Loss is more

Exploring the weight space of a perceptron via enhanced sampling techniques

UNIVERSITÀ DI TRENTO

ECT* - BRIDGING SCALES 2024

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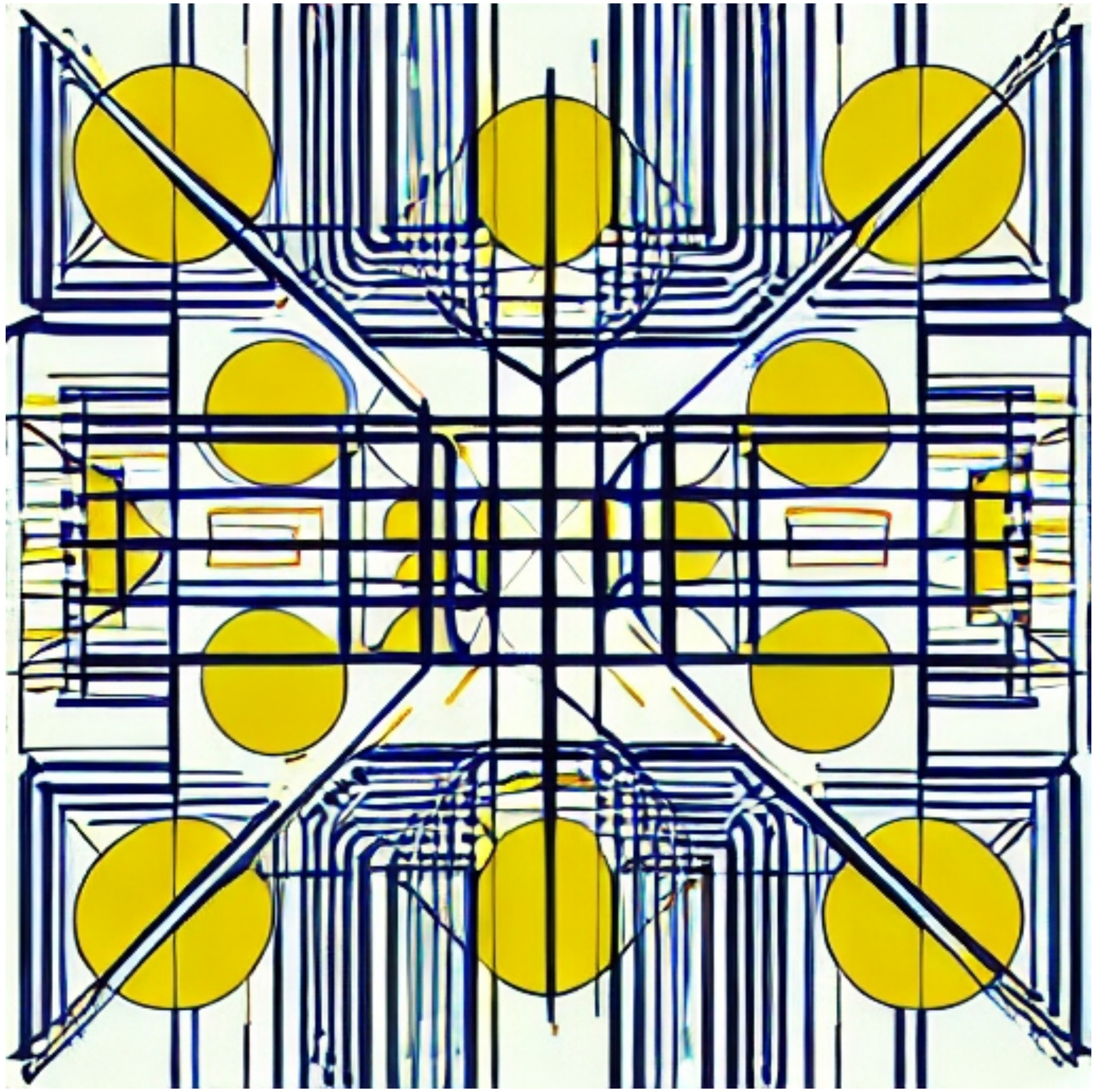
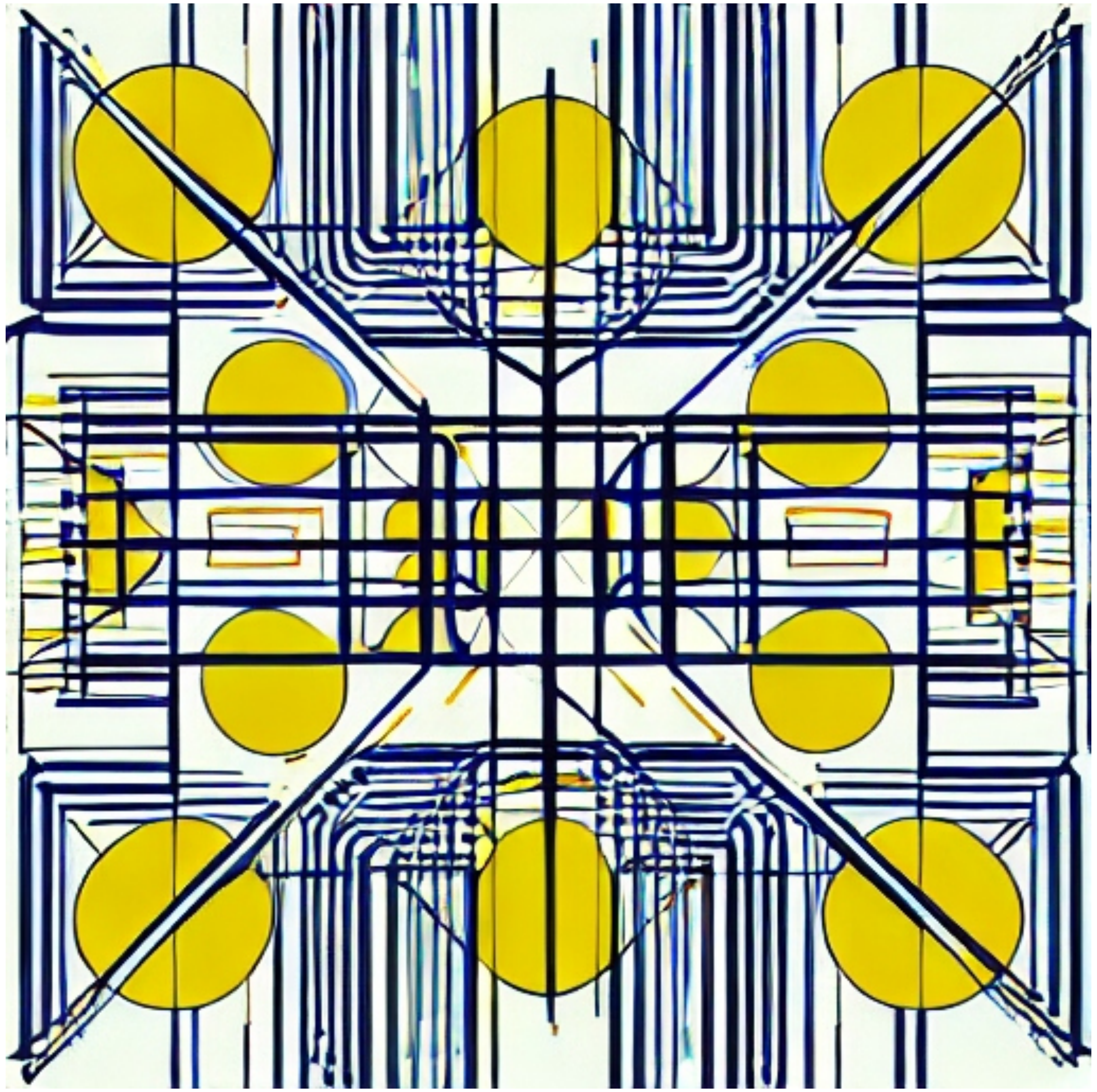
HOW DO NETWORKS LEARN?

