Tucker-1 Demixing Model

Under the Hood of Our Density Separation

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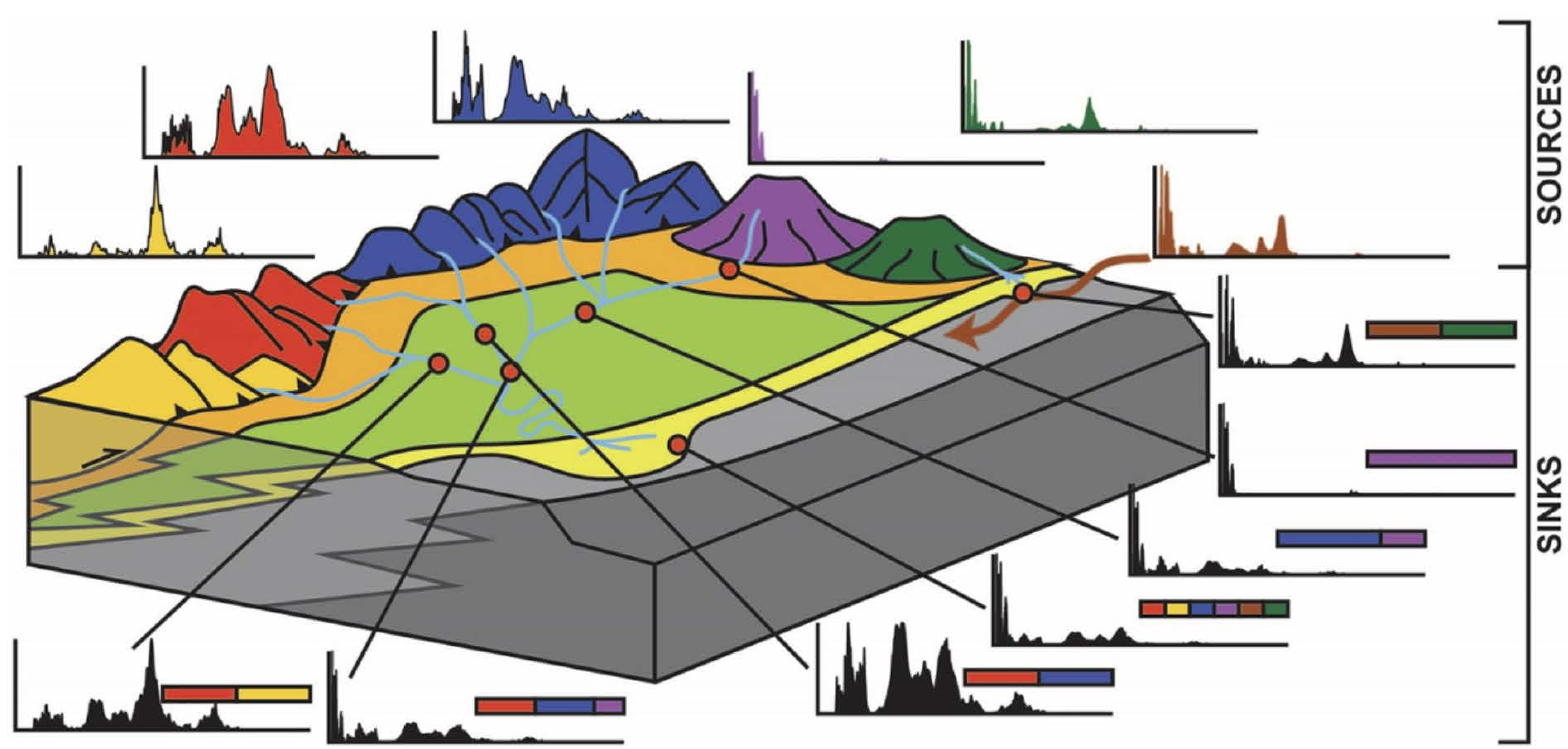
Overview

- How we frame the problem
- The model and data pipeline
- Solution and implementation
- Most of this is taken from our paper [Graham *et al.* 2025]

Physical Problem

- Source locations have their own distribution of minerals
- Rocks from these sources are mixed & deposited downstream
- Take scoops of rocks at locations downstream (sinks)
- **Goal**: Learn source distributions from the sink measurements



Framing the demixing problem

- Notation: use regular letters for scalars $a, b, \ldots$
- bold lowercase for vectors $\mathbf{a}, \mathbf{b}, \ldots$
- bold upper case for matrices/tensors $\mathbf{A}, \mathbf{B}, \ldots$

Unmix sinks $\mathbf{Y}_i$ into a small number of unknown sources $\mathbf{B}_r$ with unknown weights a_{ir}:

$$\begin{aligned}
\mathbf{Y}_1 &= a_{11}\mathbf{B}_1 + a_{12}\mathbf{B}_2 + \cdots + a_{1R}\mathbf{B}_R \\
&\vdots \\
\mathbf{Y}_I &= a_{I1}\mathbf{B}_1 + a_{I2}\mathbf{B}_2 + \cdots + a_{IR}\mathbf{B}_R
\end{aligned}$$

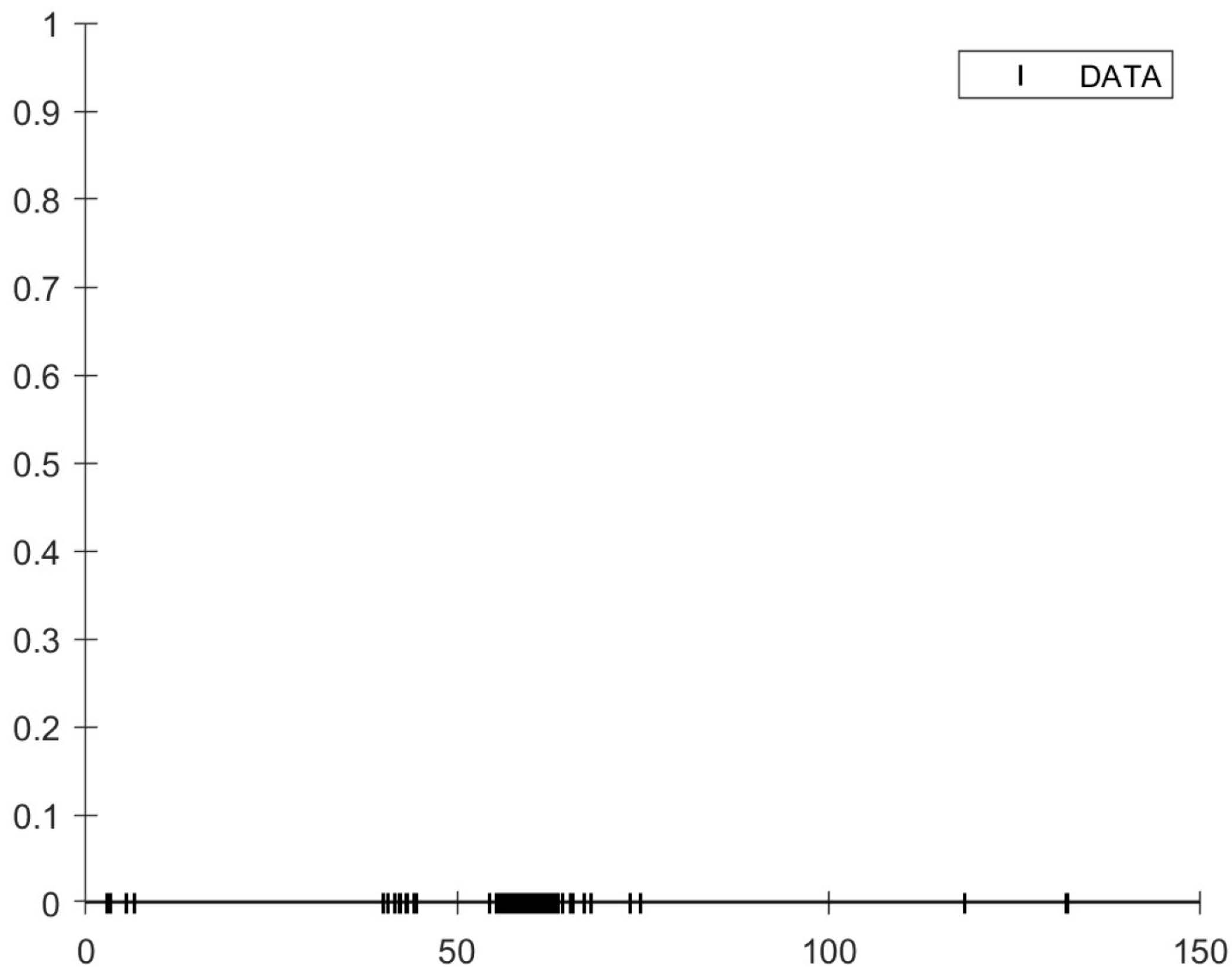
From rocks to densities $\mathbf{Y}_i$

- Sample grains of rock from many sinks
- Each grain belongs to some source
- Want to estimate the sink distributions

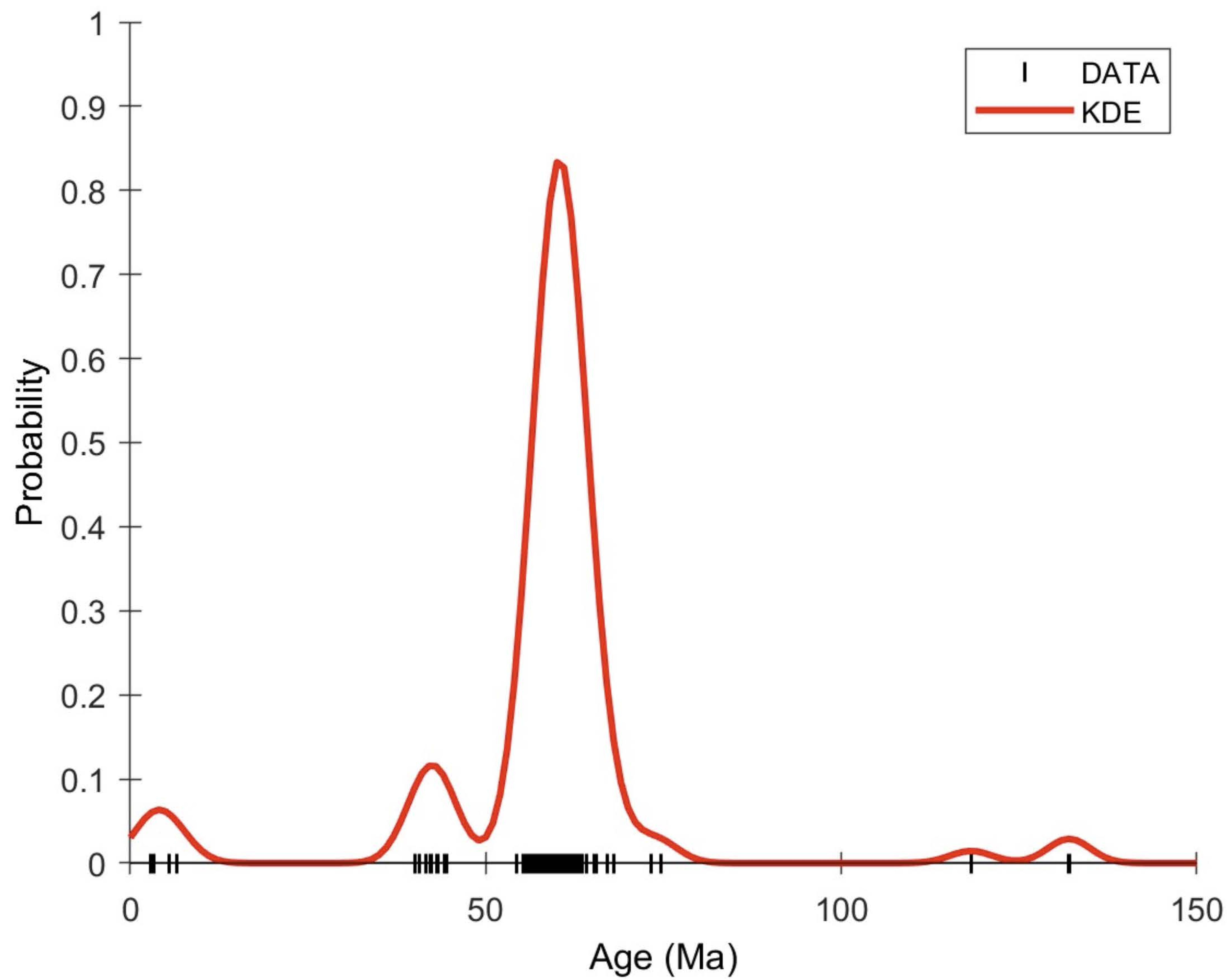
ages (MY)	**2se**	**...**
132.13	4.80	
41.53	2.98	
63.00	8.07	
43.15	2.65	
59.37	4.16	

