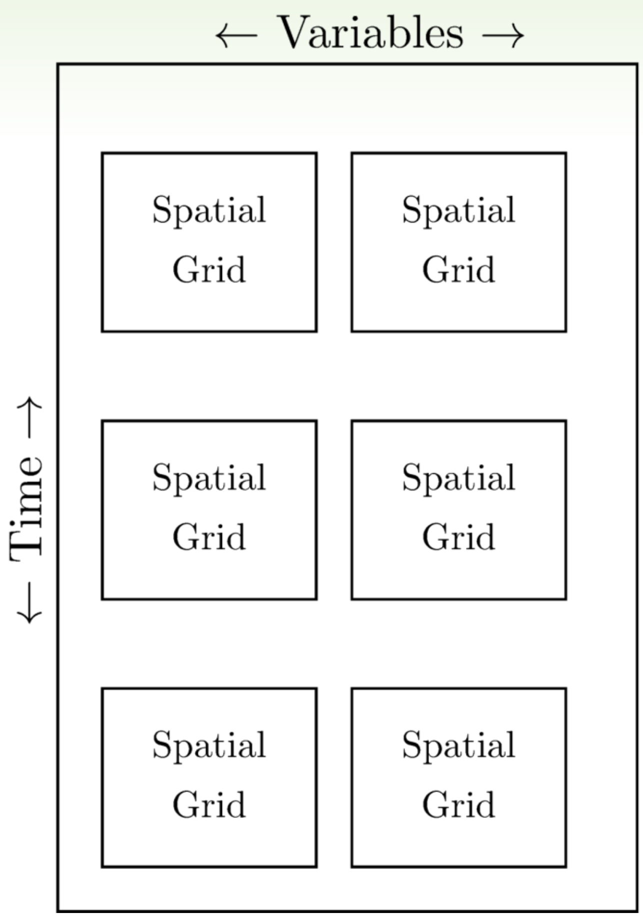
- Uses Cartesian block distribution
- Main parallel kernels
  - Gram matrix
  - Tensor-times-matrix
- Exploits clever local and global data layout
  - Communication avoiding
- Details in IPDPS'16 paper
- Code available (soon) at GitLab

TUCKERMPI

`git@gitlab.com:tensors/TuckerMPI.git`

Alicia Klinvex, Woody Austin, Grey Ballard

Combustion Simulation Results



4-way Tensor, 672 x 672 x 32 x 626

Storage: 74GB

Reduced size determined automatically to satisfy error criteria:

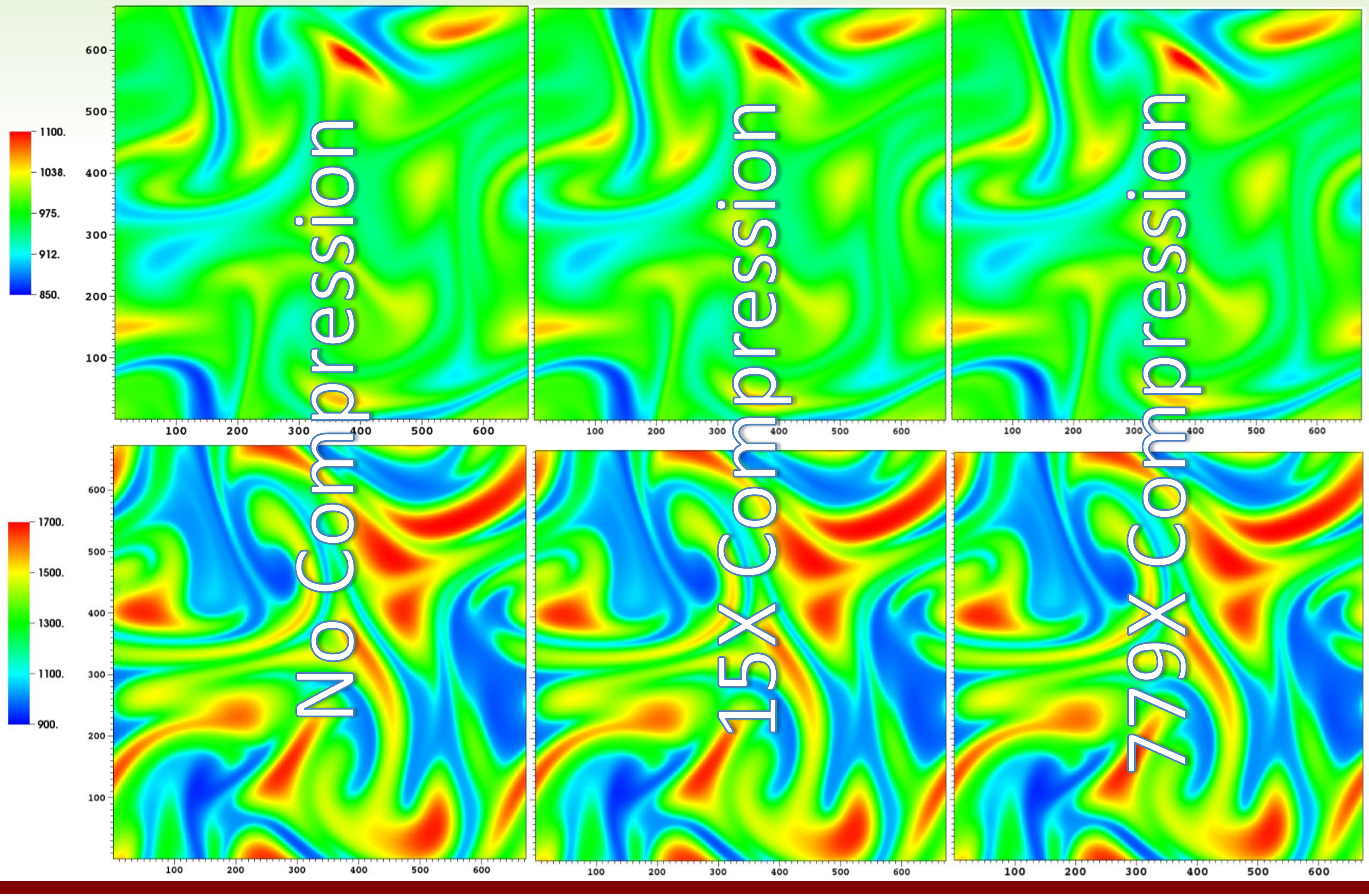
$$\|\mathcal{X} - \hat{\mathcal{X}}\| \leq \epsilon \|\mathcal{X}\|$$

Compression ratio:

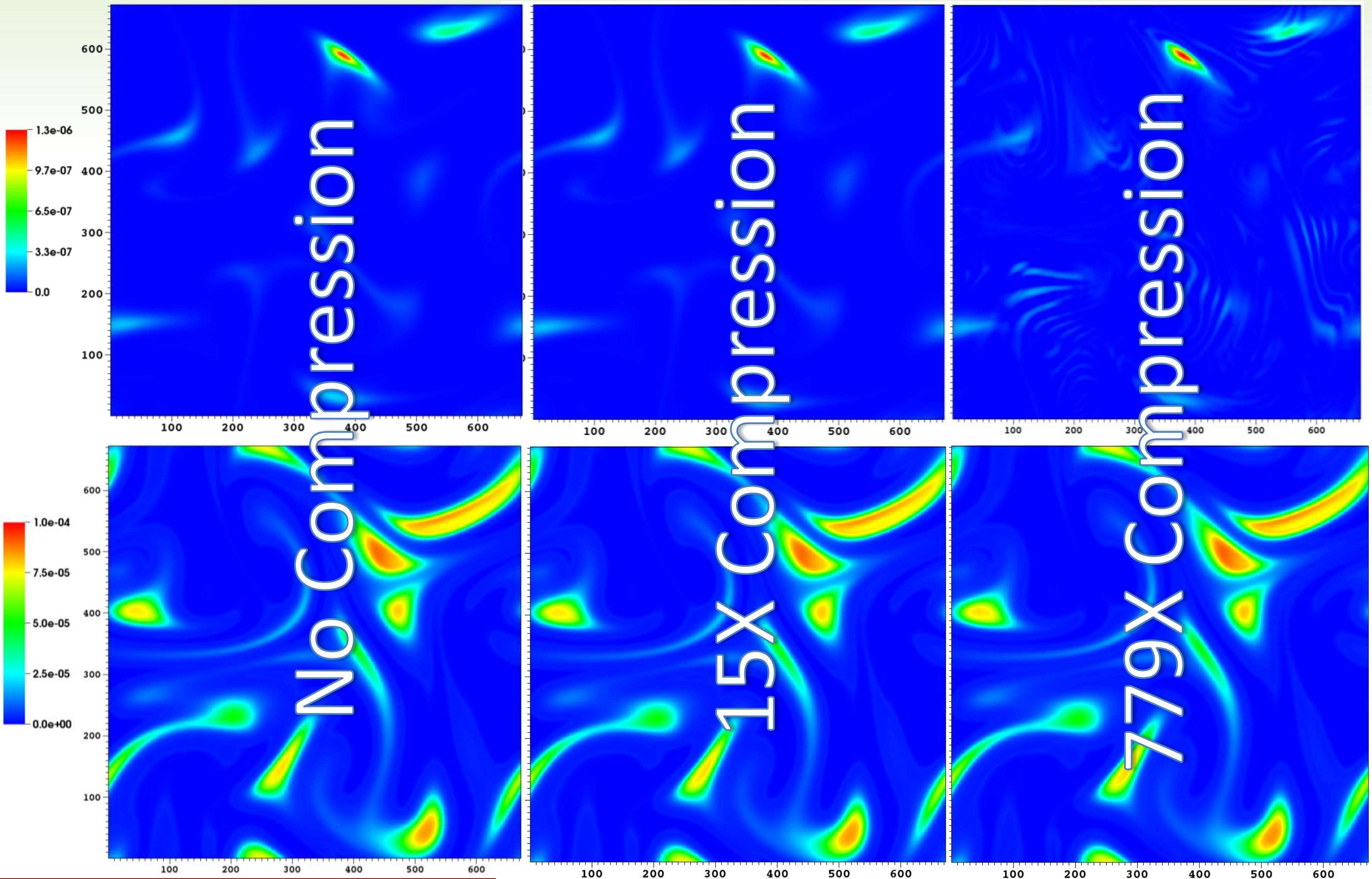
$$C = \prod_{k=1}^{N} I_n \Big/ \left(\prod_{k=1}^{N} R_n + \sum_{k=1}^{N} I_n R_n \right)$$