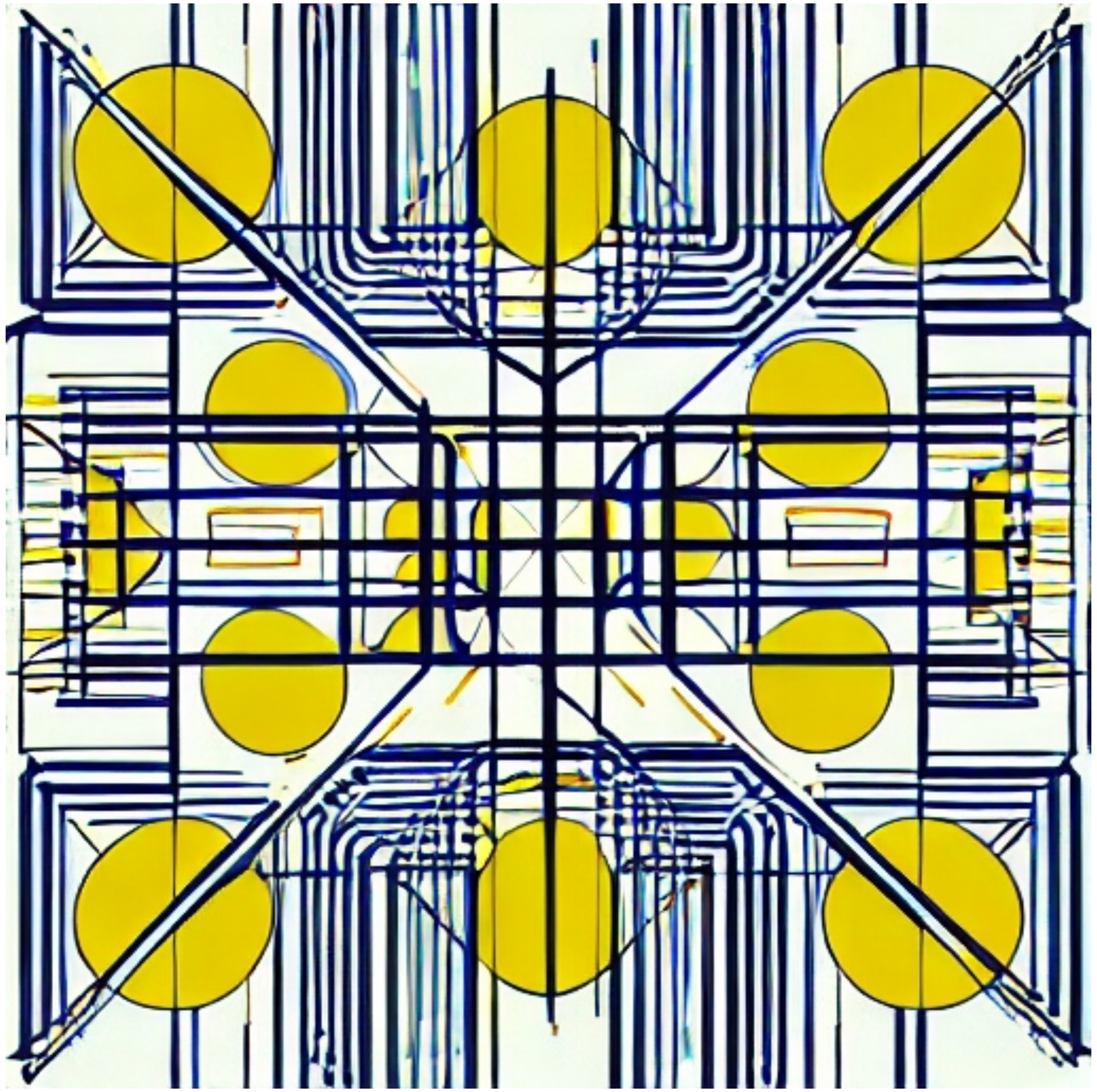


HOW DO NETWORKS LEARN?



Neural Networks identify pattern that we are not able to see

HOW DO NETWORKS LEARN?



Neural Networks identify pattern
that we are not able to see

↓

Can we identify the key data traits
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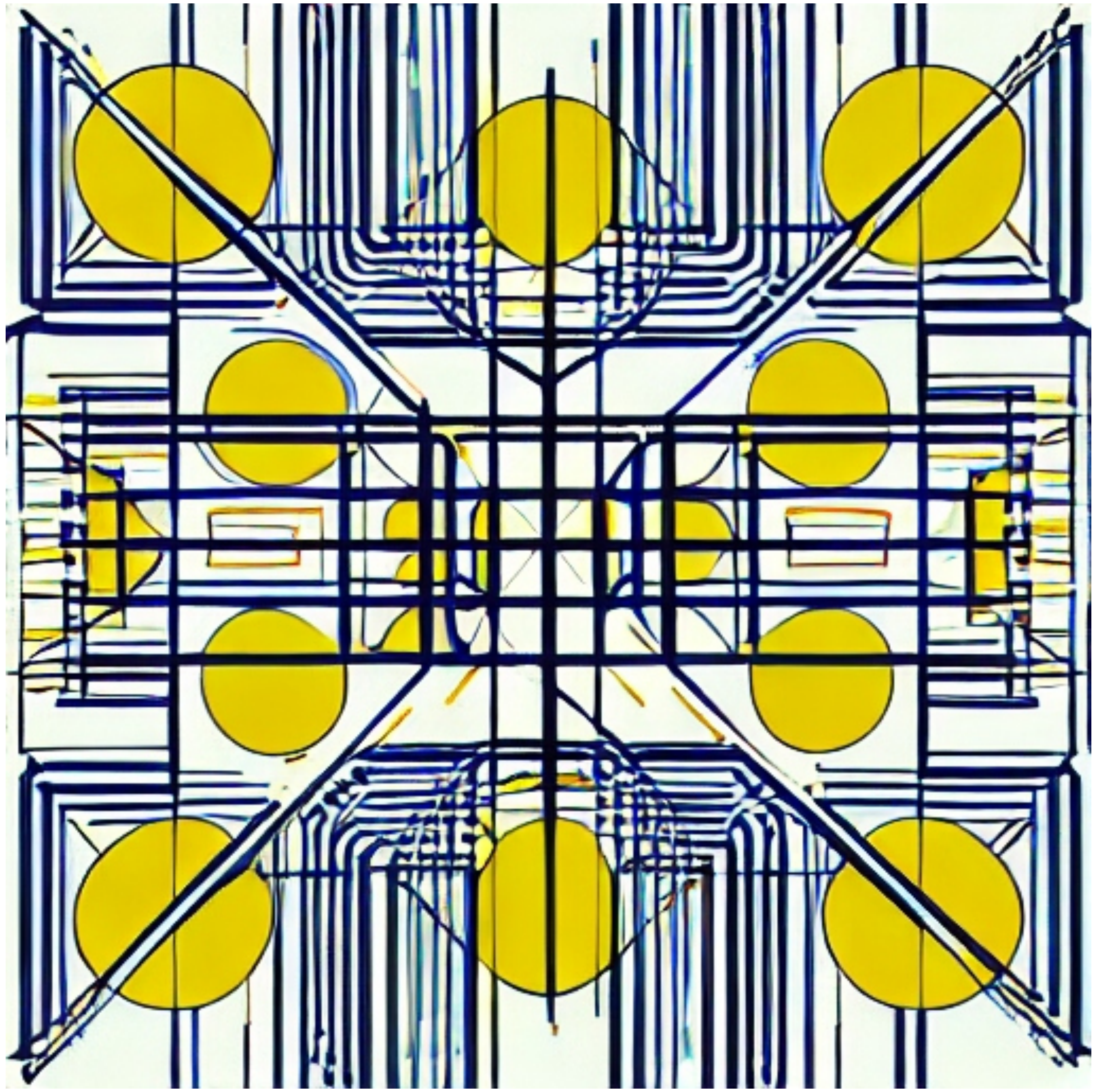
HOW DO NETWORKS LEARN?

