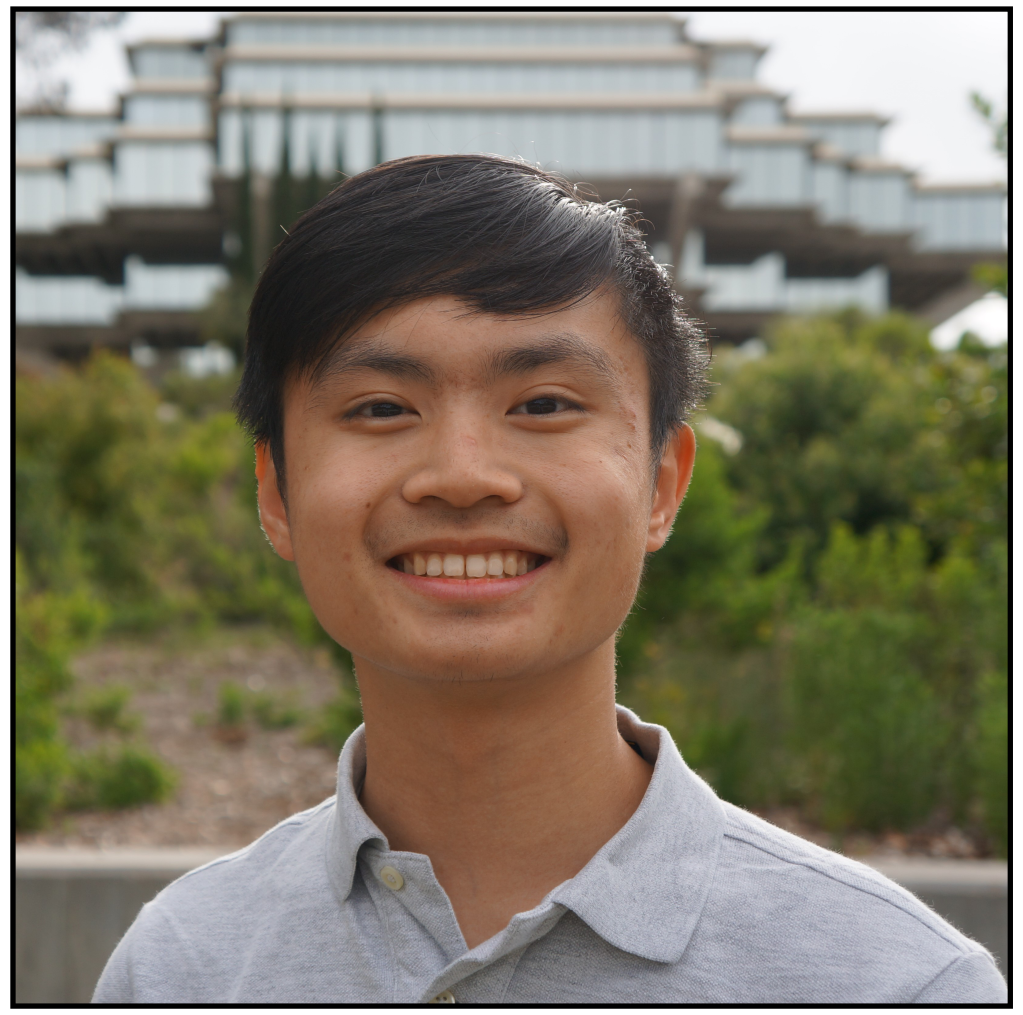
Efficient Algorithm for Sparse Fourier Transform of Generalized q-ary Functions

Darin Tsui*



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* = equal contributions

Scaling machine learning models

120B parameters

Scaling machine learning models

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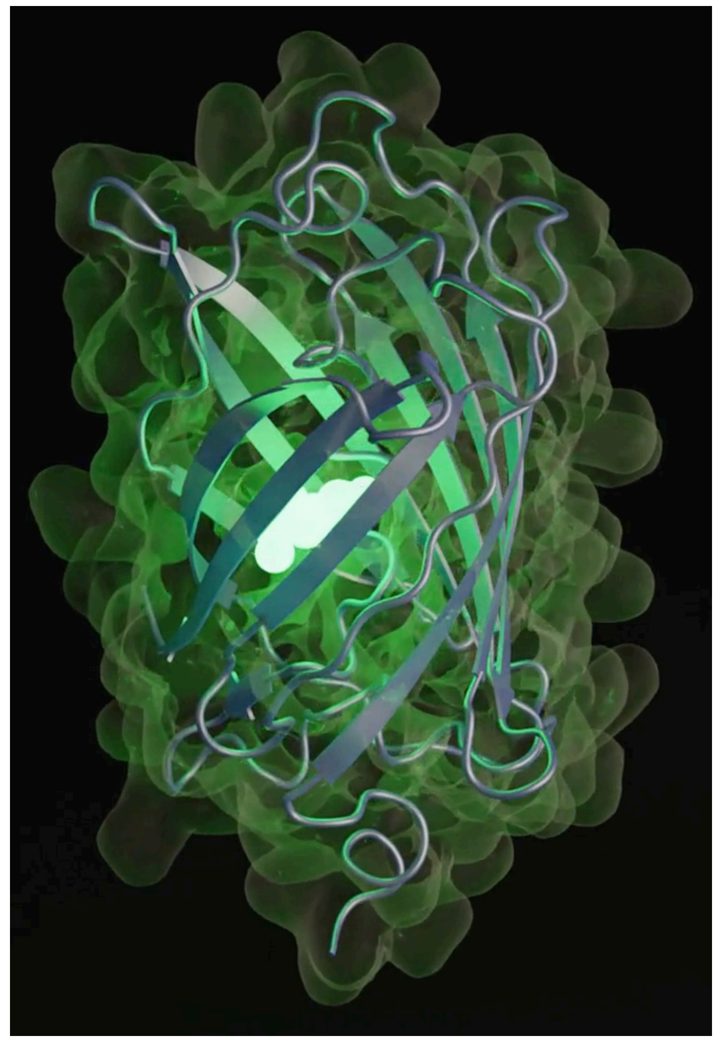
ESM3: Simulating 500 million years of evolution with a language model

Preview our paper ↗

Trained on **2.78 Billion** natural proteins

Scaling machine learning models

120B parameters



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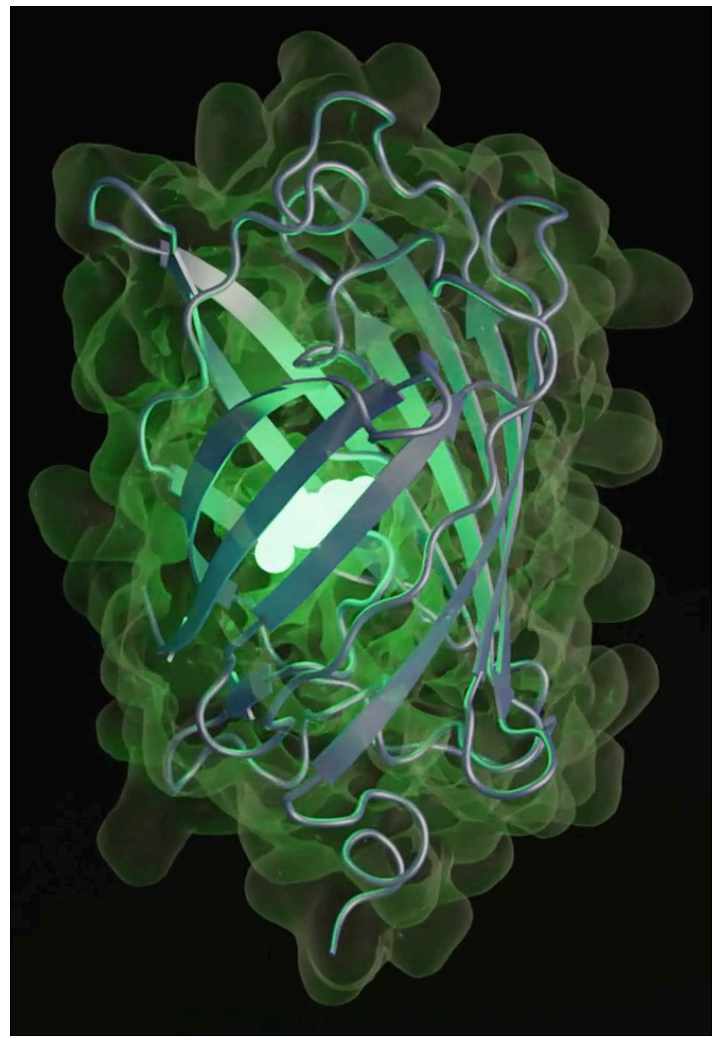

ESM3: Simulating 500 million years of evolution with a language model

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But does our power to **explain** them also **scale**?

These functions can be modeled as *q*-ary functions

$$f : \mathbb{Z}_q^n \rightarrow \mathbb{R}$$

$$f(x_1, x_2, x_3, \cdots, x_n) \rightarrow y$$

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$$f : \mathbb{Z}_q^n \to \mathbb{R}$$

$$f(x_1, x_2, x_3, \cdots, x_n) \to y$$

$$x_i \in \{0, 1, \cdots, q - 1\}$$

These functions can be modeled as *q*-ary functions

$$f : \mathbb{Z}_{20}^{n} \to \mathbb{R}$$

$$f(x_1, x_2, x_3, \cdots, x_n) \to$$ 

$$x_i \in \{P, L, S, \cdots, C\}$$

These functions can be modeled as *q*-ary functions

$$f : \mathbb{Z}_3^n \to \mathbb{R}$$

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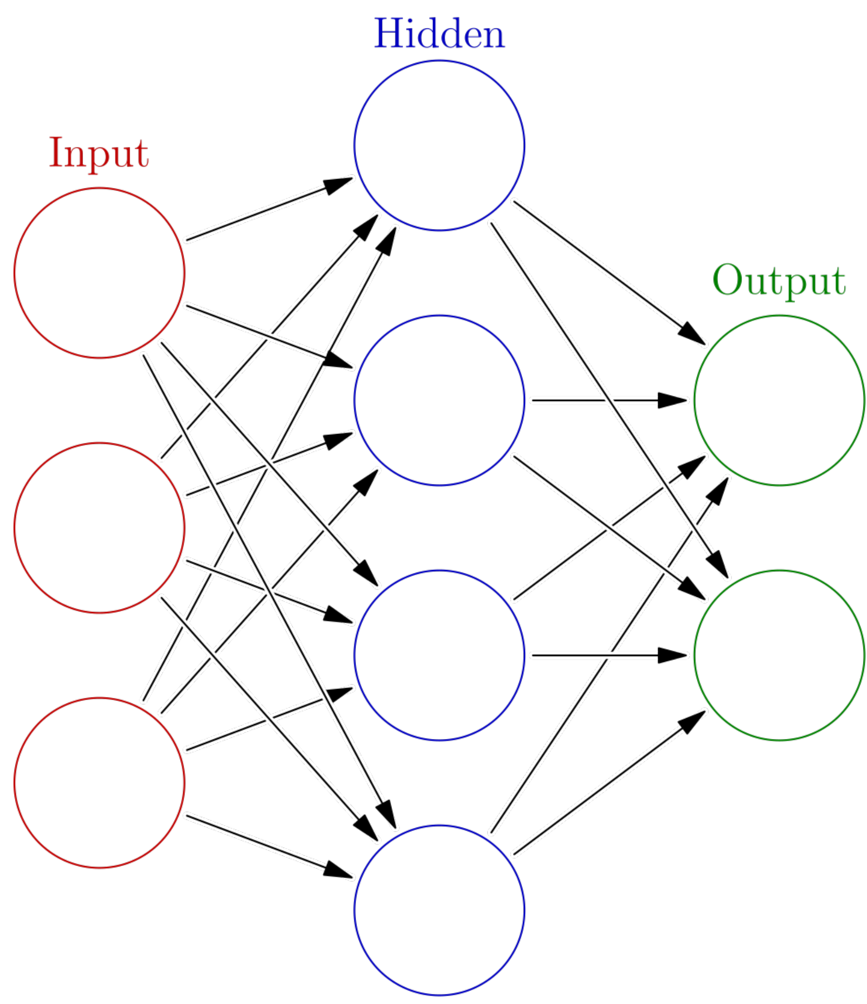


$$x_i \in \{\text{Class } 1, \text{Class } 2, \text{Class } 3\}$$

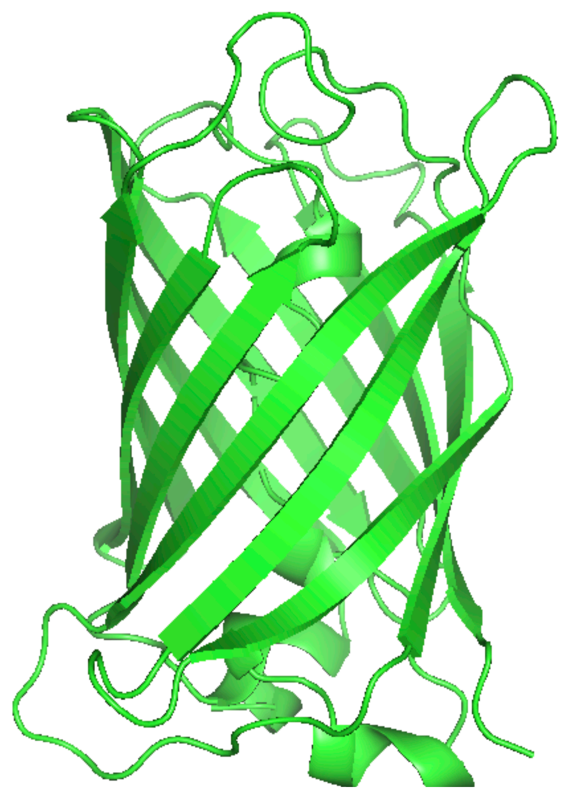
These functions can be modeled as *q*-ary functions