- Combustion simulation: HCCI Ethanol
  - 2D Spatial Grid: 672 x 672
  - Species/Variables: 32
  - Time steps: 626
- *Scaled each species by its max value*
- Experiment 1: $\epsilon = 10^{-2}$
  - New Core: 111 x 105 x 22 x 46 (<100MB)
  - Compression: 779X
- Experiment 2: $\epsilon = 10^{-4}$
  - New Core: 330 x 310 x 31 x 199 (640MB)
  - Compression: 15X

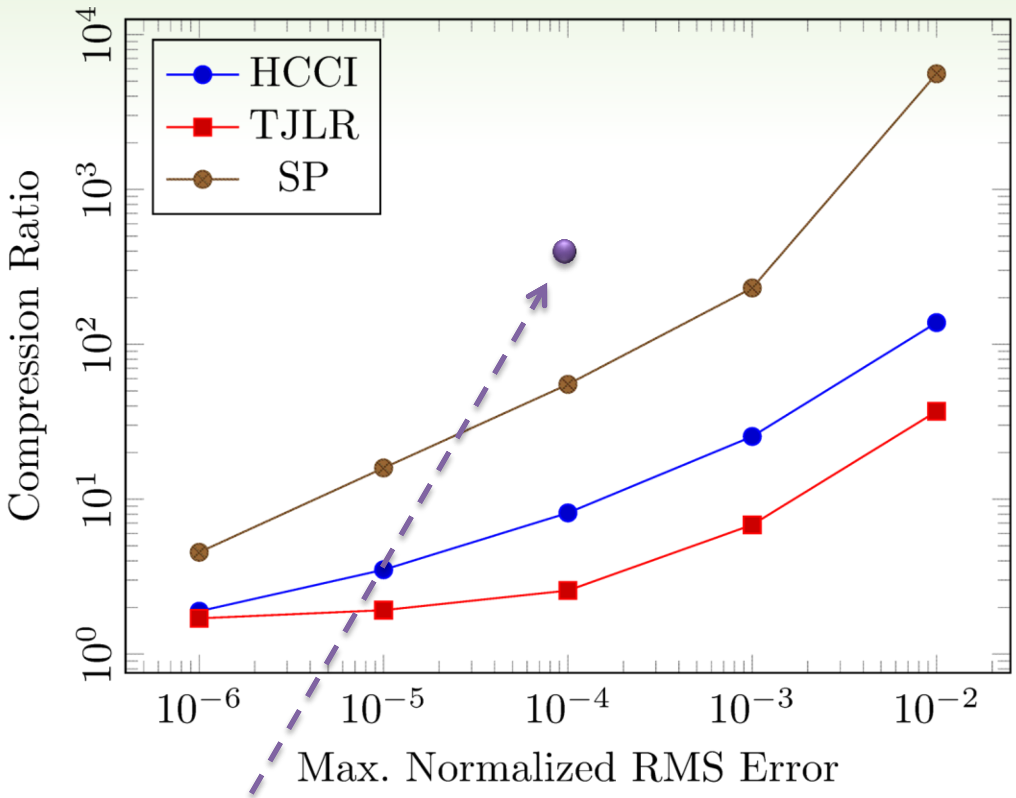
Combustion Simulation Results: Temperature @ Disparate Timesteps