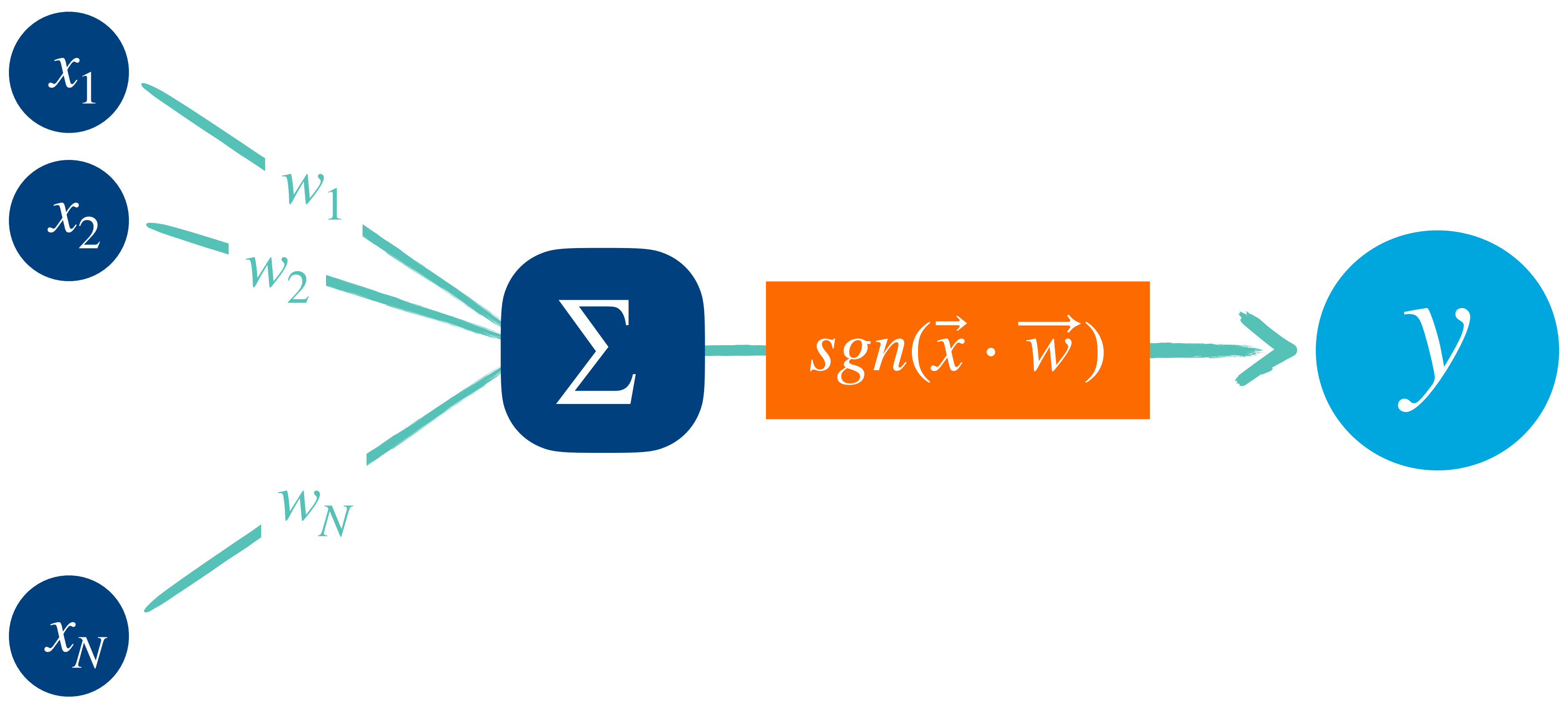


Neural Networks identify pattern that we are not able to see

Can we identify the key data traits networks learn from?

Describe the network configuration space while varying the input data structure

Perceptron



Inputs $\{x_i\}_1^P$

$$[1,1,-1,\ldots,1,-1,-1]$$
$$[-1,1,1,\ldots,-1,1,-1]$$
$$\vdots$$
$$[-1,-1,1,\ldots,-1,1,1]$$

