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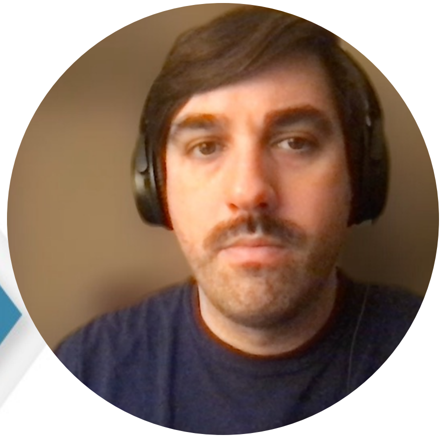

THE GENERALIZED MULTILINEAR MODEL (GMLM)

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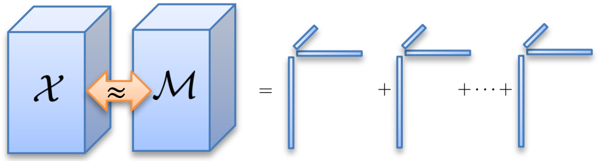
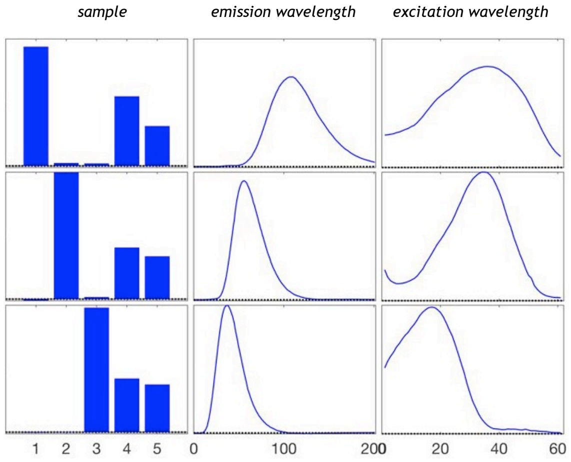
OVERVIEW

Low-Rank Tensor Decompositions



Example: Amino acid analysis

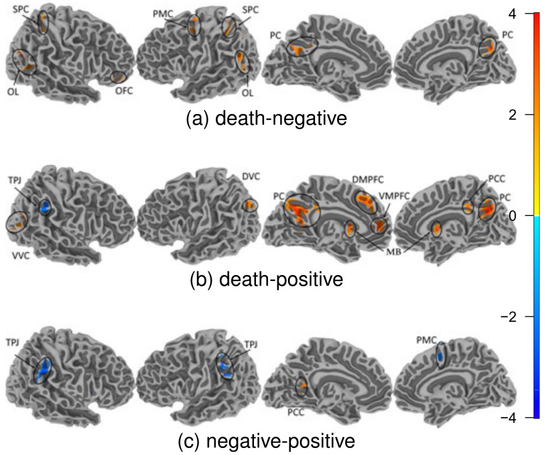


Andersen & Bro (2003)

Tensor-on-Tensor Regression Models

$$\mathcal{Y}_i = \langle \mathcal{X}_i | \mathcal{B} \rangle + \mathcal{E}_i$$

Example: Brain activity/suicide risk

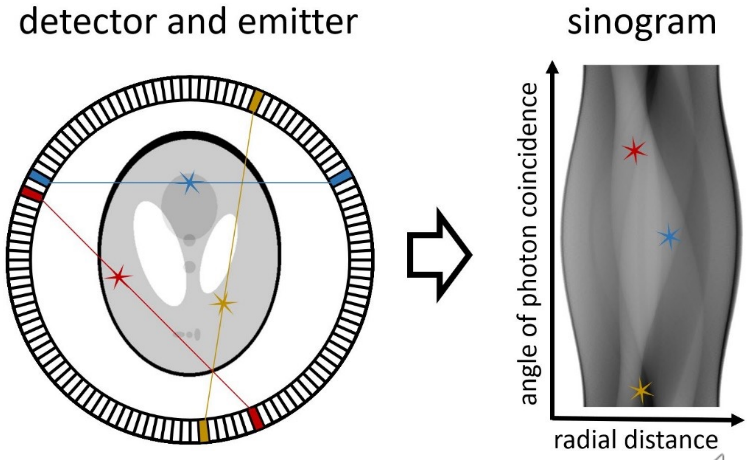


Lock (2018); Llosa & Maitra (2022)

Generalized Multilinear Models (GMLMs)

$$g\left(\mathbb{E}_{f_{\mathcal{Y}}}\left(\mathcal{Y}_i\right)\right) = \langle \mathcal{X}_i | \mathcal{B} \rangle$$