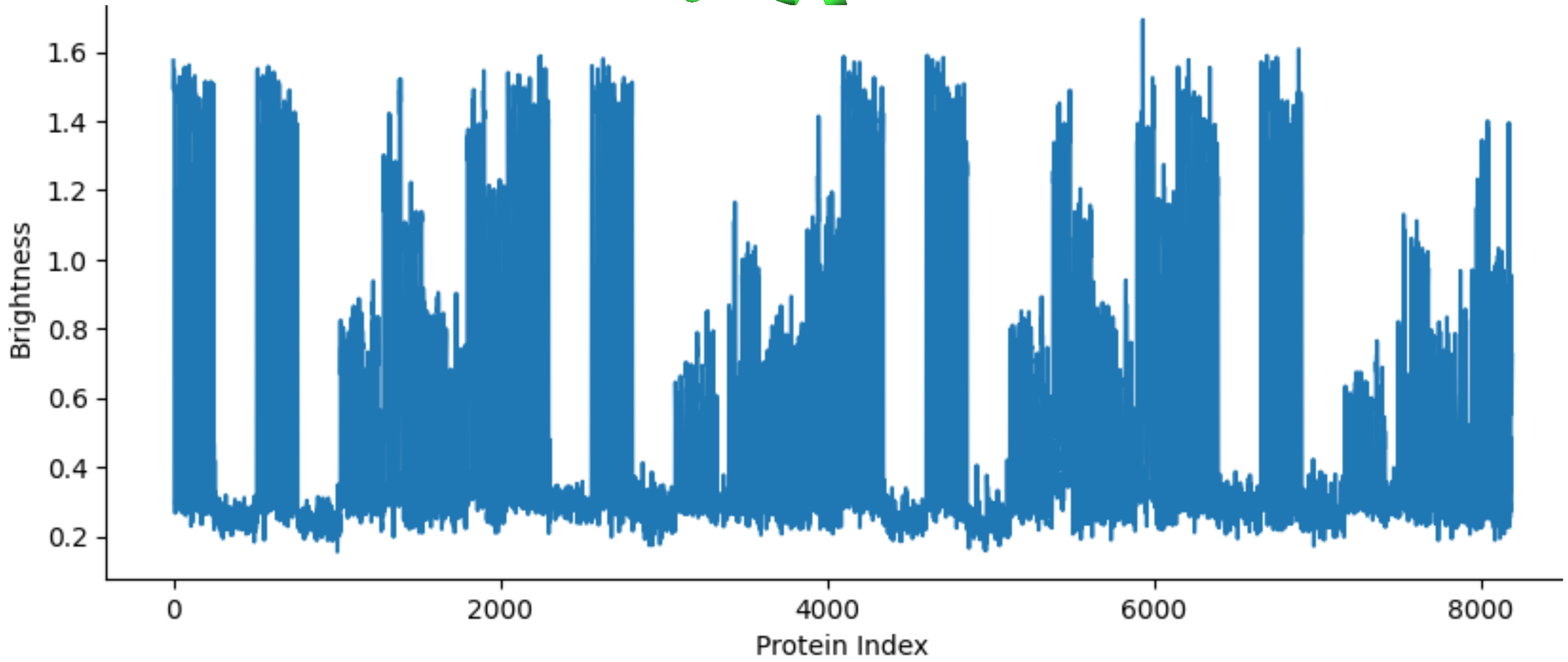
$$f : \mathbb{Z}_4^n \rightarrow \mathbb{R}$$

$$f(x_1, x_2, x_3, \cdots, x_n) \rightarrow$$ 

$$x_i \in \{\text{"love"}, \text{"hate"}, \text{"regret"}, \text{"miss"}\}$$

Many functions of interest have *sparse Fourier transforms*





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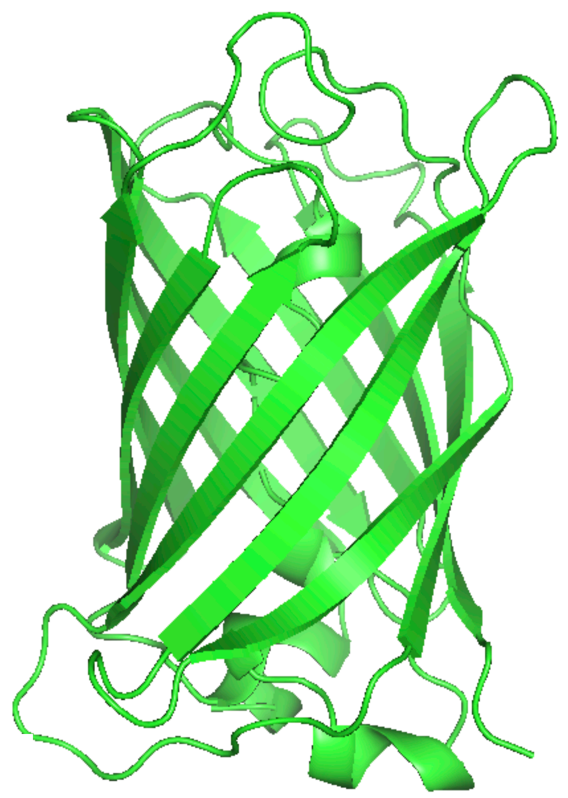
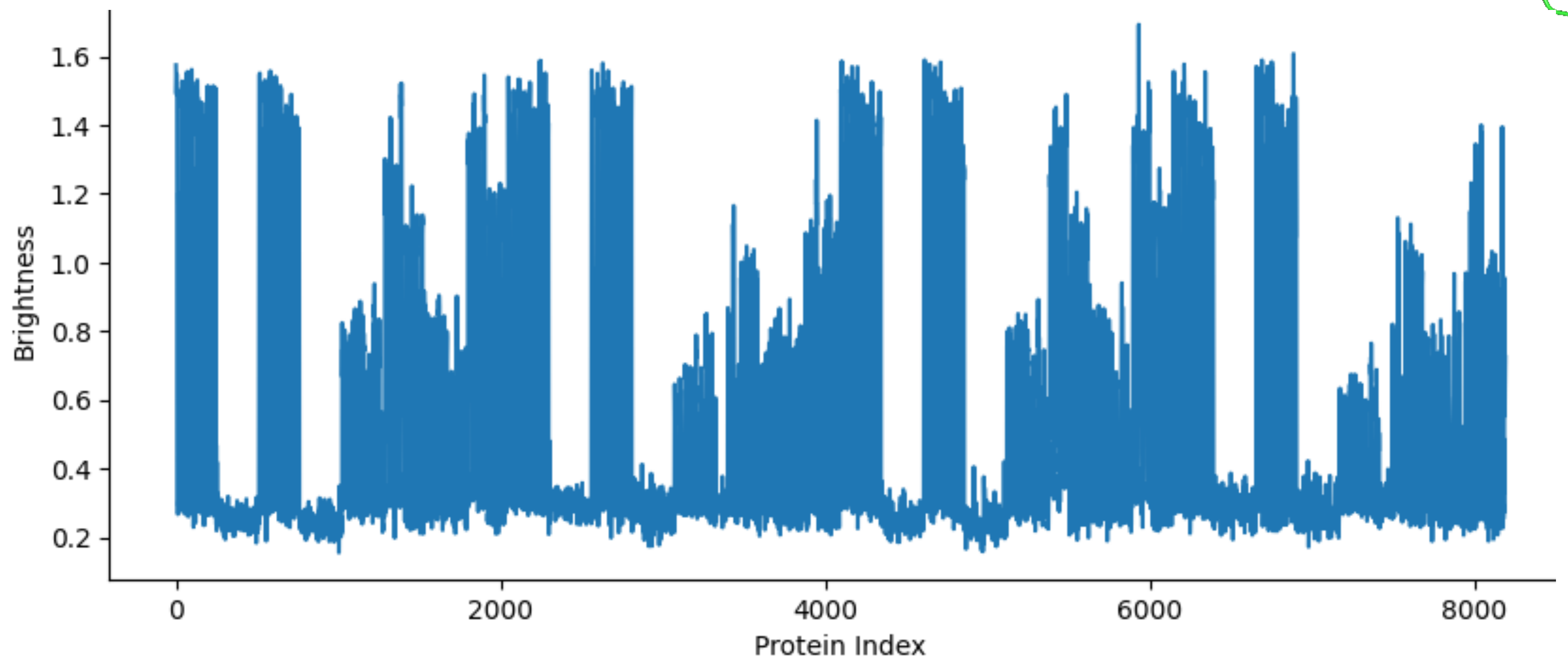
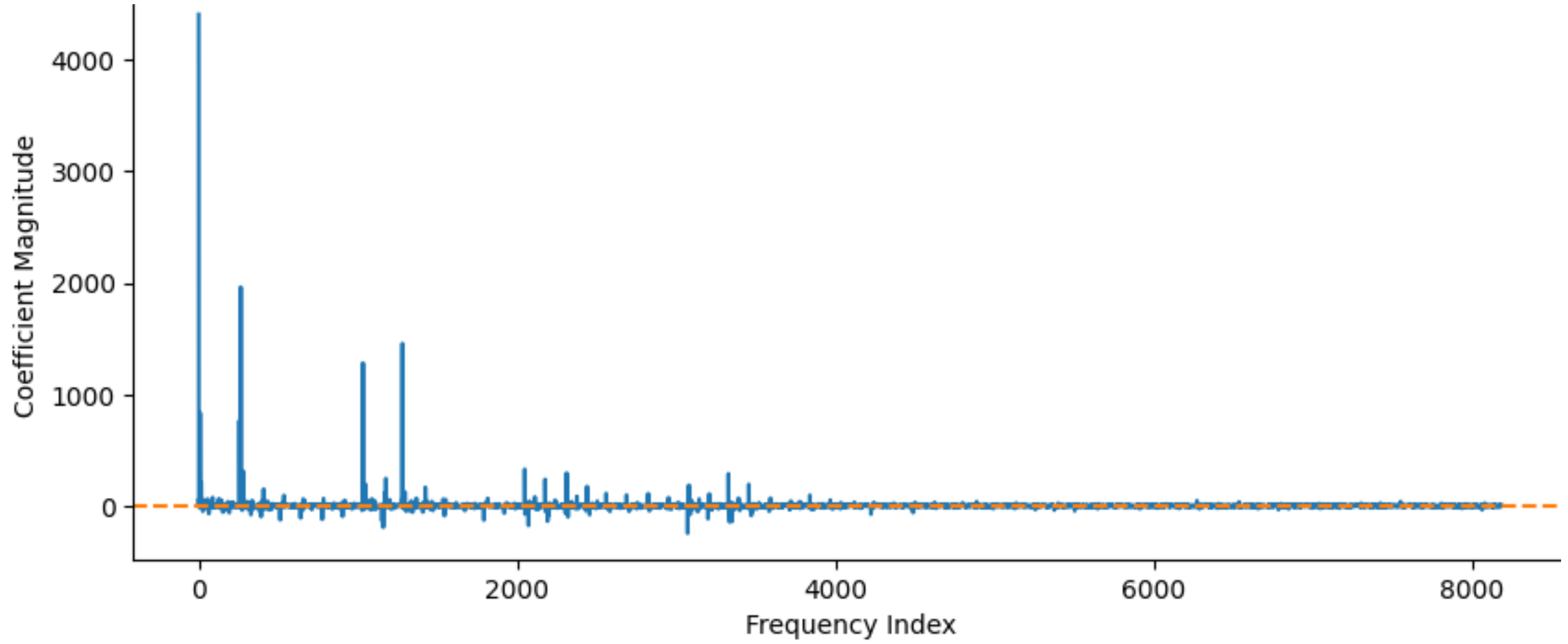