$\vdots$

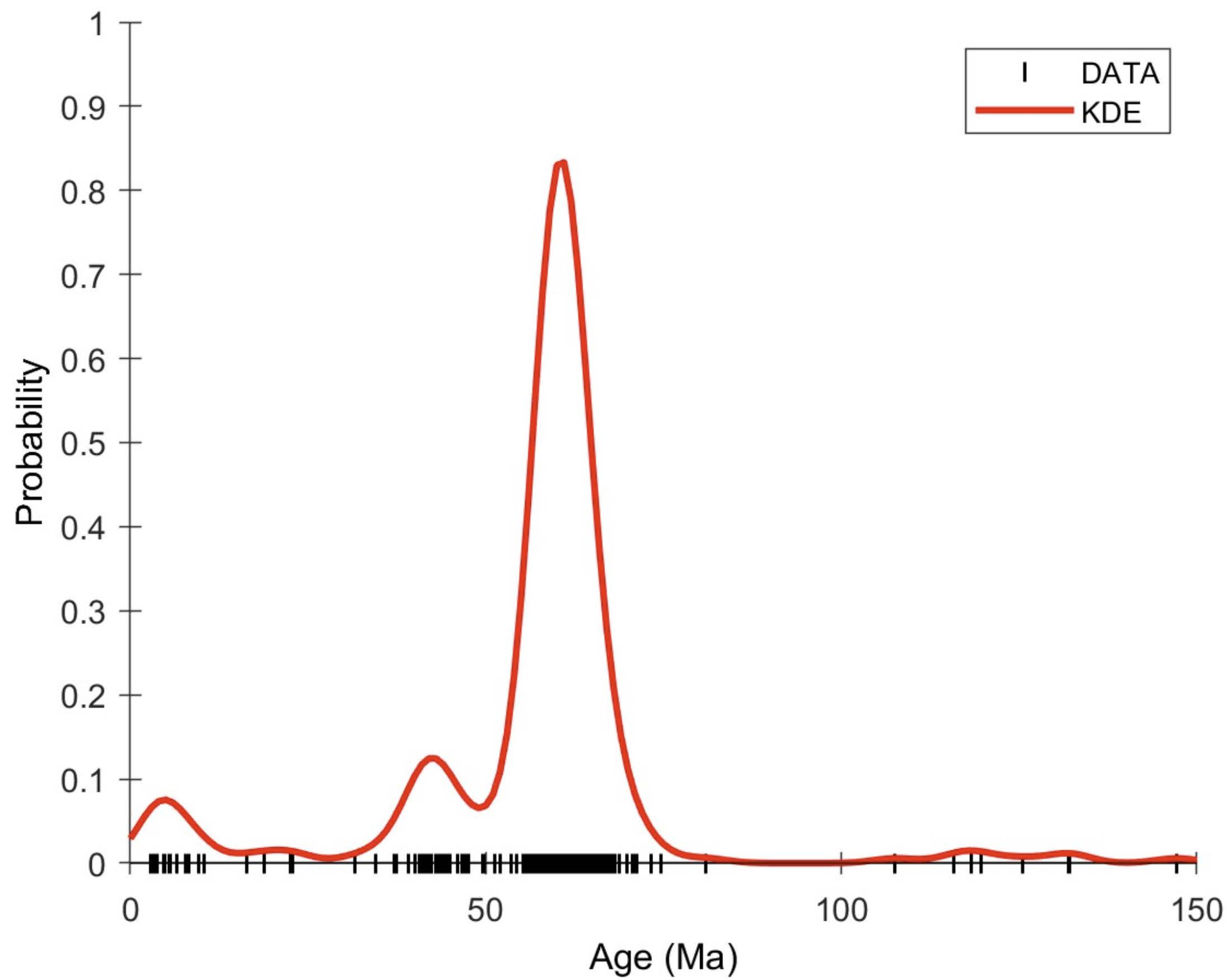
The Raw Data “Rug Plot”