Combustion Simulation Results: OH @ Disparate Timesteps



Compression on Different Data Sets



$$C = \prod_{k=1}^{N} I_n \Big/ \left(\prod_{k=1}^{N} R_n + \sum_{k=1}^{N} I_n R_n \right)$$

- HCCI: 672 x 672 x 33 x 627
- TJLR: 460 x 700 x 360 x 35 x 16
- SP: 500 x 500 x 500 x 11 x 50
- Each data set is centered and scaled for each variable/species

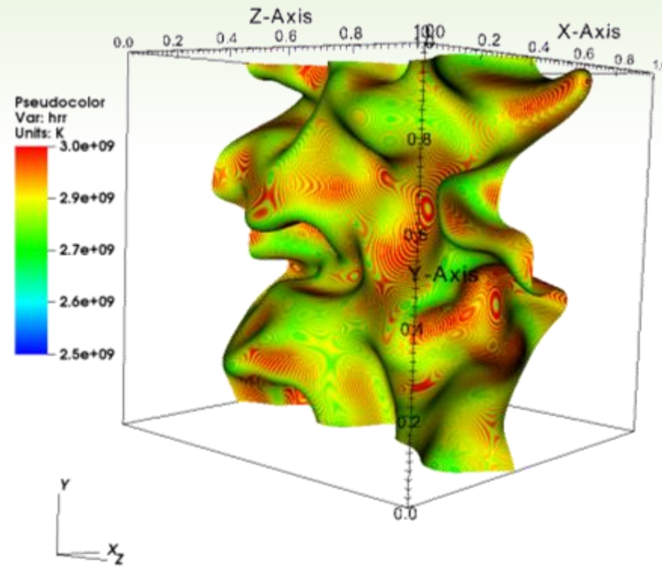
New results just in on 440 GB tensor of size 500 x 500 x 500 x 11 x 400. Achieved 410X compression at 1e-4. Run time is 58 seconds on ORNL's Rhea supercomputer (512 dual-core Intel Xeon processors with 128GB memory).

Method Supports Partial Reconstruction on Laptops, etc.

Reconstruction requires as much space as the original data!

$$\hat{\mathcal{X}} = \mathcal{G} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{U}^{(3)} \times_4 \mathbf{U}^{(4)} \times_5 \mathbf{U}^{(5)}$$

$$I_1 \times I_2 \times I_3 \times I_4 \times I_5$$



But we can just reconstruct the portion that we need at the moment:

$$\bar{\mathcal{X}} = \mathcal{G} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{C}^{(3)}\mathbf{U}^{(3)} \times_4 \mathbf{C}^{(4)}\mathbf{U}^{(4)} \times_5 \mathbf{C}^{(5)}\mathbf{U}^{(5)}$$

$$I_1 \times I_2 \times \frac{I_3}{2} \times 1 \times 1$$

$$\mathbf{C}^{(3)} = \begin{bmatrix} 1/2 & 0 & \cdots & 0 \\ 1/2 & 0 & \cdots & 0 \\ 0 & 1/2 & \cdots & 0 \\ 0 & 1/2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix} \quad \mathbf{C}^{(4)} = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{bmatrix} \quad \mathbf{C}^{(5)} = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