$$f(\mathbf{m}) \xrightarrow{\mathcal{F}} F[\mathbf{k}]$$





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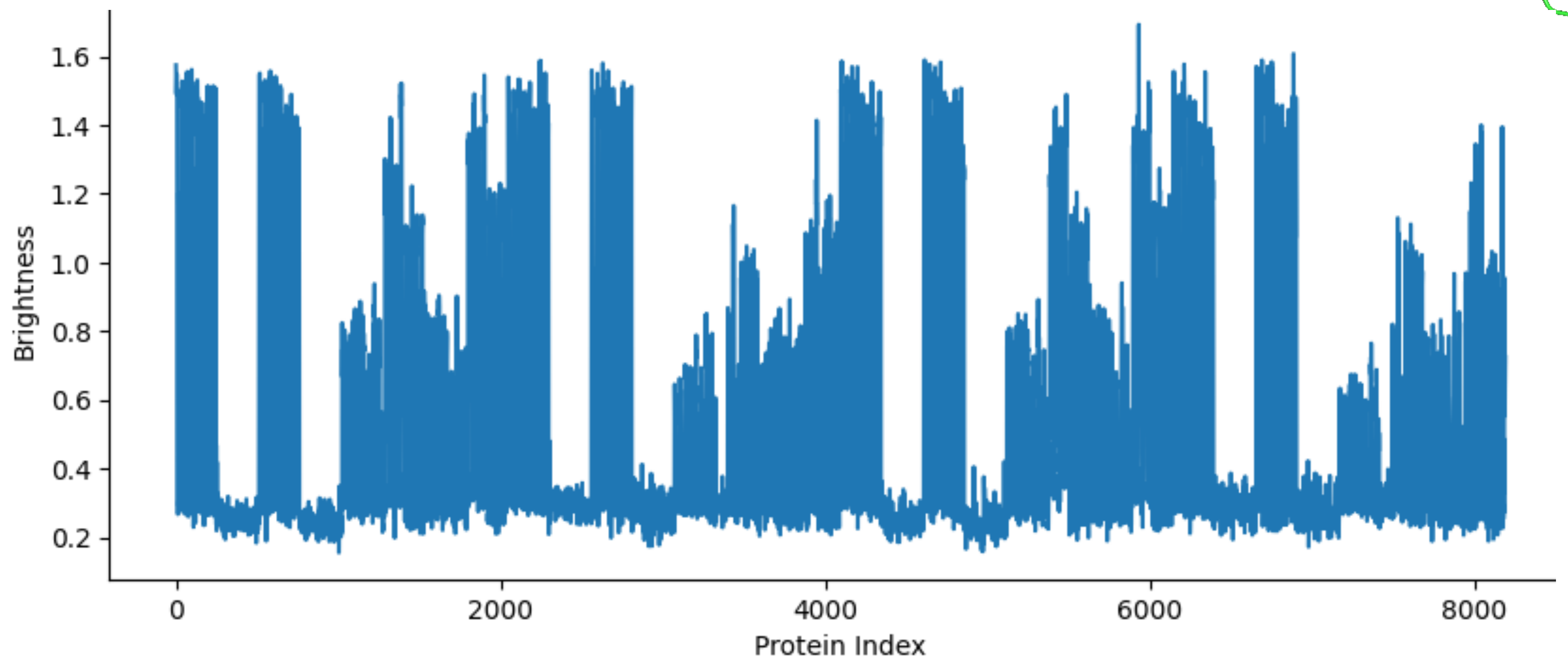

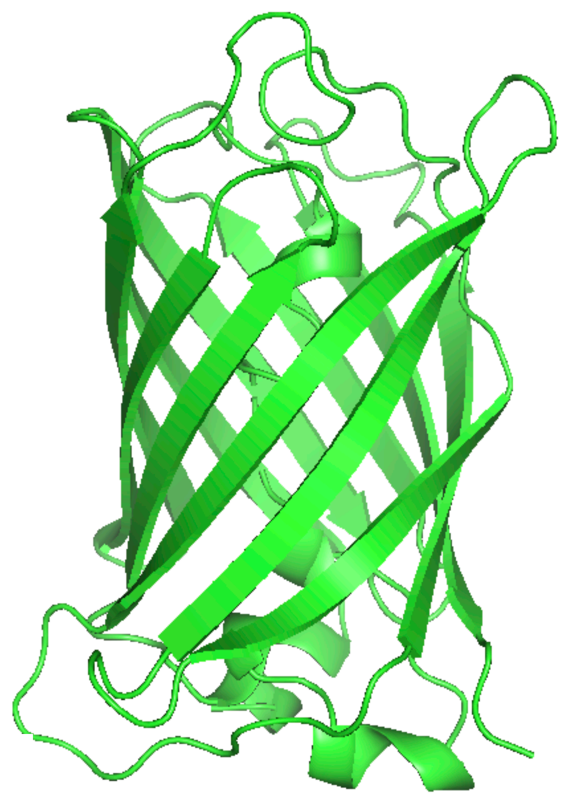

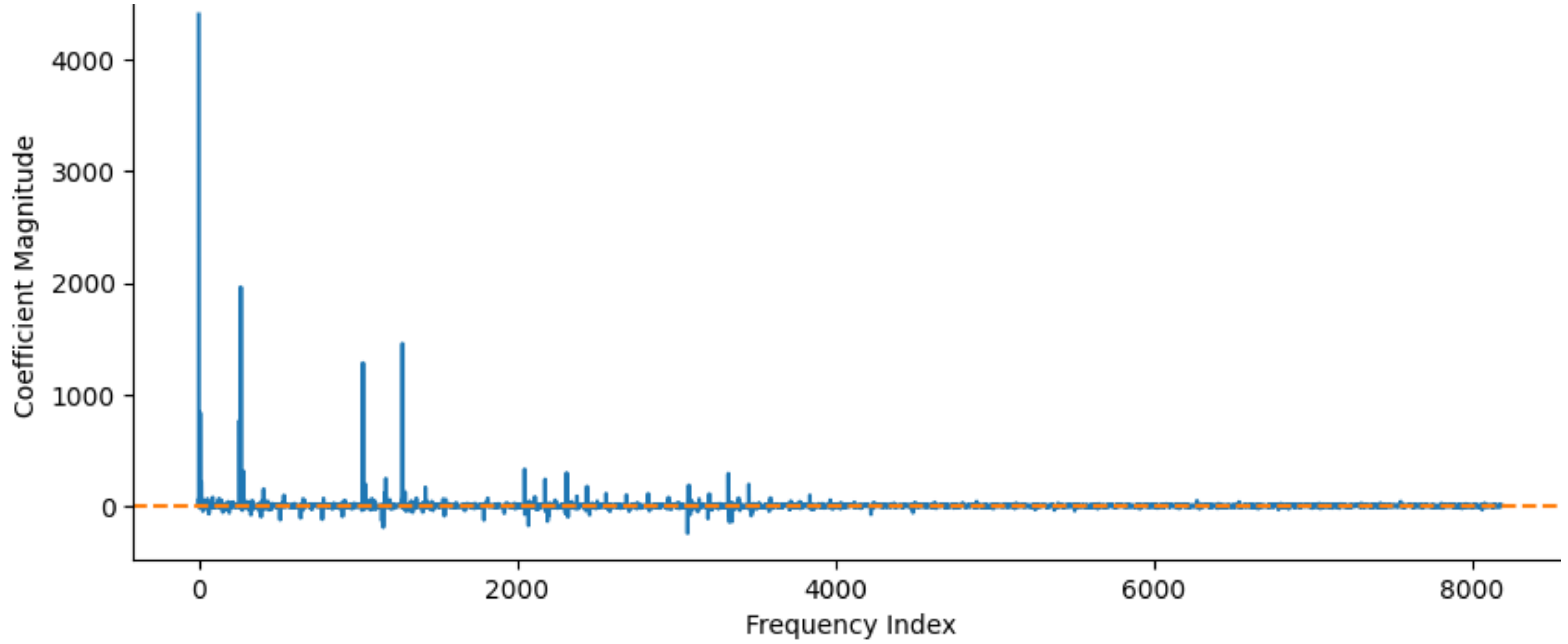

Top 40 Fourier coefficients explain **99%** of energy

Previous works

q-sft [1]: We can compute the Fourier transform of an *s*-sparse *q*-ary function with sublinear sample and computational complexity, with vanishing error probability as the function gets larger

$$F[\mathbf{k}] = \frac{1}{q^n} \sum_{\mathbf{m} \in \mathbb{Z}_q^n} f(\mathbf{m}) e^{-\frac{2j\pi}{q}}$$

[1] *Y. E. Erginbas, J. S. Kang, A. Aghazadeh, and K. Ramchandran,"Efficiently computing sparse Fourier transforms of q-ary functions," in 2023 IEEE International Symposium on Information Theory (ISIT), 2023.*

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q is fixed

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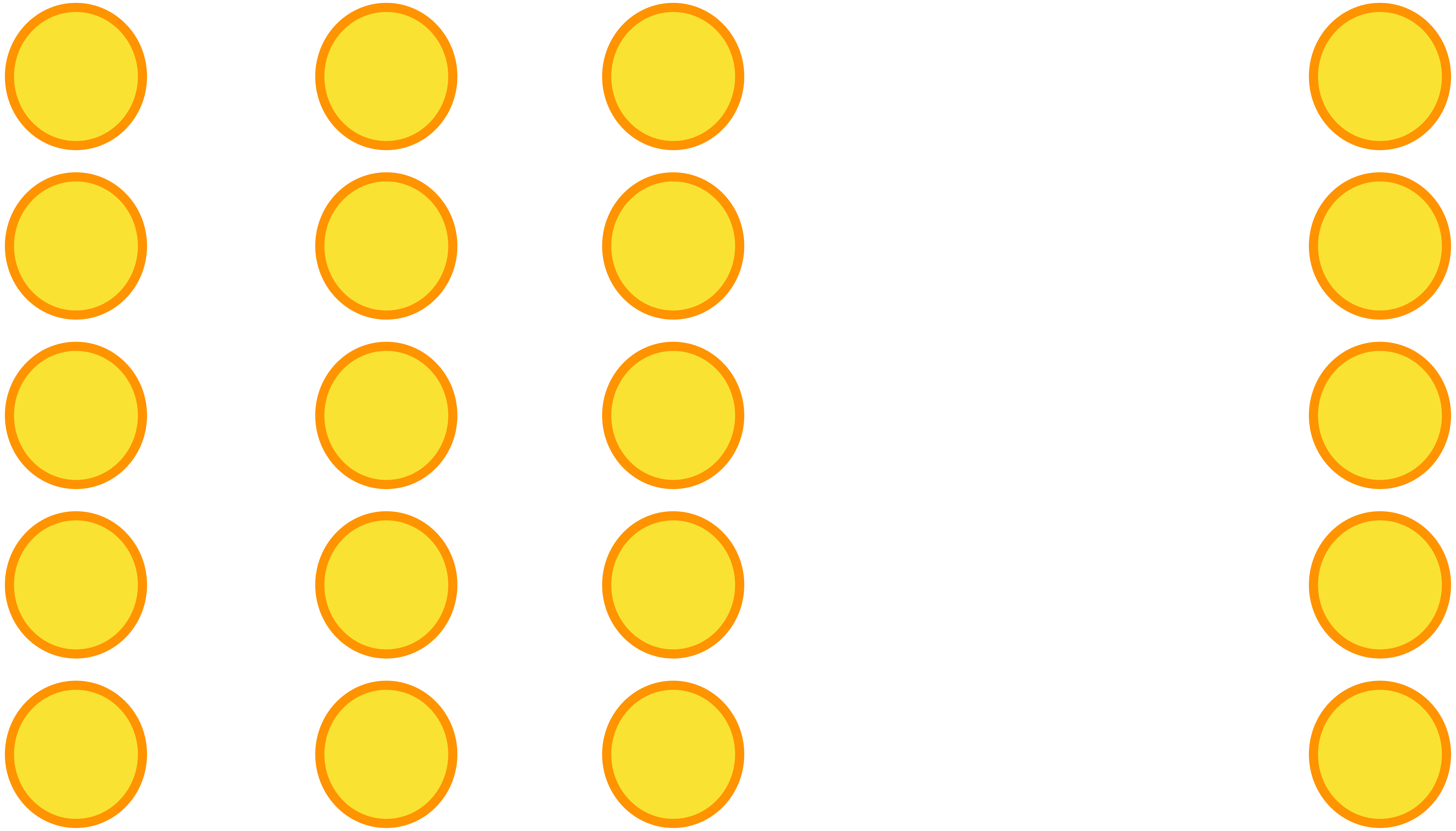
q may vary