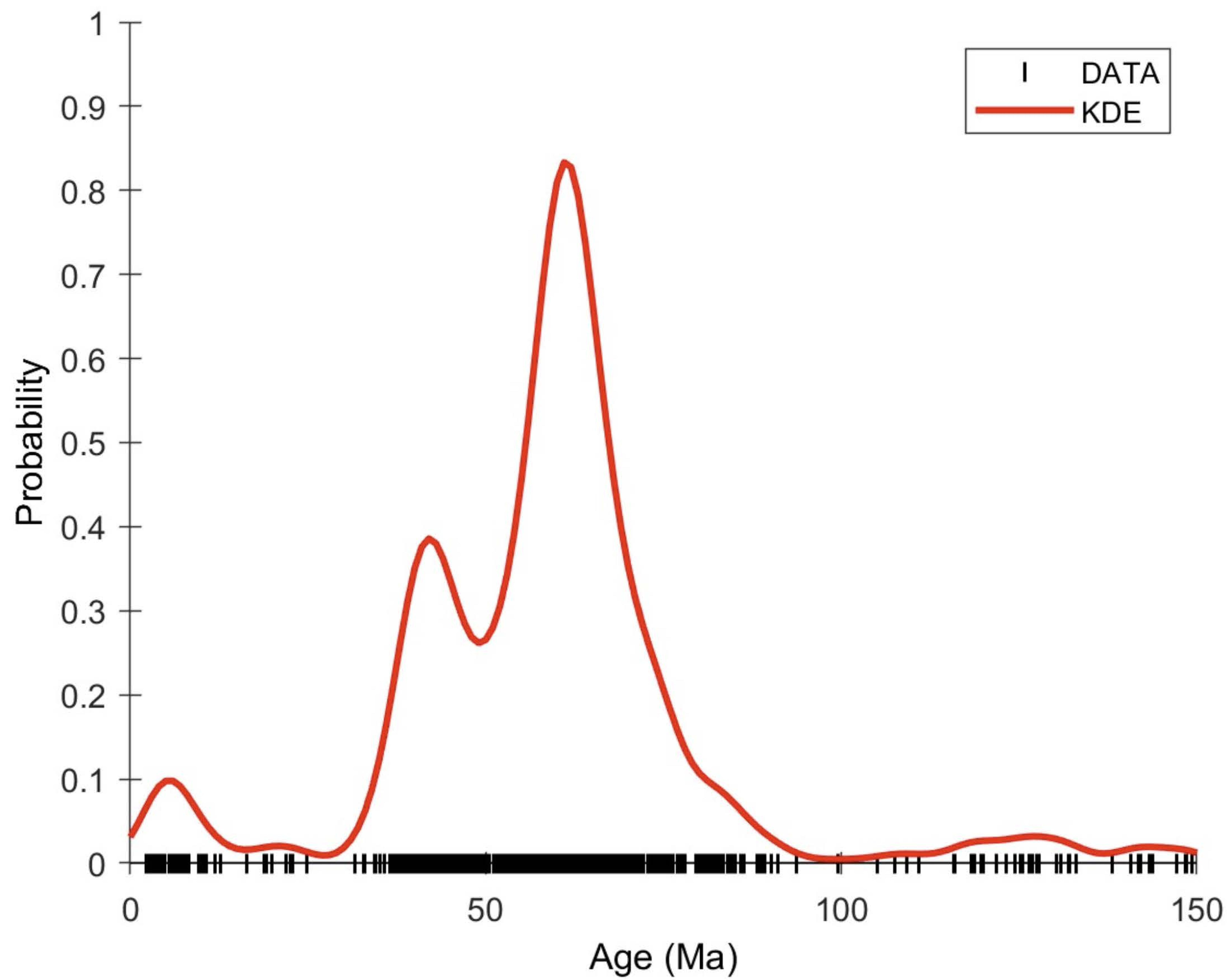
Transform Into a Smooth Density



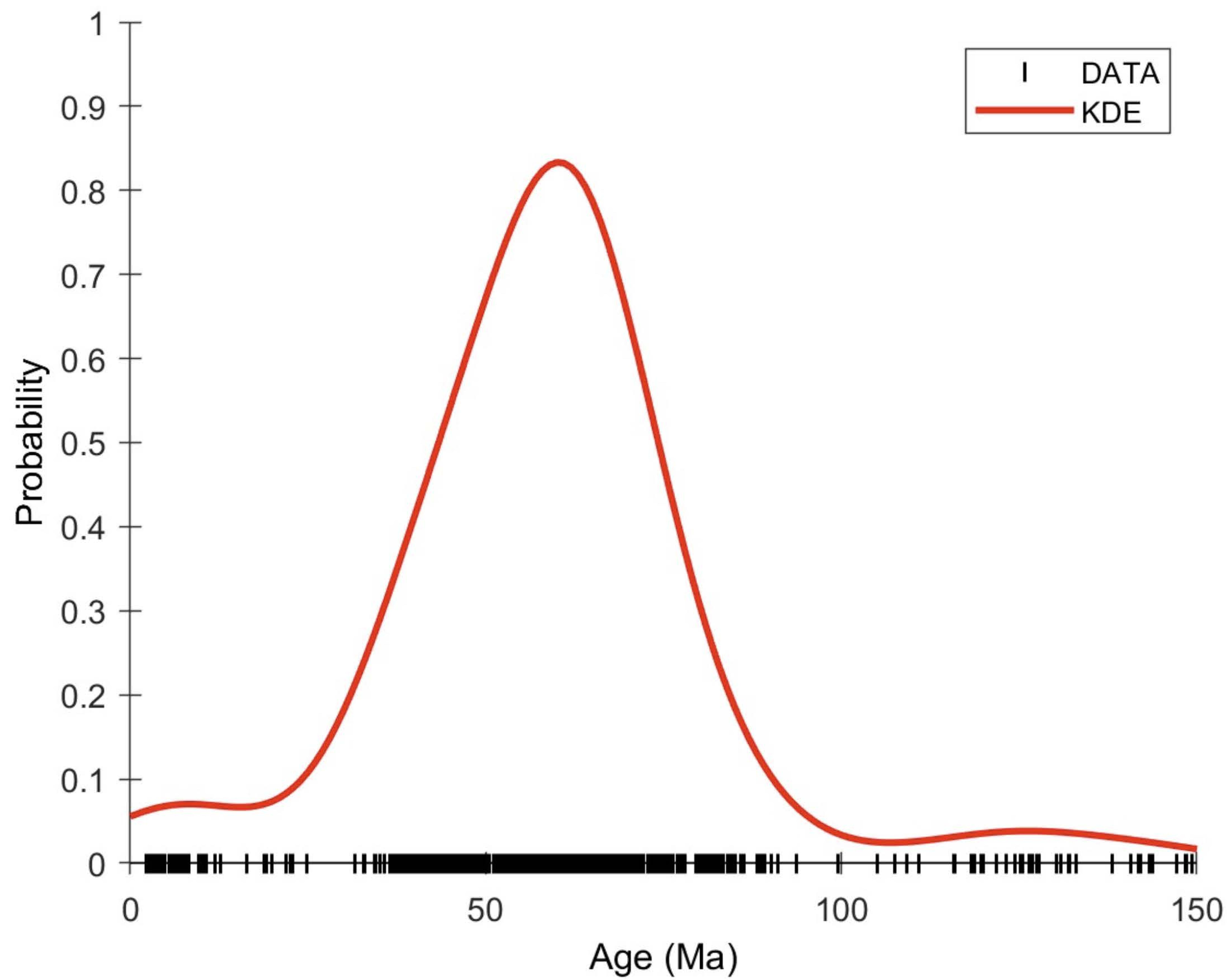
More Samples $\implies$ More Accurate



More Samples $\implies$ More Accurate

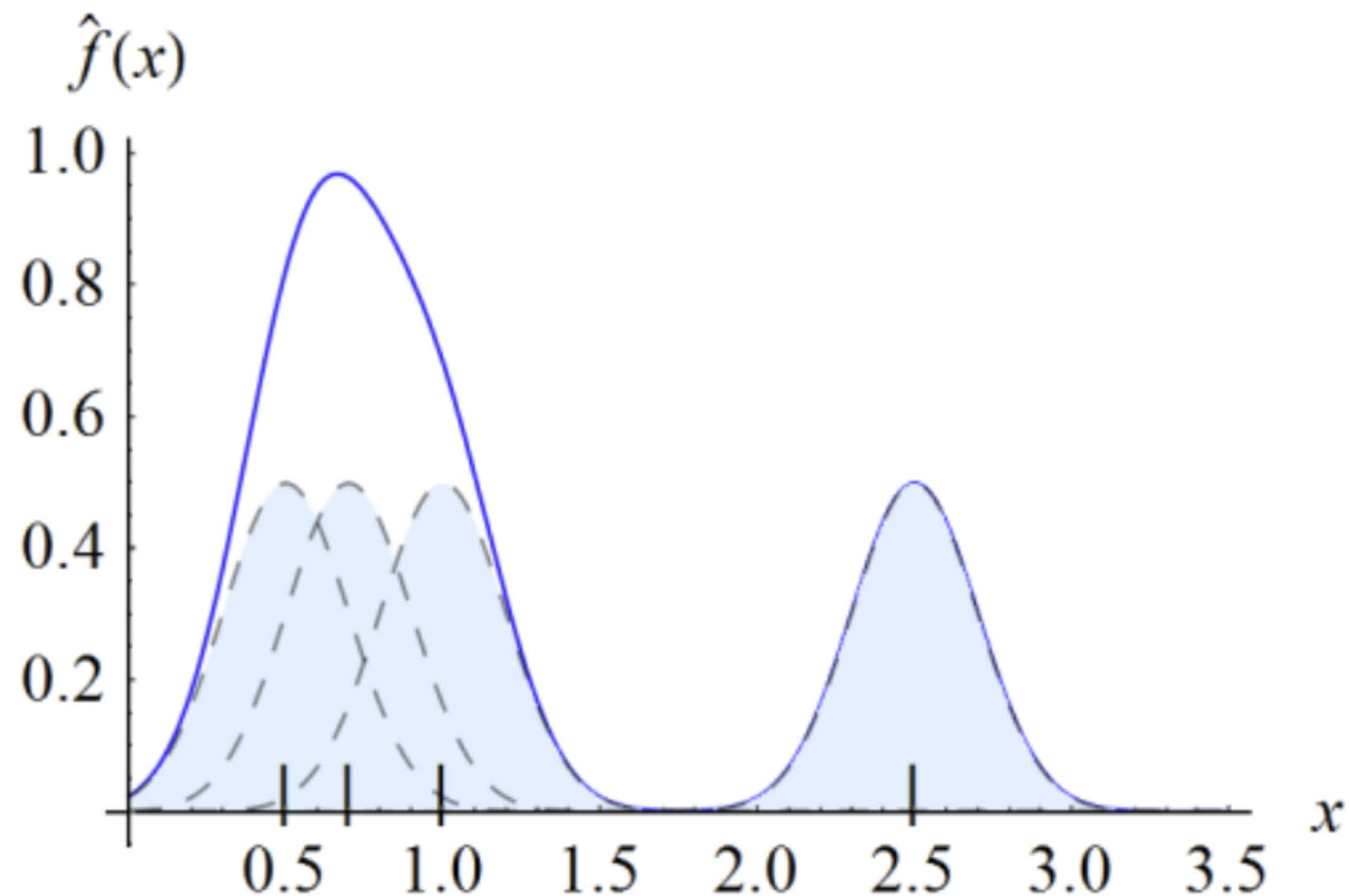


Larger bandwidth $\implies$ smoother



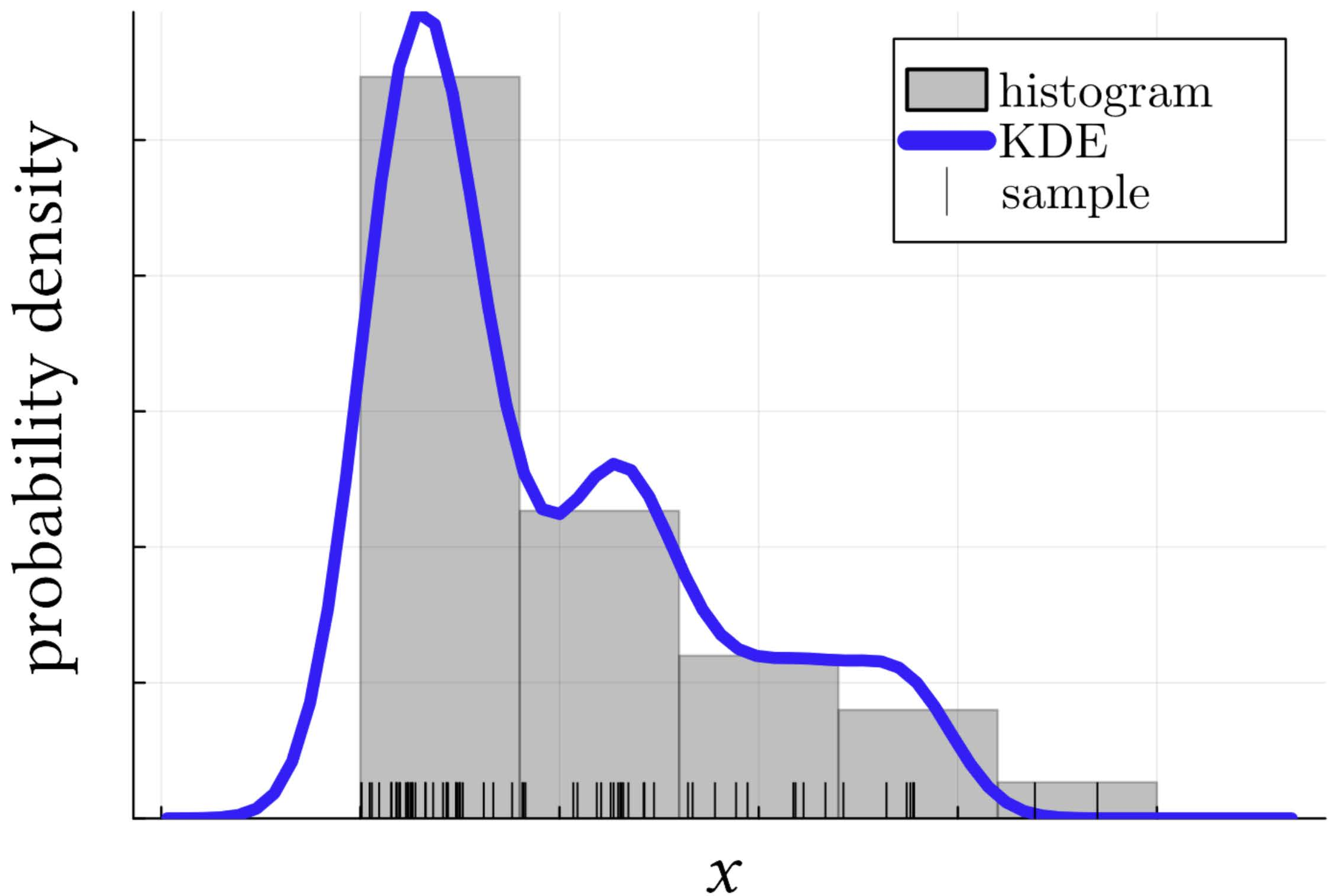
Kernel Density Estimation (KDE)

- Turns samples into distributions [Węglarczyk 2018]:



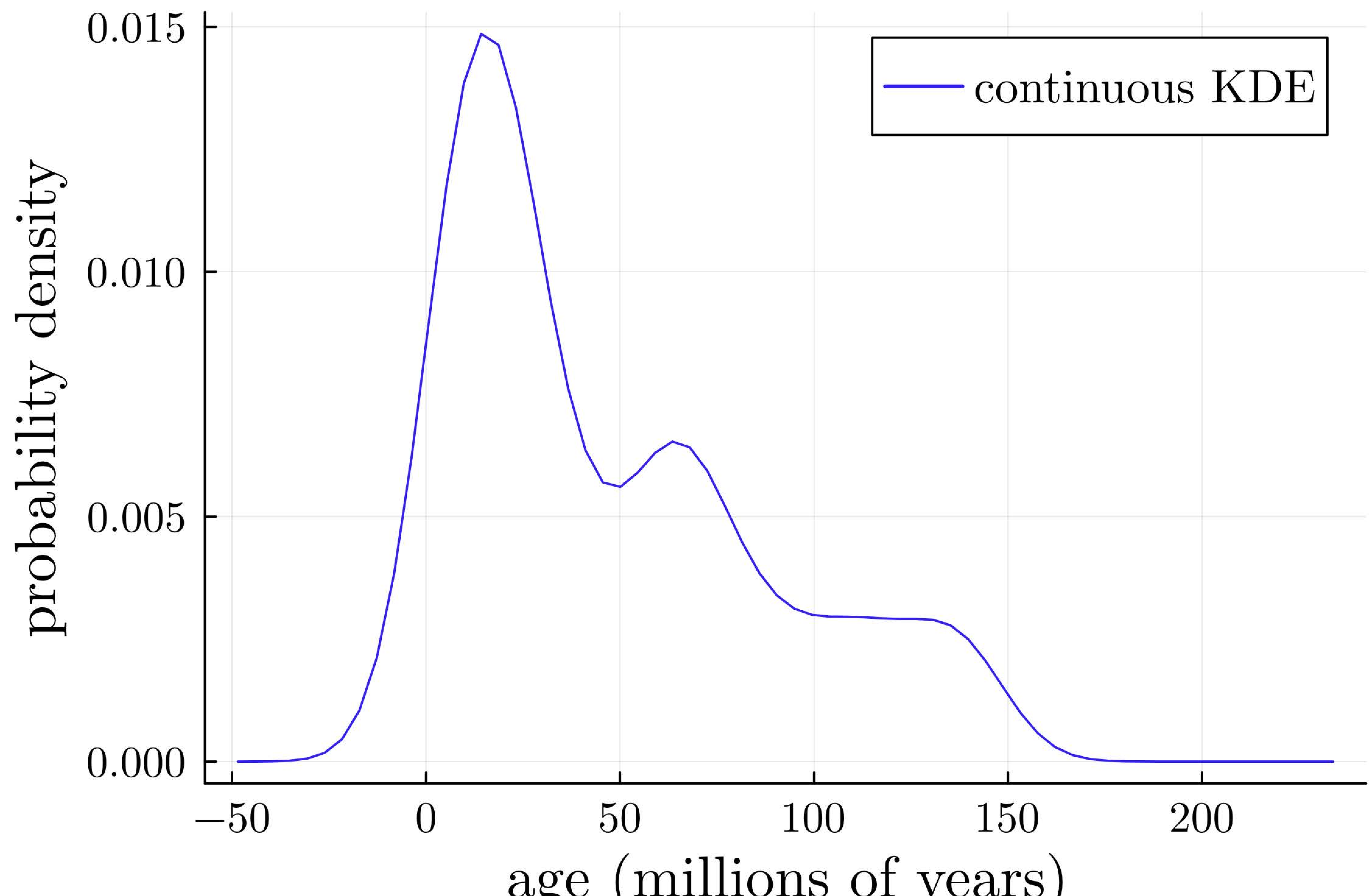
Kernel Density Estimation (KDE)