Downsample

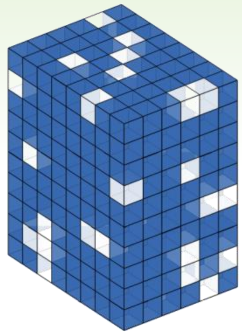
Pick single time step

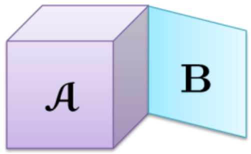
Pick single time var

A Few More Things I Didn't Have Time to Talk About…

Quick Pointers to Other Work

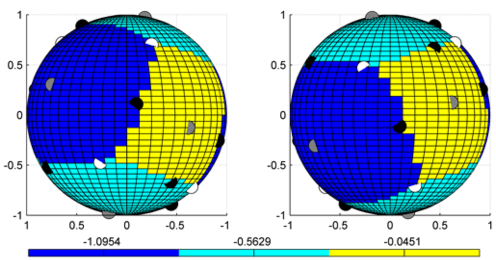
- **All-at-once Optimization (not alternating):** Acar, Dunlavy, Kolda, ***A Scalable Optimization Approach for Fitting Canonical Tensor Decompositions***, J. Chemometrics, 2011, doi:10.1002/cem.1335
- **Missing Data:** Acar, Dunlavy, Kolda, Mørup, ***Scalable Tensor Factorizations for Incomplete Data***, Chemometrics and Intelligent Laboratory Systems, 2011, doi:10.1016/j.chemolab.2010.08.004
- **Coupled Factorizations**: Acar, Kolda, Dunlavy, ***All-at-once Optimization for Coupled Matrix and Tensor Factorizations***, MLG'11, arXiv:1105.3422
- **Tensor Symmetry:** Schatz, Low, van de Geijn, Kolda, ***Exploiting Symmetry in Tensors for High Performance***, SIAM J. Scientific Computing 2014, doi:10.1137/130907215
- **Symmetric Factorizations:** Kolda, ***Numerical Optimization for Symmetric Tensor Decomposition***, Mathematical Programming B2015, doi:10.1007/s10107-015-0895-0
- **Tensor Eigenvalue Problem**
  - Kolda, Mayo, ***An Adaptive Shifted Power Method for Computing Generalized Tensor Eigenpairs***, SIAM J. Matrix Analysis and Applications 2014, doi:10.1137/140951758
  - Ballard, Kolda, Plantenga, ***Efficiently Computing Tensor Eigenvalues on a GPU***, IPDPSW'11 2011, doi:10.1109/IPDPS.2011.287
  - Kolda, Mayo, ***Shifted Power Method for Computing Tensor Eigenpairs***, SIAM J Matrix Analysis and Applications 2011, doi:10.1137/100801482
- **Link Prediction using Tensors:** Dunlavy, Kolda, Acar, ***Temporal Link Prediction using Matrix and Tensor Factorizations***, ACM Trans. Knowledge Discovery from Data, 2011, doi:10.1145/1921632.1921636
- **Tucker for Sparse Data:** Kolda, Sun, ***Scalable Tensor Decompositions for Multi-aspect Data Mining***, ICDM 2008, doi:10.1109/ICDM.2008.89





$$\mathcal{M} \approx \sum_r \lambda_r \, \mathbf{x}_r \circ \mathbf{y}_r \circ \mathbf{z}_r$$
$$\mathbf{B} \approx \mathbf{X}\mathbf{W}^{\mathsf{T}}$$

Positive Stable Basins of Attraction for 3x3x3x3 Tensors

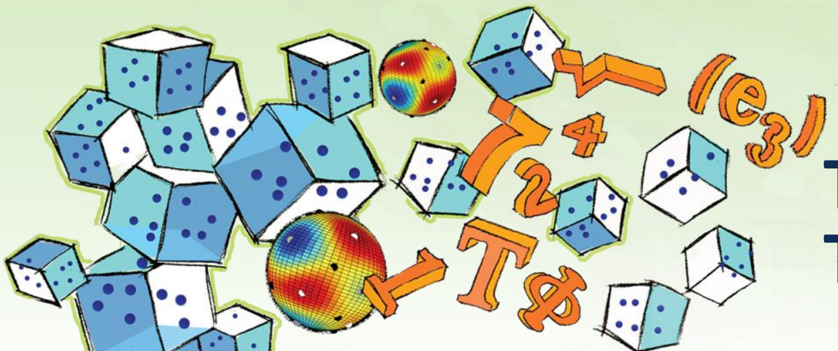


Wrapping Up…

References, Codes, Etc.