Example: PET image reconstruction

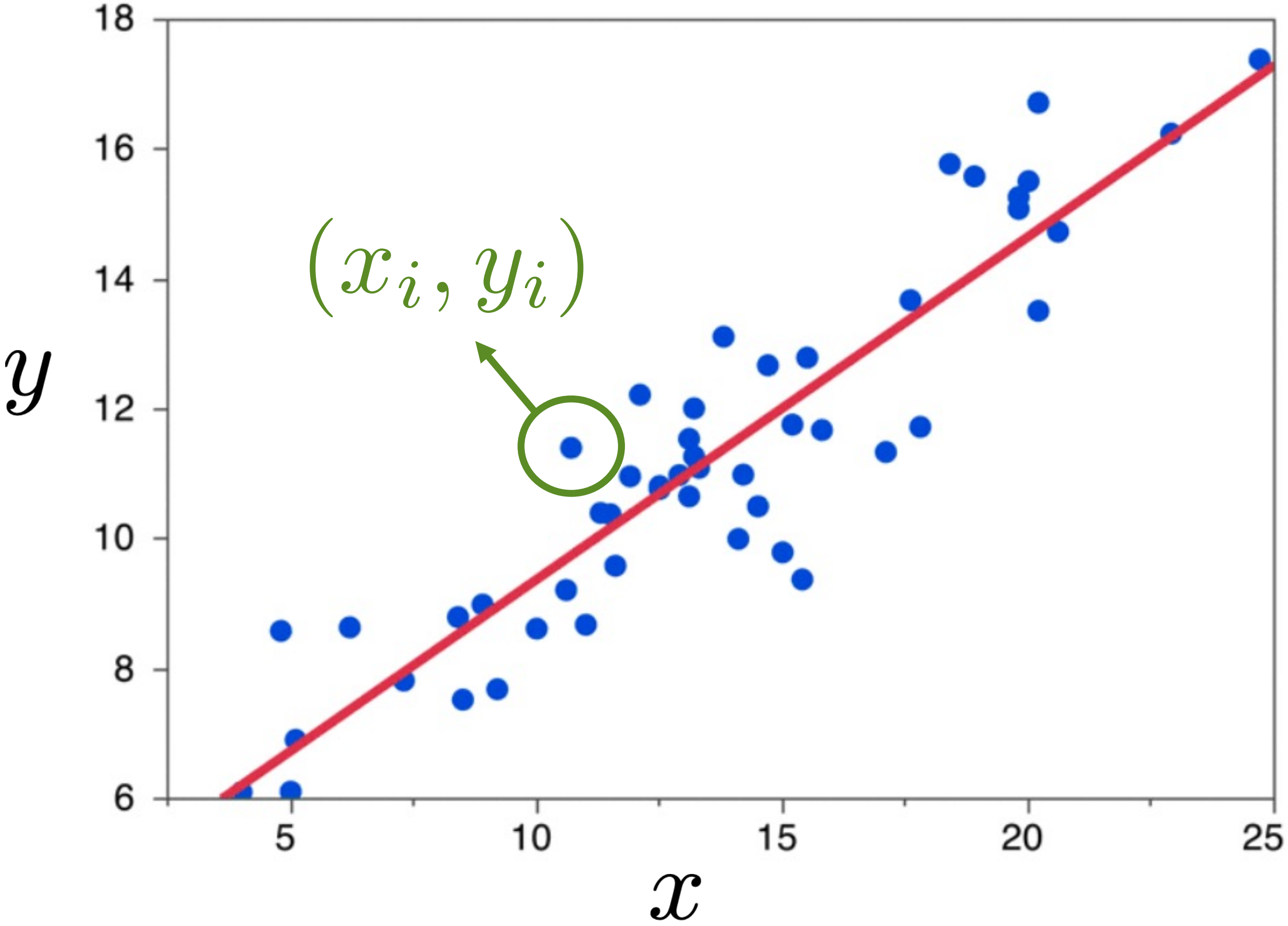


Llosa, Dunlavy, Myers, Lehoucq, Ma (2025)

OUTLINE

- Tensor-on-Tensor Regression (ToTR)
- Evolution of Generalized CP (GCP)
- Evolution of Generalized Multilinear Models (GMLMs) for ToTR
- Extending Generalized Linear Models (GLMs) to GMLMs
- Parameter Inference for GMLMs
- Example Applications

LINEAR REGRESSION



Simple linear regression:

$$y_i = \beta x_i + \epsilon_i$$

Multiple linear regression:

$$y_i = \boldsymbol{\beta}^T \mathbf{x}_i + \epsilon_i$$

TENSOR-ON-TENSOR REGRESSION

$$\langle S|T\rangle = \begin{cases} \text{inner product} & dim(S) = dim(T) \\ \text{contraction} & dim(S) \neq dim(T) \end{cases}$$

Linear regression: $$y_i = \langle \boldsymbol{x}_i | \boldsymbol{\beta} \rangle + \epsilon_i$$

Tensor regression: $$y_i = \langle \mathcal{X}_i | \mathcal{B} \rangle + \epsilon_i$$

Multivariate linear regression: $$\boldsymbol{y}_i = \langle \boldsymbol{x}_i | B \rangle + \boldsymbol{\epsilon}_i$$

Tensor-on-Tensor regression (ToTR): $$\mathcal{Y}_i = \langle \mathcal{X}_i | \mathcal{B} \rangle + \mathcal{E}_i$$

Lock (2018); Llosa & Maitra (2022)

TOTR: HOW MUCH DATA DO WE NEED TO FIT THE MODEL

$M_1 \times \cdots \times M_P \qquad N_1 \times \cdots \times N_Q$

Tensor-on-Tensor regression (ToTR):

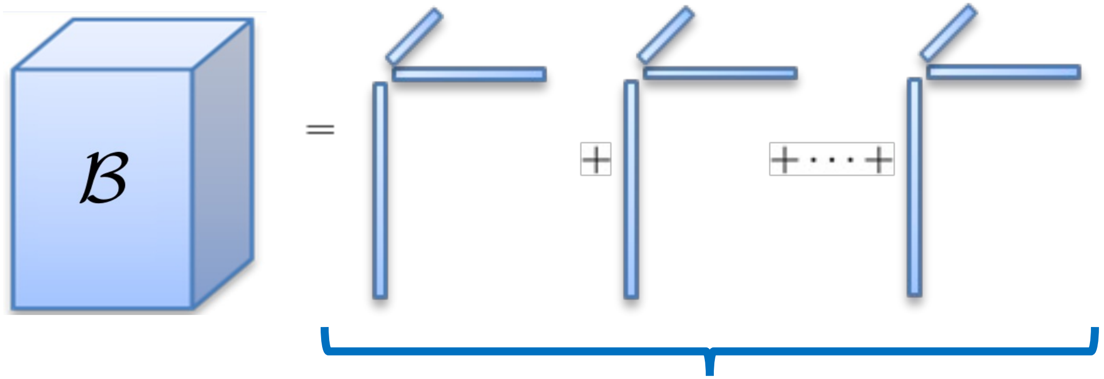
$N_1 \times \cdots \times N_Q \times M_1 \times \cdots \times M_P$

$\boxed{i = 1, 2, \ldots, n \longrightarrow \text{so many samples needed!}}$

$N_1 \times \cdots \times N_Q \times M_1 \times \cdots \times M_P$

Low-rank Canonical Polyadic (CP) Model:

Rank-1 tensor



R summands

Lock (2018); Llosa & Maitra (2022)