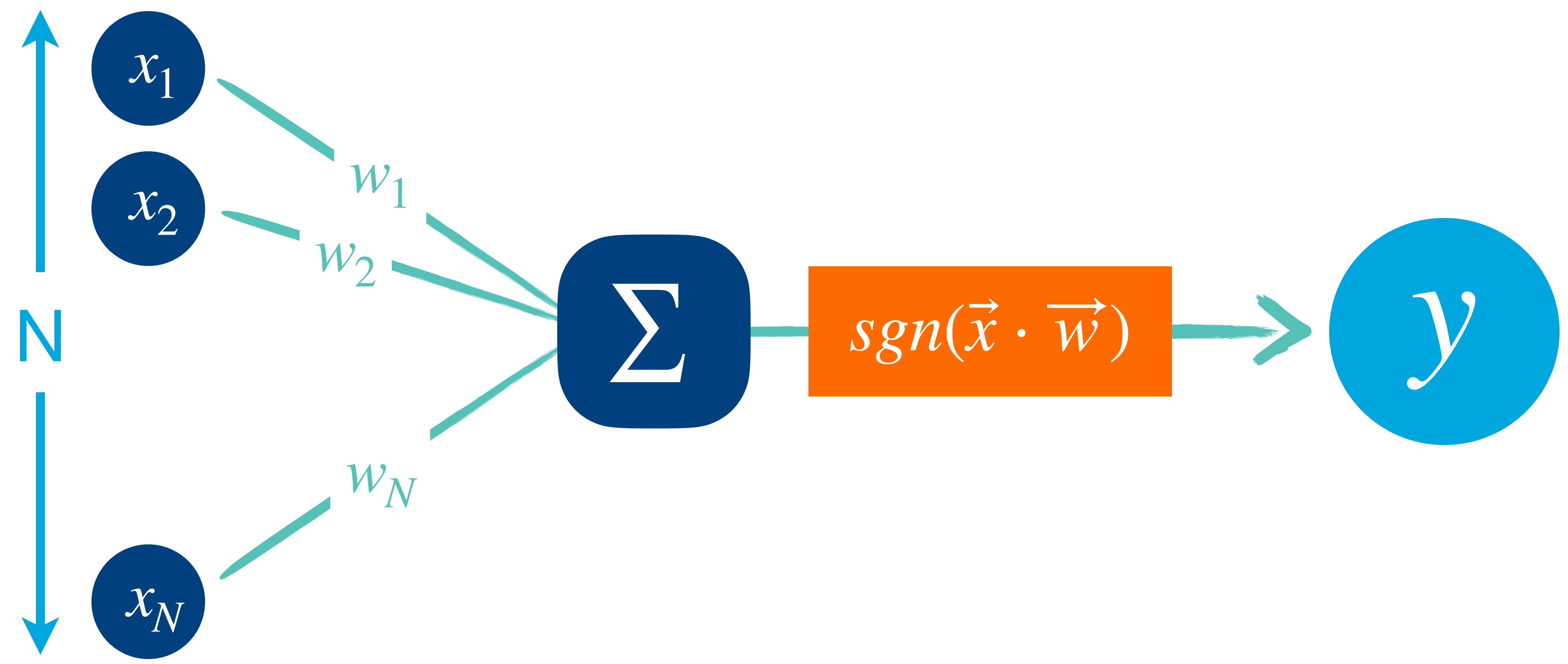
Weight vector w

$$[-1,1,-1\ \ldots,-1,-1,1]$$

Labels $\{y_i\}$

$$y_i = \text{sgn}\left(w\,x_i\right)$$

Perceptron



Inputs $\{x_i\}_1^P$

$$\begin{gathered}[1,1,-1,\ldots,1,-1,-1] \\ [-1,1,1,\ \ldots,-1,1,-1] \\ \vdots \\ [-1,-1,1,\ \ldots,-1,1,1]\end{gathered}$$

N

Weight vector w

$$[-1,1,-1\ \ldots,-1,-1,1]$$

Labels $\{y_i\}$

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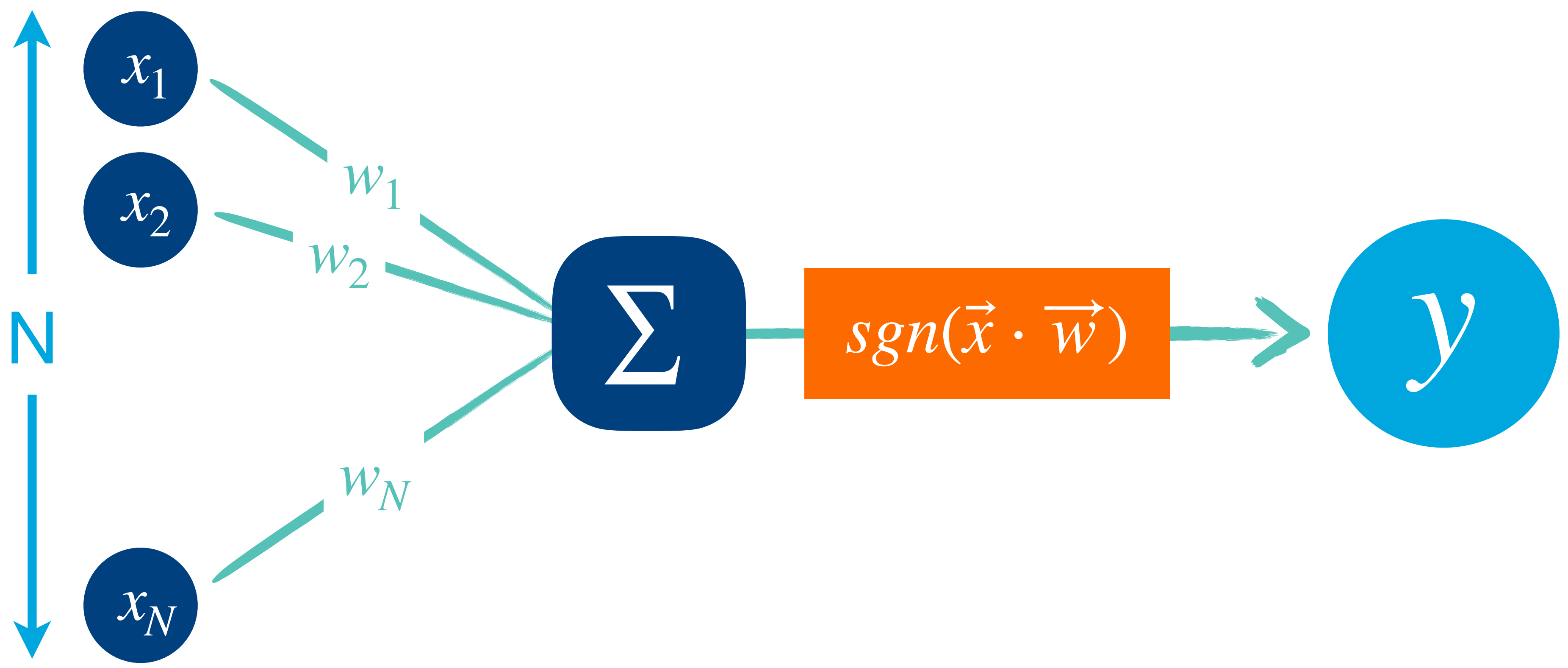
Perceptron



Inputs $\{x_i\}_1^P$

$$
\begin{array}{c}
[1,1,-1,\ldots,1,-1,-1] \\
[-1,1,1,\ \ldots,-1,1,-1] \\
\vdots \\
[-1,-1,1,\ \ldots,-1,1,1]
\end{array}
$$