- Smooth version of a histogram



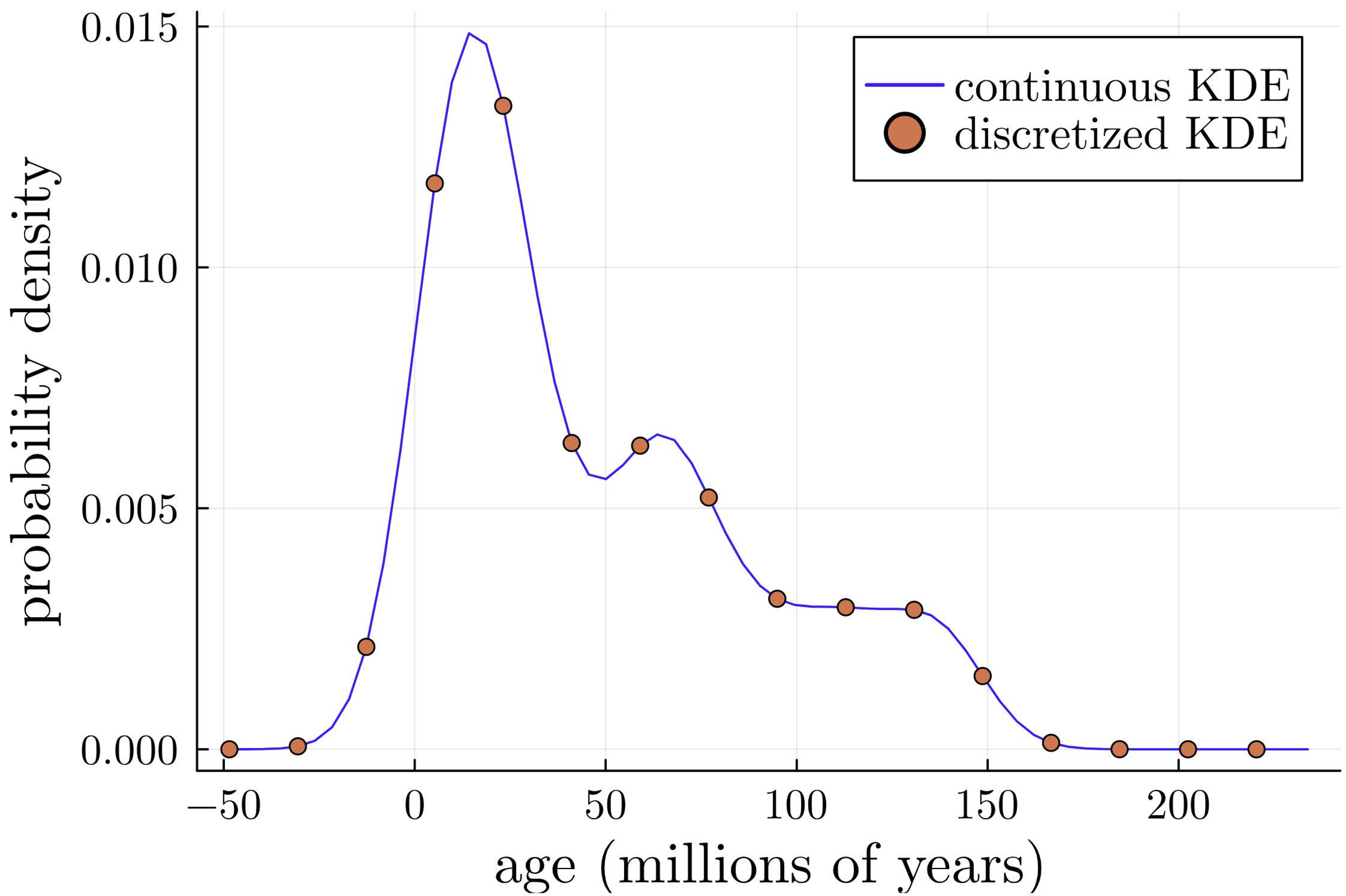
Discretizing the KDE

- Start with smooth KDE



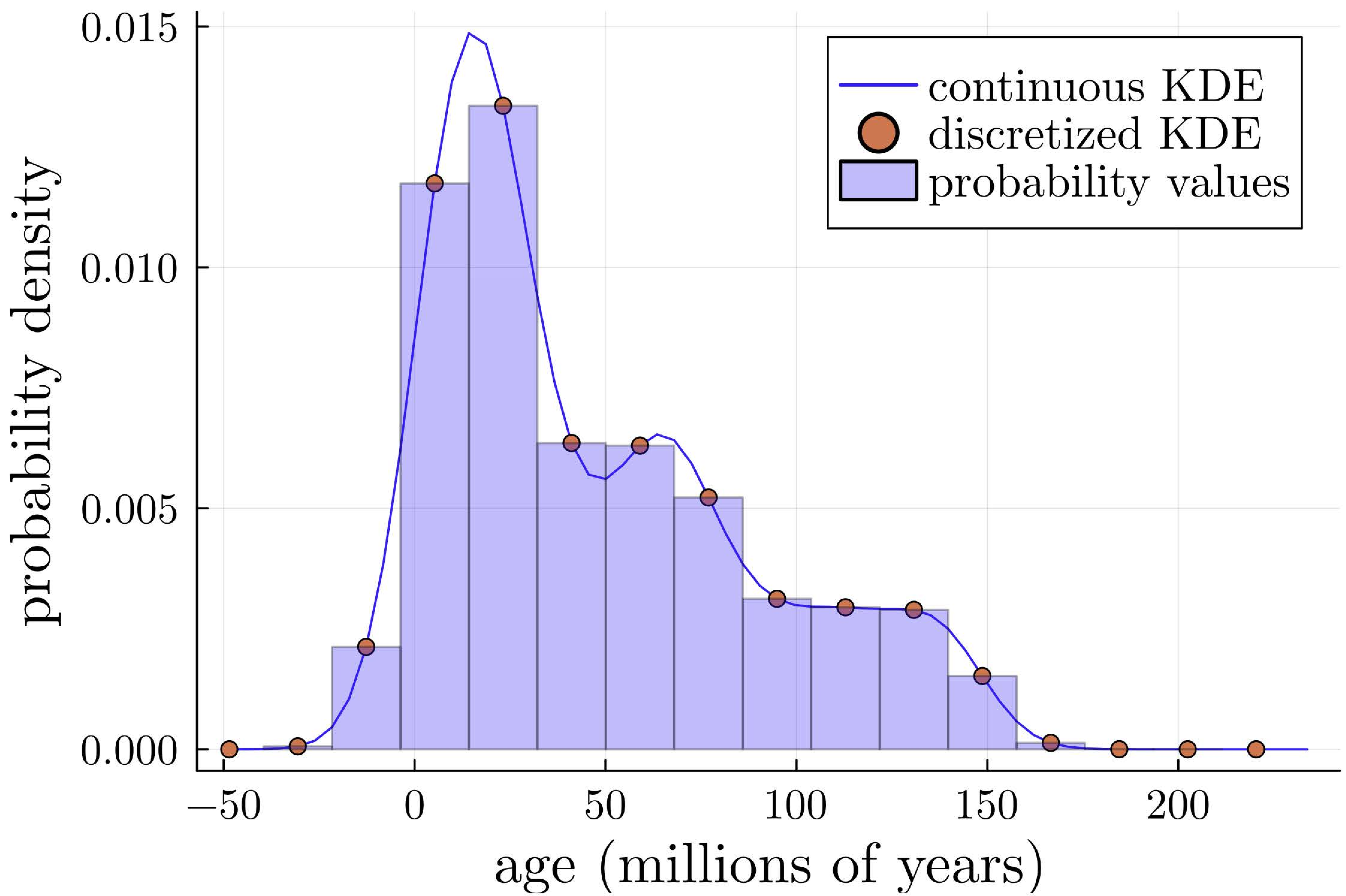
Discretizing the KDE

- Sample on a uniform grid



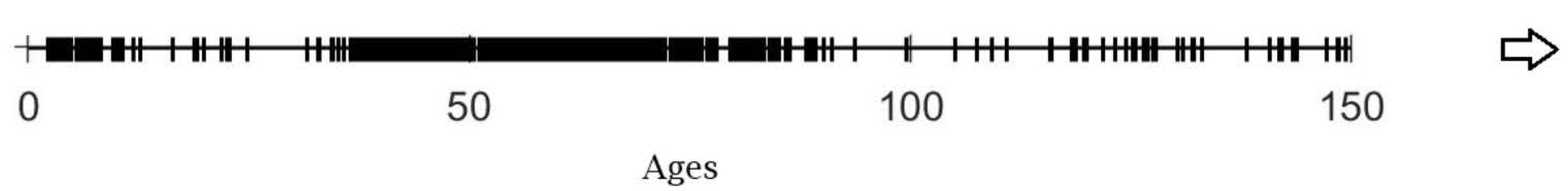
Discretizing the KDE

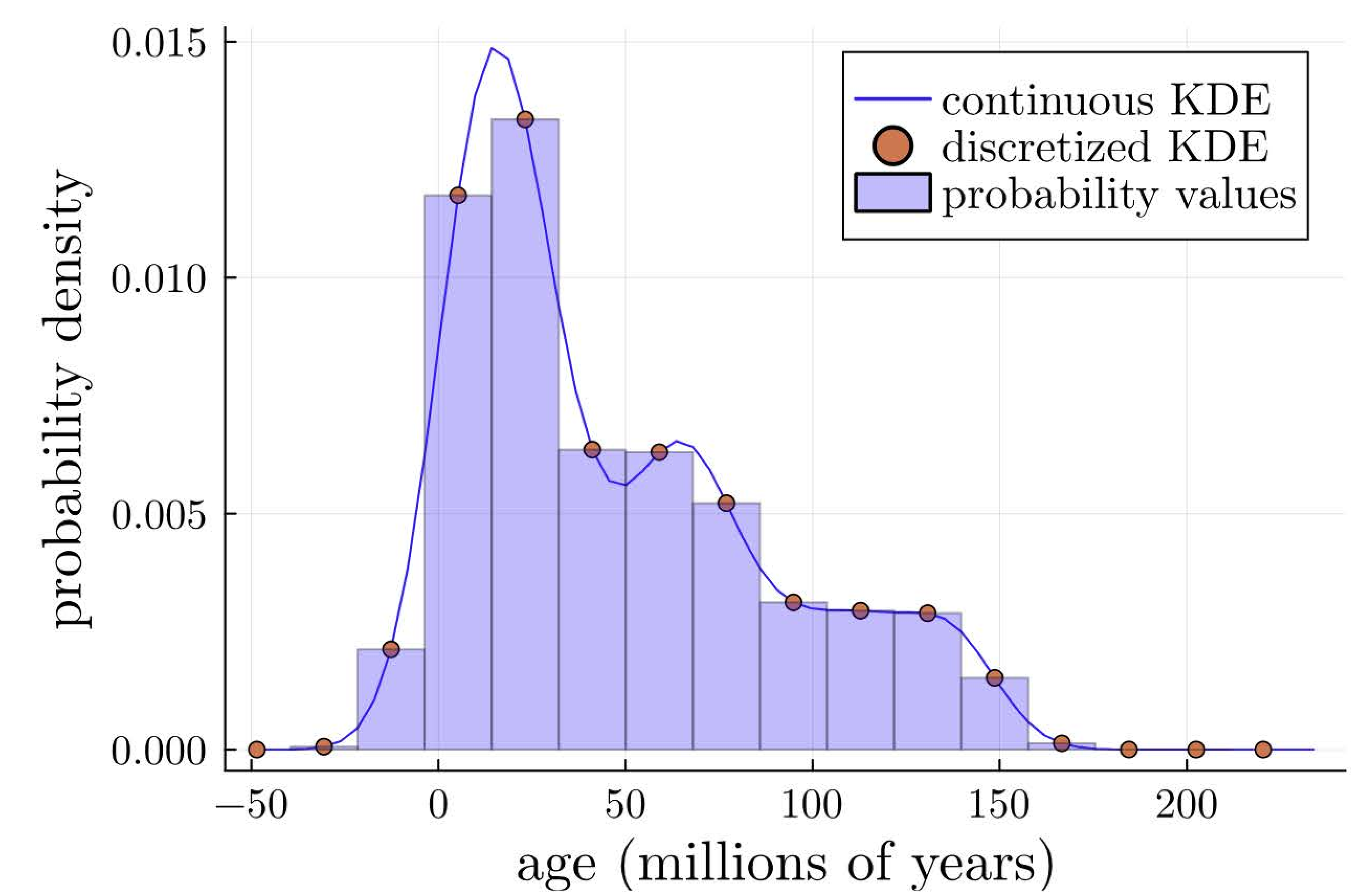
- Record the area of each box



Why do all this work?