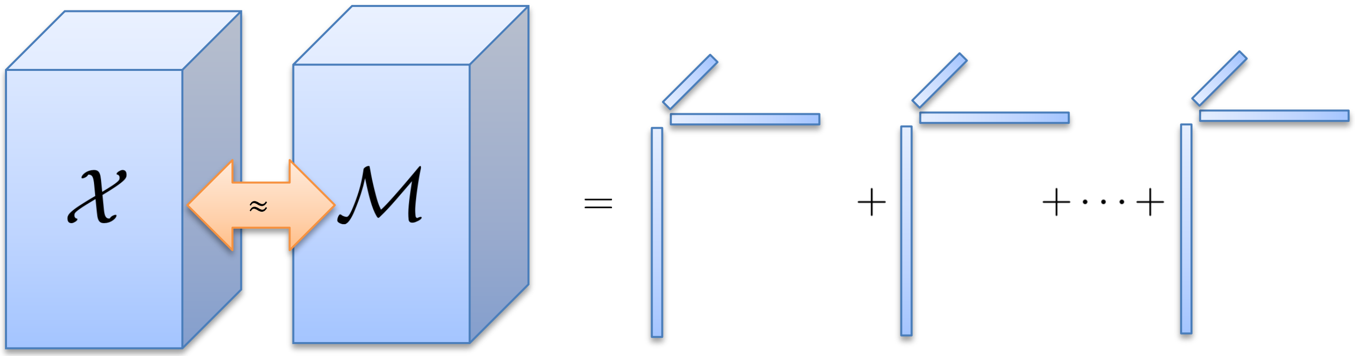
$N_1 \times R \qquad M_1 \times R$

$$\mathcal{B} = [\![V_{N_1}, \ldots, V_{N_Q}, U_{M_1}, \ldots, U_{M_P}]\!]$$

Fewer parameters $\longrightarrow$ fewer samples needed

$$\prod_p M_p \prod_q N_q \to R\left(\sum_p M_p + \sum_q N_q\right)$$

GENERALIZING CP DECOMPOSITIONS FOR D-WAY TENSORS



$$= [\![A^{(1)}, A^{(2)}, \ldots, A^{(d)}]\!] = [\![\{A^{(k)}\}_1^d]\!]$$

Multi-index for *d*-way tensors: $\boldsymbol{j} = (j_1, j_2, \ldots, j_d) \to x_{\boldsymbol{j}} = \mathcal{X}(j_1, j_2, \ldots, j_d)$

CP-ALS, CP-OPT

Carroll & Chang (1970); Harshman (1970); Acar, Dunlavy & Kolda (2011)

$$\min_{\{A^{(k)}\}_1^d} \sum_{\boldsymbol{j}} (x_{\boldsymbol{j}} - m_{\boldsymbol{j}})^2$$

$$x_{\boldsymbol{j}} \overset{indep.}{\sim} N(m_{\boldsymbol{j}}, \sigma^2)$$

CP-APR, CP-POPT

Chi & Kolda (2012); Ranadive & Baskaran (2021)

$$\min_{\{A^{(k)}\}_1^d} \sum_{\boldsymbol{j}} m_{\boldsymbol{j}} - x_{\boldsymbol{j}} \log(m_{\boldsymbol{j}})$$

$$x_{\boldsymbol{j}} \overset{indep.}{\sim} Poisson(m_i)$$

GCP

Hong, Kolda & Duersch (2020); Kolda & Hong (2020)

$$\min_{\{A^{(k)}\}_1^d} \sum_{\boldsymbol{j}} f(x_{\boldsymbol{j}}, m_{\boldsymbol{j}})$$

$$x_{\boldsymbol{j}} \overset{indep.}{\sim} P_f(m_i)$$

GENERALIZING TENSOR-ON-TENSOR REGRESSION

Tensor-on-Tensor regression (ToTR):

$$\mathcal{Y}_i = \langle \mathcal{X}_i | \mathcal{B} \rangle + \mathcal{E}_i$$

$M_1 \times \cdots \times M_P$

$N_1 \times \cdots \times N_Q$

$N_1 \times \cdots \times N_Q \times M_1 \times \cdots \times M_P$

ToTR

Lock (2018); Llosa & Maitra (2022)

$$\mathcal{Y}_i = \langle \mathcal{X}_i | \mathcal{B} \rangle + \mathcal{E}_i$$

$$\mathcal{Y}_i \sim N\left(\langle \mathcal{X}_i | \mathcal{B} \rangle, \Sigma_1, \ldots, \Sigma_P\right)$$

CP, Tucker, Tensor Train, Tensor Network, …

Poisson ToTR (PToTR)

Llosa & Dunlavy (2025)

$$\mathcal{Y}_i \sim Poisson\left(\langle \mathcal{X}_i | \mathcal{B} \rangle\right)$$

CP

GMLM

Llosa, Dunlavy, Myers, Lehoucq, Ma (2025)

$$g\left(\mathbb{E}_{f_\mathcal{Y}}\left(\mathcal{Y}_i\right)\right) = \langle \mathcal{X}_i | \mathcal{B} \rangle$$

CP

THE GENERALIZED MULTILINEAR MODEL (GMLM)

Same as in ToTR

$$g\left(\mathbb{E}_{f_{\mathcal{Y}}}\left(\mathcal{Y}_i\right)\right) = \langle \mathcal{X}_i | \mathcal{B} \rangle$$

Link Function

- $g : \mathbb{R}^{\times_{p=1}^{P} M_p} \to \mathbb{R}^{\times_{p=1}^{P} M_p}$
- Applied entry-wise
- e.g., identity, logit, log, inverse,…

Random component

- e.g., normal, binomial, Poisson, …

GENERALIZED LINEAR MODELS (GLMS)

$$y_i \sim P_{f_Y}(\psi_i), \quad \mathbb{E}(y_i) = \mu_i, \quad \mu_i = g^{-1}(\eta_i), \quad \eta_i = \boldsymbol{b}^\top \boldsymbol{x}_i$$

- y: response (independent)
- $\boldsymbol{x}$: covariate
- μ: mean response
- g: link function, relating random component and linear predictor
- $\boldsymbol{b}$: model parameters
- n samples $\rightarrow X = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]\,; \boldsymbol{y} = [y_1, \ldots, y_n]$

$$\boxed{\mathrm{GLM}(X, \boldsymbol{y})}$$

Nelder & Wedderburn (1972)

GENERALIZED LINEAR MODELS (GLMS)

$$y_i \sim P_{f_Y}(\psi_i), \quad \mathbb{E}(y_i) = \mu_i, \quad \mu_i = g^{-1}(\eta_i), \quad \eta_i = \boldsymbol{b}^\top \boldsymbol{x}_i$$

