

Density Separation with Tensor Factorization

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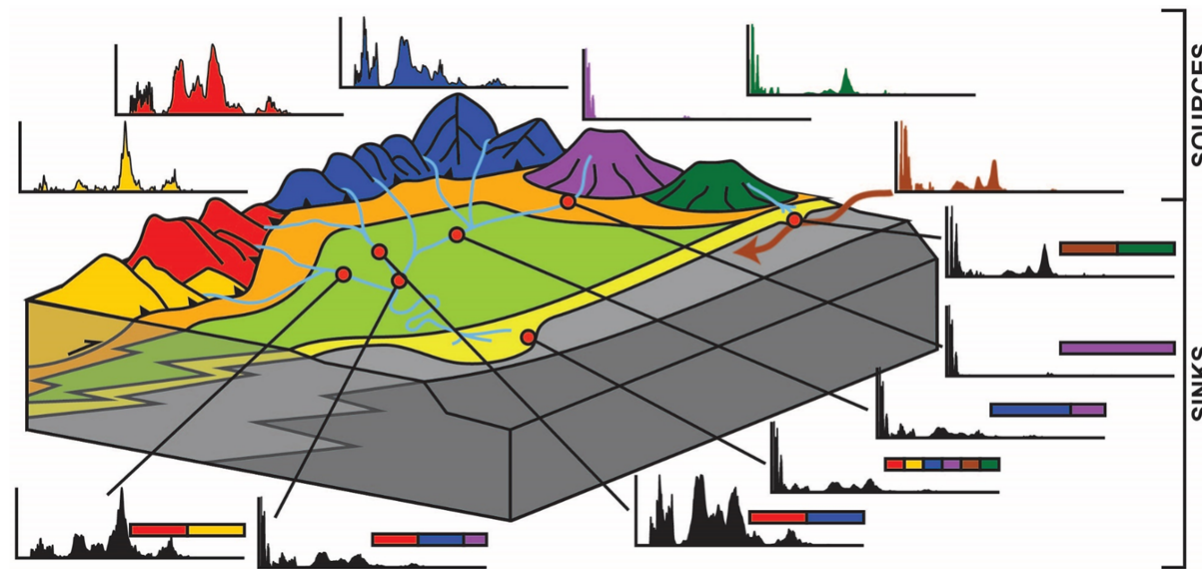
Talk Overview

- Motivation & Examples
- Generic Problem
- Solution Method
- Results

Motivation & Examples

Application 1: Geology¹

- Source locations have their own distribution of minerals
- Rocks from these sources are mixed & deposited downstream
- Take scoops of rocks at locations downstream, called “sinks”

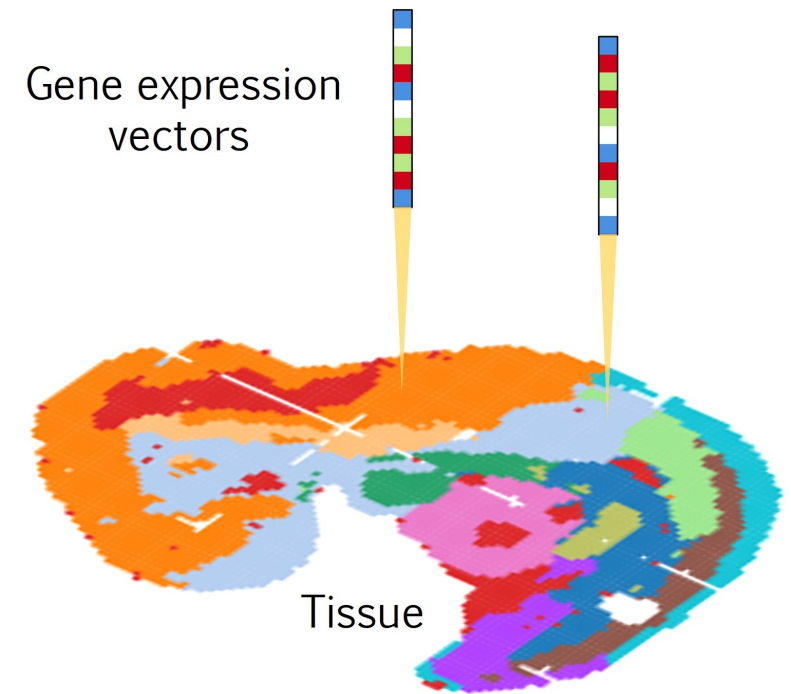


Modeling the Physical Problem

- Want to “un-mix” the measured sink distribution
- **Goal:** Estimate the mixing proportions and source distributions

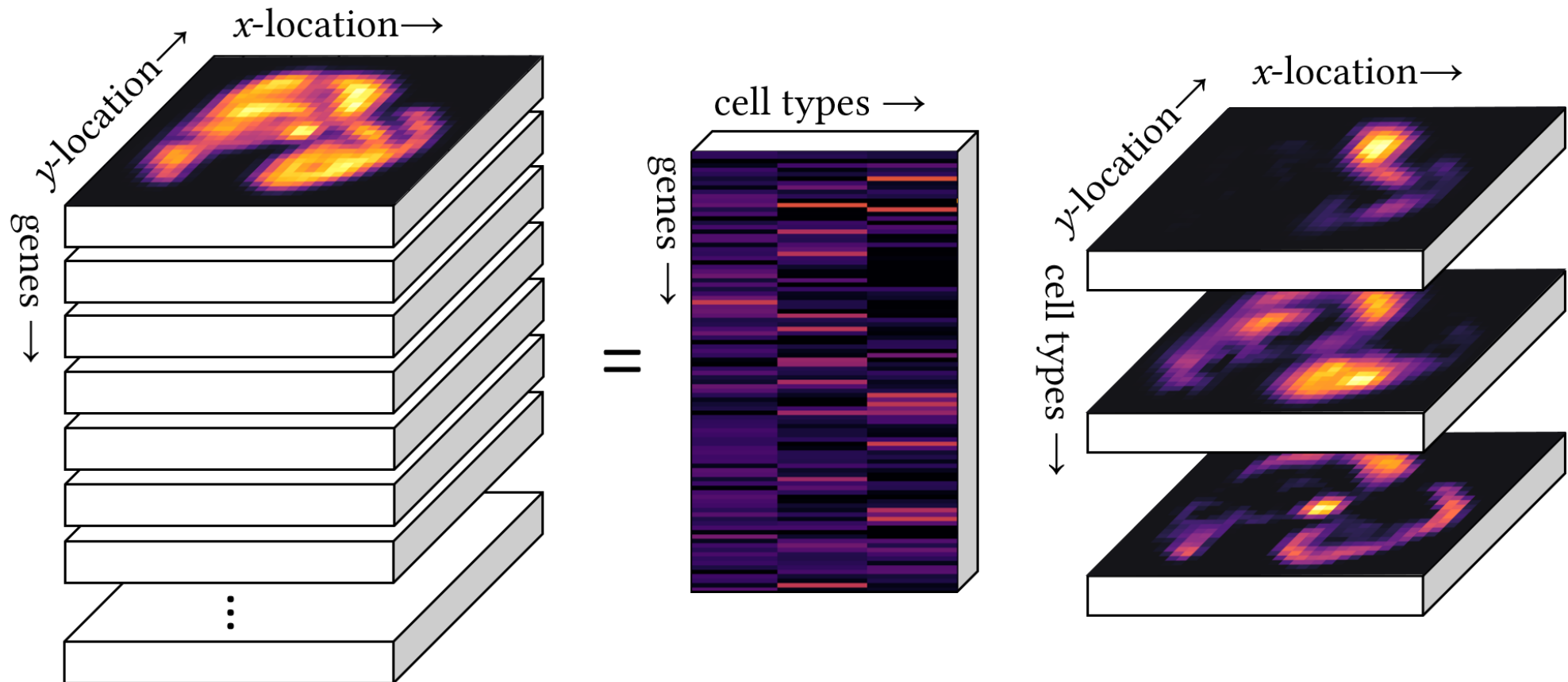
Application 2: Transcriptomics

- Perform single-cell sequencing for multiple embryos throughout development
- Label cells (heart, brain, etc.) at each time point
- **Goal:** Given gene expressions at each cell, cluster cells that have similar gene expressions