$$f(x_1, x_2, x_3, \cdots, x_n) \rightarrow y$$



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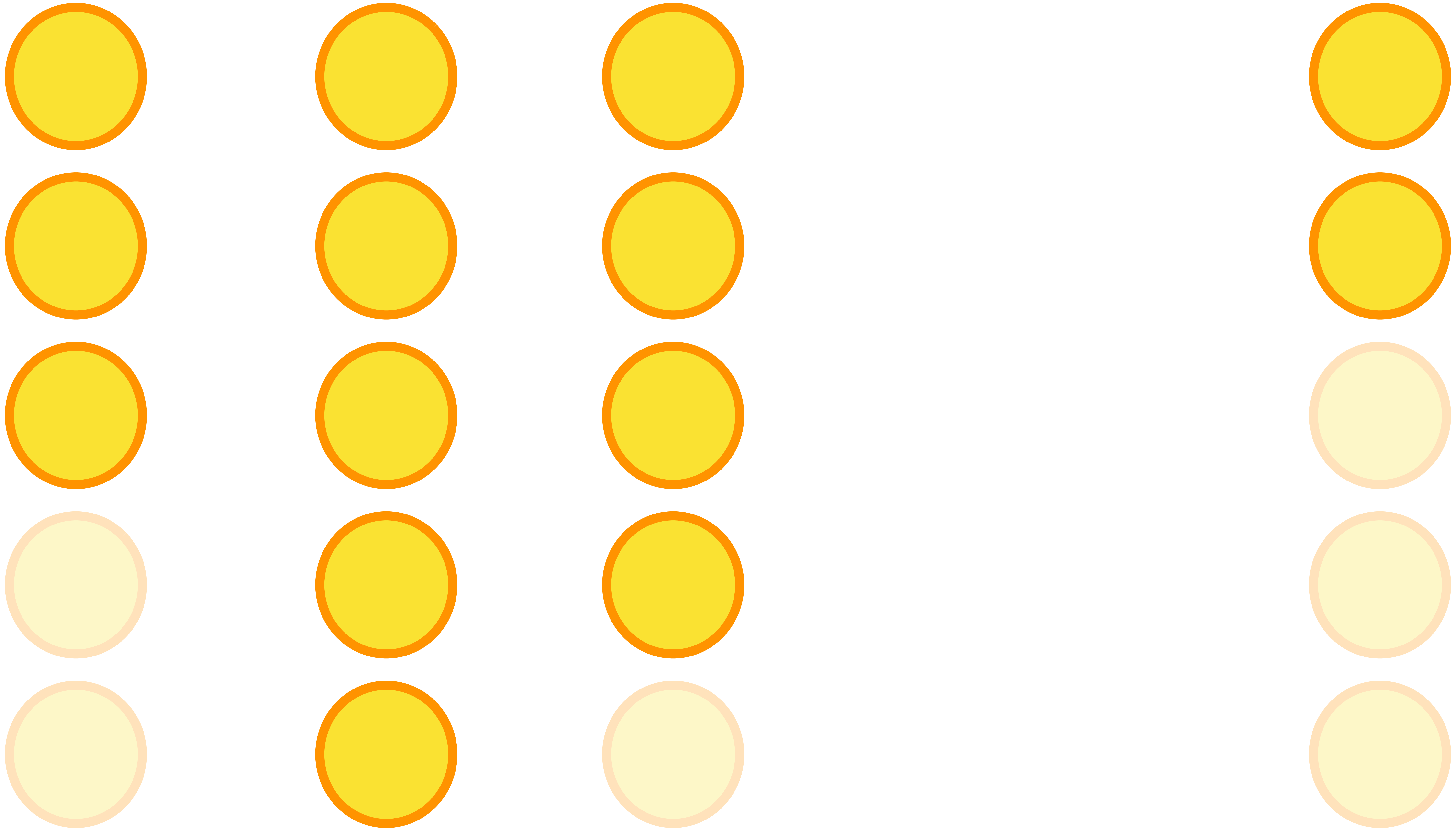
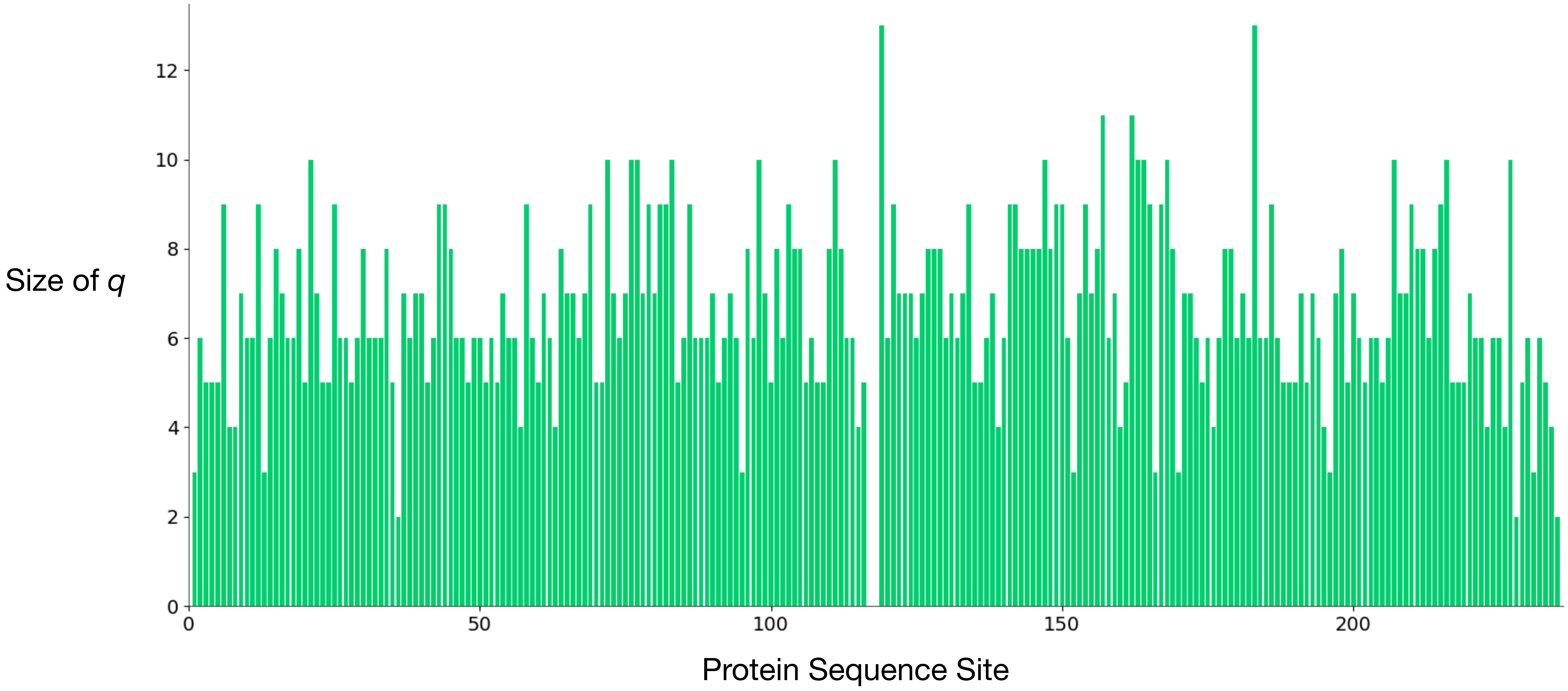


Generalized *q*-ary functions

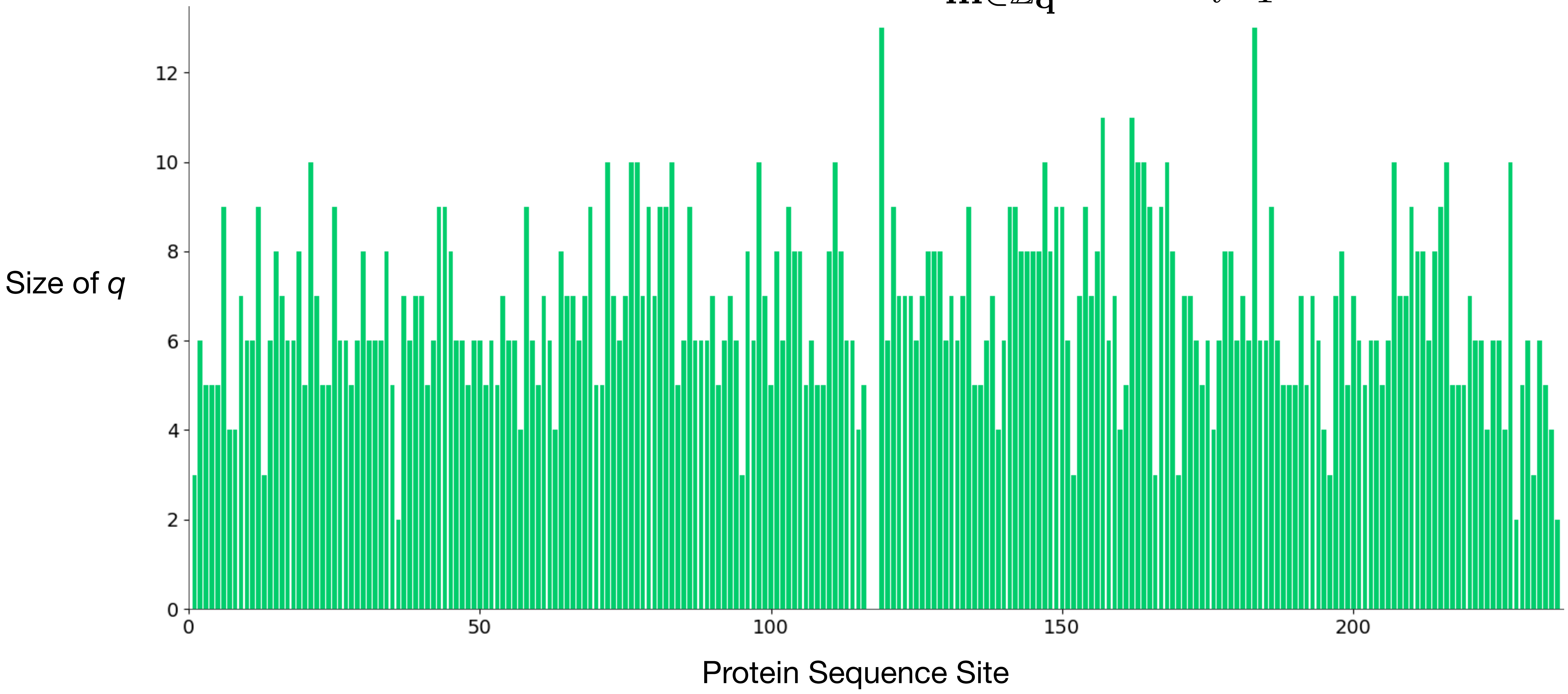
$$\mathbb{Z}_{\mathbf{q}} \triangleq \mathbb{Z}_{q_1} \times \mathbb{Z}_{q_2} \times \cdots \times \mathbb{Z}_{q_n}$$



Generalized *q*-ary functions

$$\mathbb{Z}_{\mathbf{q}} \triangleq \mathbb{Z}_{q_1} \times \mathbb{Z}_{q_2} \times \cdots \times \mathbb{Z}_{q_n}$$

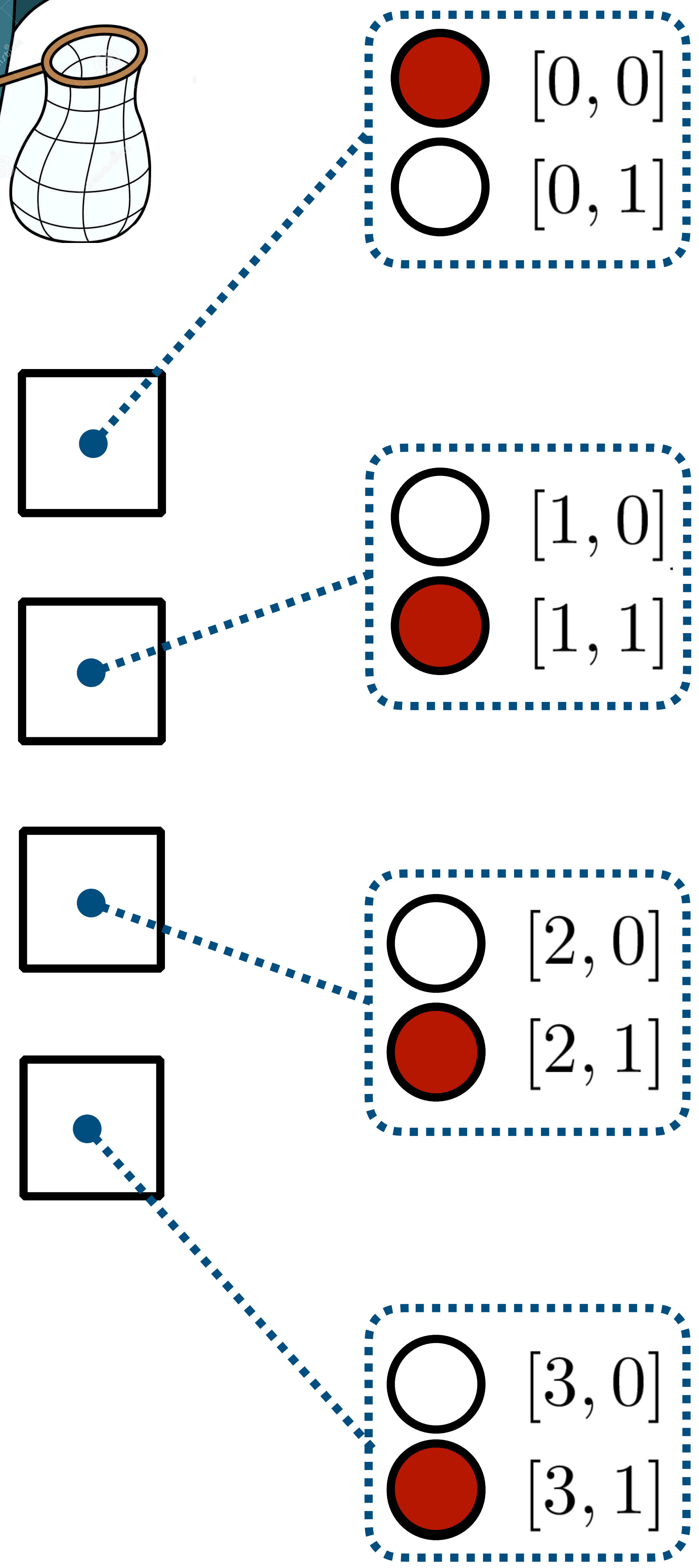
$$F[\mathbf{k}] = \frac{1}{\prod_{i=1}^{n} q_i} \sum_{\mathbf{m} \in \mathbb{Z}_{\mathbf{q}}} f(\mathbf{m}) \prod_{i=1}^{n} e^{-\frac{2j\pi}{q_i}}$$