- **Overview**
  - T. G. Kolda and B. W. Bader, ***Tensor Decompositions and Applications***, SIAM Review, Vol. 51, No. 3, pp. 455-500, September 2009, doi:10.1137/07070111X
  - B. W. Bader and T. G. Kolda, ***Efficient MATLAB Computations with Sparse and Factored Tensors***, SIAM Journal on Scientific Computing, Vol. 30, No. 1, pp. 205-231, December 2007, doi:10.1137/060676489
- **Randomization for CP**
  - C. Battaglino, G. Ballard, and T. G. Kolda, ***A Practical Randomized CP Tensor Decomposition***, coming soon!
- **Poisson Tensor Factorization (Count Data)**
  - E. C. Chi and T. G. Kolda, ***On Tensors, Sparsity, and Nonnegative Factorizations***, SIAM Journal on Matrix Analysis and Applications, Vol. 33, No. 4, pp. 1272-1299, December 2012, doi:10.1137/110859063
  - S. Hansen, T. Plantenga and T. G. Kolda, ***Newton-Based Optimization for Kullback-Leibler Nonnegative Tensor Factorizations***, Optimization Methods and Software, Vol. 30, No. 5, pp. 1002-1029, April 2015, doi:10.1080/10556788.2015.1009977, arXiv:1304.4964
- **Parallel Tucker for Compression**
  - W. Austin, G. Ballard and T. G. Kolda, ***Parallel Tensor Compression for Large-Scale Scientific Data***, IPDPS'16: Proceedings of the 30th IEEE International Parallel and Distributed Processing Symposium, pp. 912-922, May 2016, doi:10.1109/IPDPS.2016.67, arXiv:1510.06689
- **Codes**
  - Tensor Toolbox for MATLAB: http://www.sandia.gov/~tgkolda/TensorToolbox/
  - TuckerMPI: https://gitlab.com/tensors/TuckerMPI

Tensors are a Foundational Tool for Data Analysis



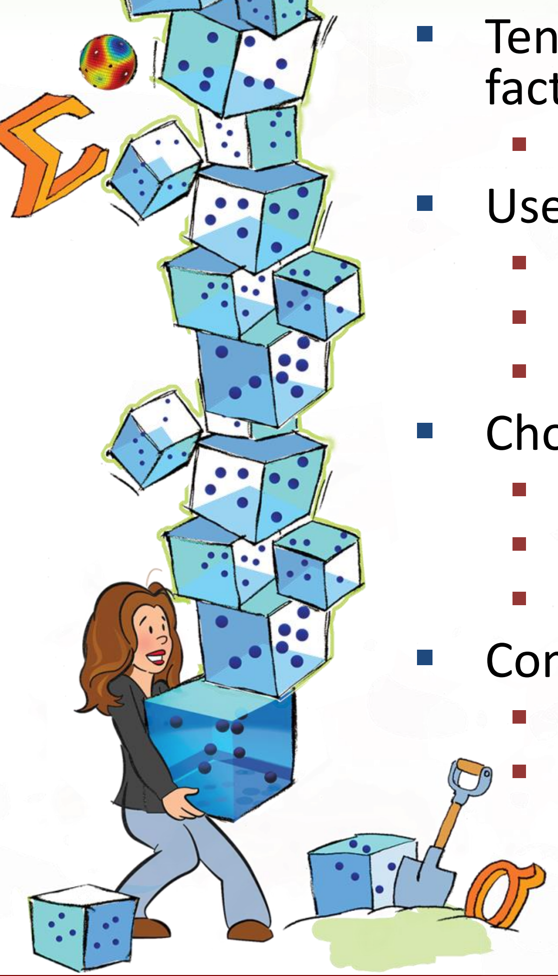
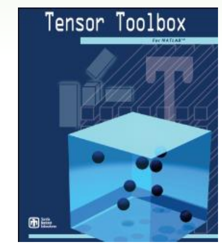
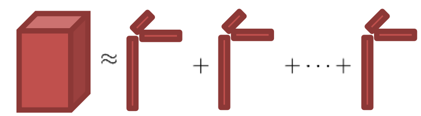


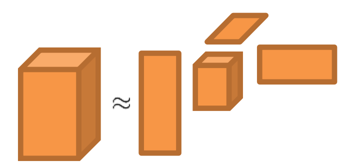
Illustration by Chris Brigman

- Tensor decomposition extends matrix factorization
  - SVD, PCA, NMF, etc.
- Useful for data analysis
  - Mouse neuron activity
  - Enron emails
  - CFD simulation data compression
- Choice of decompositions
  - Canonical polyadic (CP) decomposition
  - Poisson tensor factorization
  - Tucker decomposition
- Computational advances
  - Randomization
  - Parallelization