P

N

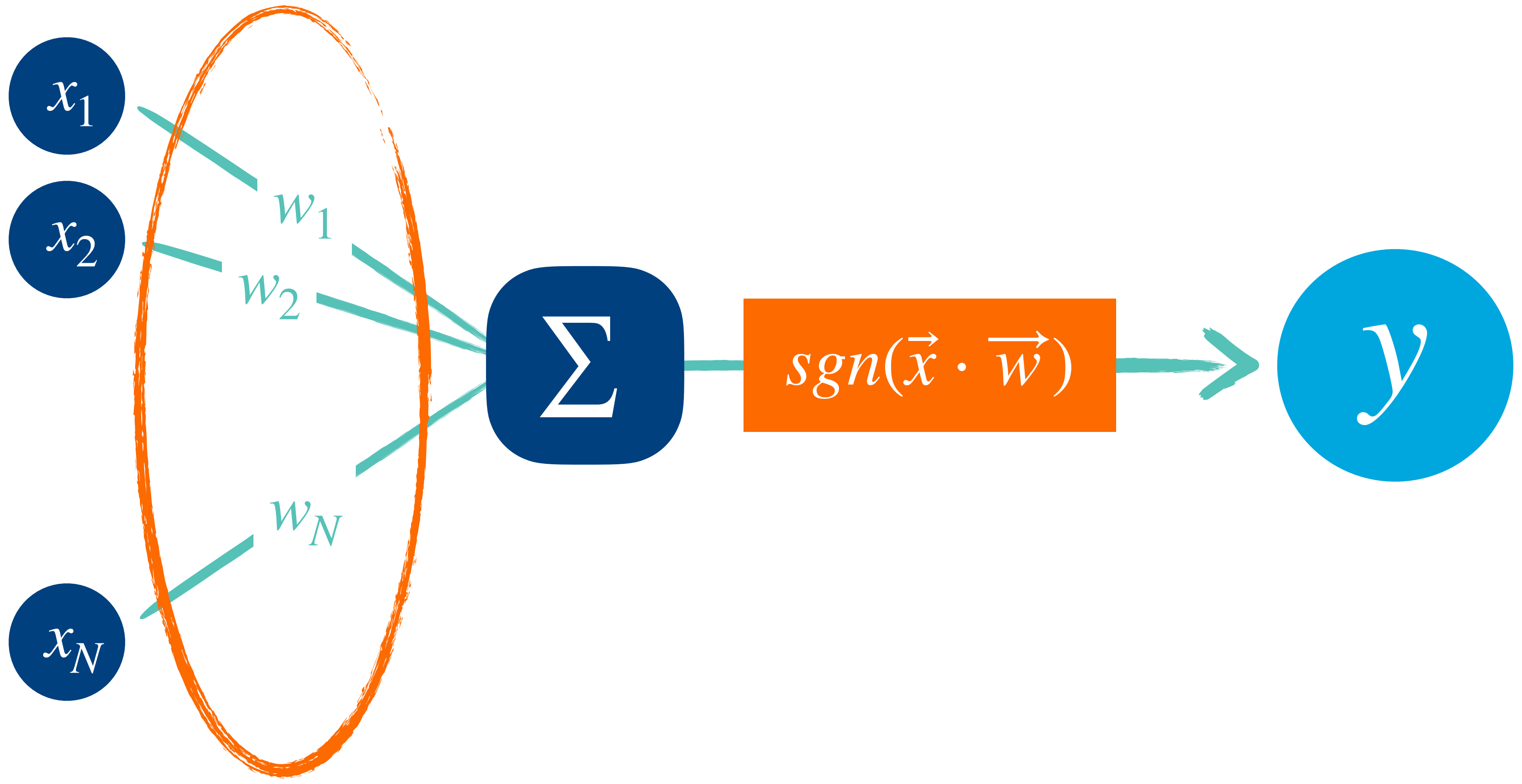
Weight vector w

$$[-1,1,-1\ \ldots,-1,-1,1]$$

Labels $\{y_i\}$

$$y_i = \mathrm{sgn}\left(w\, x_i\right)$$

Perceptron



Inputs $\{x_i\}_1^P$

$$\begin{array}{c} [1,1,-1,\ldots,1,-1,-1] \\ [-1,1,1,\ \ldots,-1,1,-1] \\ \vdots \\ [-1,-1,1,\ \ldots,-1,1,1] \end{array}$$

P

N

Weight vector w

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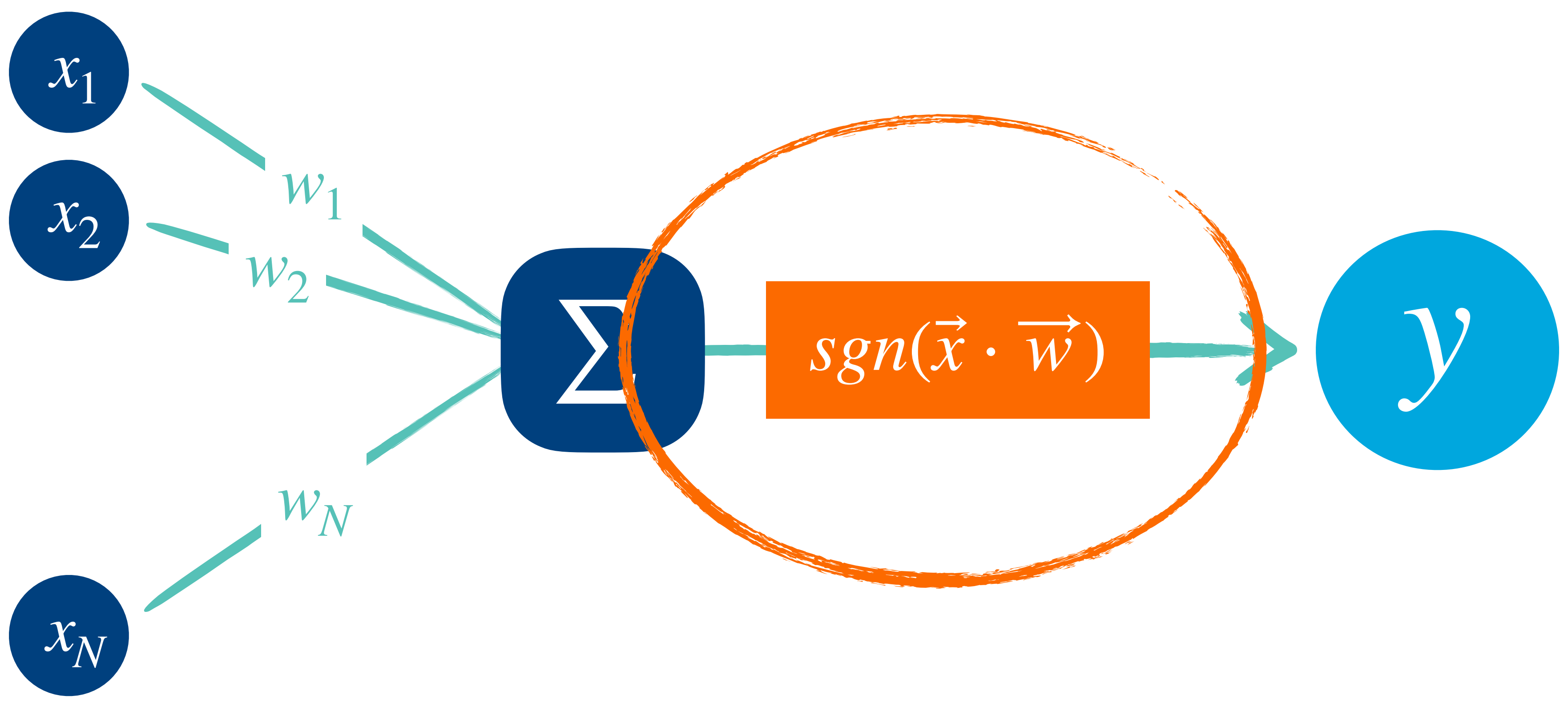

Inputs $\{x_i\}_1^P$

$$[1,1,-1,\ldots,1,-1,-1]$$
$$[-1,1,1,\ \ldots,-1,1,-1]$$
$$\vdots$$
$$[-1,-1,1,\ \ldots,-1,1,1]$$

