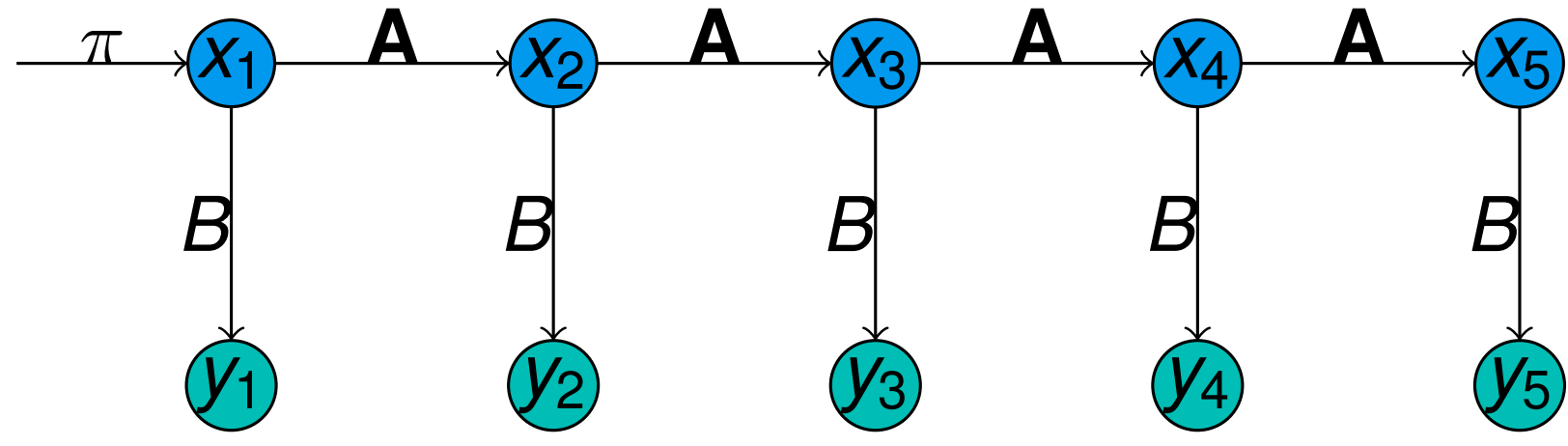


Hidden Markov Model



- ▶ **HMM**
 π, \mathbf{A} - Markov chain, B - emission matrix,
- ▶ **GaussianHMM**
 π, \mathbf{A} - Markov chain, B - family of Gaussian distributions,
- ▶ **DenseHMM [1] & GaussianDenseHMM [2]**
 π, \mathbf{A} - obtained from embedding, B - emission matrix or a family of Gaussian distributions,
- ▶ **FlowHMM [3]**
 π, \mathbf{A} - Markov chain, B - family of normalizing flow models,
- ▶ ...

Co-occurrence matrix for discrete emission

Empirical co-occurrence matrix:

$$\mathbf{Q}_{vw}^{gt} = \frac{\#\{t: y_t = v, y_{t+1} = w\}}{T-1}$$

Example:

Sequence from HMM (letters are observations, colors are hidden states) with underlined co-occurrences of the values a and b :

$a, c, \underline{a}, b, b, c, a, \underline{a}, b, c, b, c, d, c, b, b.$

Counts the co-occurrences for each pair of values:

	a	b	c	d
a	1	2	1	0
b	0	2	3	0
c	2	2	0	1
d	0	0	1	0

Co-occurrence matrix derived from model parameters:

$$\mathbf{Q}_{vw} = P(Y_t = v, Y_{t+1} = w) = \sum_{i=1}^N \sum_{j=1}^N P(X_t = i) B_i(v) \mathbf{A}_{ij} B_j(w).$$

Let us assume that π is the stationary distribution of the Markov chain:

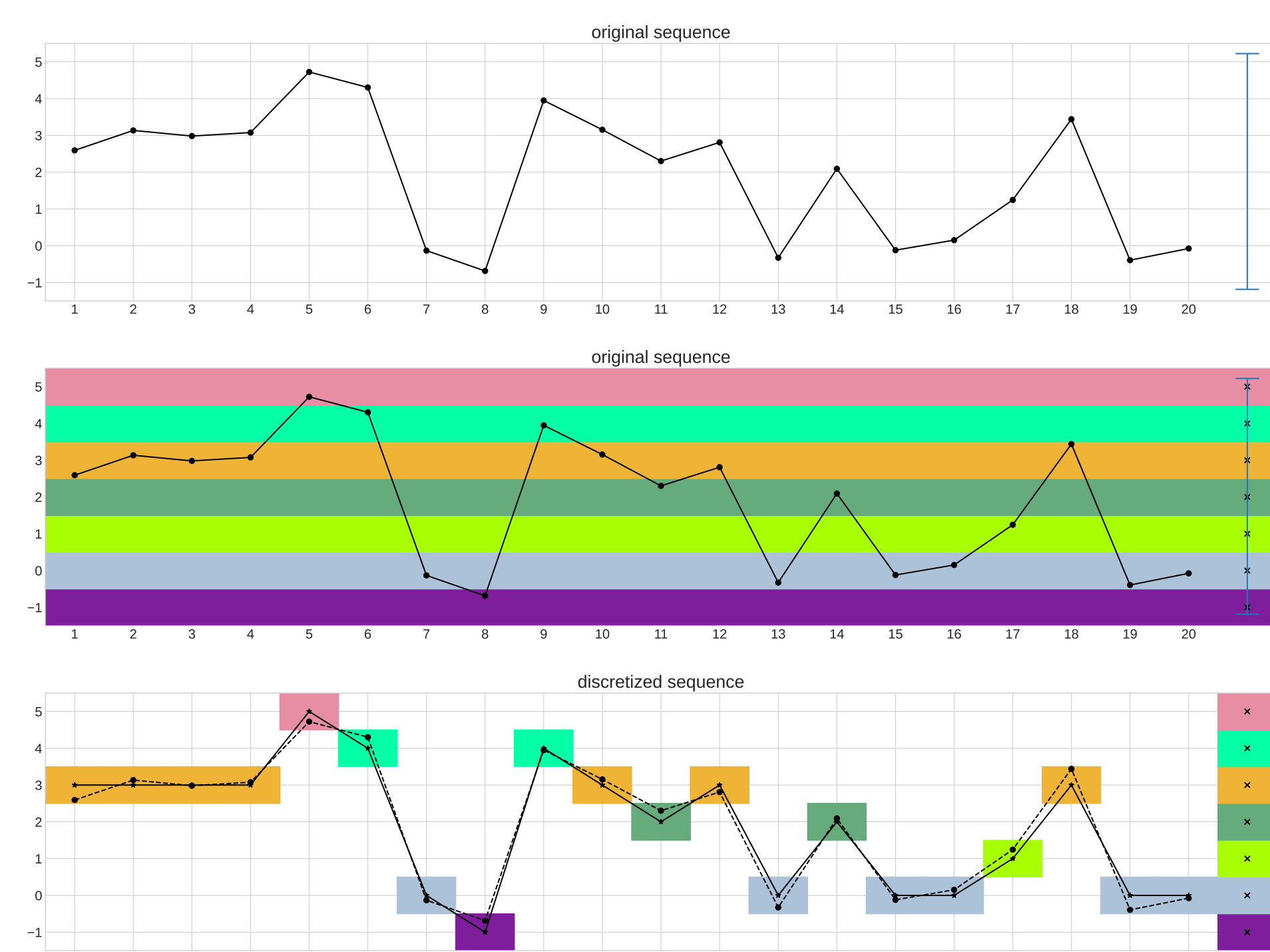
$$\mathbf{Q}_{vw} = \sum_{i=1}^N \sum_{j=1}^N \pi_i B_{iv} \mathbf{A}_{ij} B_{jw},$$

$$\mathbf{Q} = \mathbf{B}^T \mathbf{S} \mathbf{B}, \text{ where } \mathbf{S}_{ij} = \pi_i \mathbf{A}_{ij}(1)$$