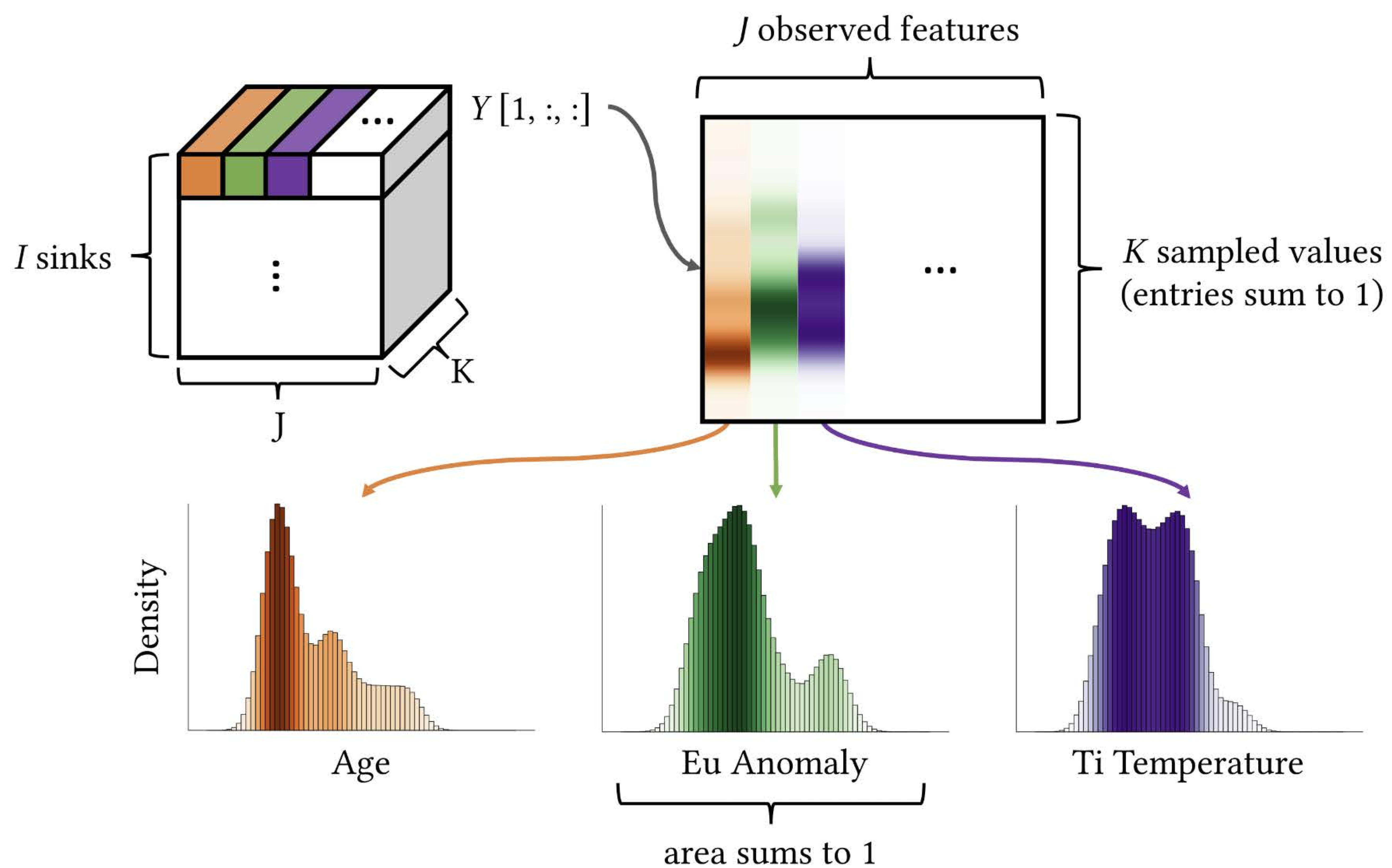
- This constructs density estimate for each feature in each sink
- Why use KDEs over histogram?
  - The size and smoothness of each KDE is the same
  - # of samples can be different across sinks and features





Data Tensor Y

- Lay KDEs along each fibre
  - i is the sink (different locations)
  - j is the feature (different elements)



Framing the demixing problem

Now we have $\mathbf{Y}$! Onto finding $\mathbf{A}$ and $\mathbf{B}$…

$$\begin{aligned}\mathbf{Y}_1 &= a_{11}\mathbf{B}_1 + a_{12}\mathbf{B}_2 + \cdots + a_{1R}\mathbf{B}_R \\ &\vdots \\ \mathbf{Y}_I &= a_{I1}\mathbf{B}_1 + a_{I2}\mathbf{B}_2 + \cdots + a_{IR}\mathbf{B}_R.\end{aligned}$$

Framing the demixing problem

$$
\begin{aligned}
\mathbf{Y}_1 &= a_{11}\mathbf{B}_1 + a_{12}\mathbf{B}_2 + \cdots + a_{1R}\mathbf{B}_R \\
&\vdots \\
\mathbf{Y}_I &= a_{I1}\mathbf{B}_1 + a_{I2}\mathbf{B}_2 + \cdots + a_{IR}\mathbf{B}_R
\end{aligned}
$$

The system of equations becomes the equation $\mathbf{Y} = \mathbf{A}\mathbf{B}$

$$
\begin{bmatrix} \leftarrow & \mathbf{Y}_1 & \rightarrow \\ \leftarrow & \mathbf{Y}_2 & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{Y}_I & \rightarrow \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1R} \\ a_{21} & a_{22} & \dots & a_{2R} \\ \vdots & & & \vdots \\ a_{I1} & a_{I2} & \dots & a_{IR} \end{bmatrix} \begin{bmatrix} \leftarrow & \mathbf{B}_1 & \rightarrow \\ \leftarrow & \mathbf{B}_2 & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{B}_R & \rightarrow \end{bmatrix}
$$

Finding A and B with Tucker-1

- Factorize $\mathbf{Y}$ into a mixing matrix $\mathbf{A}$ times a source tensor $\mathbf{B}$ using the Tucker-1 factorization model [Kolda *et al.* 2009]
- $\mathbf{Y} = \mathbf{AB} = \mathbf{B} \times_1 \mathbf{A}$ with the entry-wise equation
- $\mathbf{Y}[i, j_1, \ldots, j_N] = \sum_{r=1}^{R} \mathbf{A}[i, r] \cdot \mathbf{B}[r, j_1, \ldots, j_N]$

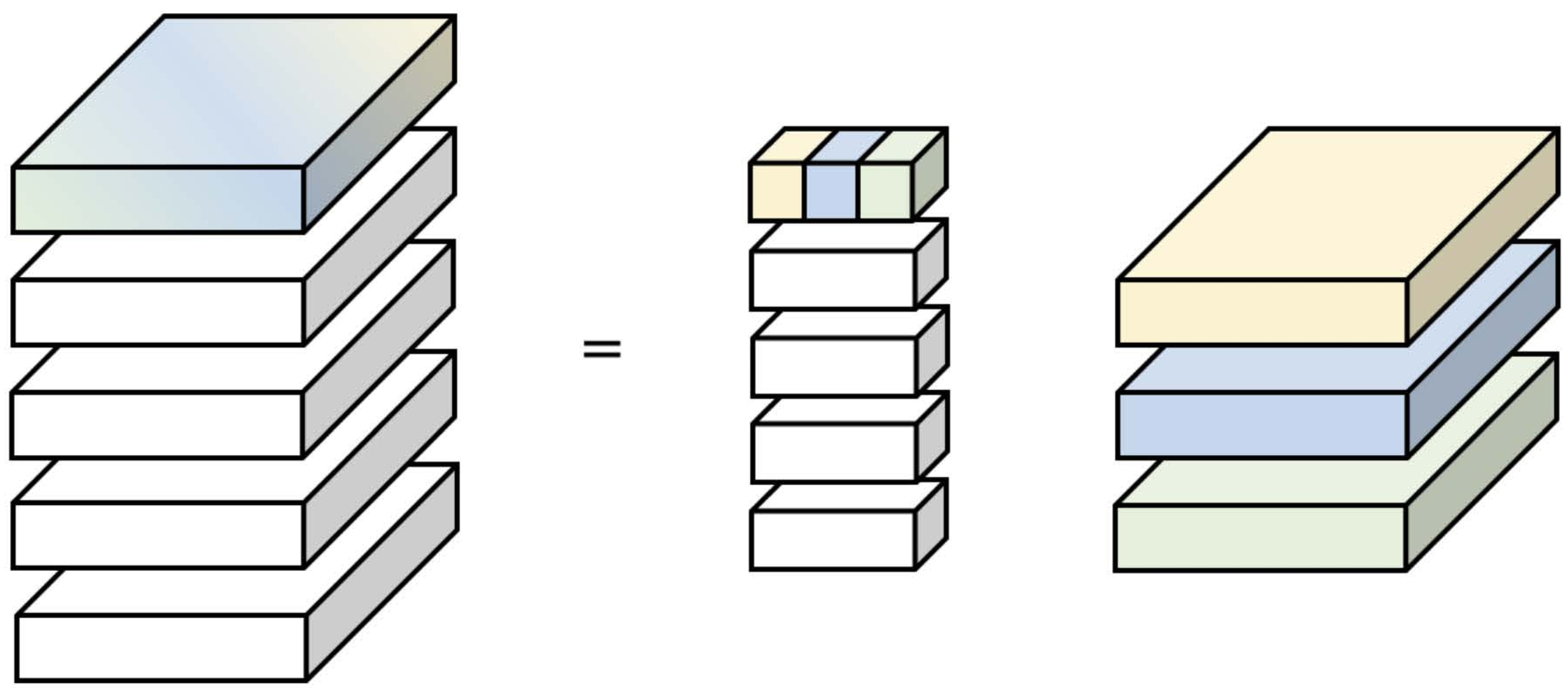


Figure 1: Example Tucker-1 decomposition for a 3rd-order tensor.