Loglikelihood:

$$\ell(\boldsymbol{b}) = \sum_{i=1}^{n} \log f_Y(\psi_i)$$

Gradient:

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{b}} \ell(\boldsymbol{b}) &= \sum_{i=1}^{n} \frac{\partial}{\partial \boldsymbol{b}} \log f_Y(\psi_i) \\ &= \sum_{i=1}^{n} \underbrace{\left[\frac{\partial}{\partial \boldsymbol{b}} \eta_i\right]}_{\boldsymbol{x}_i} \underbrace{\left[\frac{\partial}{\partial \eta_i} \mu_i\right] \left[\frac{\partial}{\partial \mu_i} \psi_i\right] \left[\frac{\partial}{\partial \psi_i} \log f_Y(\psi_i)\right]}_{\text{weight } i} \end{aligned}$$

Nelder & Wedderburn (1972)

THE GENERALIZED MULTILINEAR MODEL (GMLM)

Same as in ToTR

$$g\left(\mathbb{E}_{f_{\mathcal{Y}}}\left(\mathcal{Y}_i\right)\right) = \langle \mathcal{X}_i | \mathcal{B} \rangle$$

Link Function

- $g : \mathbb{R}^{\times_{p=1}^{P} M_p} \to \mathbb{R}^{\times_{p=1}^{P} M_p}$
- Applied entry-wise
- e.g., identity, logit, log, inverse,…

Random component

- Exponential dispersion family:

$$\log f_{\mathcal{Y}}(\psi) = \sum_{\boldsymbol{j}} \left(\frac{\mathcal{Y}_{\boldsymbol{j}}\psi_{\boldsymbol{j}} - b(\psi_{\boldsymbol{j}})}{a(\delta_{\boldsymbol{j}})} + C \right)$$

- e.g., normal, binomial, Poisson, …

Extends the Generalized Linear Model (GLM) to tensors

Nelder & Wedderburn (1972)

FROM GLM TO GMLM

$$\mathcal{Y}_i \sim P_{f_{\mathcal{Y}}}(\psi_i), \quad \mathbb{E}(\mathcal{Y}_i) = \mu_i, \quad \mu_i = g^{-1}(\eta_i), \quad \eta_i = \langle \mathcal{X}_i | \mathcal{B} \rangle$$

where $\mathcal{Y}_i, \psi_i, \mu_i, \eta_i$ are all tensors of size $M_1 \times \cdots \times M_P$

Low-rank constraint: $\mathcal{B} = [\![V_1, \ldots, V_{N_Q}, U_1, \ldots, U_{M_P}]\!]$

Loglikelihood: $\ell(\boldsymbol{\theta}) = \sum_{i,\boldsymbol{j}} \log f_{\mathcal{Y}}(\psi_{i,\boldsymbol{j}})$

Gradient: $\frac{\partial}{\partial \boldsymbol{\theta}} \ell(\boldsymbol{\theta}) = \left[\left(\frac{\partial}{\partial \operatorname{vec}(V_1)} \ell(\boldsymbol{\theta}) \right)^\top \ldots \left(\frac{\partial}{\partial \operatorname{vec}(U_P)} \ell(\boldsymbol{\theta}) \right)^\top \right]^\top$

where $\boldsymbol{\theta} = [\ \operatorname{vec}(V_1)^\top \ldots\ \operatorname{vec}(V_Q)^\top\ \operatorname{vec}(U_1)^\top \ldots\ \operatorname{vec}(U_P)^\top]^\top$

GMLM: MAXIMUM LIKELIHOOD ESTIMATION

Stack all $\mathcal{Y}_i, \mathcal{X}_i$ into $\mathcal{Y} \in \mathbb{R}^{(\times_{p=1}^{P} M_p)\times n}, \mathcal{X} \in \mathbb{R}^{(\times_{q=1}^{Q} N_q)\times n}$. Use $\mathrm{GLM}(X, \boldsymbol{y})$ as follows:

- **Row-based inference** for U_p, where $W = \mathcal{X}_{(Q+1)}(\odot_q V_q)$:

Khatri-Rao Product

$$U_p[j_p, :] \leftarrow \mathrm{GLM}\left(X = \mathrm{reshape}\left[\left(\bigodot_{k\neq p} U_k\right) \odot W\right],\ \boldsymbol{y} = (Y_{(p)}[j_p, :])^\top\right)$$

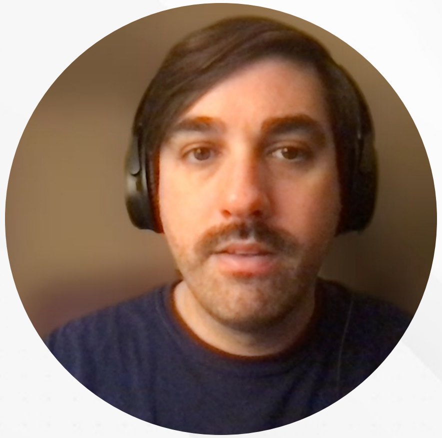
- **Factor-based inference** for V_q, where $W_q = \mathcal{X}_{(Q+1,q)}(\odot_{k\neq q} V_k)$:

$$\mathrm{vec}(V_q) \leftarrow \mathrm{GLM}\left(X = \mathrm{reshape}\left[\left(\bigodot_{p} U_p\right) \odot W_q\right],\ \boldsymbol{y} = \mathrm{vec}(\mathcal{Y})\right)$$

1 outer iteration

NOTE: Leverage iteratively reweighted least squares (IRLS) to solve each GLM.

EXAMPLE APPLICATIONS



PARAMETER INFERENCE VALIDATION: SIMULATED DATA

$$g\left(\mathbb{E}_{f_{\mathcal{Y}}}\left(\mathcal{Y}_i\right)\right) = \langle \mathcal{X}_i | \mathcal{B} \rangle$$

Gaussian distribution, identity link:

- 4 different camelid images
- 150 noisy samples of each

- $\mathcal{Y}_i$: 87 x 106 (*pixel height* x *width*)
- $\mathcal{X}_i$: 4 x 3 (*camelid* x *RGB channel*)
- $\mathcal{B}$: 4 x 3 x 87 x 106

Can recover original images from noisy samples using GMLM with sufficiently high rank of parameter tensor.