GFast: Efficiently computing generalized *q*-ary Fourier transforms

Theorem. We can recover a $N = \prod_{i=1}^{n} q_i$ -dimensional generalized *q*-ary function whose Fourier is s-sparse

- with **sample complexity** $O(sn^2)$
- with **computational complexity** $O(sn^2 \log N)$
- assumption: interactions chosen **uniformly** at random
- high probability guarantee + robust to noise



- Key strategy
  - smart subsampling
  - small Fourier transform
  - sparse graph codes

fix one position, enumerate the rest

$$\begin{array}{l} \quad\;\; q_1 \;\; q_2 \\ \mathbf{q} = [4, 2] \\ n = 2 \text{ sites} \\ N = 4 \times 2 = 8 \end{array}$$

$$\underset{\mathbf{y}}{\begin{bmatrix} 6 \\ -2 \\ 0 \\ 4 \\ 2 \\ 2 \\ 0 \\ 4 \end{bmatrix}} = \underbrace{\overset{\mathbf{W}}{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & w_2 & 1 & w_2 & 1 & w_2 & 1 & w_2 \\ 1 & 1 & w_4 & w_4 & w_4^2 & w_4^2 & w_4^3 & w_4^3 \\ 1 & w_2 & w_4 & w_4 w_2 & w_4^2 & w_4^2 w_2 & w_4^3 & w_4^3 w_2 \\ 1 & 1 & w_4^2 & w_4^2 & 1 & 1 & w_4^2 & w_4^2 \\ 1 & w_2 & w_4^2 & w_4^2 w_2 & 1 & w_2 & w_4^2 & w_4^2 w_2 \\ 1 & 1 & w_4^3 & w_4^3 & w_4^2 & w_4^2 & w_4 & w_4 \\ 1 & w_2 & w_4^3 & w_4^3 w_2 & w_4^2 & w_4^2 w_2 & w_4 & w_4 w_2 \end{bmatrix}}}_{\text{generalized } q\text{-ary Fourier transform matrix}} \overset{\mathbf{x}}{\begin{bmatrix} 2 \\ 0 \\ 0 \\ 1 \\ 0 \\ 2 \\ 0 \\ 1 \end{bmatrix}}$$

$$\omega_{q_i} = e^{\frac{2\pi j}{q_i}}$$

$y = f([x_1, x_2])$

x_1	x_2	y
0	0	2
0	1	2
1	0	0
1	1	4
2	0	6
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$n = 2$ sites

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$$\underset{\mathbf{y}_T}{\begin{bmatrix} 6 \\ 0 \\ 2 \\ 0 \end{bmatrix}} = \underset{\mathbf{W}_T}{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & w_4 & w_4 & w_4^2 & w_4^2 & w_4^3 & w_4^3 \\ 1 & 1 & w_4^2 & w_4^2 & 1 & 1 & w_4^2 & w_4^2 \\ 1 & 1 & w_4^3 & w_4^3 & w_4^2 & w_4^2 & w_4 & w_4 \end{bmatrix}} \underset{\mathbf{x}}{\begin{bmatrix} \color{red}{2} \\ 0 \\ 0 \\ \color{red}{1} \\ 0 \\ \color{red}{2} \\ 0 \\ \color{red}{1} \end{bmatrix}}$$

regularly subsampled FT matrix

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take small Fourier transform

$$\begin{array}{cc} q_1 & q_2 \end{array}$$
$$\mathbf{q} = [4, 2]$$
$$n = 2 \text{ sites}$$
$$N = 4 \times 2 = 8$$

$$\mathbf{y}_T \quad \frac{1}{4}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & w_4 & w_4^2 & w_4^3 \\ 1 & w_4^2 & 1 & w_4^2 \\ 1 & w_4^3 & w_4^2 & w_4 \end{bmatrix} \times \quad \mathbf{W}_T \quad \mathbf{x}$$

$$\begin{bmatrix} 6 \\ 0 \\ 2 \\ 0 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & w_4 & w_4 & w_4^2 & w_4^2 & w_4^3 & w_4^3 \\ 1 & 1 & w_4^2 & w_4^2 & 1 & 1 & w_4^2 & w_4^2 \\ 1 & 1 & w_4^3 & w_4^3 & w_4^2 & w_4^2 & w_4 & w_4 \end{bmatrix}}_{\textbf{regularly}\text{ subsampled FT matrix}} \begin{bmatrix} 2 \\ 0 \\ 0 \\ 1 \\ 0 \\ 2 \\ 0 \\ 1 \end{bmatrix}$$

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$$\frac{1}{4}\mathbf{W}_{4\times 4}\mathbf{y}_T$$

$$\downarrow$$

$$\begin{bmatrix} 2 \\ 1 \\ 2 \\ 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\text{induced sparse graph}} \overset{\mathbf{x}}{\begin{bmatrix} 2 \\ 0 \\ 0 \\ 1 \\ 0 \\ 2 \\ 0 \\ 1 \end{bmatrix}}$$

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take small Fourier transform

Fourier

transformed samples

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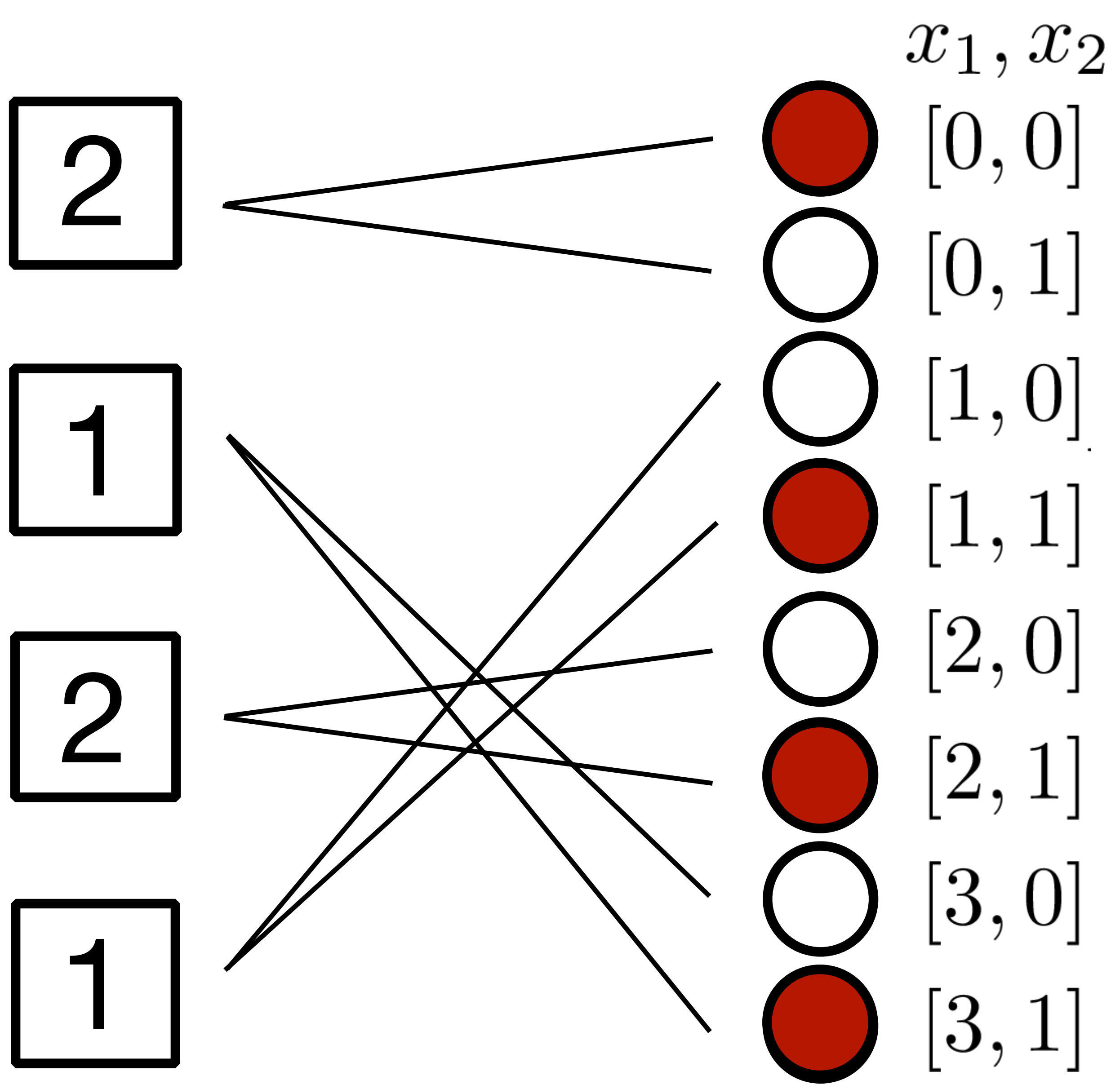
$$\begin{bmatrix}2\\1\\2\\1\end{bmatrix} = \underbrace{\begin{bmatrix}1&1&0&0&0&0&0&0\\0&0&0&0&0&0&1&1\\0&0&0&0&1&1&0&0\\0&0&1&1&0&0&0&0\end{bmatrix}}_{\text{induced sparse graph}} \overset{\mathbf{x}}{\begin{bmatrix}\color{red}{2}\\0\\0\\\color{red}{1}\\0\\\color{red}{2}\\0\\\color{red}{1}\end{bmatrix}} \longrightarrow$$



<u>sparse bipartite graph</u>
#edges ~ #nodes

new set of samples

$$\mathbf{q} = [\overset{q_1}{4}, \overset{q_2}{2}]$$

$$n = 2 \text{ sites}$$

$$N = 4 \times 2 = 8$$

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new set of position patterns

$$q_1 \;\; q_2$$
$$\mathbf{q} = [4, 2]$$
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$$\mathbf{y}_T = \mathbf{W}_T \, \mathbf{x}$$

$$\begin{bmatrix} 6 \\ -2 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & w_2 & 1 & w_2 & 1 & w_2 & 1 & w_2 \end{bmatrix}}_{\text{regularly subsampled FT matrix}} \begin{bmatrix} 2 \\ 0 \\ 0 \\ 1 \\ 0 \\ 2 \\ 0 \\ 1 \end{bmatrix}$$

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take small Fourier transform

$$\begin{array}{cc} q_1 & q_2 \end{array}$$

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$$\mathbf{y}_T \qquad \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & w_2 \end{bmatrix} \times \qquad \mathbf{W}_T \qquad \mathbf{x}$$

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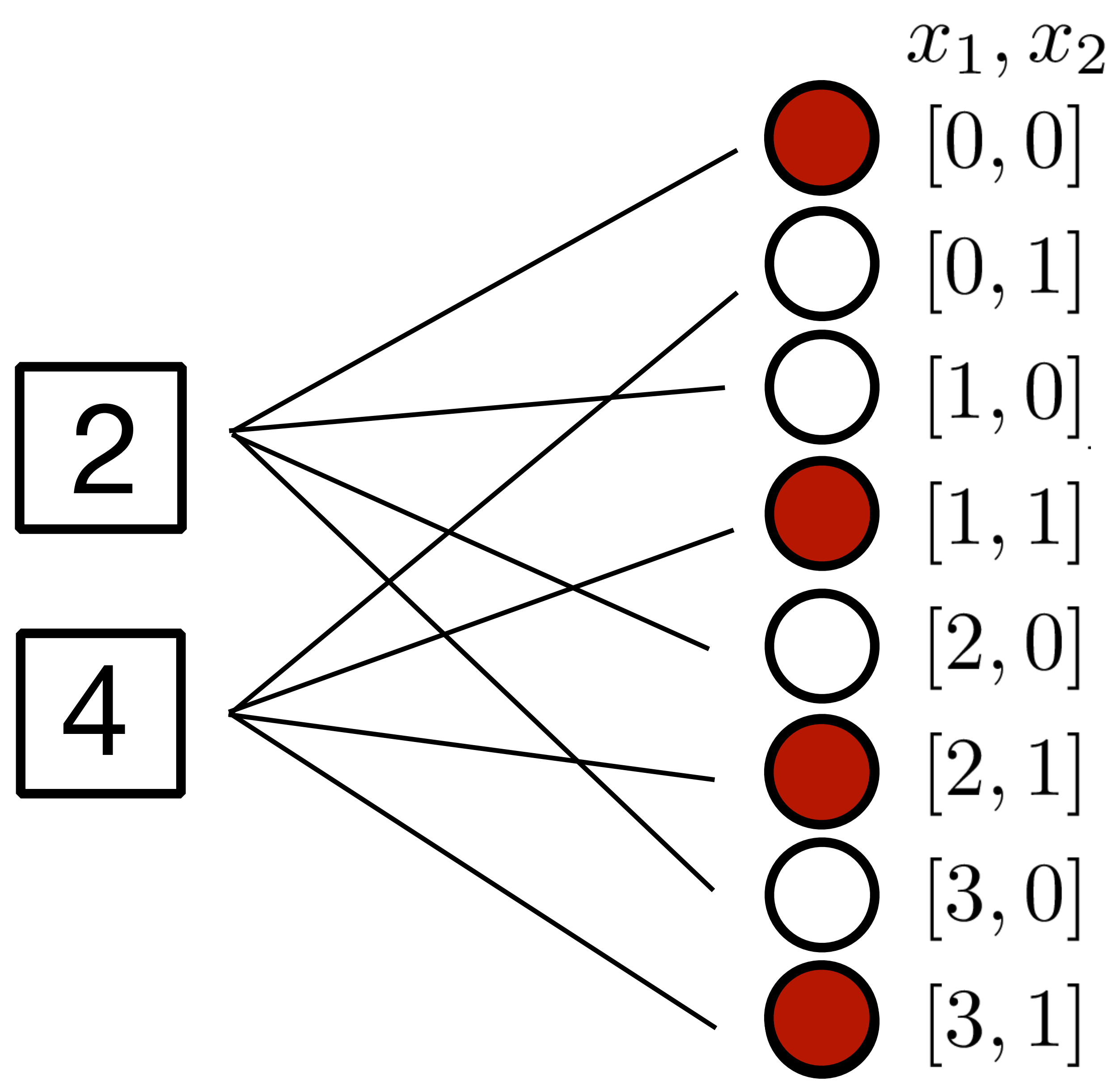
take small Fourier transform