BlockTensorFactorization.jl

Least-Squares Optimization

Minimize the error between the model $\mathbf{B} \times_1 \mathbf{A}$ and the data $\mathbf{Y}$:

$$\min_{\mathbf{A},\mathbf{B}} \ell(\mathbf{A}, \mathbf{B}) := \frac{1}{2}\|\mathbf{B} \times_1 \mathbf{A} - \mathbf{Y}\|_F^2 \quad \text{s.t} \quad \mathbf{A} \text{ in } \mathcal{C}_{\mathbf{A}},\ \mathbf{B} \text{ in } \mathcal{C}_{\mathbf{B}}.$$

Basic use:

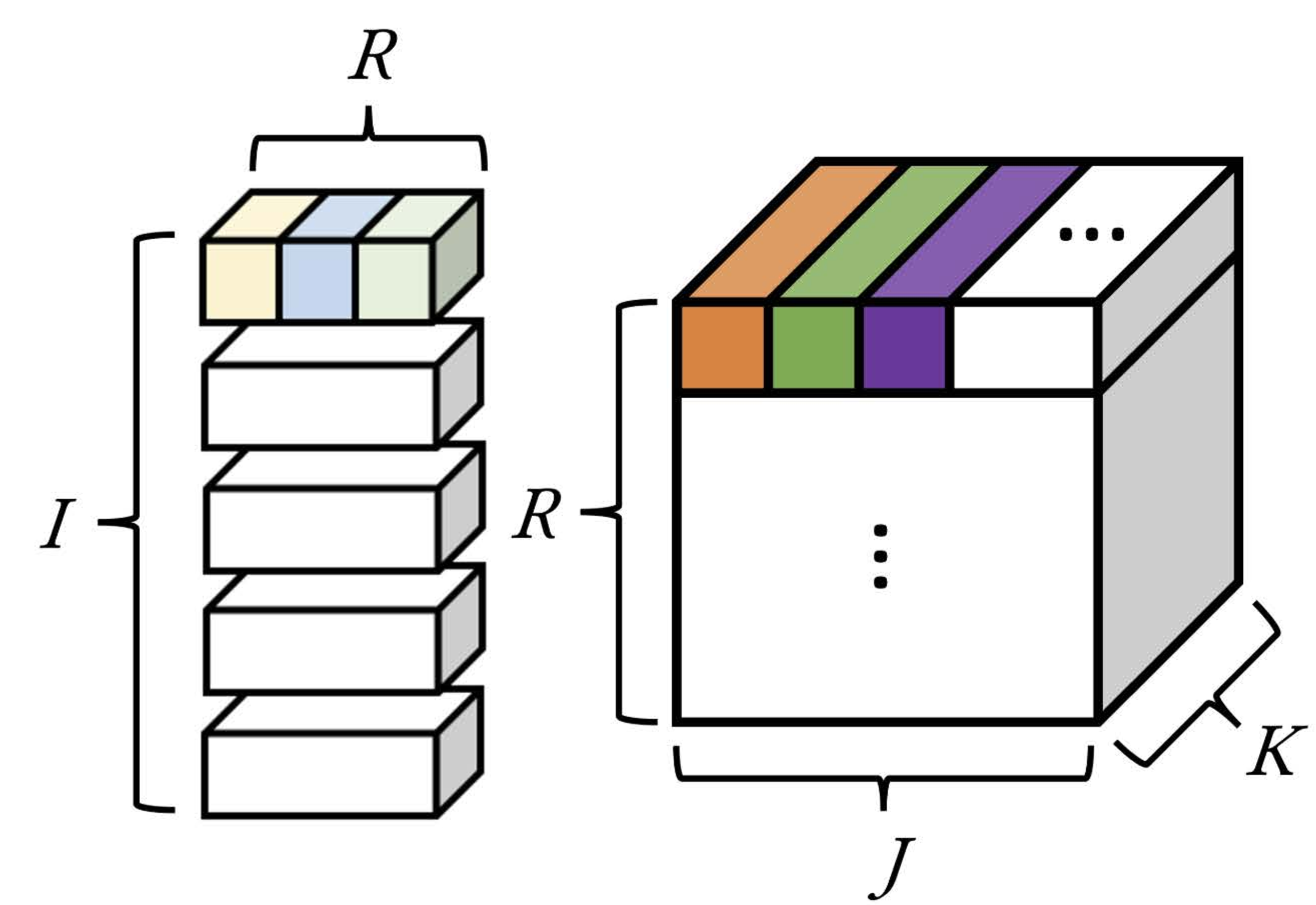
```
options = (rank=3, model=Tucker1, constraints=[B_constraint, A_constraint])

decomposition, stats, kwargs = factorize(Y; options...)

(B_out, A_out) = factors(decomposition)
```

Algorithm: Constraints

$$\mathcal{C}_{\mathbf{A}} = \Delta^I_R = \left\{ \mathbf{A} \in \mathbb{R}_+^{I\times R} \middle| \sum_{r=1}^R \mathbf{A}[i,r] = 1, \text{ for all } i \right\}$$

$$\mathcal{C}_{\mathbf{B}} = \Delta^{RJ}_K = \left\{ \mathbf{A} \in \mathbb{R}_+^{R\times J\times K} \middle| \sum_{k=1}^K \mathbf{B}[r,j,k] = 1, \text{ for all } r,j \right\}$$

- Rows of $\mathbf{A}$ and fibres of $\mathbf{B}$ need to be nonnegative and sum to one
- Ensures their product is a probability distribution




```
constraint_A = simplex_rows!
constraint_B = simplex_12slices!
```

Algorithm: Alternating Descent

- Start with a guess for $\mathbf{A}^0$ and $\mathbf{B}^0$. Then for $t = 1, 2, \ldots$

$$\mathbf{A}^{t+1} = P_{\Delta_R^I}(\mathbf{A}^t - \frac{1}{L_{\mathbf{A}}} \nabla_{\mathbf{A}} \ell(\mathbf{A}^t, \mathbf{B}^t))$$
$$\mathbf{B}^{t+1} = P_{\Delta_K^{RJ}}(\mathbf{B}^t - \frac{1}{L_{\mathbf{B}}} \nabla_{\mathbf{B}} \ell(\mathbf{A}^{t+1}, \mathbf{B}^t))$$

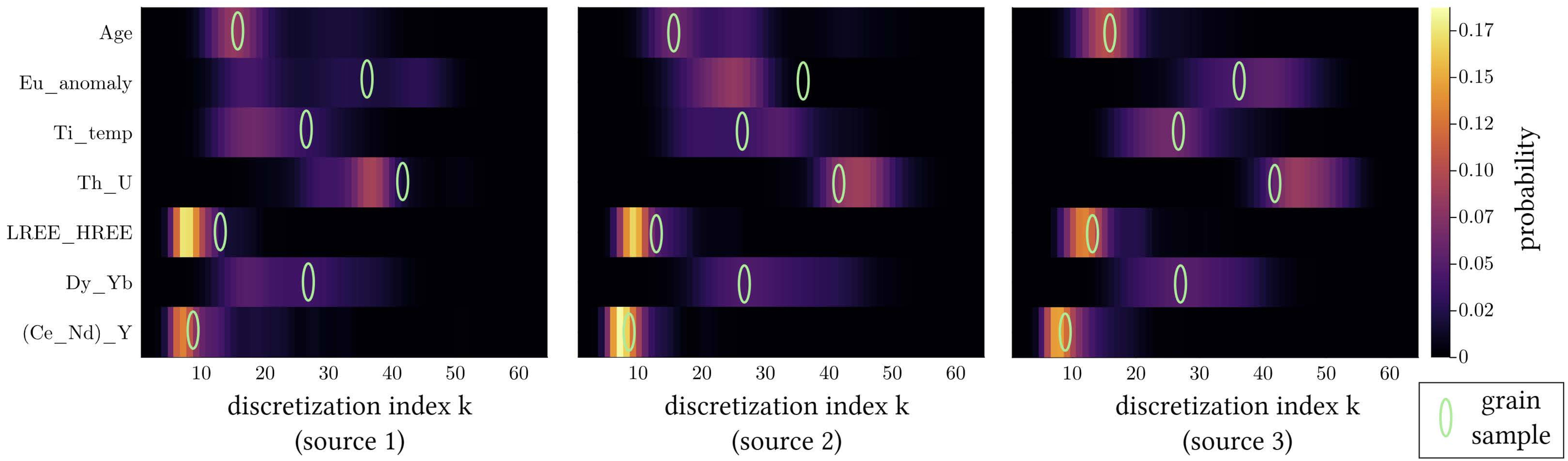
- Converges to a *block-wise* minimum and stationary point

$$\ell(\mathbf{A}^*, \mathbf{B}^*) \leq \min_{\mathbf{A} \in \mathcal{C}_{\mathbf{A}}, \mathbf{B} \in \mathcal{C}_{\mathbf{B}}} \{\ell(\mathbf{A}^*, \mathbf{B}), \ell(\mathbf{A}, \mathbf{B}^*)\}$$

The Bells and Whistles

Labelling Grains

- Categorize each grain **g** according to its most likely source
- Learned distribution sources $\mathbf{B}_r$:



Labelling Grains

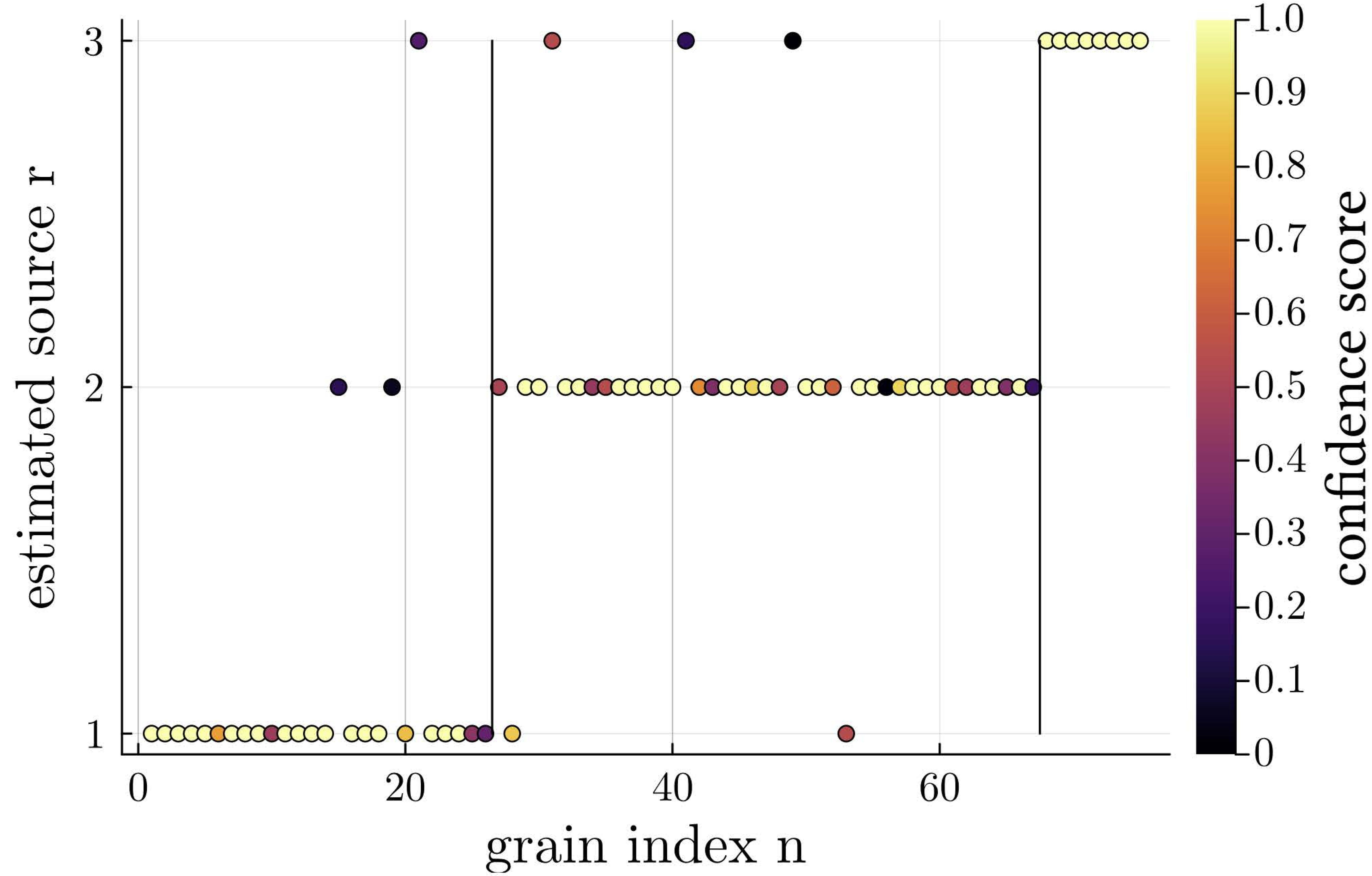
- Approximate the probability that a grain came from source r

$$p_r = \mathbb{P}(\mathbf{g} \in \mathcal{V}_{\mathbf{g}} \mid \mathbf{g} \sim \mathbf{B}_r) \approx \prod_{j=1}^{J} \mathbf{B}[r, j, \hat{k}_j]$$