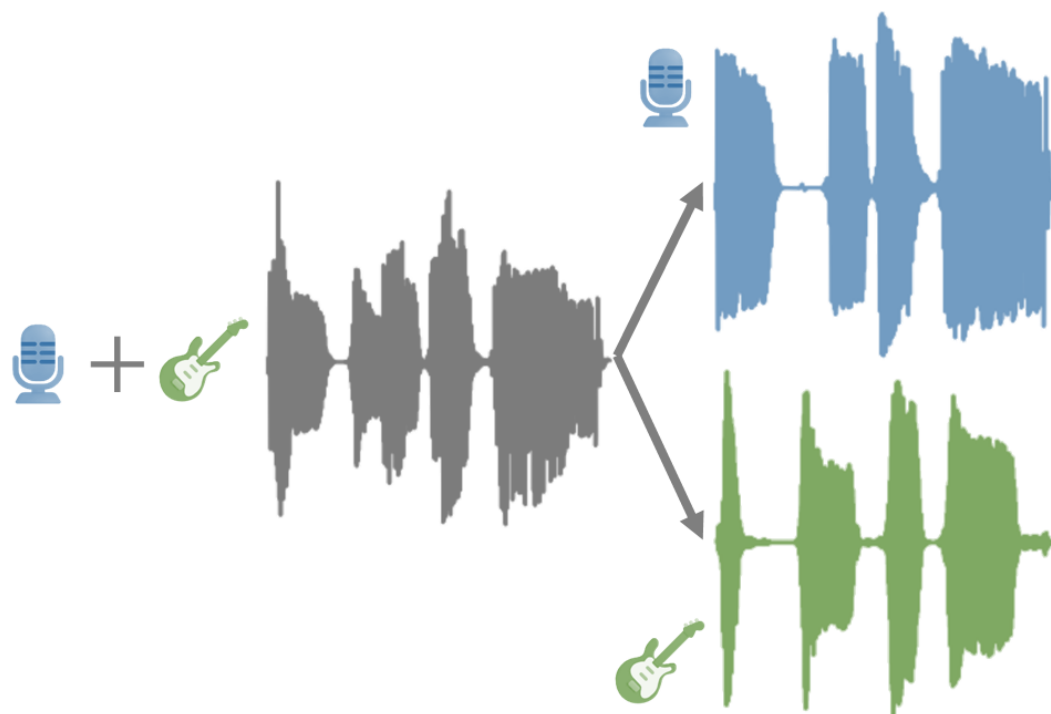
Modeling the problem

- **Goal:** Learn gene expressions and distribution of each cell type



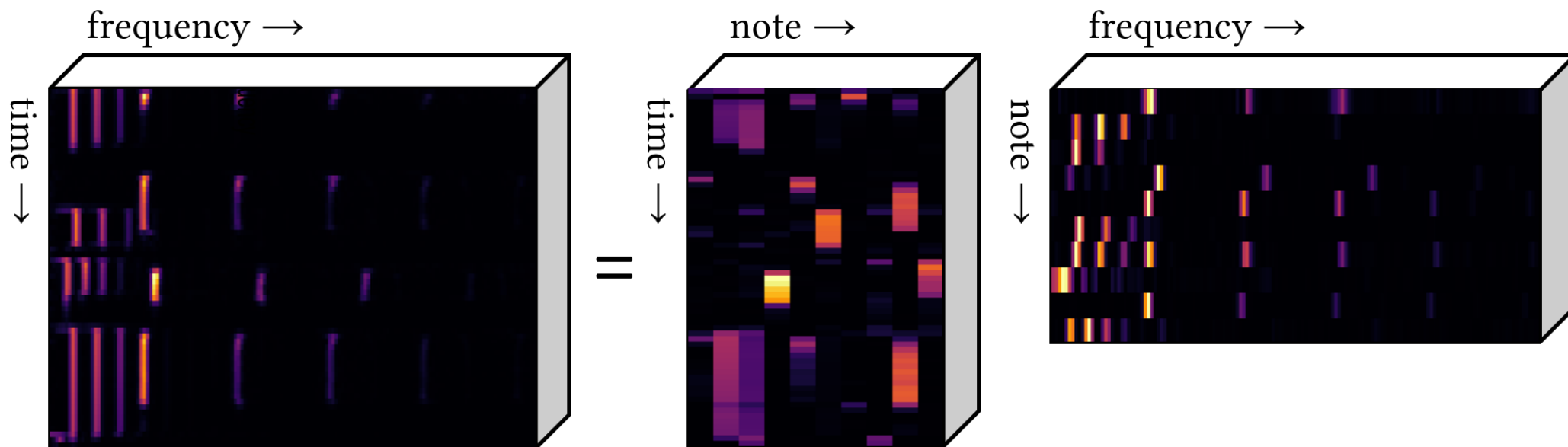
Application 3: Music Decomposition

- Rebalance or isolate instruments from a single recording
- Learn what each note sounds like (frequency spectrum)
- **Goal:** Separate audio mixture by frequency spectrums



Modeling Music Decomposition

- Take short-time Fourier transform of audio recording
- **Goal:** Learn the frequencies and amplitudes of each note



Generic Problem

Joint Signal Decomposition

- Given mixtures $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_I$
- Find mixing coefficients a_{ij} and sources $\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_R$

$$\mathbf{y}_1 = a_{11}\mathbf{b}_1 + a_{12}\mathbf{b}_2 + \dots + a_{1R}\mathbf{b}_R$$

$$\mathbf{y}_2 = a_{21}\mathbf{b}_1 + a_{22}\mathbf{b}_2 + \dots + a_{2R}\mathbf{b}_R$$

$$\vdots$$

$$\mathbf{y}_I = a_{I1}\mathbf{b}_1 + a_{I2}\mathbf{b}_2 + \dots + a_{IR}\mathbf{b}_R$$

Other Decomposition Approaches

Parametrised Basis

- Fixed basis: $y = \sum_{b \in \mathcal{B}} a_b b$
 - Fourier and short-time Fourier transform (Gröchenig 2001)
 - Wavelets (Benedetto and Frazier 1993; Daubechies et al. 2011)
 - Frame decomposition (Benedetto and Frazier 1993, Ch. 7)
 - Atomic decomposition (Chen et al. 2001; Fan et al. 2022)
 - Dictionary learning* (Tošić and Frossard 2011)
- Random basis: $y = \sum_r a_r b_r$ where $b_r \sim \mathcal{B}$
 - Random feature models $b_r(x) = f(\langle \omega_r, x \rangle + \phi_r)$, where $(\omega_r, \phi_r) \sim \Omega \times \Phi$ (Rahimi and Recht 2008; Hashemi et al. 2023)
 - Sparse random mode decomposition (Richardson et al. 2023)

Other Decomposition Approaches

Parametrised Basis

- Great if you know a *good* basis for your data!
 - Data becomes sparse in your basis
 - Basis elements having meaningful interpretations (e.g. Fourier frequencies)
- Otherwise, sources b_r may not be meaningful

Other Decomposition Approaches

Data-driven

- Intrinsic Mode Functions: $y = \sum_r b_r$ where $b_r(t) = a_r(t) \sin(\phi_r(t))$
 - Empirical mode decomposition ([Huang et al. 1998](#))
 - Empirical wavelet transform ([Gilles 2013](#))
 - Variational mode decomposition ([Dragomiretskiy and Zosso 2014](#))
- Supervised learning: learn parameters θ so that $F_\theta(\mathbf{y}) = (\mathbf{b}_r)_r$
 - Convolutional neural networks ([Zhu et al. 2019](#))
 - Long short-term memory networks ([Cao et al. 2019](#))
 - Autoencoders ([Karamatlı et al. 2019](#))
- Dictionary learning ([Tošić and Frossard 2011](#))

Other Decomposition Approaches

Data-driven

- Intrinsic Mode Functions
 - Effective for frequency-amplitude modulated sources b_r
- Supervised learning
 - ★ State-of-the-art ★
 - Need lots of data with known decompositions
 - Must retrain on data for each application