Fourier

transformed samples

$$\frac{1}{2}\mathbf{W}_{2\times 2}\mathbf{y}_T \rightarrow \begin{bmatrix}2\\4\end{bmatrix} = \underbrace{\mathbf{W}_T}_{} \mathbf{x}$$

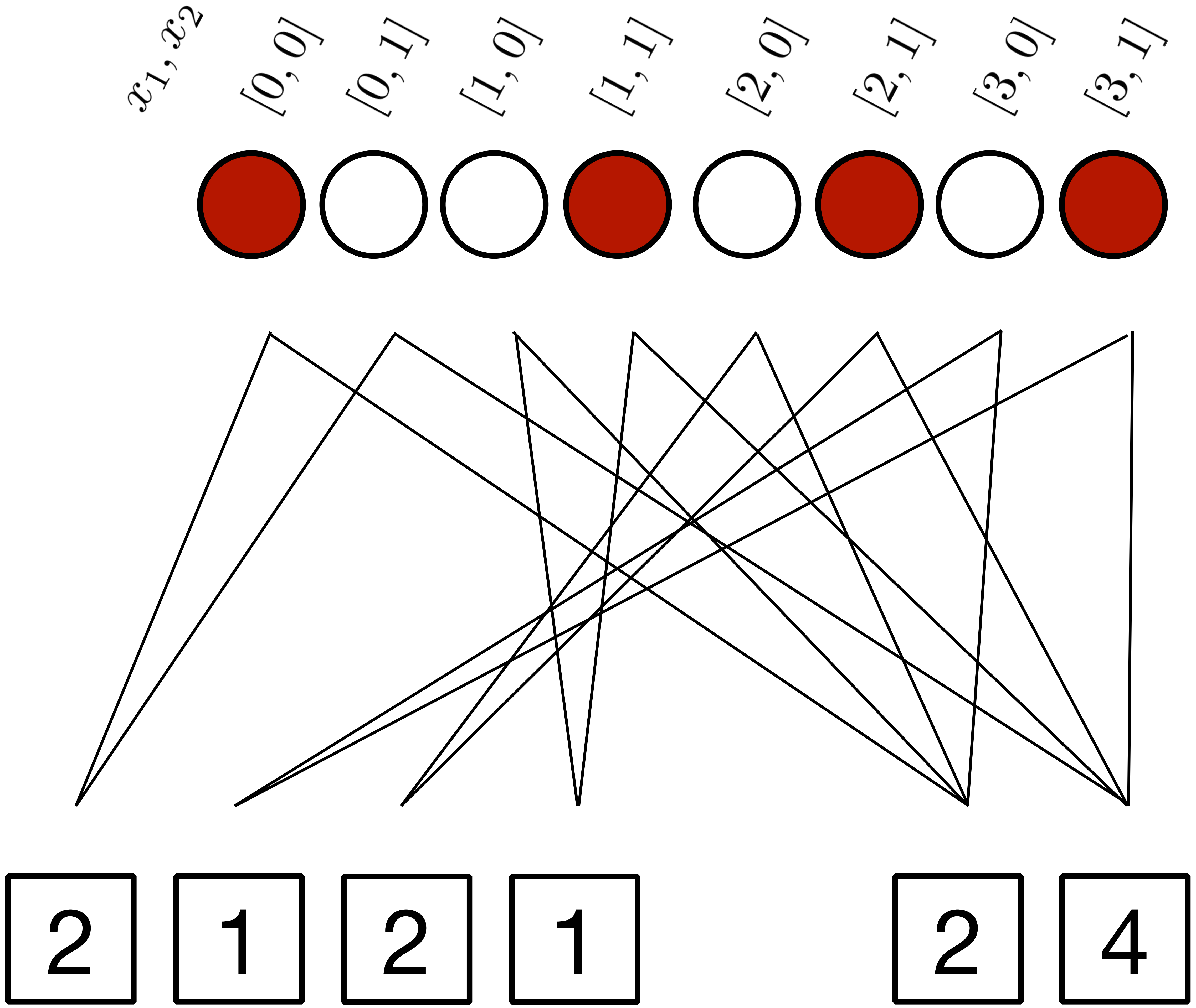
$$\begin{bmatrix}2\\4\end{bmatrix} = \underbrace{\begin{bmatrix}1 & 0 & 1 & 0 & 1 & 0 & 1 & 0\\0 & 1 & 0 & 1 & 0 & 1 & 0 & 1\end{bmatrix}}_{\text{induced sparse graph}} \begin{bmatrix}\color{red}{2}\\0\\0\\\color{red}{1}\\0\\\color{red}{2}\\0\\\color{red}{1}\end{bmatrix}$$



sparse bipartite graph

#edges ~ #nodes

Peel interactions one by one



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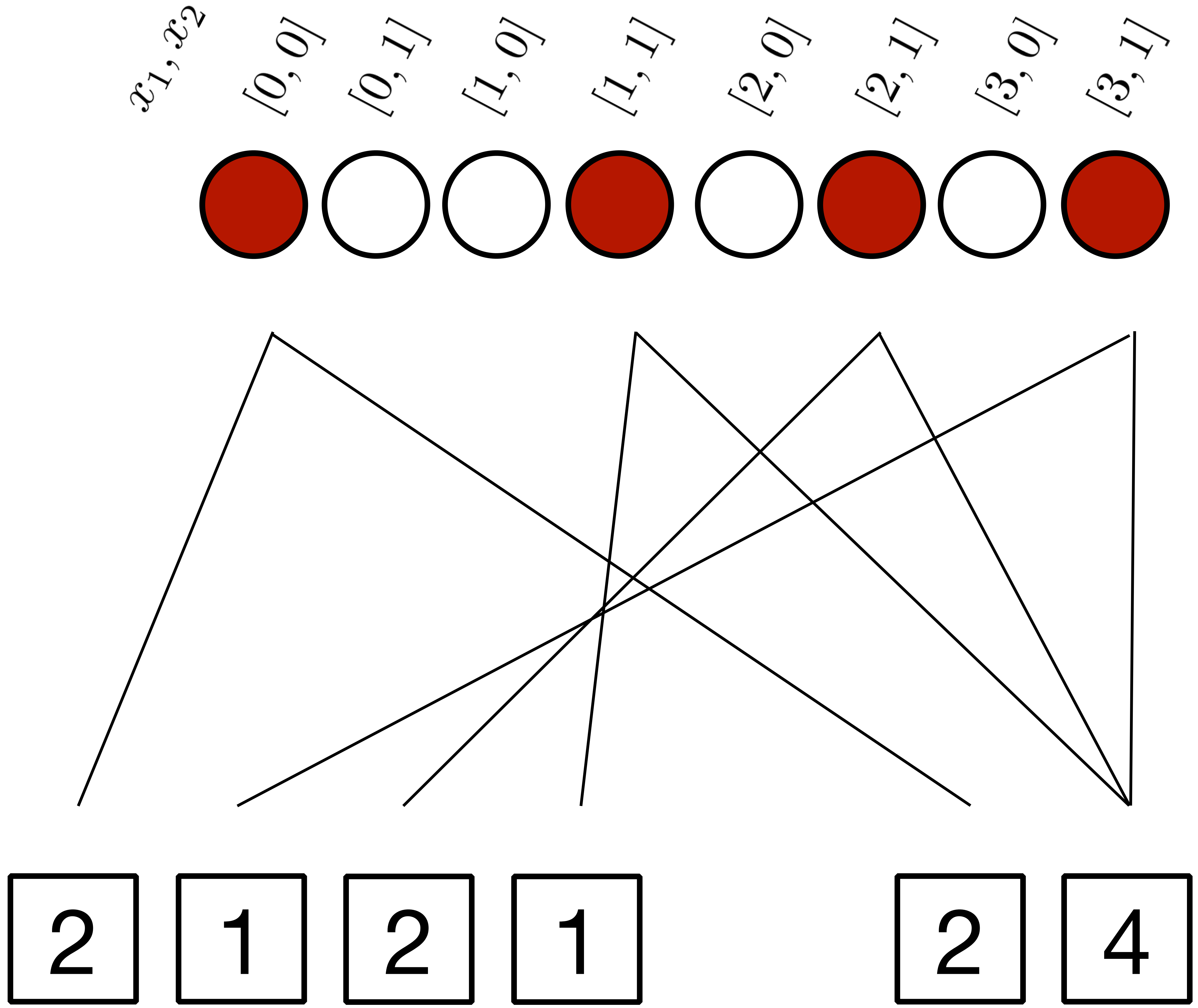

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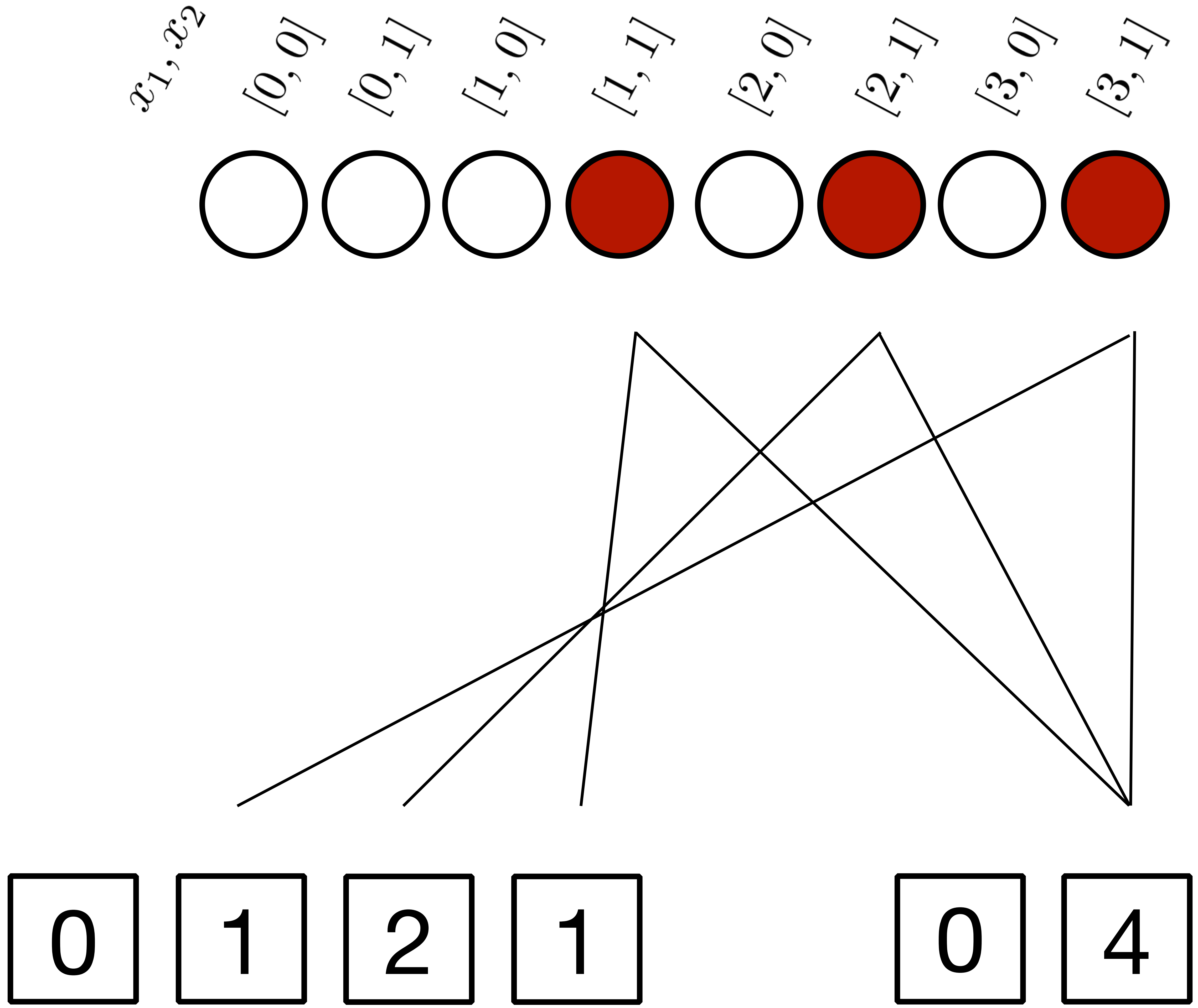