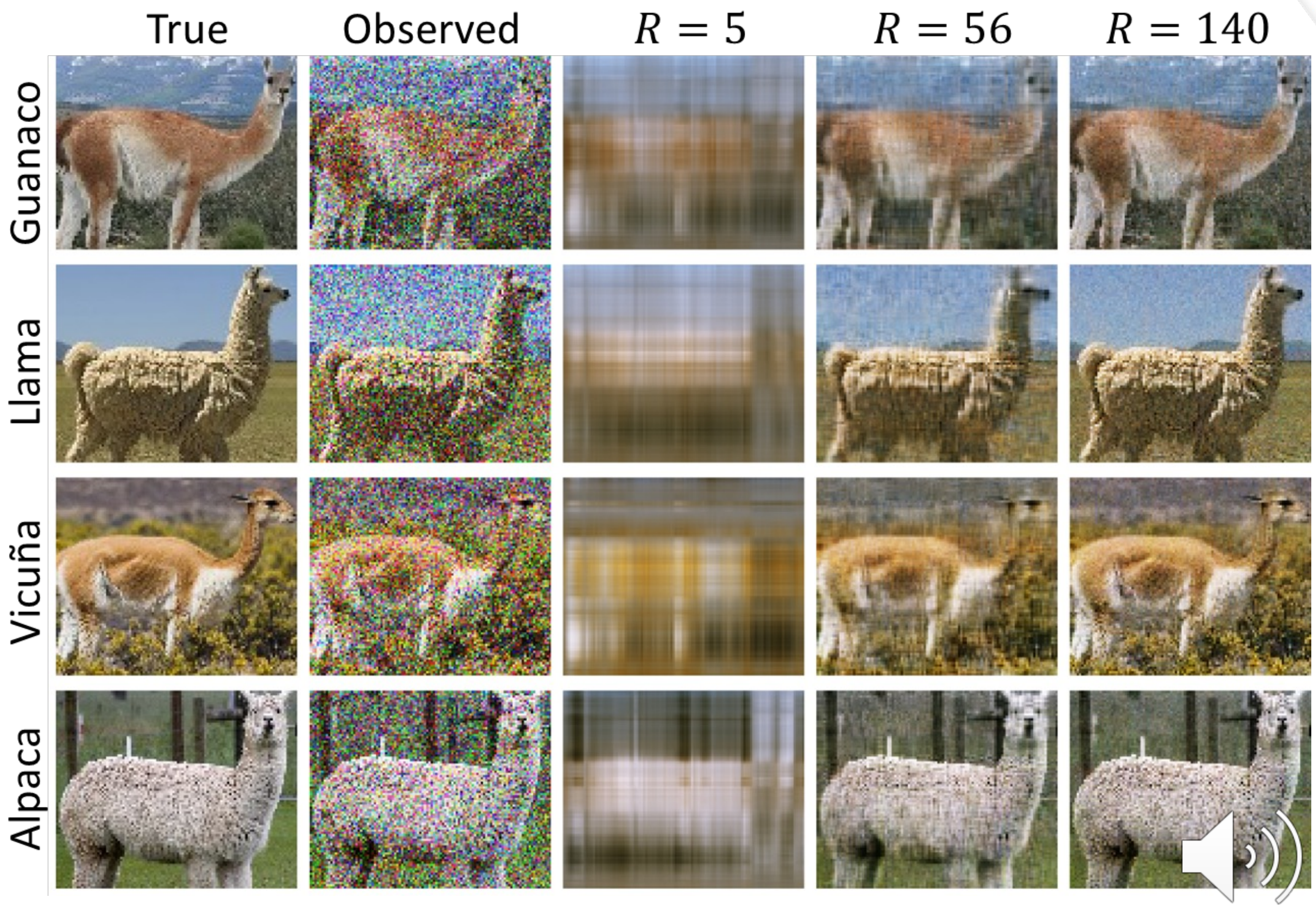


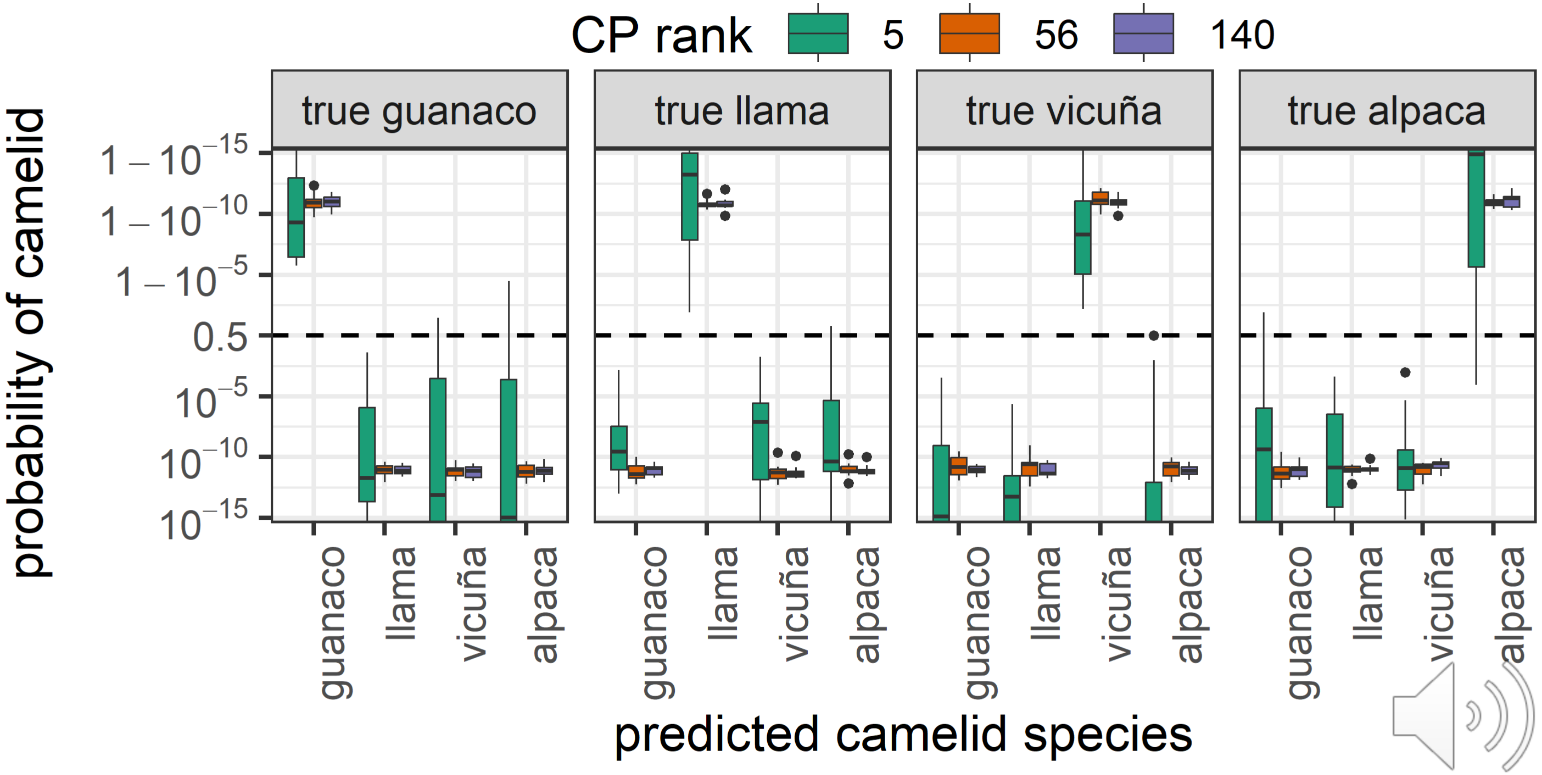
IMAGE CLASSIFICATION (PREDICTION): SIMULATED DATA

$$g\left(\mathbb{E}_{f_{\mathcal{X}}}\left(\mathcal{X}_i\right)\right) = \langle \mathcal{Y}_i | \mathcal{B} \rangle$$

Bernoulli distribution, logit link:

- 4 different camelid images
- 150 noisy samples of each

- $\mathcal{Y}_i$: 87 x 106 (*pixel height* x *width*)
- $\mathcal{X}_i$: 4 x 1 (*camelid* x *RGB channel*)
- $\mathcal{B}$: 87 x 106 x 4 x 1



Can accurately predict image classifications from noisy samples using GMLM with sufficiently high rank of parameter tensor.

POSITRON EMISSION TOMOGRAPHY RECONSTRUCTION

Poisson distribution, identity link:

- Poisson distribution for number of photon coincidences in sinogram
- Radon basis $\mathcal{K}$ is a 4D tensor with combined dimensions of Y and B
- Element-wise formulation (ML-EM) [1]:

$$y_{i_1 i_2} \overset{ind.}{\sim} \text{Poisson}(\langle B, K_{i_1 i_2} \rangle)$$

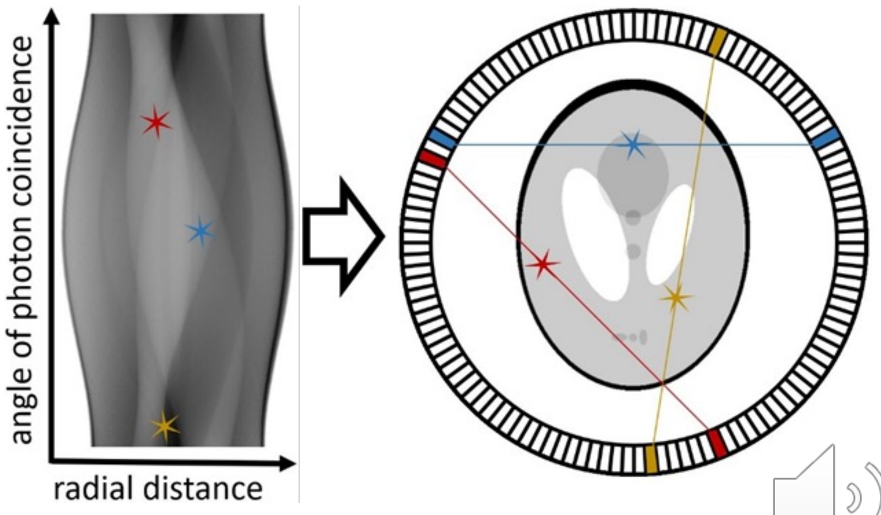
- Ill-posed without additional restrictions [2]
- Here $K_{i_1 i_2}$ is one matrix slice of $\mathcal{K}$
- **New: 4D PET model (volume across time):**

$$Y_{i_1, i_2} \overset{ind.}{\sim} \text{Poisson}(\langle K_{i_1, i_2} | \mathcal{B} \rangle)$$

$$Y \sim \text{Poisson}(\langle \overbrace{B|\mathcal{K}}^{\text{Radon transform of } B} \rangle)$$