Joint Signal Decomposition

- Given mixtures $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_I$
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$$\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_I \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1R} \\ a_{21} & a_{22} & \dots & a_{2R} \\ \vdots & & & \vdots \\ a_{I1} & a_{I2} & \dots & a_{IR} \end{bmatrix} \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_R \end{bmatrix}$$

Joint Signal Decomposition

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Our approach

Matrix and Tensor Factorization

- Principle component analysis ([Pearson 1901](#); [Abdi and Williams 2010](#))
- Independent component analysis ([Comon 1994](#); [Hyvarinen 1999](#))
- Nonnegative matrix factorization ([Cohen and Rothblum 1993](#); [Gillis 2020](#))
- **Tensor decompositions** ([Kolda and Bader 2009](#))
- Why?
 - Interpretability
 - Minimal assumptions on sources b_r
 - No training step, so less data needed
 - *Unsupervised* learning

Tucker-1 Decomposition

- A generalization of rank- R matrix factorization
- $\mathbf{Y} = \mathbf{AB}$ • $Y_{ijk} = \sum_{r=1}^R A_{ir} B_{rjk}$ • $\mathbf{Y}_i = \sum_{r=1}^R A_{ir} \mathbf{B}_r$

Tucker-1 Decomposition

- A generalization of rank- R matrix factorization

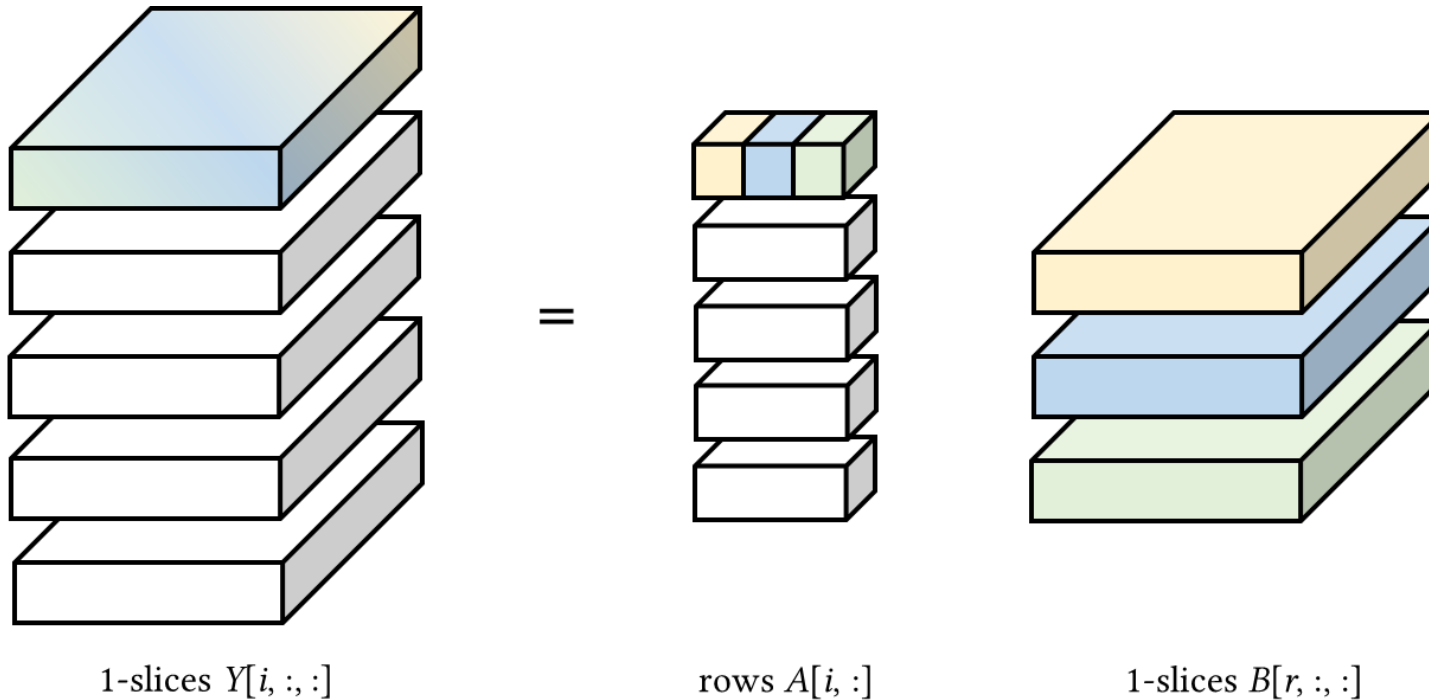
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Tucker-1 Decomposition

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- $\mathbf{Y}_i = \sum_{r=1}^R A_{ir} \mathbf{B}_r$



Properties of the model

Should be *low rank*

- Need more mixtures $\mathbf{y}_i$ than sources $\mathbf{b}_r$ ($I > R$)
- Otherwise, there's too many solutions for a_r and $\mathbf{b}_r$
- For example,

$$\mathbf{y} = a_1 \mathbf{b}_1 + a_2 \mathbf{b}_2 + \cdots + a_R \mathbf{b}_R$$

- has the unhelpful solution $a_1 = 1$ and $\mathbf{b}_1 = \mathbf{y}$, where the rest of the coefficients $a_r = 0$ for $r = 2, \dots, R$

Properties of the model

Should be *scaled*

- Need to scale coefficients a_{ir} or sources $\mathbf{b}_r$ (or both)
- Otherwise, decomposition is not unique and unbounded

- For example,

$$\mathbf{Y} = \mathbf{A}\mathbf{B} = (c\mathbf{A}) \left(\frac{1}{c}\mathbf{B}\right) = (\mathbf{A}\mathbf{C}) (\mathbf{C}^{-1}\mathbf{B})$$

- for all positive $c > 0$, or $R \times R$ invertible matrix $\mathbf{C}$
- Common scales include normalizing columns/rows of $\mathbf{A}$ or slices of $\mathbf{B}$

Solution Method

First, we need our densities y_i

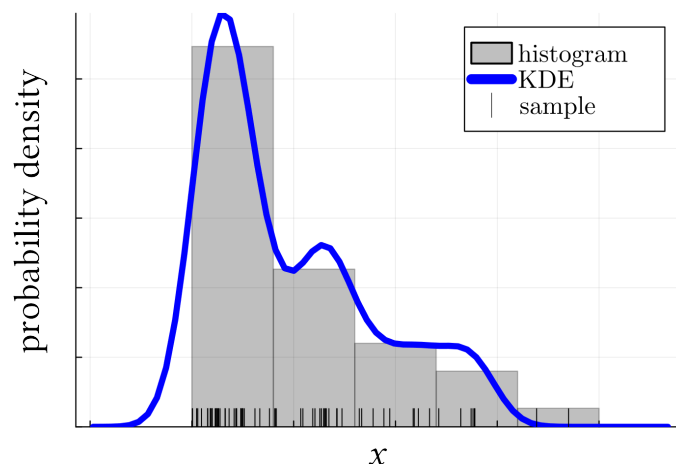
- Often cannot measure our mixture densities y_i directly
- Typical problem:
 - given i.i.d. samples $s_i^n \sim \mathcal{Y}_i$ for $n = 1, \dots, N_i$
 - each distribution $\mathcal{Y}_i$ is a convex mixture of the (the same) source distributions $\mathcal{B}_R$: $\mathcal{Y}_i = a_{i1}\mathcal{B}_1 + \dots + a_{iR}\mathcal{B}_R$
 - estimate mixing coefficients a_{ir} and probability density functions b_r for the distributions $\mathcal{B}_R$
- In other words, “ $\mathbb{P}(s \sim \mathcal{B}_r | s \sim \mathcal{Y}_i) = a_{ir}$ ”