Discretization of continuous values

Let us define a (minimal) hypercube $\hat{\mathcal{Y}}$ containing all observed values $y_{1:T}$ and fix $M^D \in \mathbb{N}$. Let us define a discrete set $\mathcal{Y}^D = \{v_1^D, \dots, v_{M^D}^D\}$, $v_i^D \in \hat{\mathcal{Y}}$. **Discretization [4]** is a function $\mathcal{D}: \mathbb{R}^m \rightarrow \mathcal{Y}^D$:

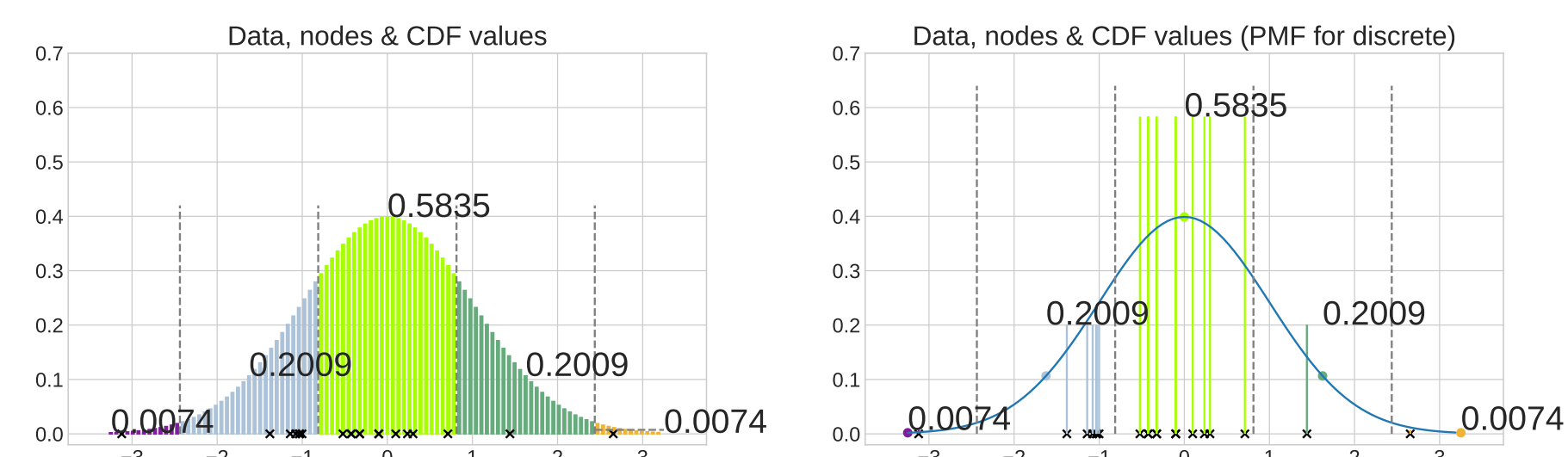
$$\mathcal{D}(y) = \arg \min_{v \in \mathcal{Y}^D} \|y - v\|.$$



One needs also to discretize the probabilities; see Eq. (3), (4).

Exact probabilities in discretization

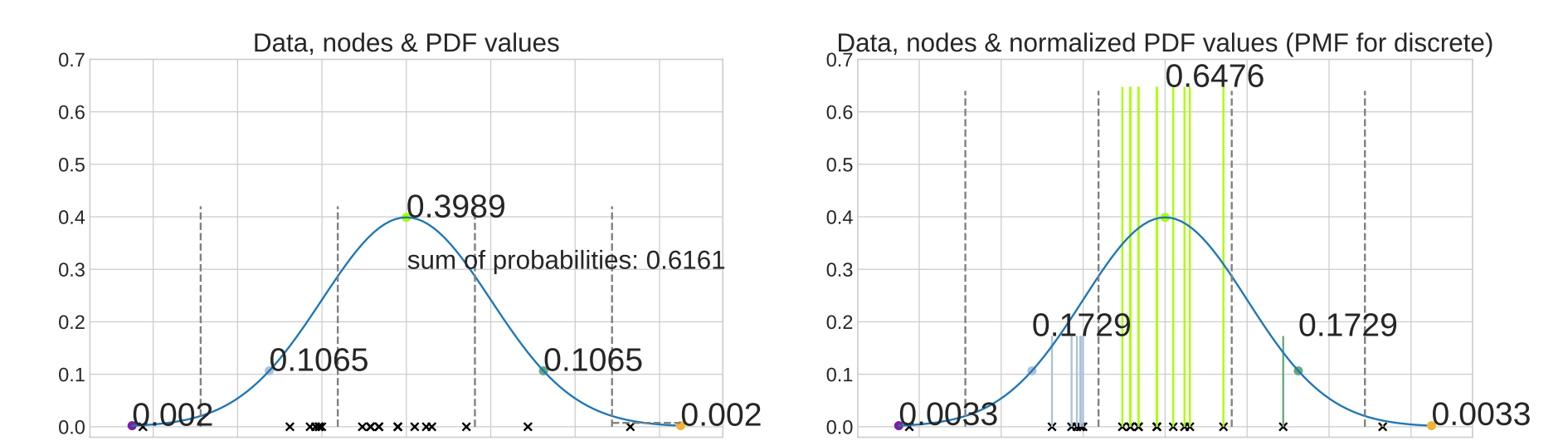
$$P(\mathcal{D}(y) = v^D | x = i) = \int_{\{y: \mathcal{D}(y) = v^D\}} B_i(y) dy \quad (3)$$