- $\mathcal{V}_{\mathbf{g}} = \left[x_{1\hat{k}_1}, x_{1(\hat{k}_1+1)}\right] \times \cdots \times \left[x_{J\hat{k}_J}, x_{J(\hat{k}_J+1)}\right]$ is the box that contains the measured grain
- Label based on the most likely probability $\hat{r} = \text{argmax}_r p_r$

Labelling Grains

- Estimated source for many grains:
- Grains are ordered by their true source in this example



Label Confidence Score

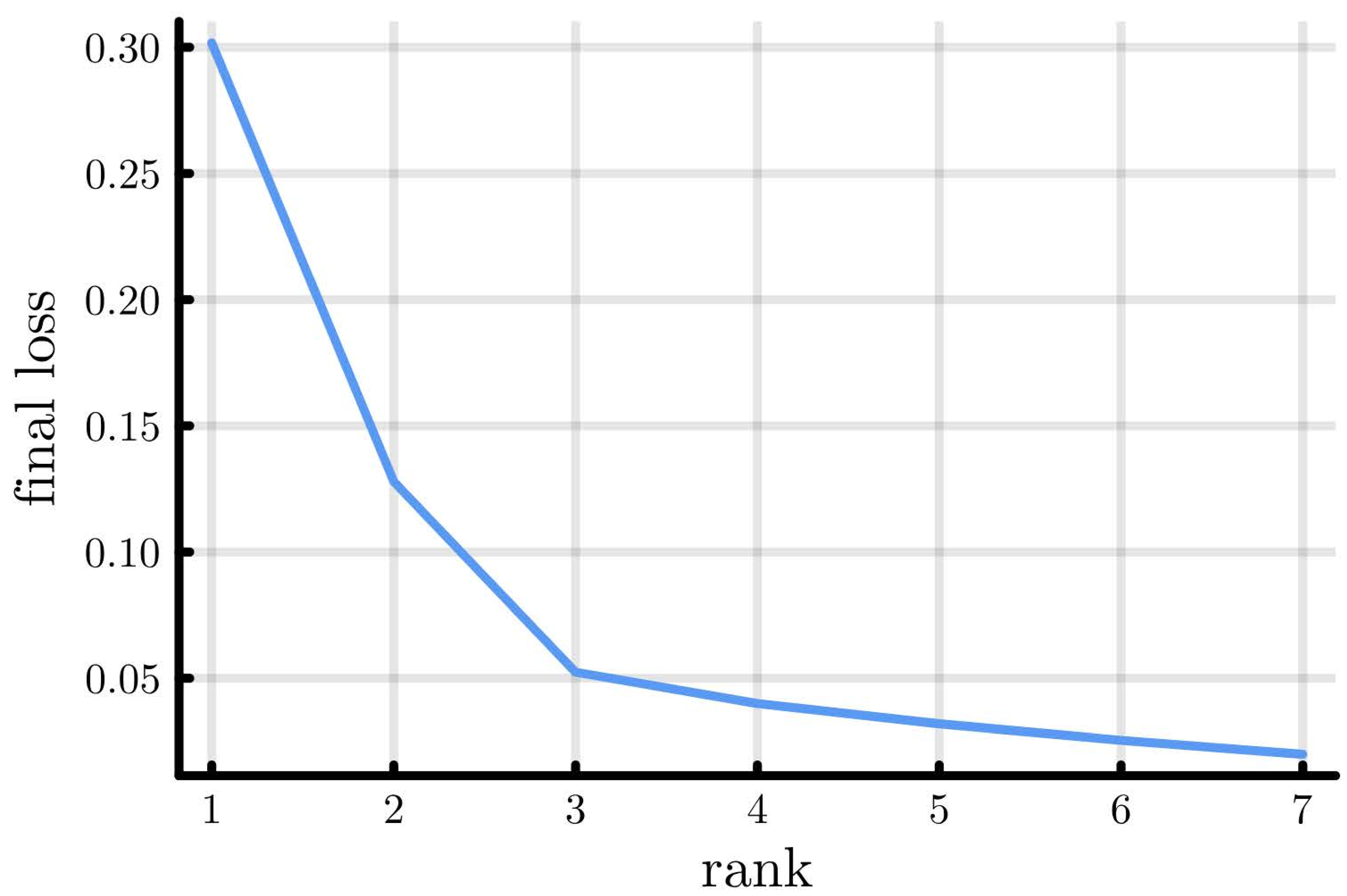
- Give a confidence score for the grain labels using the log-ratio of the top two estimated probabilities

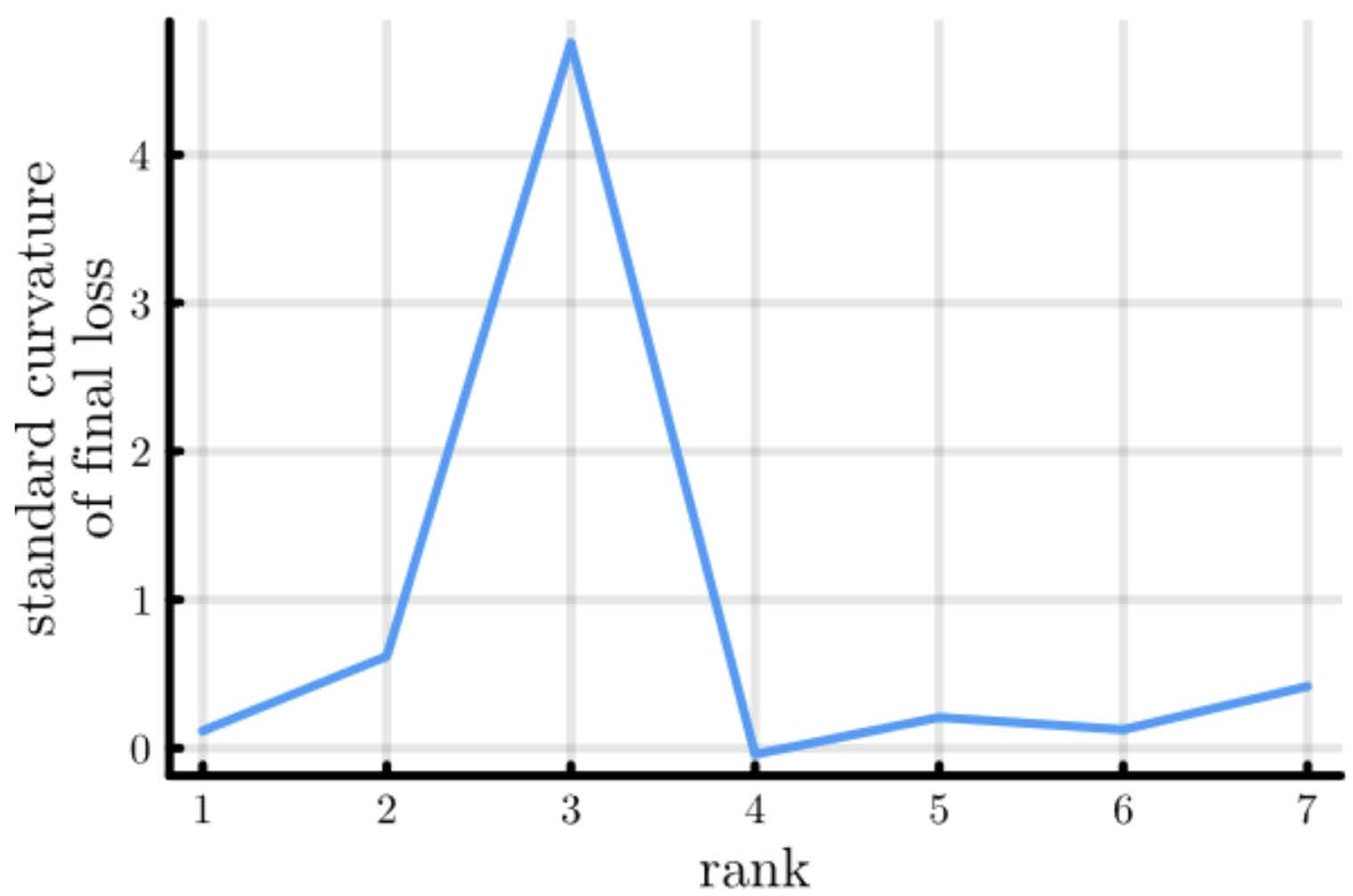
$$\text{confidence score} = \log_{10}\left(\frac{p_{(1)}}{p_{(2)}}\right)$$

- score ≥ 1 means it's at least 10 times as likely the grain came from source $\hat{r}$ than any other source
- score ≈ 0 means there's a similar probability the grain came from a difference source

Estimating Rank

- Usually we need to know R in advance
- Can estimate it based on an accuracy and simplicity trade-off





Estimating Rank

- Let $f(r) = \|\mathbf{X}_r^* - \mathbf{Y}\|_F / \|\mathbf{Y}\|_F$ be final relative error with a rank r factorization
- Pick the r at the maximum curvature [Satopaa *et al.* 2011]

$$\hat{R} = \arg\max_r \kappa_f(r) := \frac{f''(r)}{(1 + (f'(r))^2)^{3/2}}$$

```
options = (model=Tucker1, constraints=[B_constraint, A_constraint])

# Will try to factorize at many ranks and pick the "best" one
decomposition, stats, kwargs = rank_detect_factorize(Y; options...)

estimated_rank = kwargs[:rank]
```

Multi-Scaled Decomposition

- Use `continuous_dims` to optimize over multiple scales
- Often faster, and leads to smoother results

```
factorize(Y; continuous_dims=[3], options...)
# Third dimension K is continuous in our model
```