Density Estimation from samples

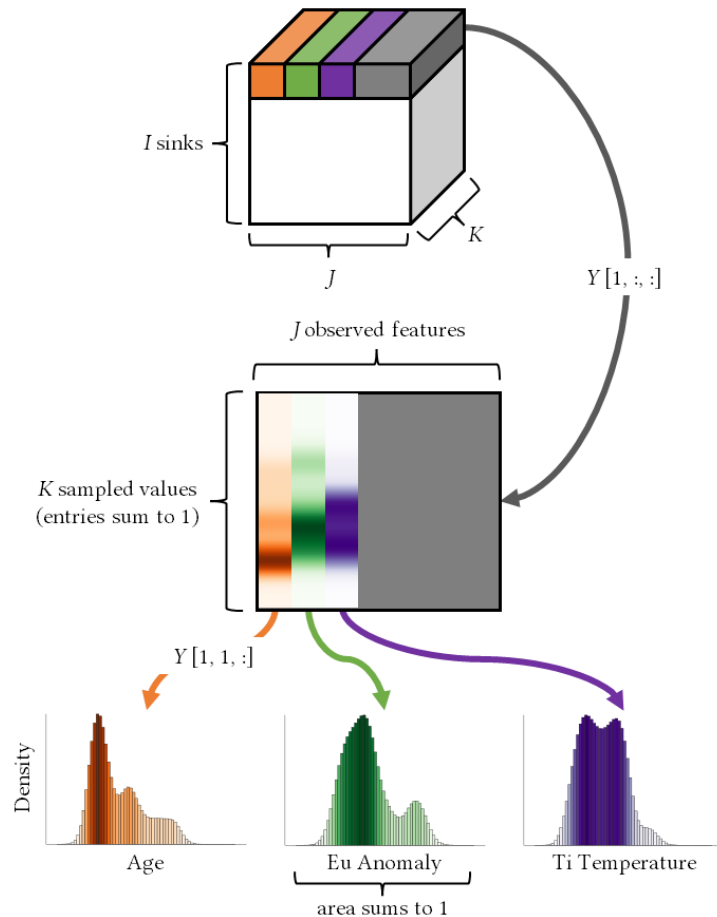
- *if* we knew what the sources look like...
- ...parametrize sources and optimize parameters with
 - expectation maximization (Dempster et al. 1977)
 - method of moments (Pearson 1936)
 - e.g, Gaussian mixture models (Lindsay and Basak 1993)
- *otherwise* we need a nonparametric estimation

Density Estimation from samples

- Kernel density estimation ([Rosenblatt 1956](#); [Parzen 1962](#))
- $y(x) = \frac{1}{N_i} \sum_{n=1}^{N_i} k\left(\frac{x-s^n}{h}\right)$ is the KDE from samples s^n
- k is the *kernel* and h is the *bandwidth*



Higher Order KDE & Tensors

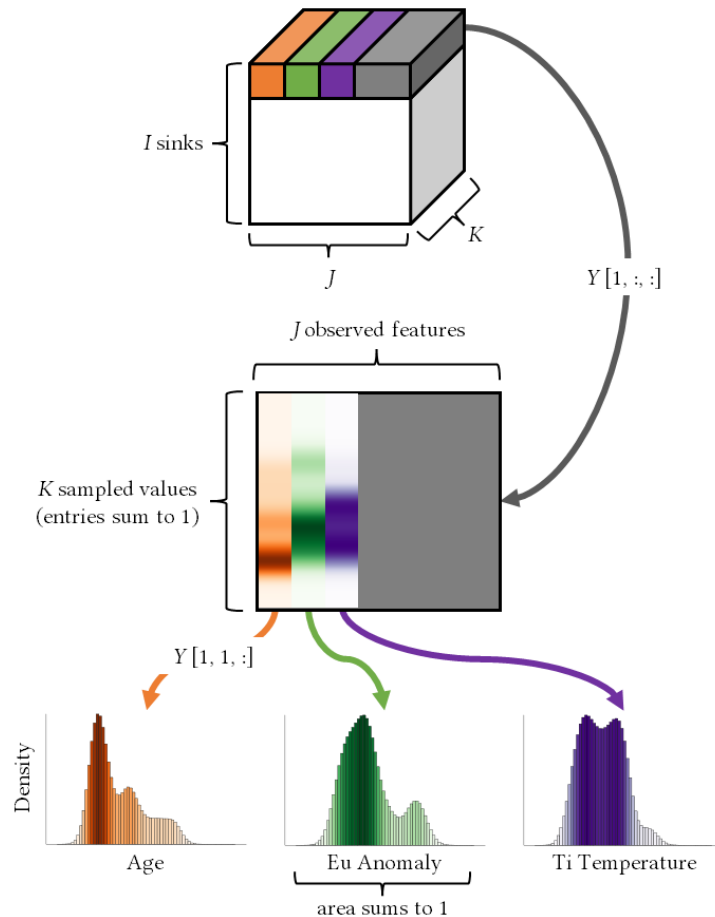


- If *independent* features
 - store discretized 1-dim KDEs for each sink i and feature j in $\mathbf{Y}_{ij}$:
- Doing it this way, reduces the size of the data
 - J -dim KDEs¹ (I of them) is more expensive to compute than IJ cheaper 1-dim KDEs
 - IK^J to IJK tensor entries

Higher Order KDE & Tensors

Contributions / advancements

- Perform this source separation on all features jointly
- Model that scales well to arbitrary number of features J
- Size of problem is independent of number of samples collected



Source separation model

$$\min_{\mathbf{A}, \mathbf{B}} \left\{ \ell(\mathbf{A}, \mathbf{B}) := \frac{1}{2} \|\mathbf{Y} - \mathbf{AB}\|_F^2 \mid \mathbf{A} \in \Delta_{\mathbf{A}}, \mathbf{B} \in \Delta_{\mathbf{B}} \right\}$$

$\|\cdot\|_F^2$ squared Frobenius norm (sum-of-squares)

$\Delta_{\mathbf{A}}$ non-negative entries & rows sum to 1

$\Delta_{\mathbf{B}}$ non-negative entries & fibres $\mathbf{B}_{ij}$: sum to 1

- Nonnegativity implies it's NP hard¹ 😞
- Simplex implies a bounded feasible set 😊
- Not convex, but *block*-convex and smooth