- ▶ find the region boundaries (the set of observations resulting in a given discrete value)
- ▶ integrate the PDF within the region

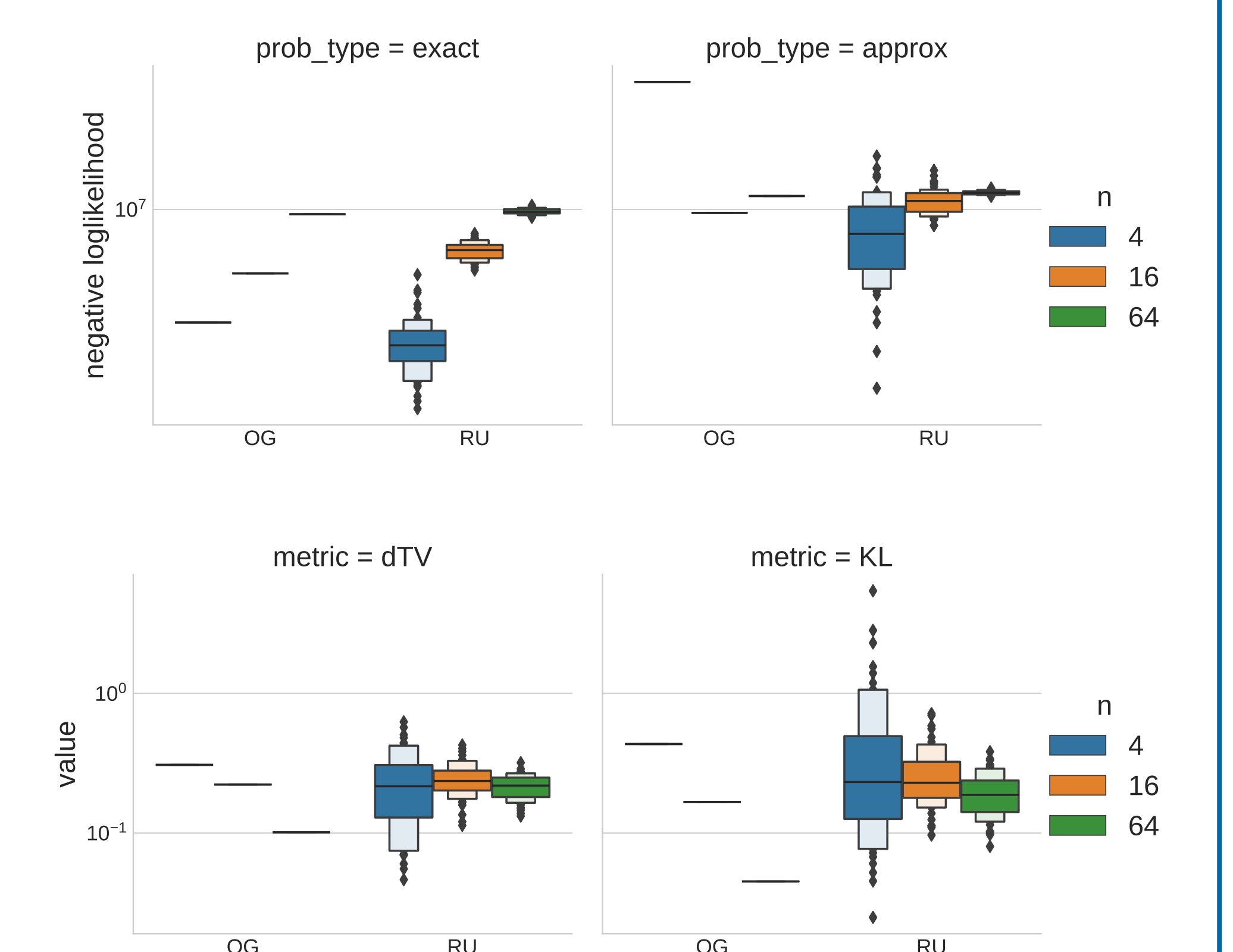
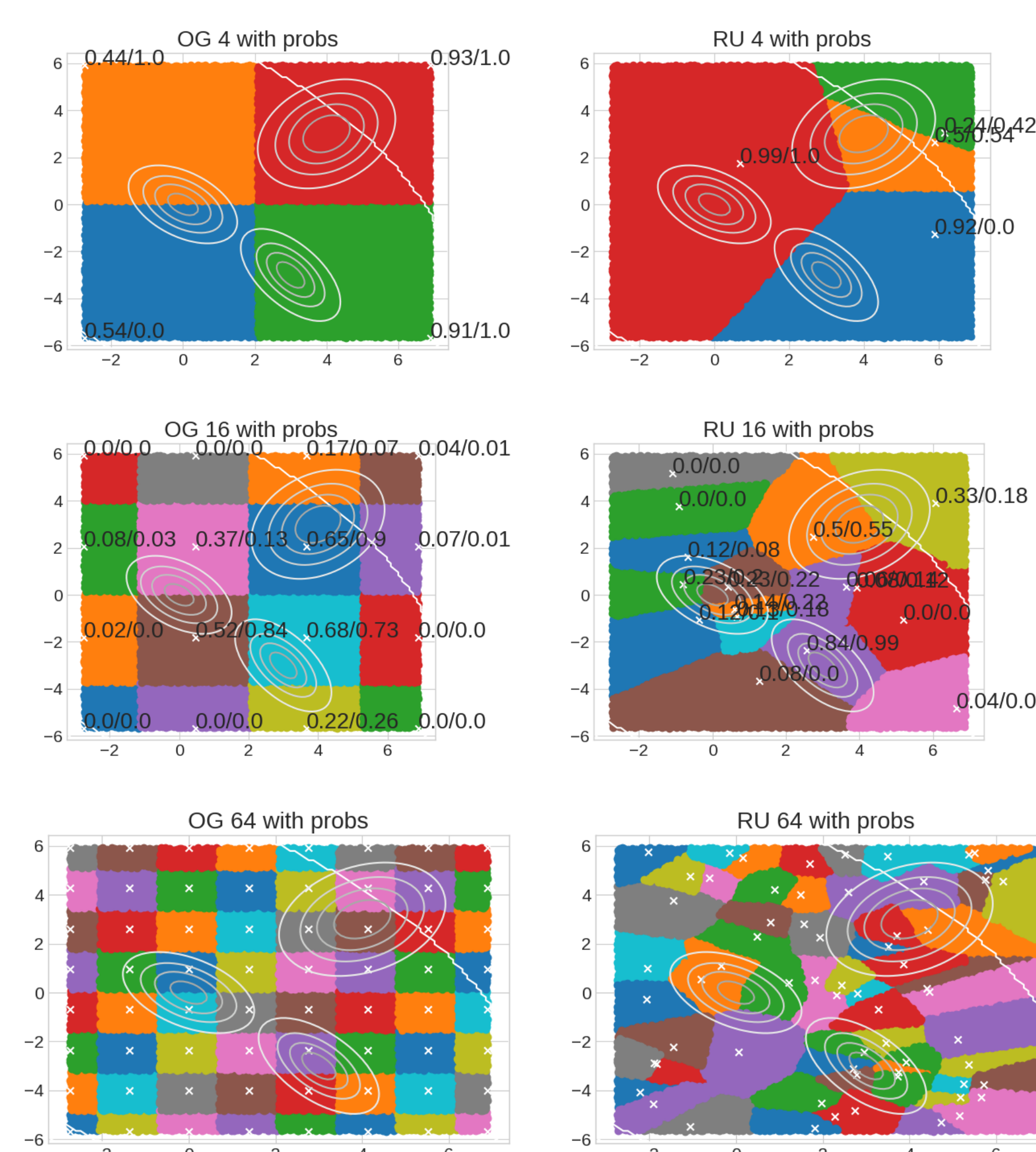
Approximate probabilities in discretization