P

N

Weight vector w

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Labels $\{y_i\}$

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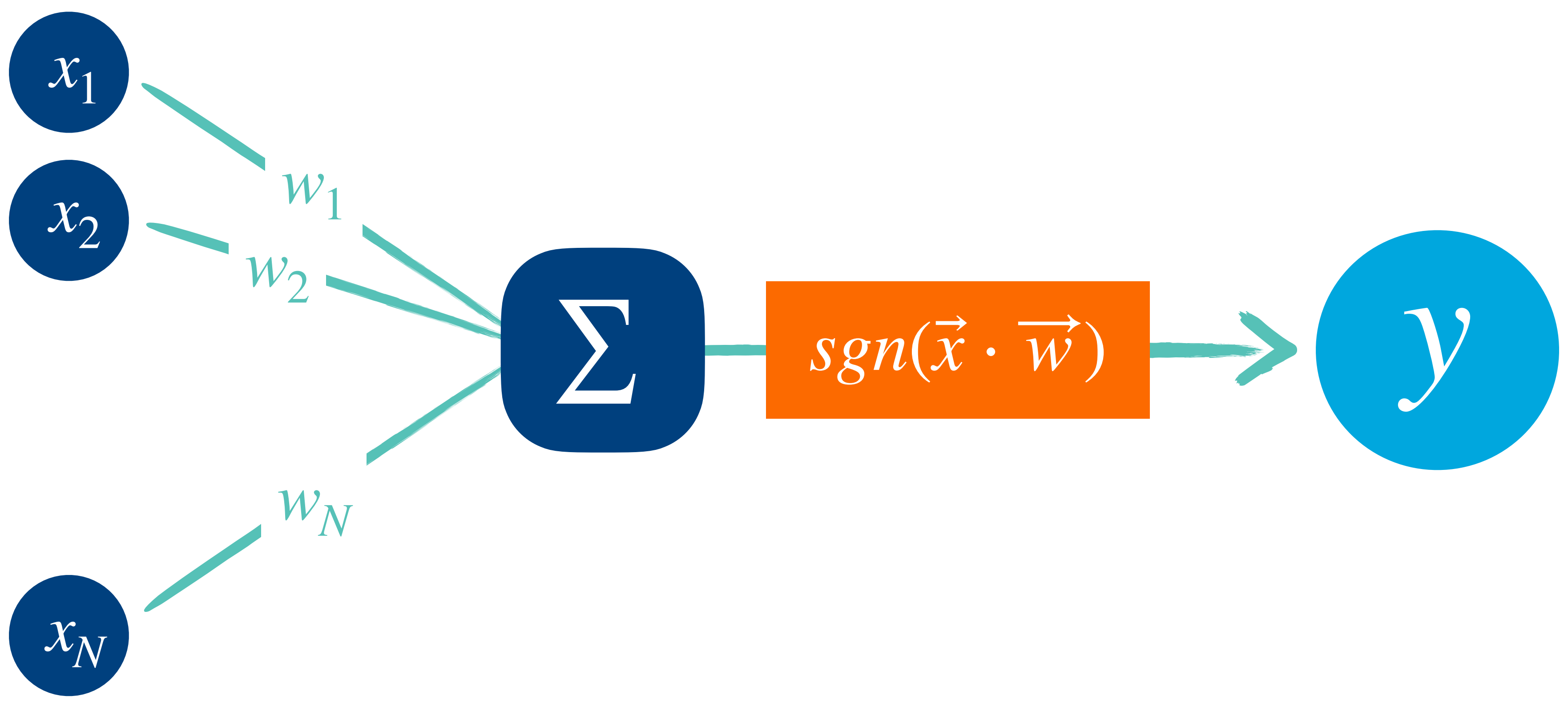
Perceptron



Energy

$$E_w = \sum_i^P \Theta\left(-y_i \cdot \mathrm{sgn}\left(w\, x_i\right)\right)$$

Entropy

$$S(\bar{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \bar{E})\right)$$

Inputs $\{x_i\}_1^P$

$$\begin{array}{cc} & \begin{bmatrix}1,1,-1,\ldots,1,-1,-1\end{bmatrix} \\ P & \begin{bmatrix}-1,1,1,\ \ldots,-1,1,-1\end{bmatrix} \\ & \vdots \\ & \begin{bmatrix}-1,-1,1,\ \ldots,-1,1,1\end{bmatrix} \\ & N \end{array}$$