Block Coordinate Descent

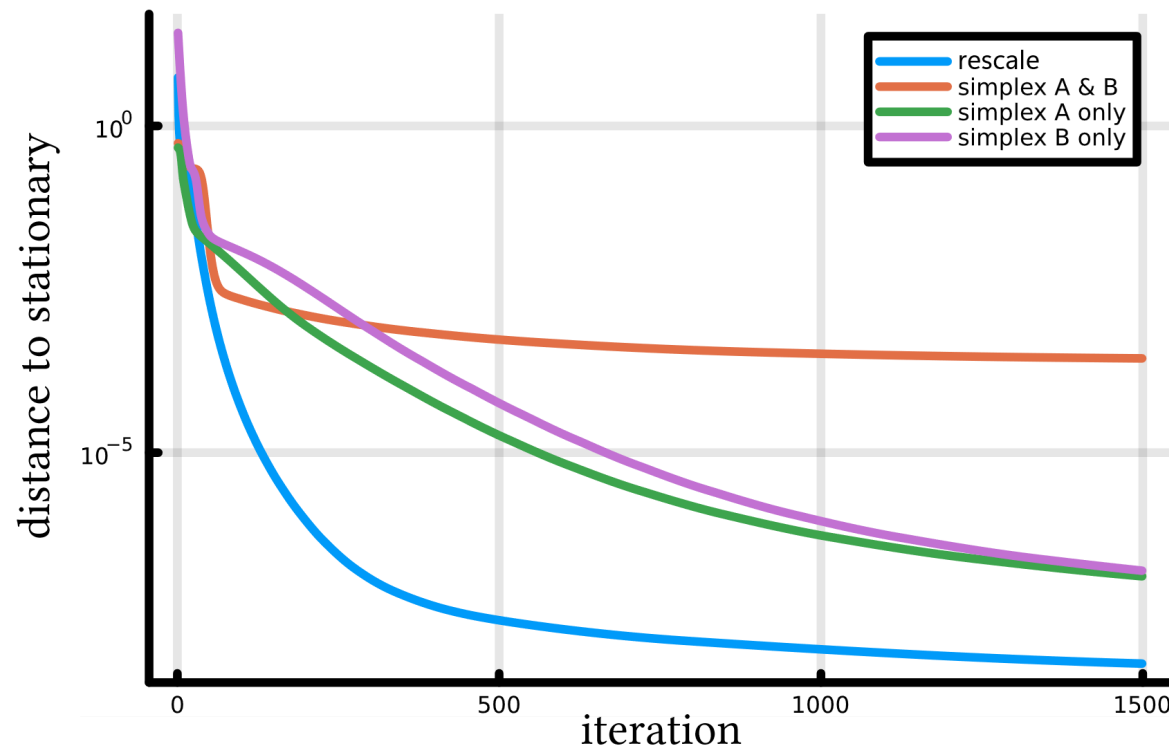
- Alternately update $\mathbf{A}$ and $\mathbf{B}$ via projected gradient descent¹
 - $\mathbf{A}^{t+1} = P_{\Delta_{\mathbf{A}}}(\mathbf{A}^t - \frac{1}{L_{\mathbf{A}}} \nabla_{\mathbf{A}} \ell(\mathbf{A}^t, \mathbf{B}^t))$
 - $\mathbf{B}^{t+1} = P_{\Delta_{\mathbf{B}}}(\mathbf{B}^t - \frac{1}{L_{\mathbf{B}}} \nabla_{\mathbf{B}} \ell(\mathbf{A}^{t+1}, \mathbf{B}^t))$
- Convergence to nash equilibria $(\mathbf{A}^*, \mathbf{B}^*)$
 - *block-wise* min: $\ell(\mathbf{A}^*, \mathbf{B}^*) \leq \min(\ell(\mathbf{A}^*, \mathbf{B}), \ell(\mathbf{A}, \mathbf{B}^*))$
- Also stationary: $0 \in \partial(\ell + \delta_{\Delta_{\mathbf{A}} \times \Delta_{\mathbf{B}}})(\mathbf{A}^*, \mathbf{B}^*)$

Rescaling trick

- Relax constraints to
 - $\mathbf{A} \geq 0, \mathbf{B} \geq 0$
 - $\frac{1}{J} \sum_{jk} B_{rjk} = 1$ for all r (vs $\sum_k B_{rjk} = 1$ for all r, j)
- Updates now look like:
 - $\mathbf{A}^{t+1/2} = (\mathbf{A}^t - \frac{1}{L_A} \nabla_{\mathbf{A}} \ell(\mathbf{A}^t, \mathbf{B}^t))_+$
 - $\mathbf{B}^{t+1/2} = (\mathbf{B}^t - \frac{1}{L_B} \nabla_{\mathbf{B}} \ell(\mathbf{A}^{t+1/2}, \mathbf{B}^t))_+$
 - $\mathbf{B}^{t+1} = \mathbf{C}^{-1} \mathbf{B}^{t+1/2}$ and $\mathbf{A}^{t+1} = \mathbf{A}^{t+1/2} \mathbf{C}$
 - where $C_{rr} = \frac{1}{J} \sum_{jk} B_{rjk}$

Rescaling vs simplex projection

- Compare stationary condition $\text{dist}(0, \partial(\ell + \delta_{\geq 0})(\mathbf{A}, \mathbf{B}))$ every iteration for different constraint methods

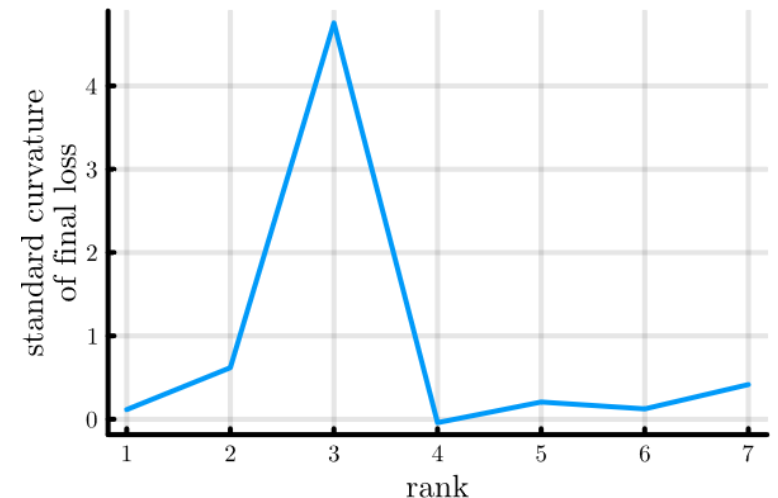
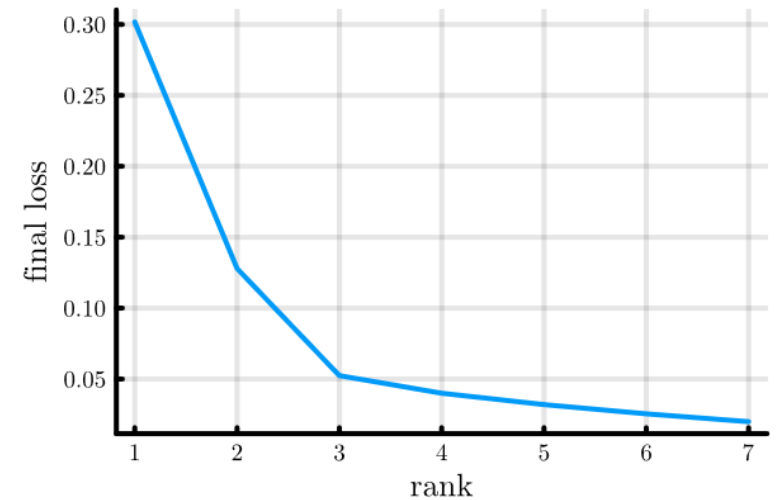


Estimating the rank

- Try many ranks $R = 1, \dots, R_{\max}$
- Compare the objective as a function of the rank

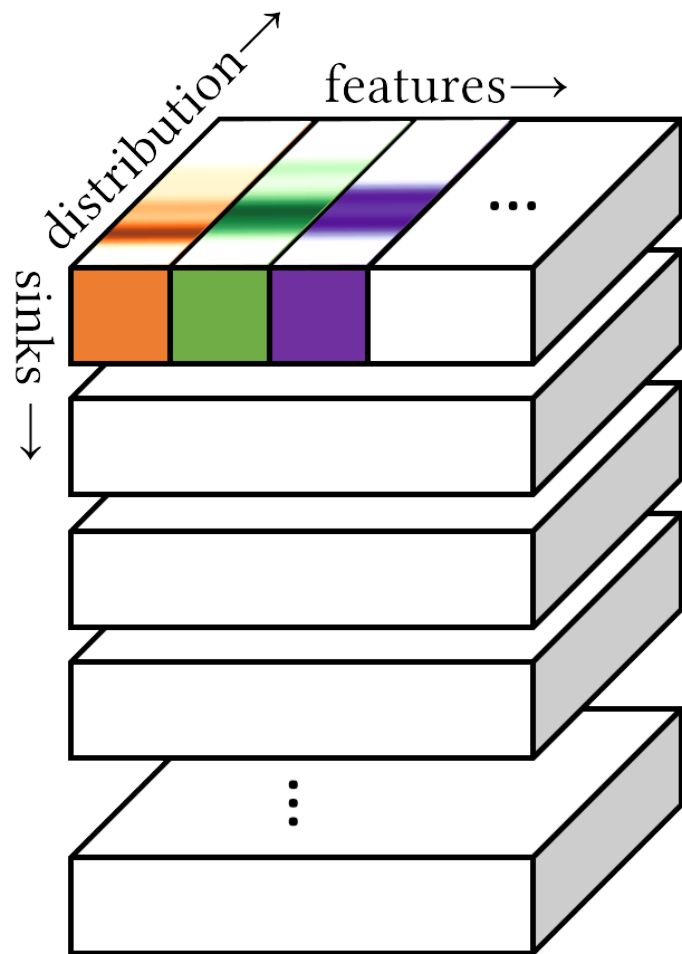
$$\ell(R) = \|\mathbf{Y} - \mathbf{A}_R \mathbf{B}_R\|_F^2$$