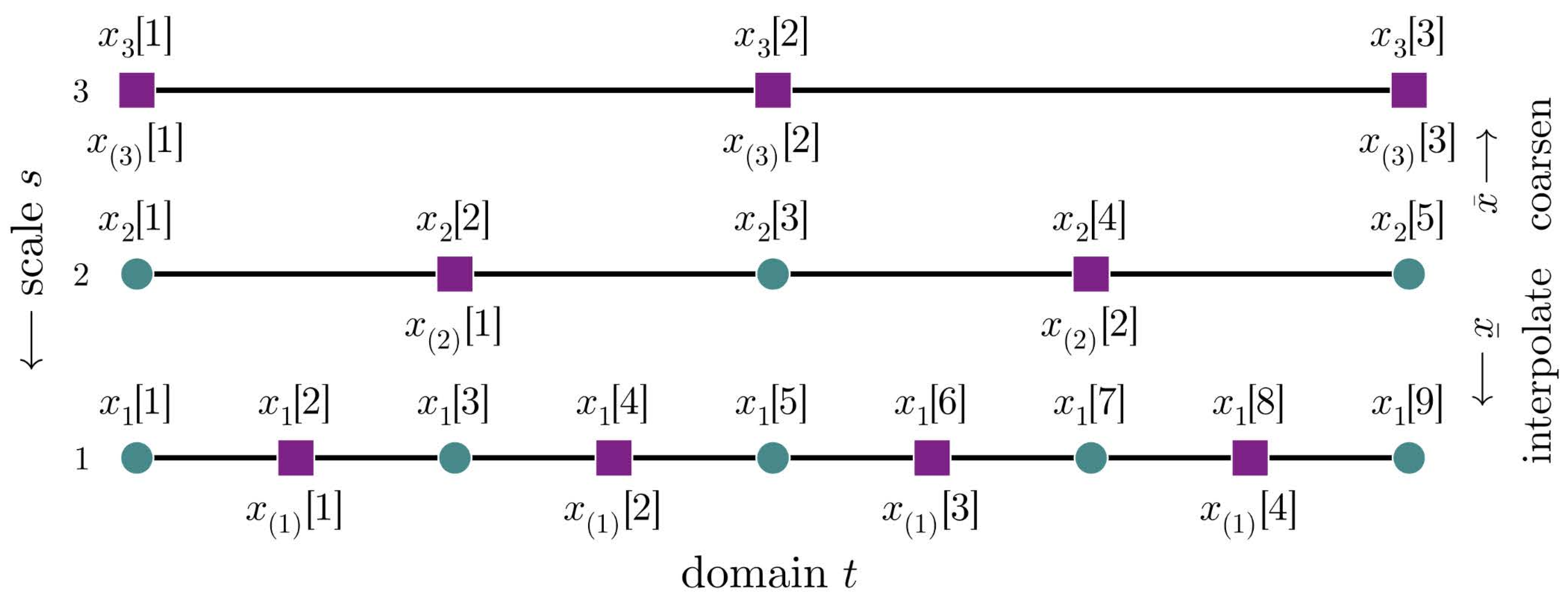


Figure 2: Rather than discretizing the mixtures $\mathbf{Y}_i$ on a fine grid from the start, optimize over a cheaper, coarse discretization with fewer points and gradually refine.

References

[1] N. Graham, N. Richardson, M. P. Friedlander, and J. Saylor, "Tracing Sedimentary Origins in Multivariate Geochronology via Constrained Tensor Factorization," *Mathematical Geosciences*, Feb. 2025.

[2] S. Węglarczyk, "Kernel density estimation and its application," *ITM Web of Conferences*, vol. 23, 2018.

[3] T. G. Kolda and B. W. Bader, "Tensor Decompositions and Applications," *SIAM Rev.*, vol. 51, no. 3, Aug. 2009.

[4] V. Satopaa, J. Albrecht, D. Irwin, and B. Raghavan, "Finding a "Kneedle" in a Haystack: Detecting Knee Points in System Behavior," in *2011 31st International Conference on Distributed Computing Systems Workshops*, Jun. 2011.

Try our code here!

https://github.com/MPF-Optimization-Laboratory/BlockTensorFactorization.jl

Extra Slides

Many more extra features…

- Momentum and second-order acceleration like Block-lipschitz constants (Hessian approximations)
- Rank detection
- Other factorizations like full Tucker, CP-Decomposition, custom
- Other constraints like p-norms, interval, linear, custom
- Other block update order: fully random, partial random

Rescaling trick

- Relax simplex constraints to $\mathbf{A} \geq 0, \mathbf{B} \geq 0$
- and $\frac{1}{J}\sum_{jk} \mathbf{B}[r, j, k] = 1$ for all r. Old constraints were $\sum_k \mathbf{B}[r, j, k] = 1$ for all r, j

Updates now look like:

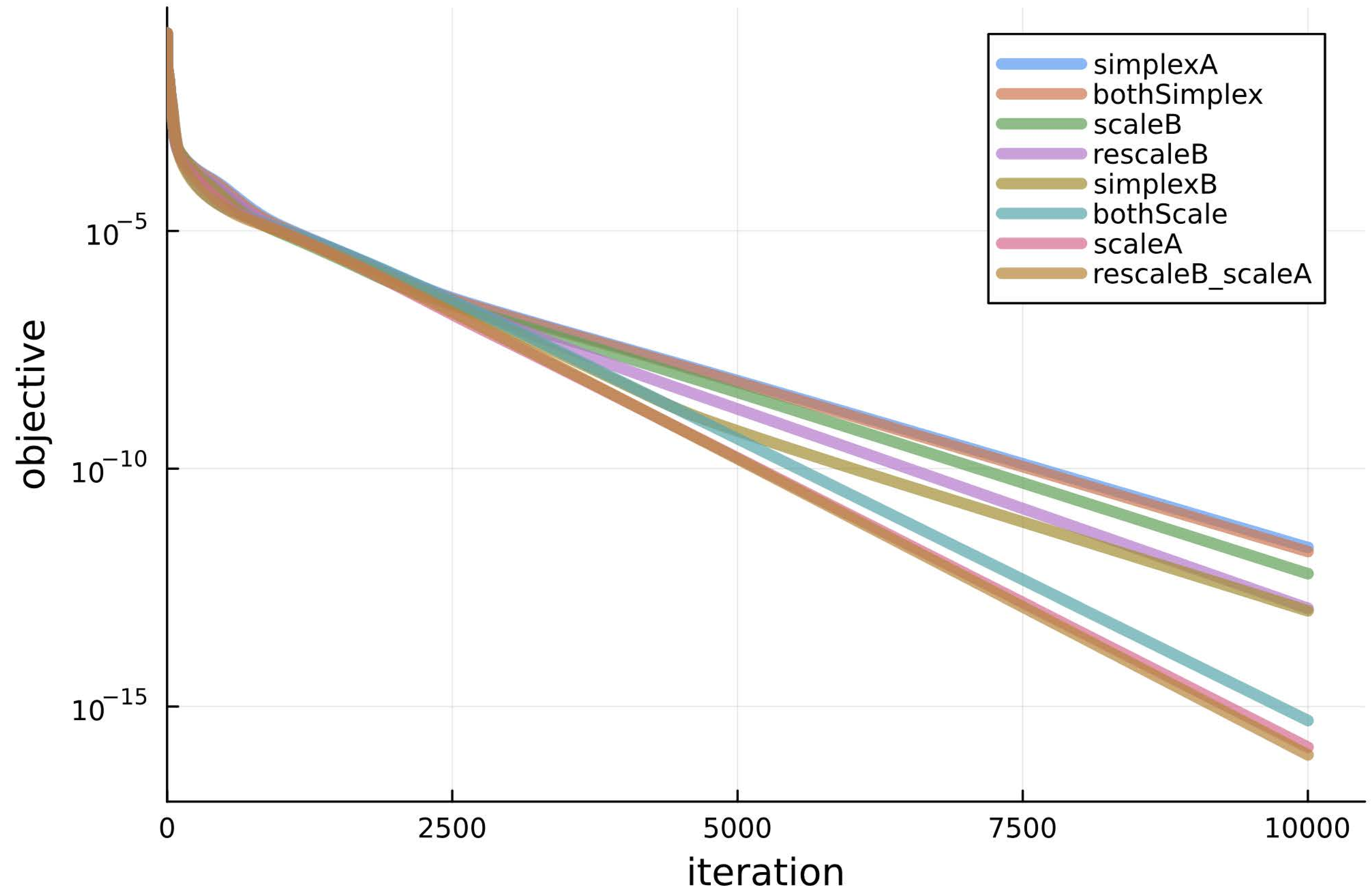
- $\mathbf{A}^{t+1/2} = (\mathbf{A}^t - \frac{1}{L_{\mathbf{A}}}\nabla_{\mathbf{A}}\ell(\mathbf{A}^t, \mathbf{B}^t))_+$
- $\mathbf{B}^{t+1/2} = (\mathbf{B}^t - \frac{1}{L_{\mathbf{B}}}\nabla_{\mathbf{B}}\ell(\mathbf{A}^{t+1/2}, \mathbf{B}^t))_+$
- $\mathbf{B}^{t+1} = \mathbf{C}^{-1}\mathbf{B}^{t+1/2}$ and $\mathbf{A}^{t+1} = \mathbf{A}^{t+1/2}\mathbf{C}$
- where $\mathbf{C}[r, r] = \frac{1}{J}\sum_{jk} \mathbf{B}[r, j, k]$

Examples of Constraints

```
l1scale_average12slices! = ScaledNormalization(l1norm;
    whats_normalized=each1slice, scale=size2)

nonnegative! = Entrywise(ReLU, isnonnegative)

scaleB_rescaleA! = ConstraintUpdate(
    0, # the zeroth factor
    l1scale_average12slices! ∘ nonnegative!;
    whats_rescaled = x -> eachcol(factor(x, 1))
)

constraint_A = nonnegative!
constraint_B = scaleB_rescaleA!
```

Rescaling vs simplex projection

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



Block-Lipschitz Constant

$$a_{n,r}^{t+1} \leftarrow P_{\mathcal{C}_{n,r}}\left(a_{n,r}^{t} - \frac{1}{L_{n,r}^{t}} \nabla f_{n,r}^{t}(a_{n,r}^{t})\right),$$

where

$f_{n,r}^{t}(a) = \frac{1}{2}\left\|[\mathbf{B}; \mathbf{A}_1^{t+1}, \ldots, \mathbf{A}_{n-1}^{t+1}, A_{n,r}^{t}(a), \mathbf{A}_{n+1}^{t}, \ldots, \mathbf{A}_N^{t}] - \mathbf{Y}\right\|_F^2$

and

$$\mathbf{A}_{n,r}^{t}(a) = \begin{bmatrix} \uparrow & & \uparrow & \uparrow & \uparrow & & \uparrow \\ a_{n,1}^{t+1} & \cdots & a_{n,r-1}^{t+1} & a & a_{n,r+1}^{t} & \cdots & a_{n,R_n}^{t} \\ \downarrow & & \downarrow & \downarrow & \downarrow & & \downarrow \end{bmatrix}.$$

Block-Lipschitz Constant

$$\mathbf{A}_n^{t+1} \leftarrow P_{\mathcal{C}_n}\left(\mathbf{A}_n^t - \nabla f_n^t(\mathbf{A}_n^t)(\hat{\mathbf{L}}_n^t)^{-1}\right),$$

where

$$f_n^t(a) = \frac{1}{2}\left\|[\mathbf{B}; \mathbf{A}_1^{t+1}, \dots, \mathbf{A}_{n-1}^{t+1}, \mathbf{A}_n^t, \mathbf{A}_{n+1}^t, \dots, \mathbf{A}_N^t] - \mathbf{Y}\right\|_F^2$$

and

$$\hat{\mathbf{A}}_n^t = \begin{bmatrix} \uparrow & & \uparrow & \uparrow & \uparrow & & \uparrow \\ a_{n,1}^t & \cdots & a_{n,r-1}^t & a_{n,r}^t & a_{n,r+1}^t & \cdots & a_{n,R_n}^t \\ \downarrow & & \downarrow & \downarrow & \downarrow & & \downarrow \end{bmatrix}.$$

Momentum

Before a gradient step, we move $\mathbf{A}$ further in the direction of travel

$$\begin{aligned}\hat{\mathbf{A}}_n^t &\leftarrow \mathbf{A}_n^t + \omega_n^t(\mathbf{A}_n^t - \mathbf{A}_n^{t-1}) \\ &= \mathbf{A}_n^t(\mathrm{id}_{R_n} + \omega_n^t) - \mathbf{A}_n^{t-1}\omega_n^t\end{aligned}$$

where the amount of momentum is determined by

$$\omega_n^t \leftarrow \min\left(\hat{\omega}^t, \delta\sqrt{\hat{\mathbf{L}}_n^{t-1}(\hat{\mathbf{L}}_n^t)^{-1}}\right).$$

Methods for estimating rank

- Can be one of…
- `:spline`, default and often accurate
- `:finite_differences`, faster but less accurate
- `:circles`, fastest and smallest memory footprint, but more sensitive to results from factorize
- `:breakpoints`, picks the rank R that fits the model

$$f(r) = a + b(\min(r, R) - R) + c(\max(r, R) - R)$$

to the final errors