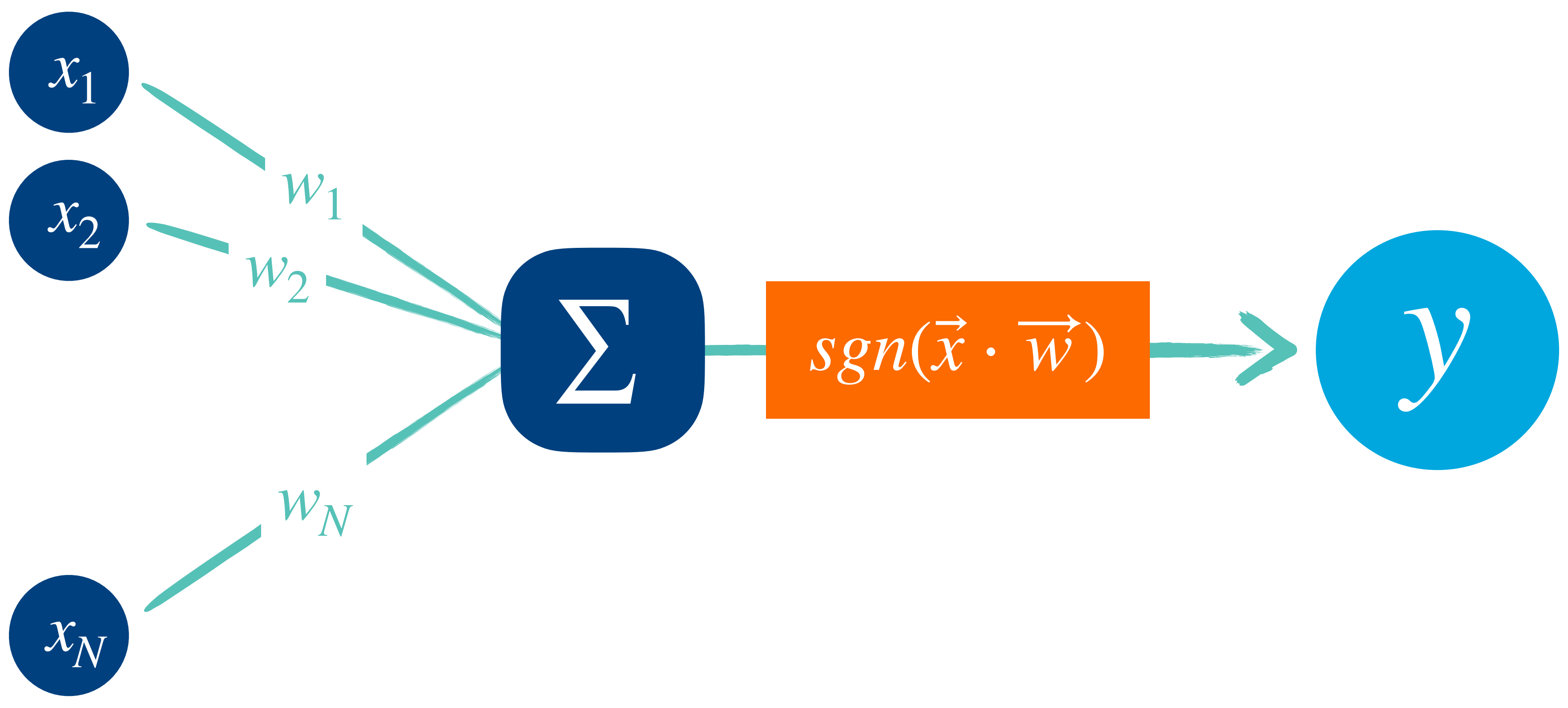
Weight vector w

$$\begin{bmatrix}-1,1,-1\ \ldots,-1,-1,1\end{bmatrix}$$

Labels $\{y_i\}$

$$y_i = \mathrm{sgn}\left(w\, x_i\right)$$

Perceptron



Inputs $\{x_i\}_1^P$

$[1,1,-1,\dots,1,-1,-1]$
$[-1,1,1,\dots,-1,1,-1]$
$\vdots$
$[-1,-1,1,\dots,-1,1,1]$

P

N

Weight vector w

$[-1,1,-1 \dots,-1,-1,1]$

Labels $\{y_i\}$

$$y_i = \mathrm{sgn}\left(w\, x_i\right)$$

Energy

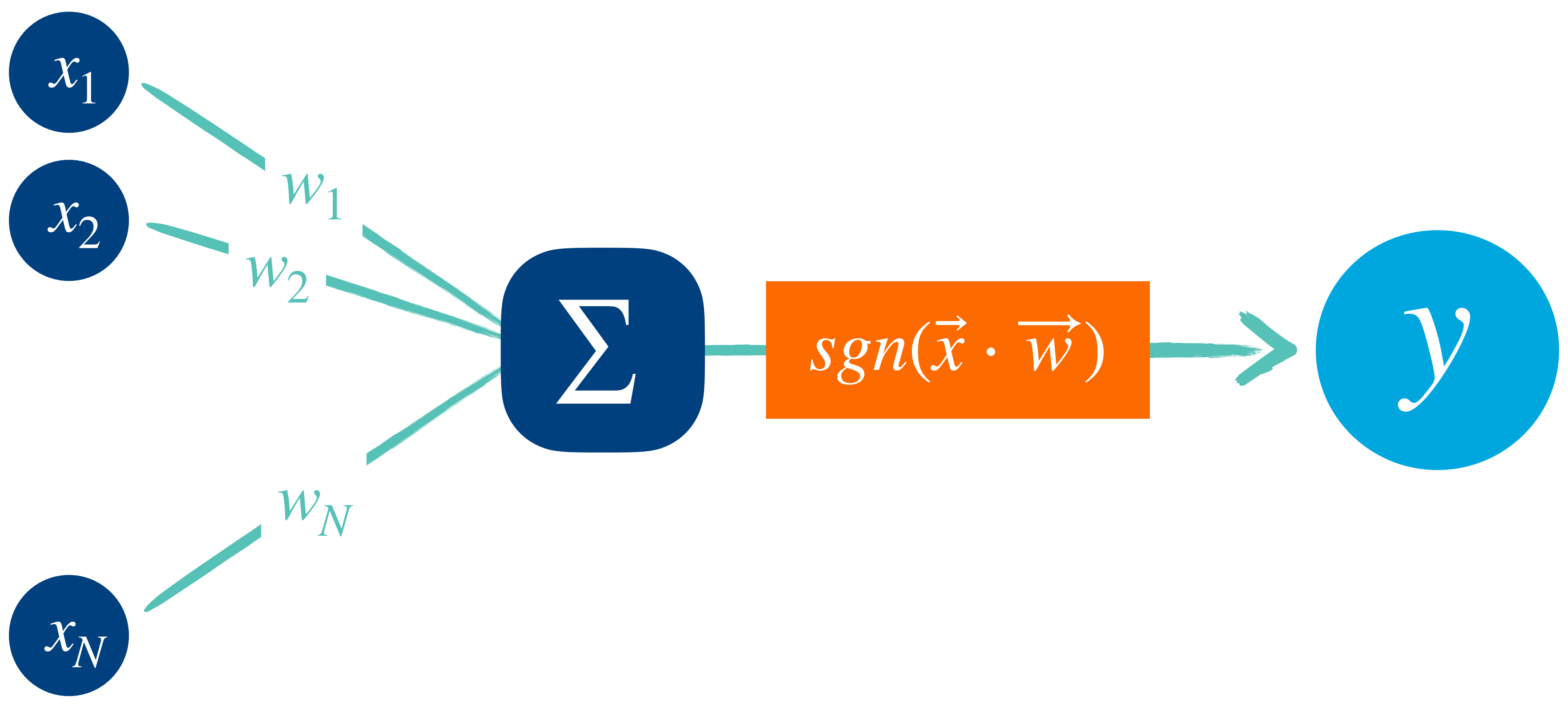
$$E_w = \sum_i^P \Theta\left(-y_i \cdot \mathrm{sgn}\left(w\, x_i\right)\right)$$

Number of Errors

Entropy

$$S(\overline{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \overline{E})\right)$$

Perceptron



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Number of Errors

Entropy

$$\boxed{S(\overline{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \overline{E})\right)}$$

Inputs $\{x_i\}_1^P$

$$P \left\{ \begin{array}{l} [1,1,-1,\ldots,1,-1,-1] \\ [-1,1,1,\ \ldots,-1,1,-1] \\ \vdots \\ [-1,-1,1,\ \ldots,-1,1,1] \end{array} \right.$$