Observed sinogram containing counts

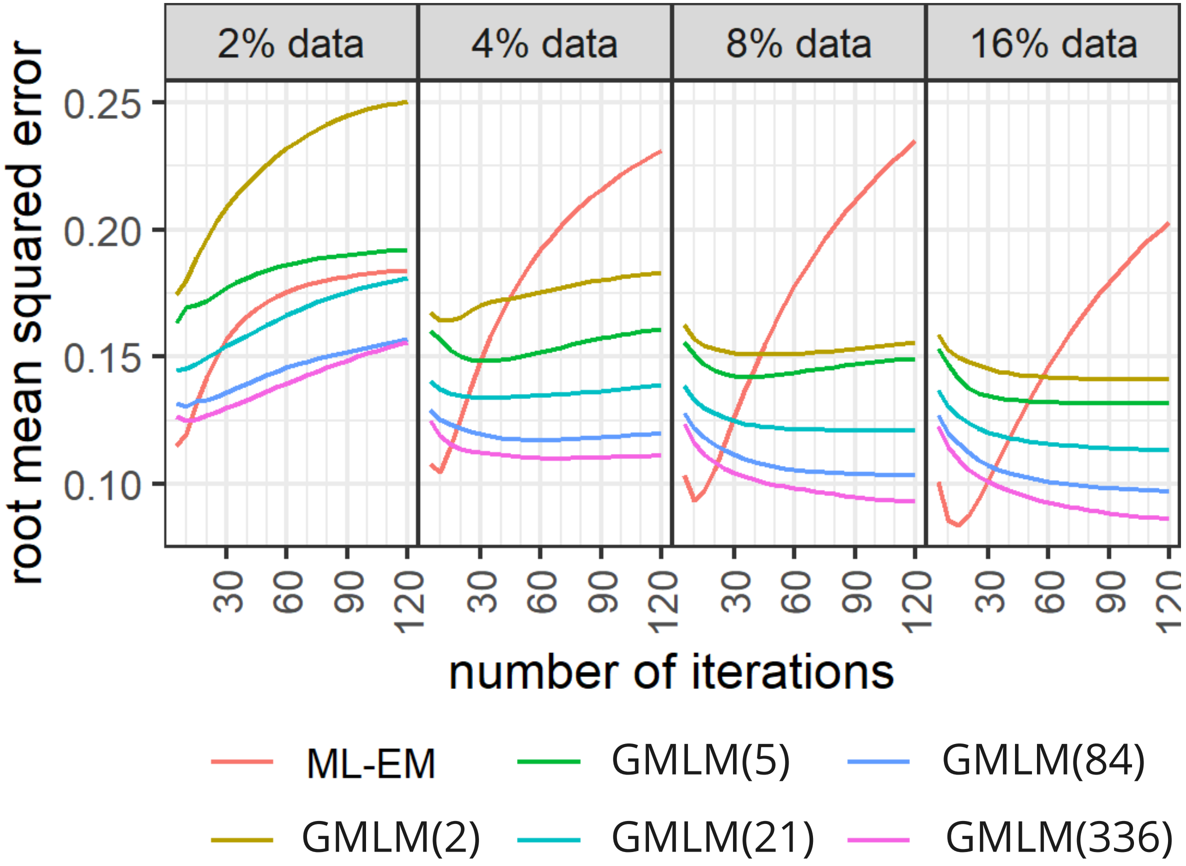
Image to reconstruct

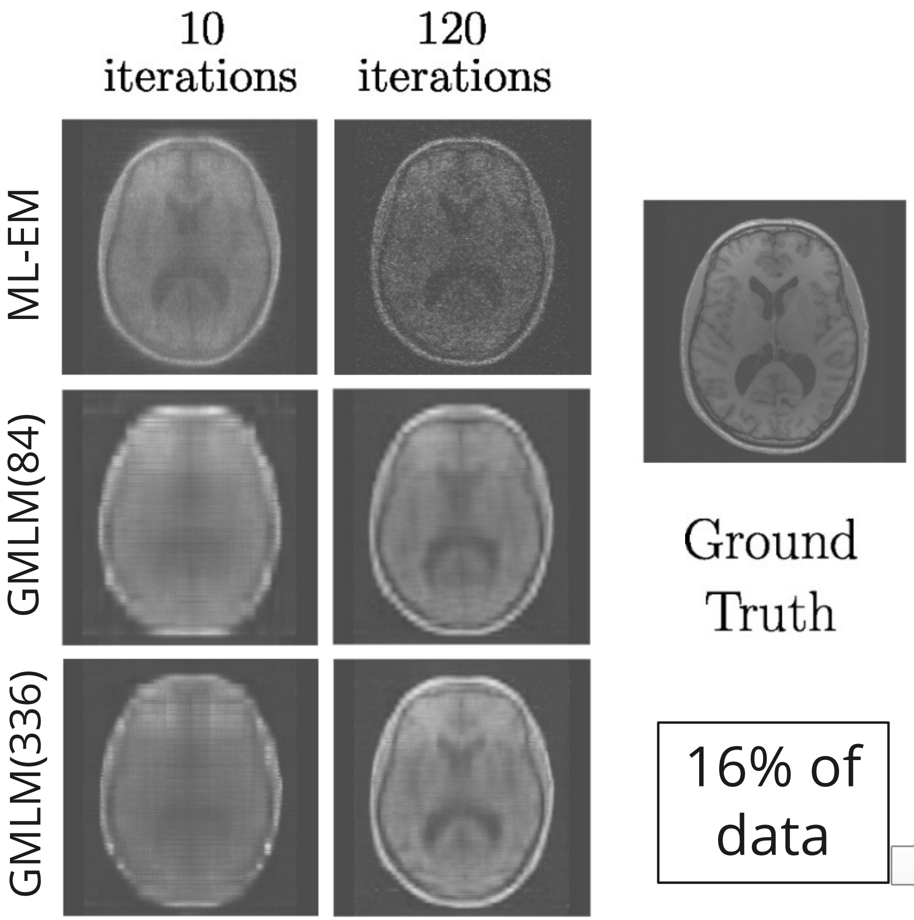


[1] Shepp & Vardi (1982); [2] Snyder, et al. (1987)

POSITRON EMISSION TOMOGRAPHY RECONSTRUCTION

- 4-way tensor data: four MRI measurements on the same subject and scanner *Hawco, et al. (2022)*
- 256 x 256 matrix slices → 256 x 1024 sinograms
- Parameters: ML-EM (no low-rank): ~ 63 million; GMLM: ~ 63 thousand (rank-84)





16% of data

TENSOR-VARIATE ANALYSIS OF VARIANCE (TANOVA)

TANOVA is a special case of ToTR ($\mathcal{X}_i$ are indicator tensors) that generalizes ANOVA

General Model	Definition	Special Case (Indicator $\mathcal{X}_i$)
Linear regression (LR)	$y_i \overset{indep.}{\sim} N(\langle \boldsymbol{x}_i \vert \boldsymbol{\beta} \rangle, \sigma^2)$	**ANOVA**
Multivariate LR	$\boldsymbol{y}_i \overset{indep.}{\sim} N(\langle \boldsymbol{x}_i \vert B \rangle, \Sigma)$	**MANOVA**
Tensor regression	$y_i \overset{indep.}{\sim} N(\langle \mathcal{X}_i \vert \mathcal{B} \rangle, \sigma^2)$	**Factorial designs**
Tensor-on-tensor regression	$\mathcal{Y}_i \overset{indep.}{\sim} N(\langle \mathcal{X}_i \vert \mathcal{B} \rangle, \Sigma_1, \ldots, \Sigma_p)$	**TANOVA**

$\mathcal{Y}_i \overset{ind.}{\sim} Poisson(\langle \mathcal{X}_i \vert \mathcal{B} \rangle)$ → **Poisson TANOVA**