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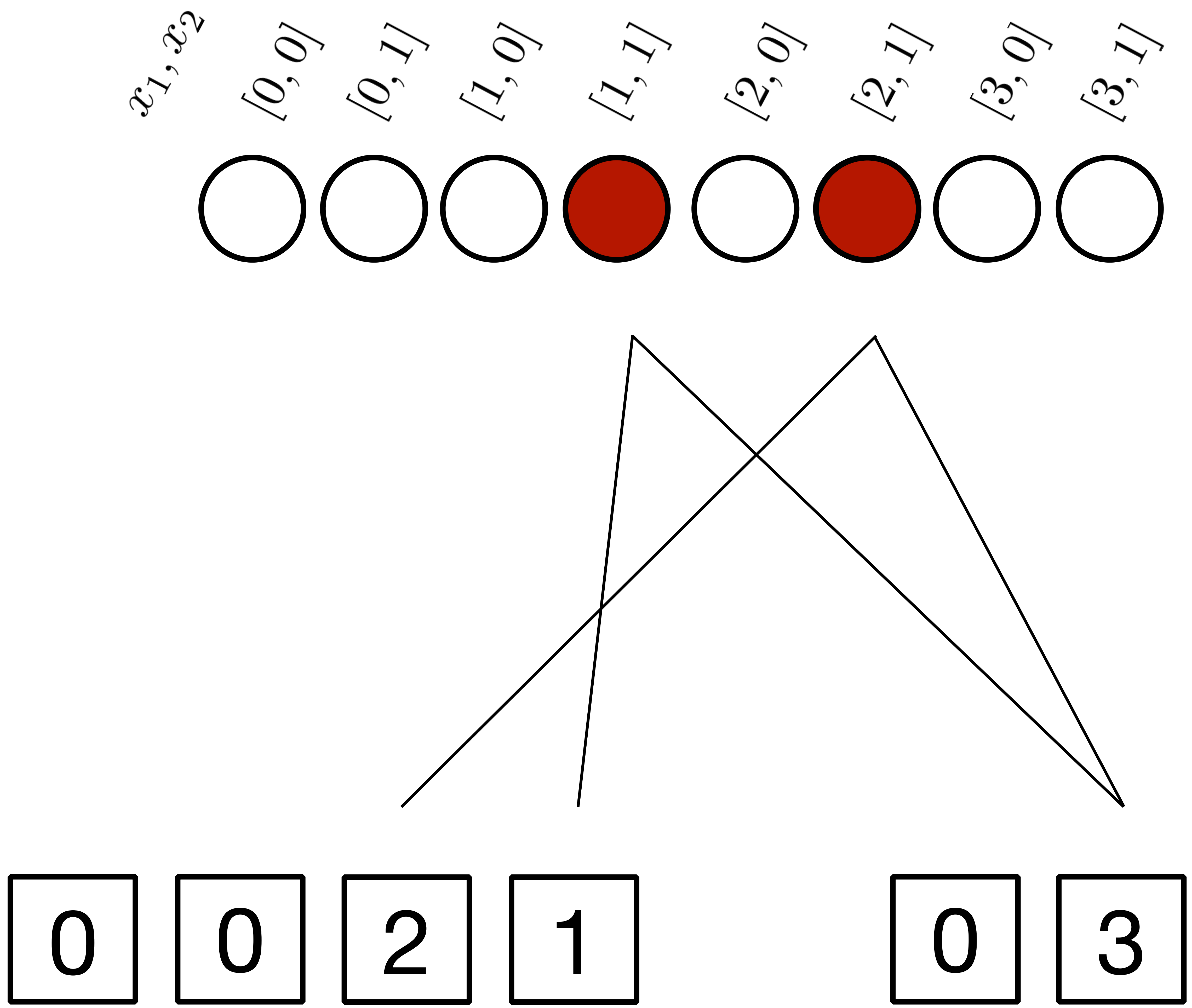

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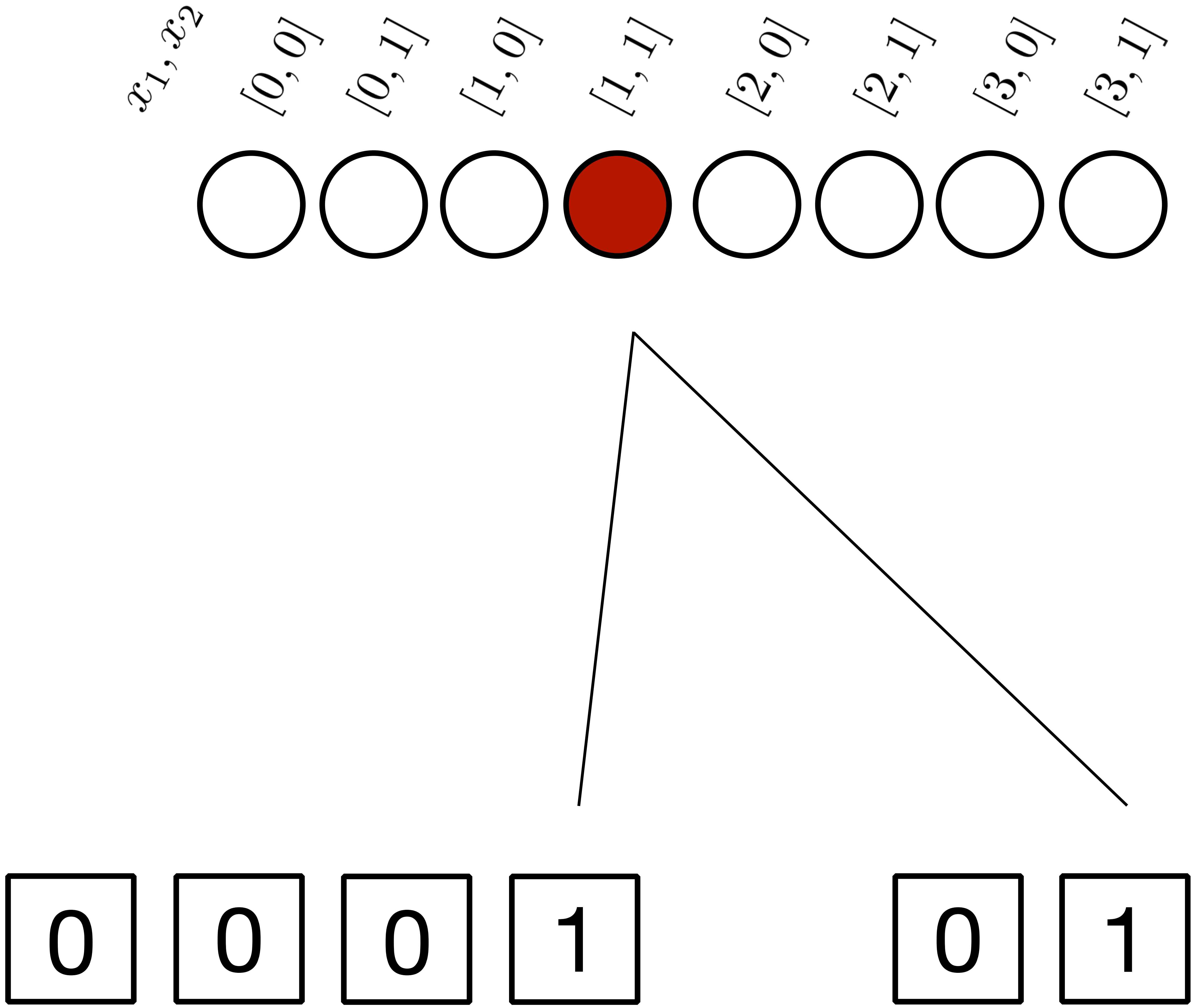

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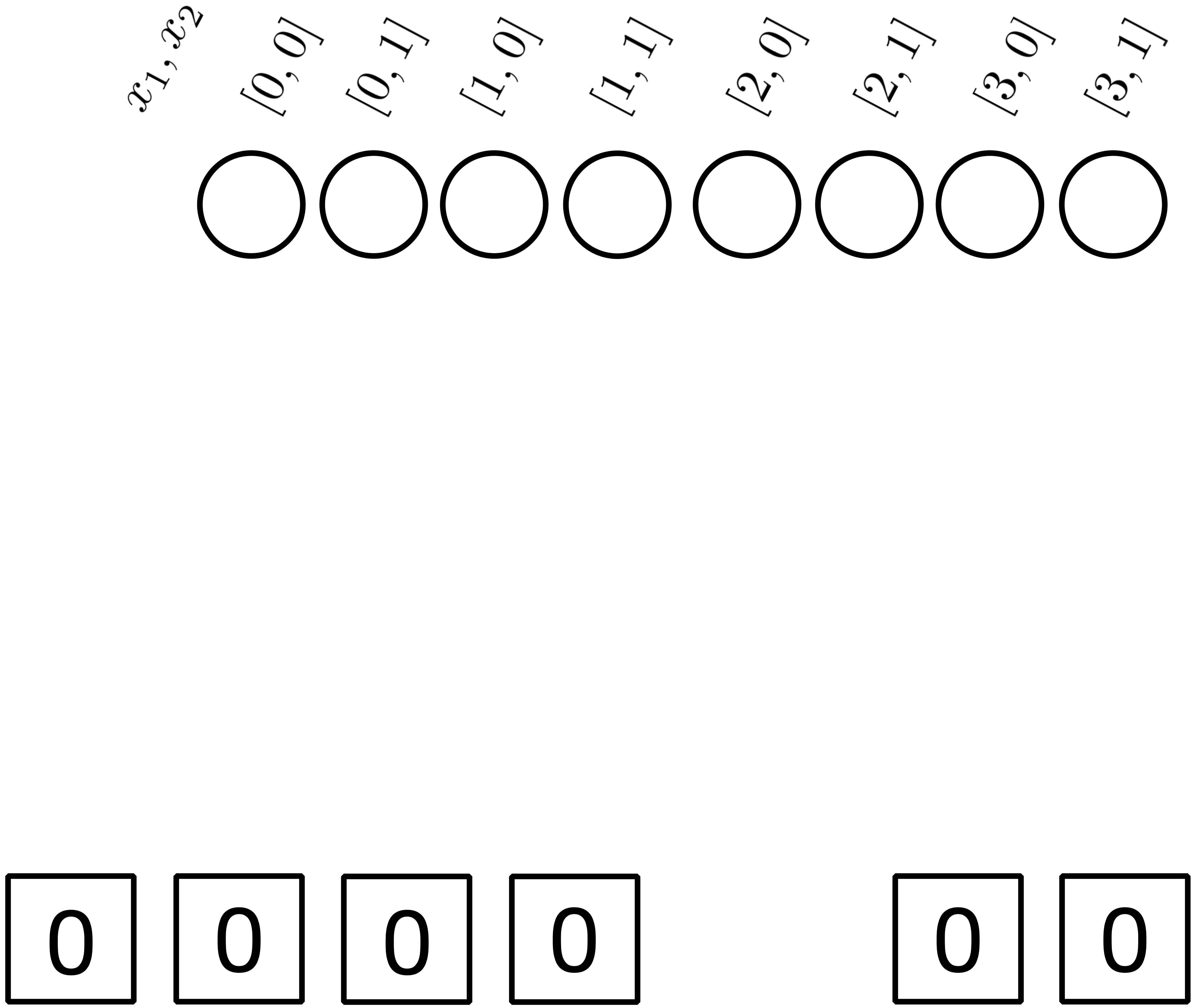