- *Occam's Razor*: Trade off between simple model (low rank R) and explanatory power (larger R)
- Select point of maximum curvature
 $\arg \max_R \ell''(R) / (1 + \ell'(R)^2)^{1.5}$

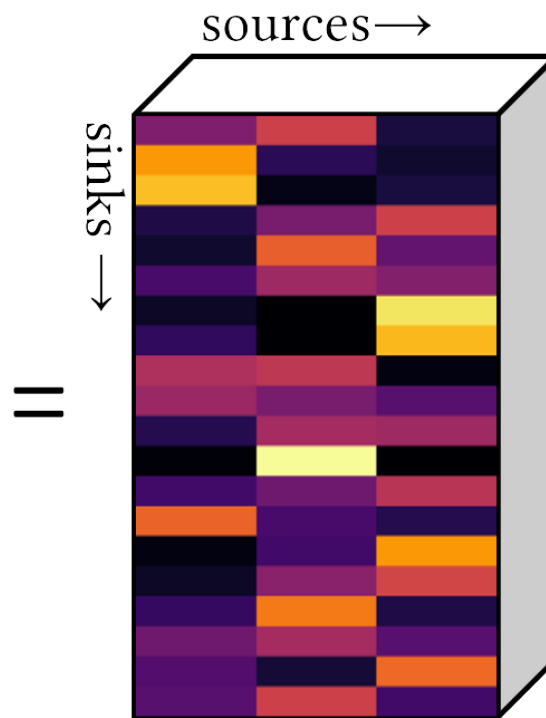


Results

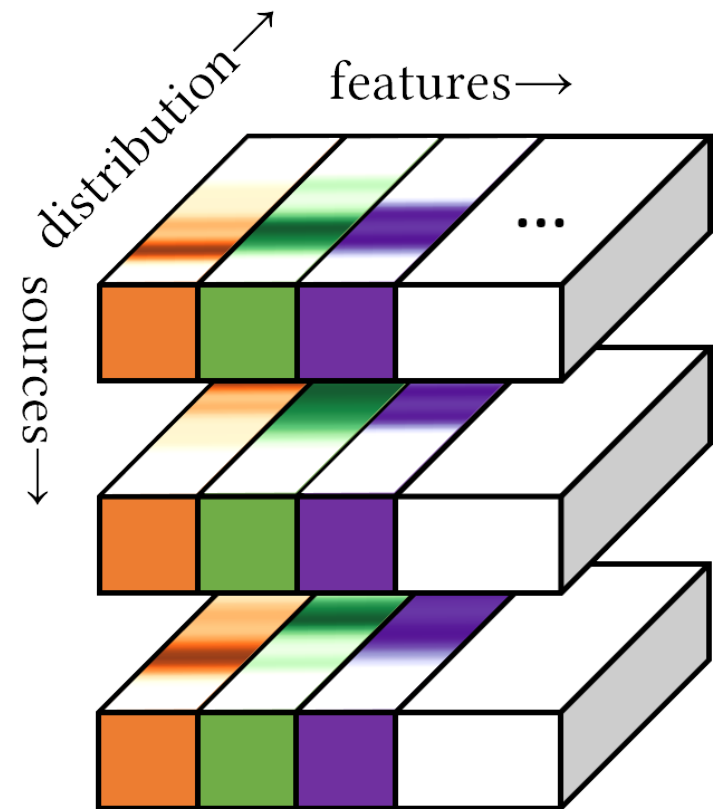
Application 1: Geology



measured distributions

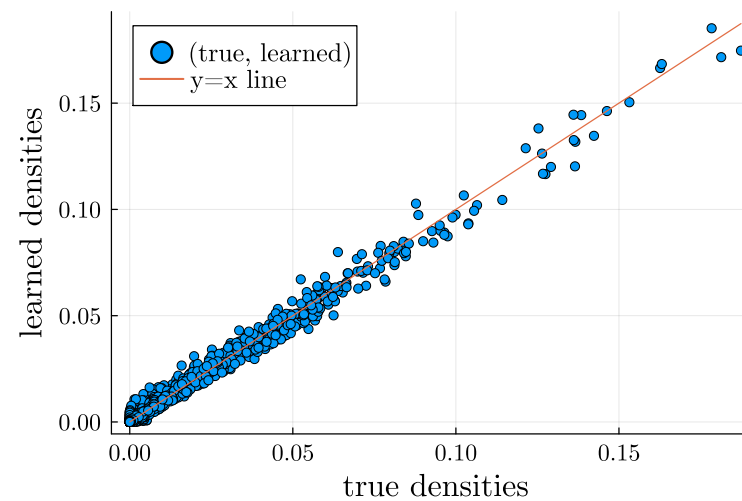
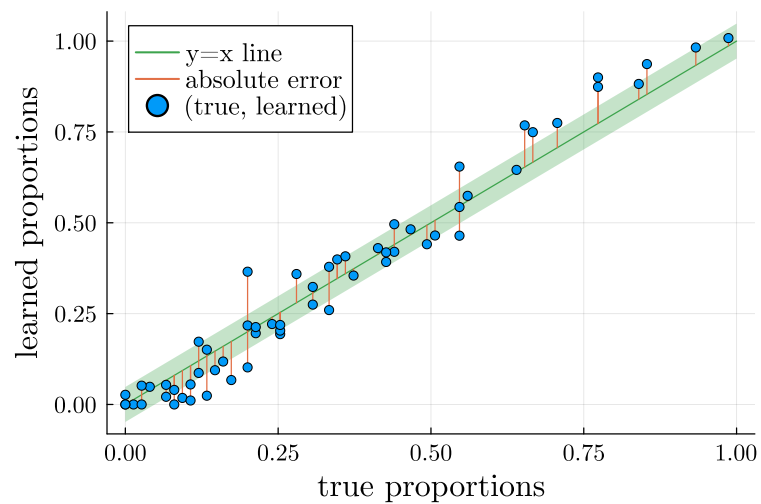