TUCKERMPI

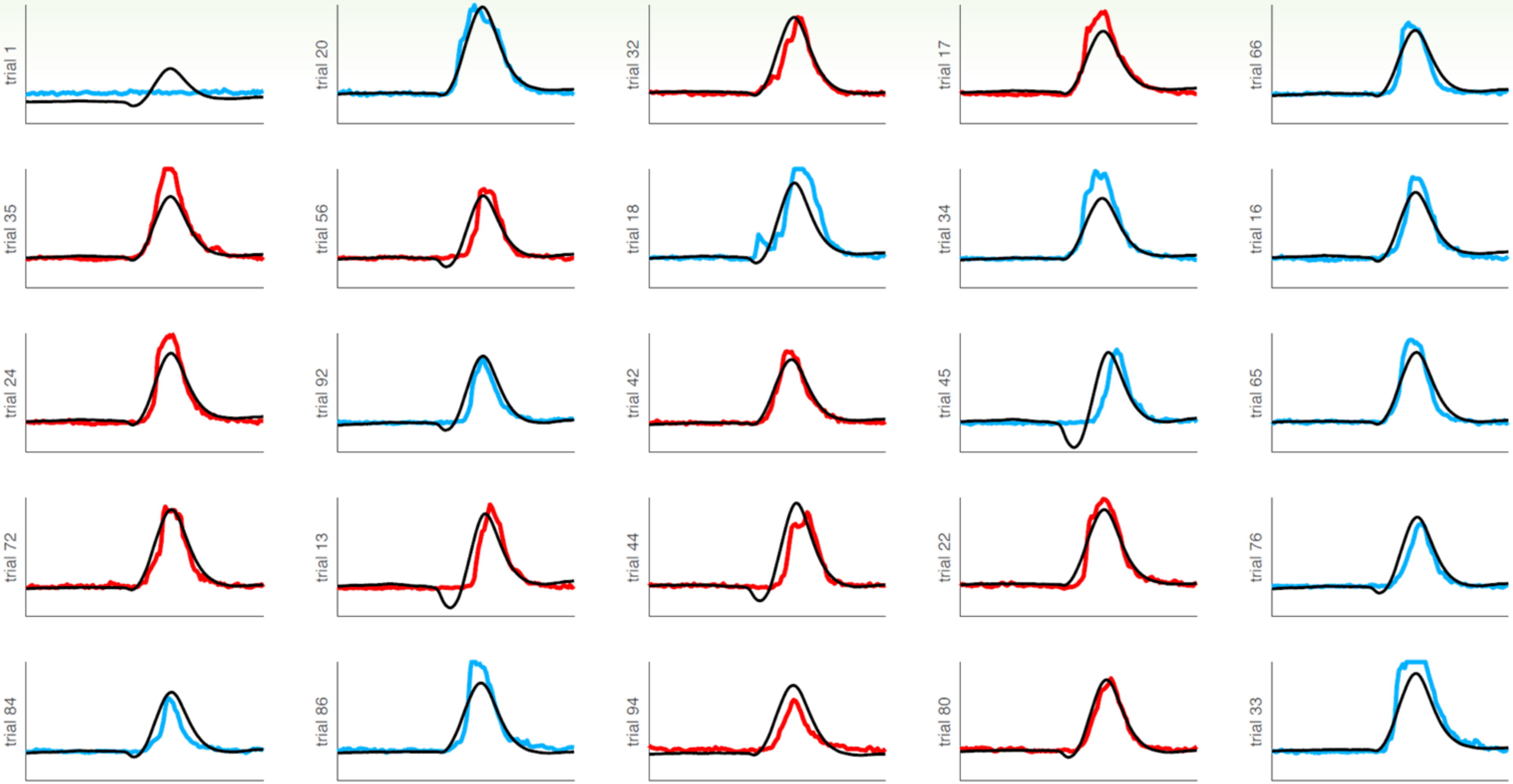


Staff, Postdoc, Intern Positions Available!

Tamara G. Kolda
tgkolda@sandia.gov
http://www.sandia.gov/~tgkolda/

Model is a Good Fit to Data

Single Neuron, Randomly Selected Trials



Coming soon: Williams, Wang, Kim, Schnitzer, Ganguli, Kolda, 2016