Llosa & Maitra (2022)

PTANOVA AND CHANGE-POINT DETECTION

Poisson-tensor change-point detection

$\mathcal{Y}_t$ changes in mean at time τ_1

$$\mathcal{Y}_t \sim \left\{ \begin{array}{ll} \text{Poisson}(\mathcal{M}_1) & t = 1, \ldots, \tau_1 \\ \text{Poisson}(\mathcal{M}_2) & t = \tau_1 + 1, \ldots, n_T \end{array} \right\}$$

- Mean before change-point: $\mathcal{M}_1$
- Mean after change-point: $\mathcal{M}_2$
- Change-point location: τ_1

Equivalent PTANOVA formulation

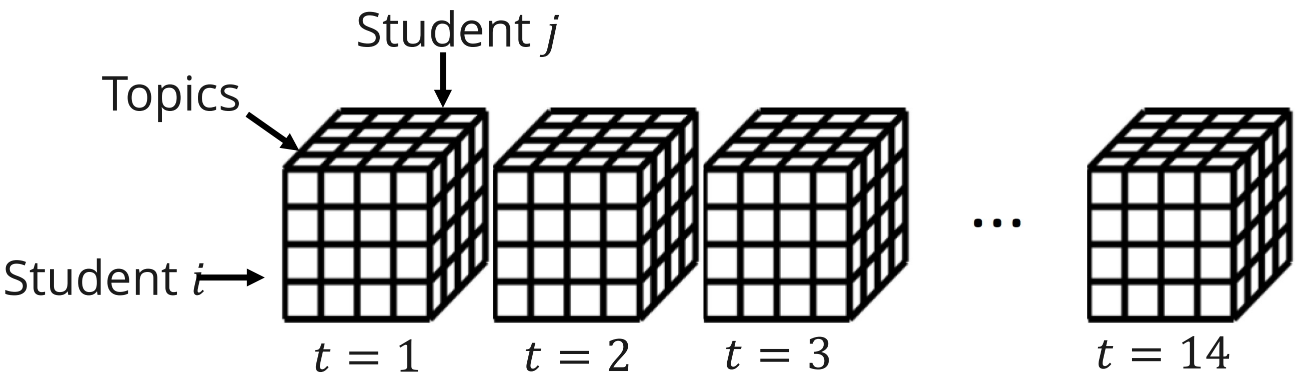
$$\mathcal{Y}_t \sim \text{Poisson}(\langle \boldsymbol{x}_t | \mathcal{B} \rangle)$$

$$\boldsymbol{x}_t = \left\{ \begin{array}{ll} (1,0)' & t = 1, \ldots, \tau_1 \\ (0,1)' & t = \tau_1 + 1, \ldots, n_T \end{array} \right\}$$

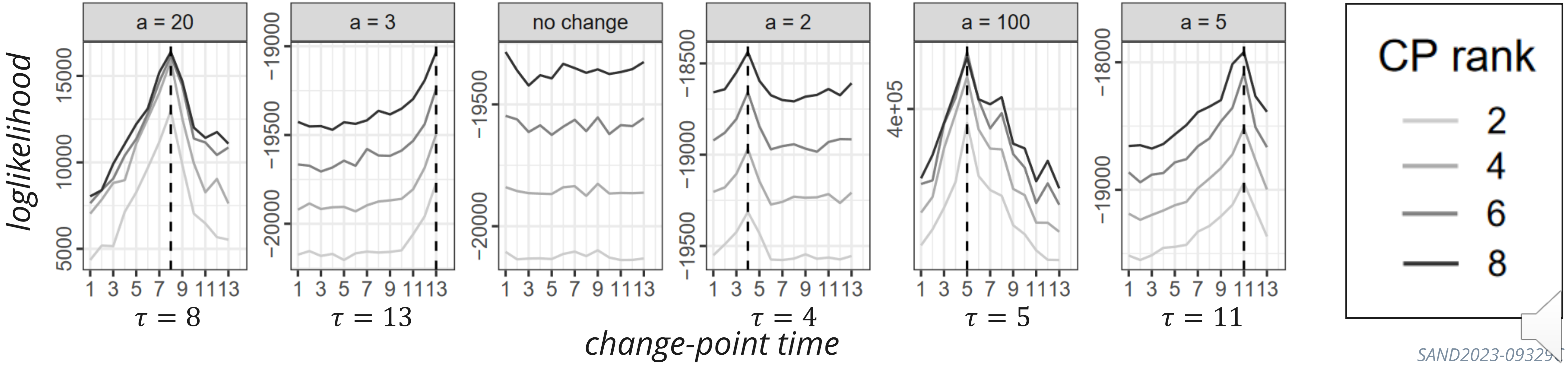
- Mean before change-point: $\langle (1,0)' | \mathcal{B} \rangle$
- Mean after change-point: $\langle (0,1)' | \mathcal{B} \rangle$
- Change-point location: τ_1

Originally solved using PToTR → Now we can perform parameter inference via GMLM

CHANGE-POINT DETECTION: SIMULATED DATA



- 10 Students talking about 15 topics over 14 time-steps: 14 count tensors of size 10 x 10 x 15.
- Event occurs at time τ that changes communication pattern:
  - All conversation generated independently from Poisson(λ), $\lambda = 5$.
  - One topic changes to Poisson($\lambda \times a$) after time τ, where $a = 1, 2, 3, 5, 20, 100$.



SUMMARY AND NEXT STEPS

- **GMLM: Generalized Multilinear Model for Tensor-on-Tensor Regression**
  - *Inference efficiency:* leverages low-rank decomposition of parameter tensor
  - *Well-posed model:* low-rank parameter tensor avoids need for regularization
  - *Reasonable computation:* leverages IRLS for alternating parameter inference subproblems

- **Future Directions**
  - *GMLM vs. GCP:* GMLM reduces to tensor decomposition with $\mathcal{X}_i = 1$
  - *Analysis of variance:* GMLM is equivalent to ANOVA with indicator $\mathcal{X}_i$
  - *Accelerating computation:* randomized IRLS
  - *Uncertainty quantification:* Fisher Information and Cramér-Rao lower bounds on variance
  - *Applications:* temporal prediction, change-point detection, imaging reconstruction

GMLM: GENERALIZED MULTILINEAR MODEL

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