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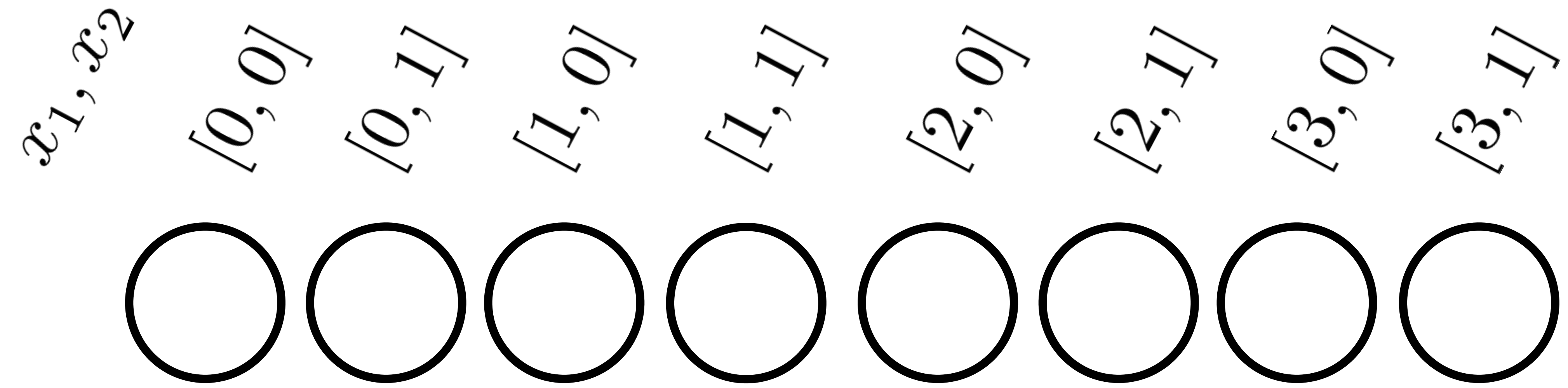
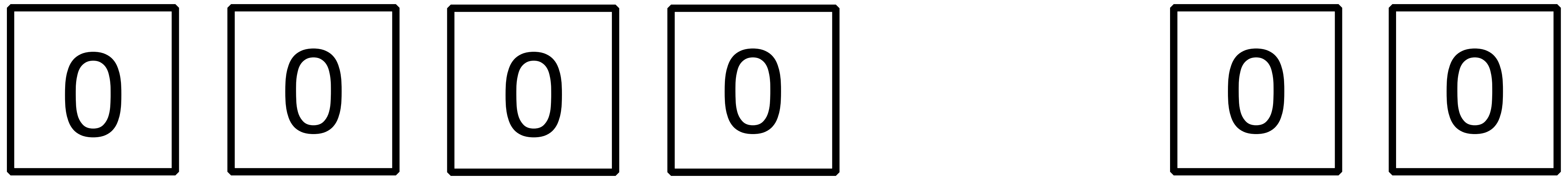
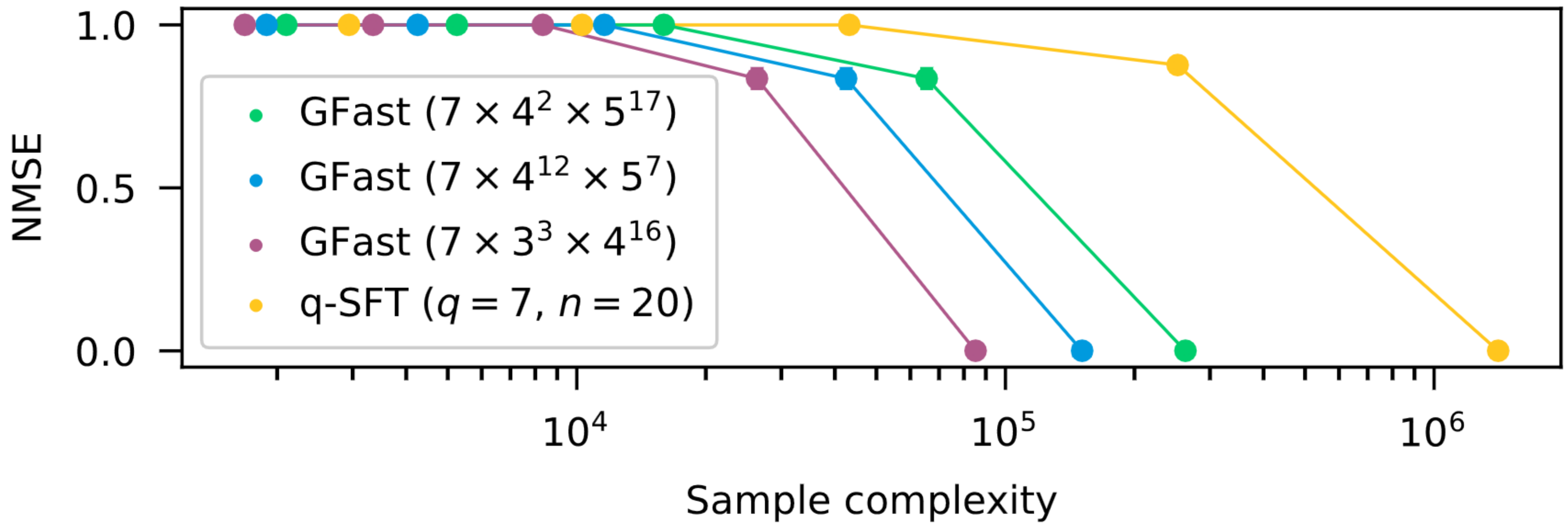


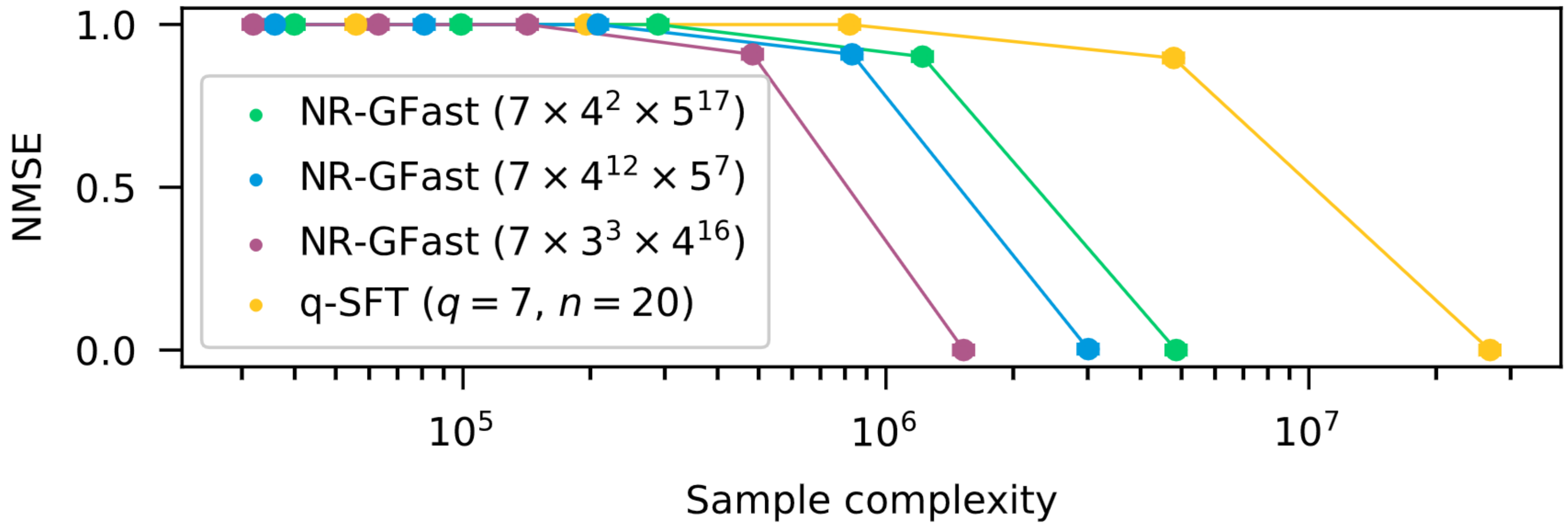
- High probability guarantees using density evolution
- Each small transform group has check node degrees that are Poisson distributed



We can save a lot if you know a bit about the model

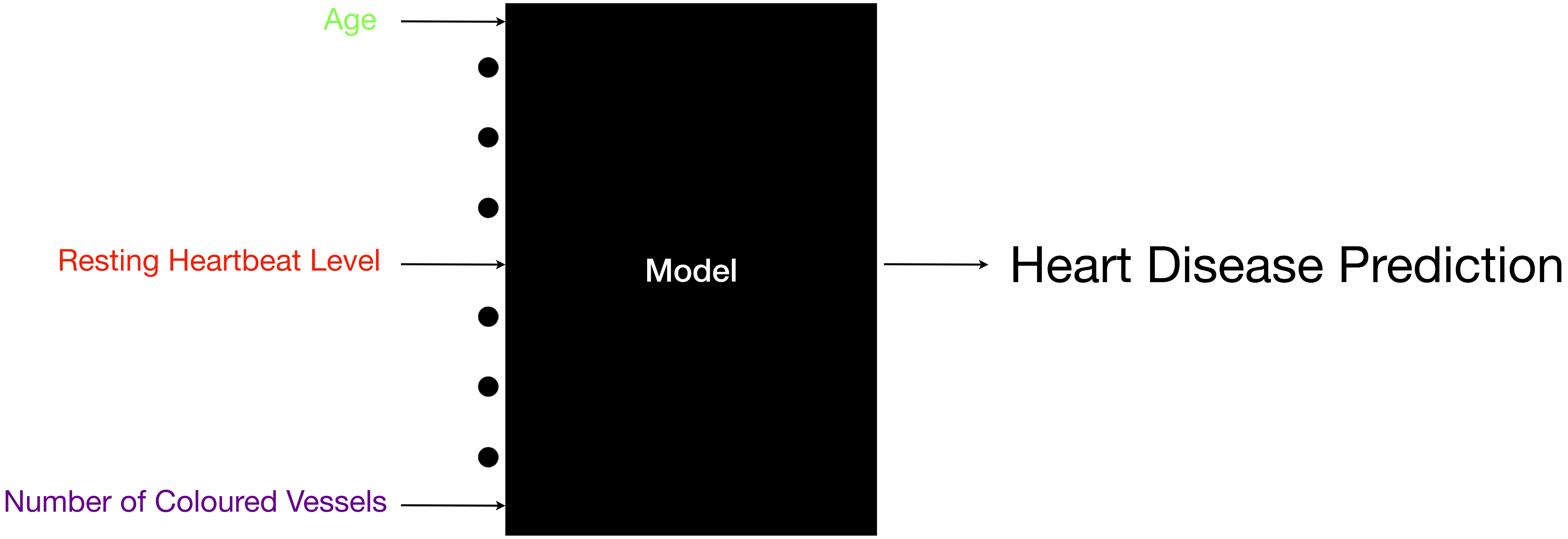


Noise-less



Noise-robust

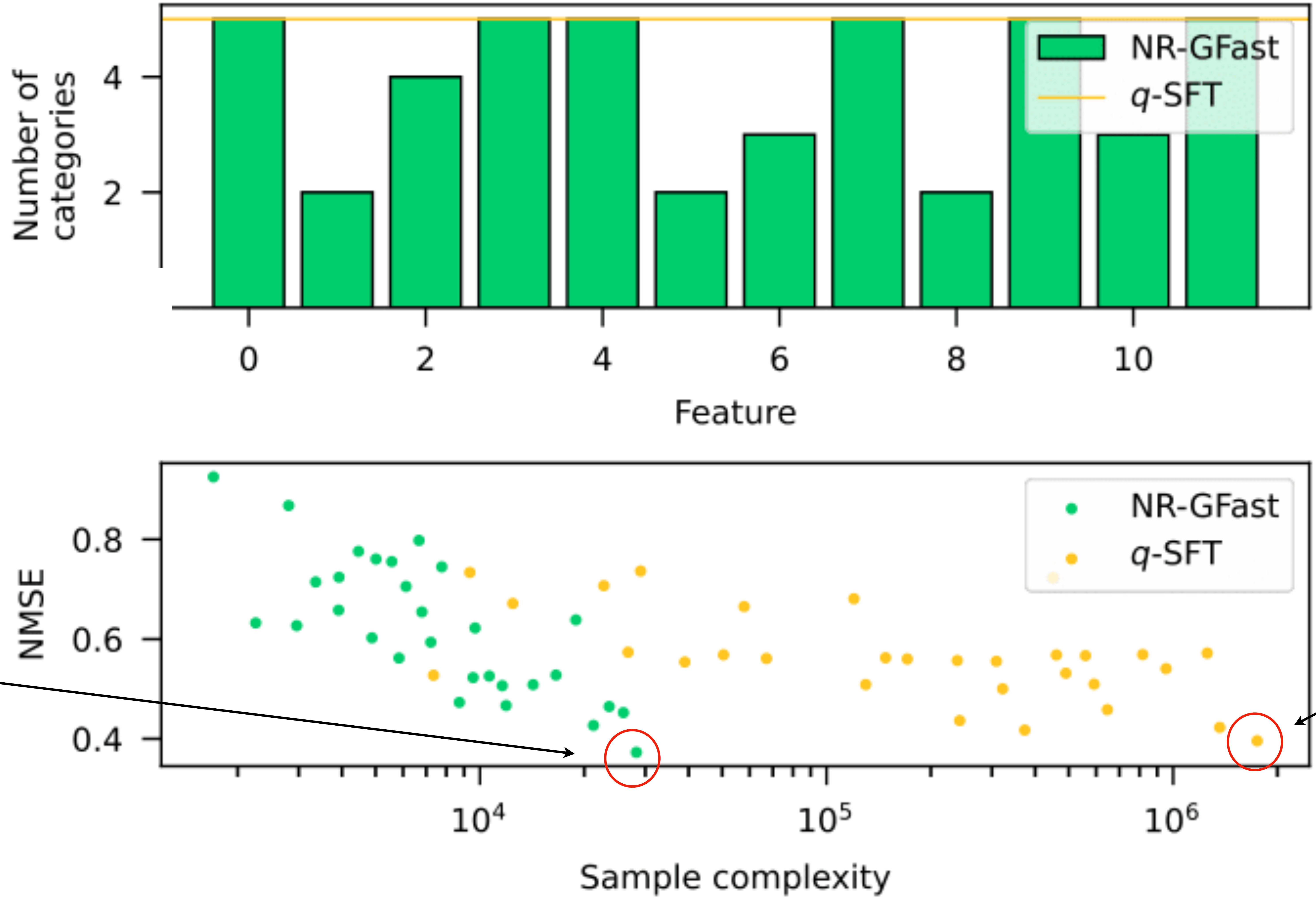
Machine learning example



$$\mathbb{Z}_5 \times \mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_5 \times \mathbb{Z}_5 \times \mathbb{Z}_2 \times \mathbb{Z}_3 \times \mathbb{Z}_5 \times \mathbb{Z}_2 \times \mathbb{Z}_5 \times \mathbb{Z}_3 \times \mathbb{Z}_5$$

q-ary: $\mathbb{Z}_5^{12}$

Treating the function as *q*-ary requires *61x* more samples to achieve similar accuracy



28,000 samples

1.75 million samples

Thanks!

arXiv

Github