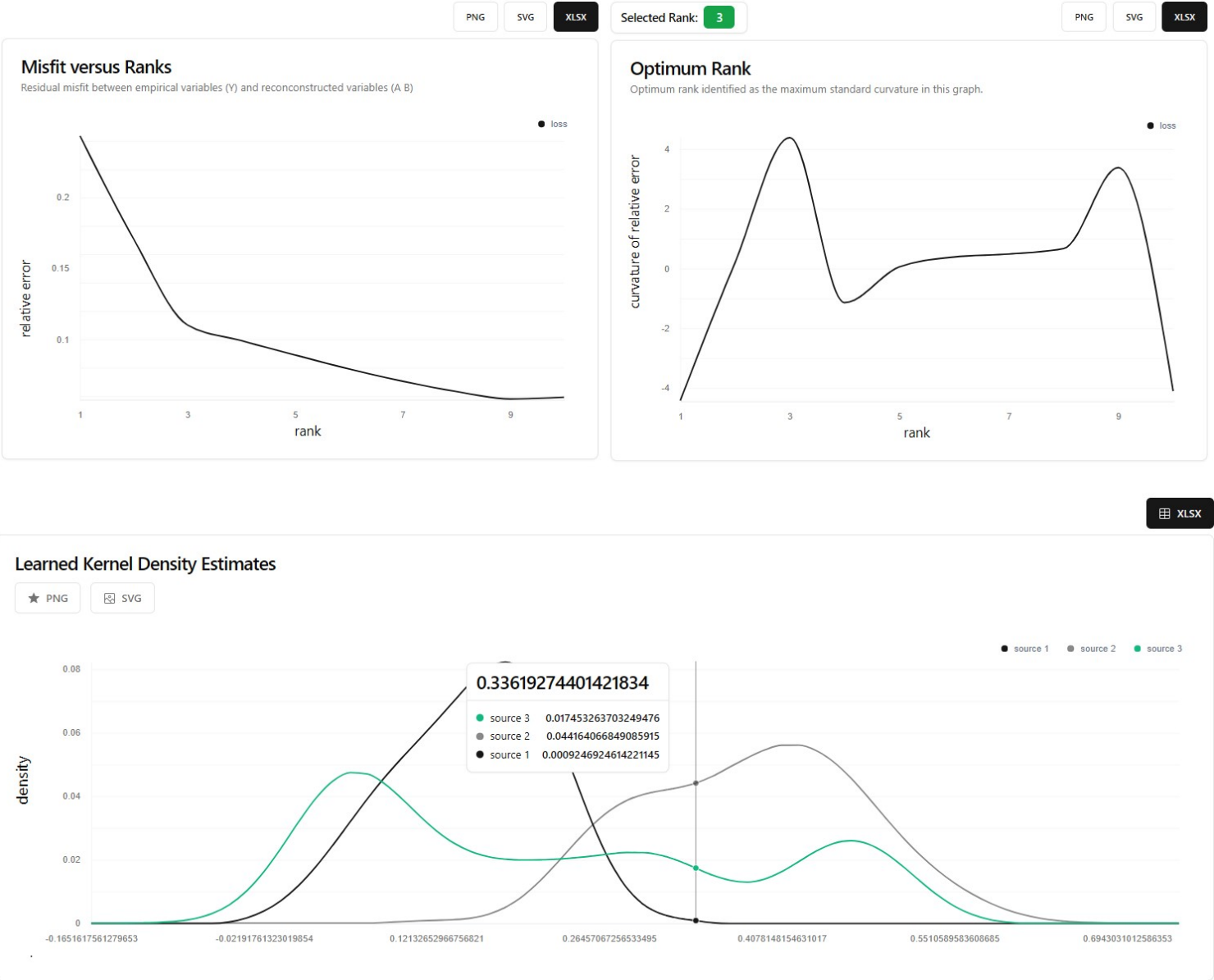
mixing proportions



source distributions

Application 1: Geology



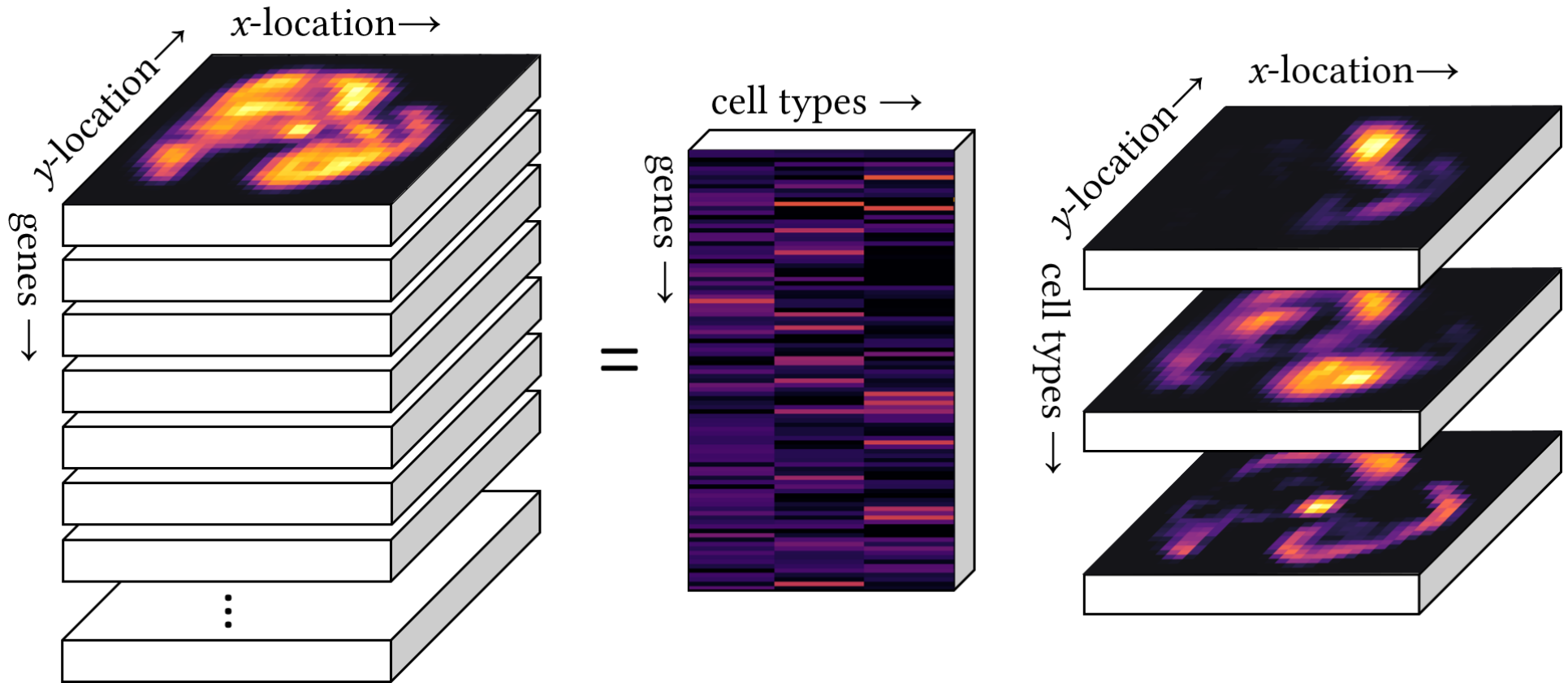


Density Separation with Tensor Factorization

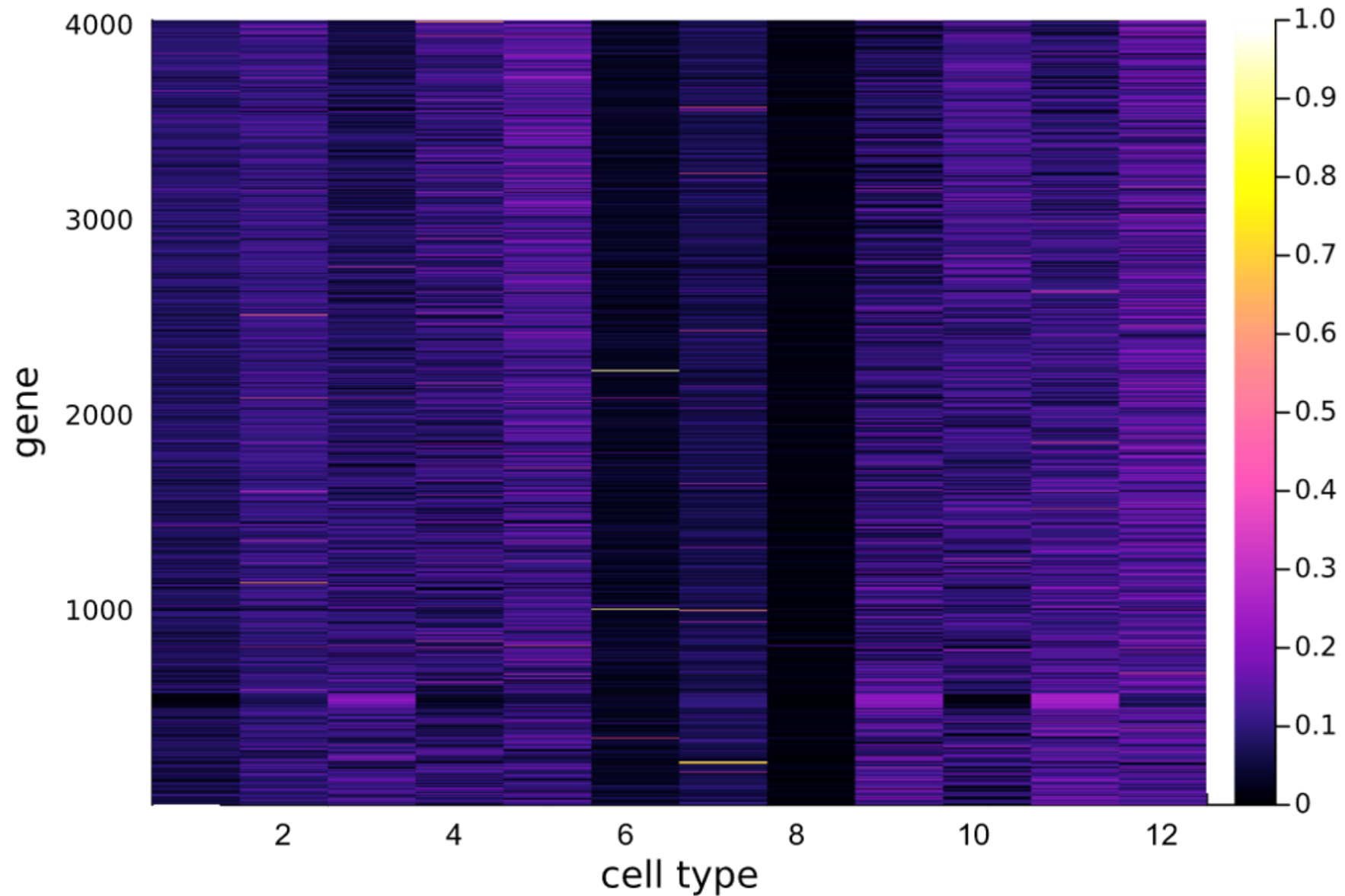
Application 2: Transcriptomics

- constraint modification: horizontal slices are normalized

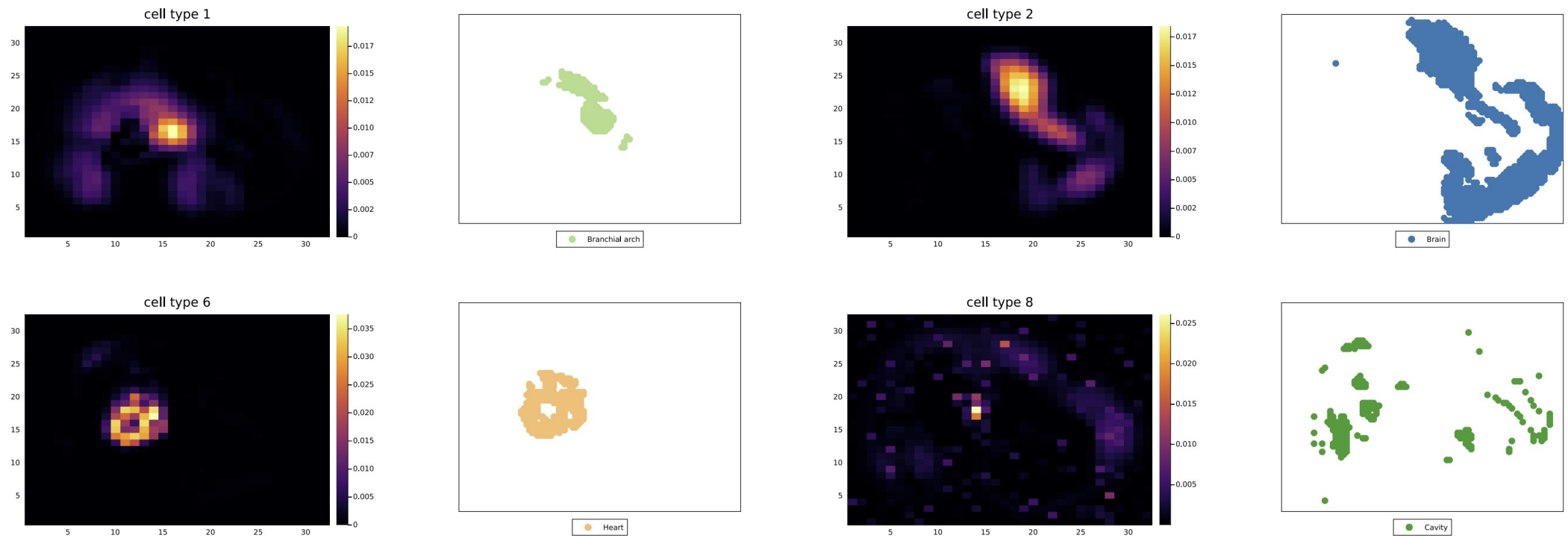
$$\sum_{j,k} B_{r,j,k} = 1 \quad \forall r$$



Application 2: Transcriptomics



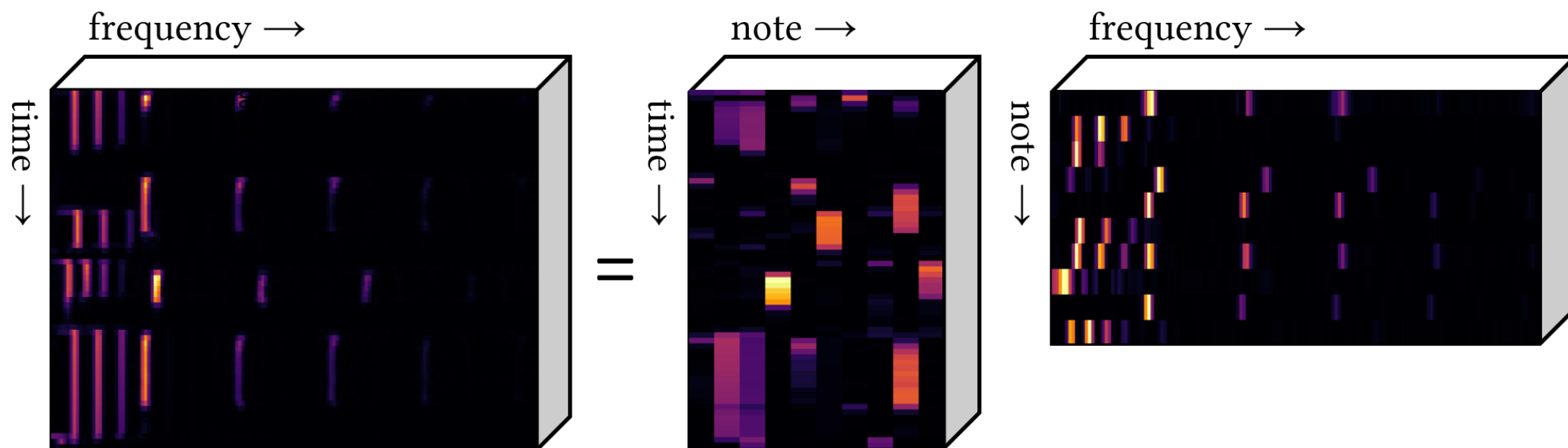
Application 2: Transcriptomics



Application 3: Music Decomposition

- constraint modification: horizontal slices are max-normalized

$$\max_j B_{r,j} = 1 \quad \forall r$$



Summary

- Combine KDE with Tucker-1 factorization into a scalable **nonparametric density decomposition** method
- **Algorithm converges** to block-minimum and stationary point
 - Open-source Julia code on GitHub: `MatrixTensorFactor.jl`
- **Practical model** applicable to many areas
 - geology, genetics, music, etc.
- Expanding code for **more decompositions**, **faster convergence** along cts. dimensions



Paper & Code

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Additional Slides

What features did we look at?

- age
- Eu anomaly
- Ti-based crystallization temperature
- Th-U ratio
- sum of light rare-earth elements over heavy rare-earth elements ($\Sigma\text{LREE}/\Sigma\text{HREE}$)
- Dy-Yb ratio
- normalized (Ce/ND)/Y ratio

Convergence Details

- when iterates are bounded
 - there are limit points
 - know this because feasible set is bounded
- when the objective function is KL
 - sequence of iterates converges to a finite limit point

How should we format our data?

Example

- When you sample $s \sim \mathcal{Y}$, do the following
 - Sample r where $r = 1$ with probability a_1 , and $r = 2$ with probability $a_2 = 1 - a_1$
 - Draw a sample from distribution $\mathcal{B}_r$
- The distribution of s is the same as $a_1\mathcal{B}_1 + a_1\mathcal{B}_2$
- So the density function y for distribution $\mathcal{Y}$ is equal to $y = a_1b_1 + a_2b_2$

Rank robustness