$$P(\mathcal{D}(y) = v^D | x = i) \approx \frac{B_i(v^D)}{\sum_{w^D \in \mathcal{Y}^D} B_i(w^D)} \quad (4)$$



- ▶ calculate the PDF function in the discrete values
- ▶ normalize the obtained PDF values (to assure obtaining a discrete probability distribution)

Comparison of exact and approximate probabilities



$$d_{TV}(\mu, \nu) = \frac{1}{2} \sum_i |\mu(v_i^D) - \nu(v_i^D)|, \quad KL(\mu || \nu) = \sum_i \mu(v_i^D) \log \frac{\mu(v_i^D)}{\nu(v_i^D)}$$

Training schema

- ▶ **EM**
- ▶ **GD**
We can use SGD, Adam, etc., for optimizing

$$\mathbf{S}, \mathbf{B} = \arg \min_{\tilde{\mathbf{S}}, \tilde{\mathbf{B}}} \|\mathbf{Q}^{gt} - \mathbf{Q}\|.$$

We optimize **unconstrained matrices $\tilde{\mathbf{S}}, \tilde{\mathbf{B}}$** and convert them via softmax:

$$\mathbf{S}, \mathbf{B} = \arg \min_{\tilde{\mathbf{S}}, \tilde{\mathbf{B}}} \left\| \mathbf{Q}^{gt} - \left(\frac{\exp(\tilde{\mathbf{B}})}{\sum_{w=1}^M \exp(\tilde{\mathbf{B}}_w)} \right)^T \frac{\exp(\tilde{\mathbf{S}})}{\sum_{i=1}^N \sum_{j=1}^N \exp(\tilde{\mathbf{S}}_{ij})} \frac{\exp(\tilde{\mathbf{B}})}{\sum_{w=1}^M \exp(\tilde{\mathbf{B}}_w)} \right\|$$

- ▶ **NMF [5]**
We will use the pseudo inverses (from Eq. (1)):

$$\mathbf{S} = \mathbf{B}^{-1} \mathbf{Q} (\mathbf{B}^T)^{-1}, \quad (2a)$$

$$\mathbf{B} = ((\mathbf{S} \mathbf{B})^{-1} \mathbf{Q})^T, \quad (2b)$$

$$\mathbf{B} = \mathbf{Q} (\mathbf{B}^T \mathbf{S})^{-1}. \quad (2c)$$

The update procedure is:

pseudo inverse > ReLU > softmax.

In each iteration, we update the following:

- ▶ \mathbf{S} with Eq. (2a)
- ▶ \mathbf{B} with Eq. (2b)
- ▶ \mathbf{S} with Eq. (2a)
- ▶ \mathbf{B} with Eq. (2c)

Conclusions

	exact	approx
fast to compute	✗	✓
available for all distributions	✗	✓
domain aware	✓	✗
accurate	✓	✗

- ▶ Many multivariate distributions don't have analytical formulas for CDFs (thus, we estimate the exact probabilities with Monte Carlo methods, which is time-consuming to perform in each training step)
- ▶ The approximation of probabilities disrupts the distribution of discrete values visibly (over 10%) and may affect the learning process.
- ▶ Exact values result in better likelihood than approximate.
- ▶ The random uniform grid is expected to work better than the ordinary grid.
- ▶ Discrete likelihood is incomparable to continuous likelihood.

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