N

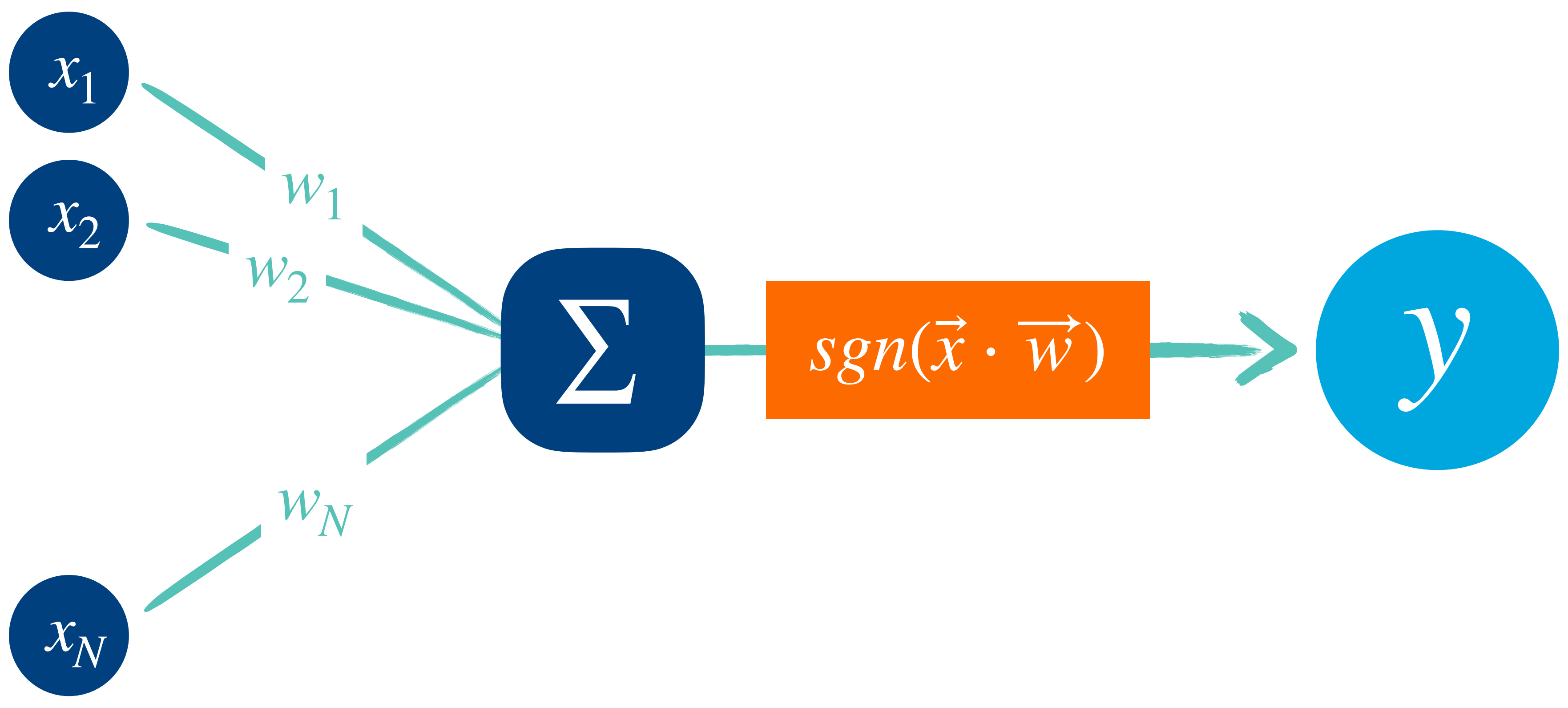
Weight vector w

$$[-1,1,-1\ \ldots,-1,-1,1]$$

Labels $\{y_i\}$

$$y_i = \mathrm{sgn}\left(w\, x_i\right)$$

Perceptron



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$$E_w = \sum_i^P \Theta\left(-y_i \cdot \mathrm{sgn}\left(w\, x_i\right)\right)$$

Number of Errors

Entropy

$$S(\bar{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \bar{E})\right)$$

N small (< 25)

Inputs $\{x_i\}_1^P$

$[1,1,-1,\ldots,1,-1,-1]$
$[-1,1,1,\ \ldots,-1,1,-1]$
$\vdots$
$[-1,-1,1,\ \ldots,-1,1,1]$

P

N

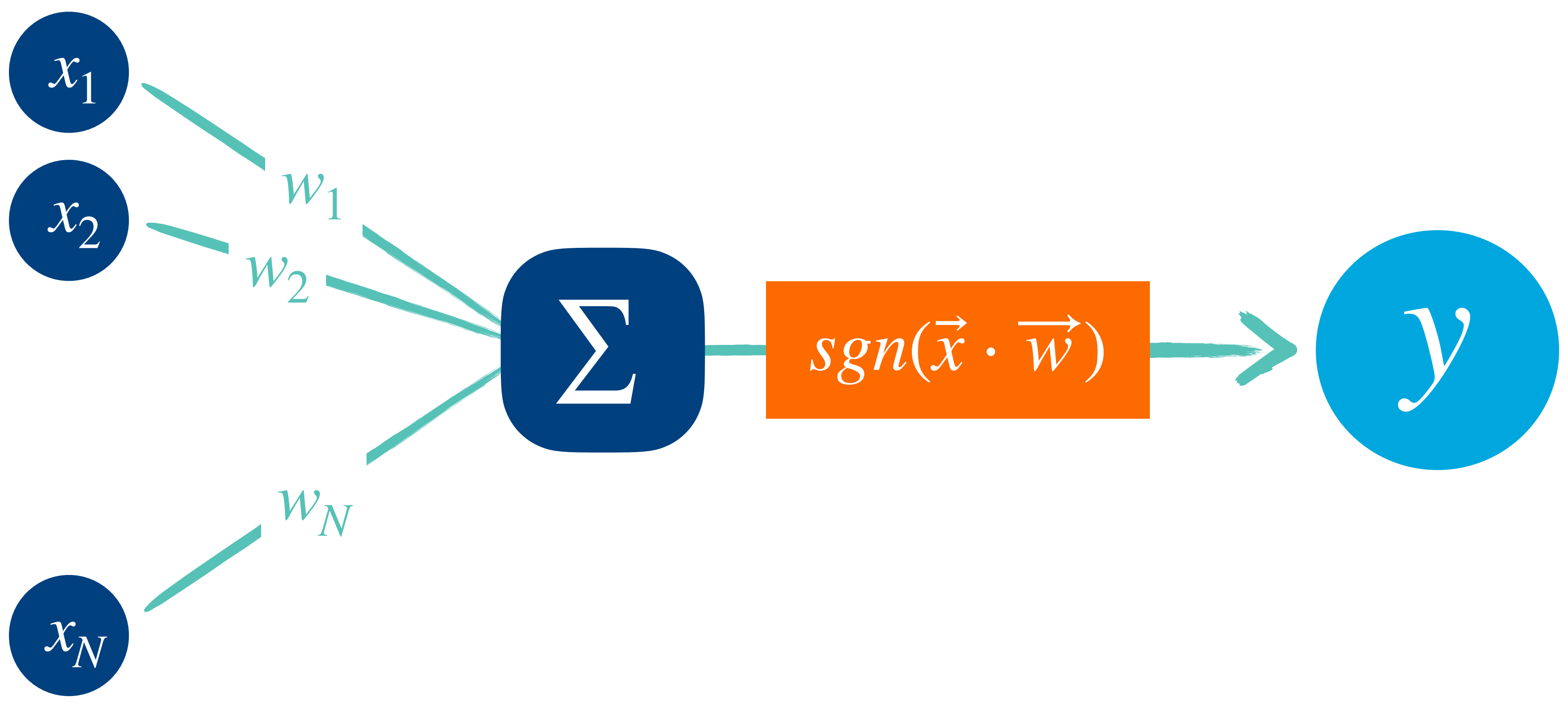
Weight vector w

$[-1,1,-1\ \ldots,-1,-1,1]$

Labels $\{y_i\}$

$$y_i = \mathrm{sgn}\left(w\, x_i\right)$$

Perceptron



Energy

$$E_w = \sum_i^P \Theta\left(-y_i \cdot \text{sgn}\left(w\, x_i\right)\right)$$

Number of Errors

Entropy

$$S(\overline{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \overline{E})\right)$$

N small (< 25) → **EASY**

Inputs $\{x_i\}_1^P$

$$\begin{array}{c} [1,1,-1,\ldots,1,-1,-1] \\ [-1,1,1,\ \ldots,-1,1,-1] \\ \vdots \\ [-1,-1,1,\ \ldots,-1,1,1] \end{array}$$

P

N

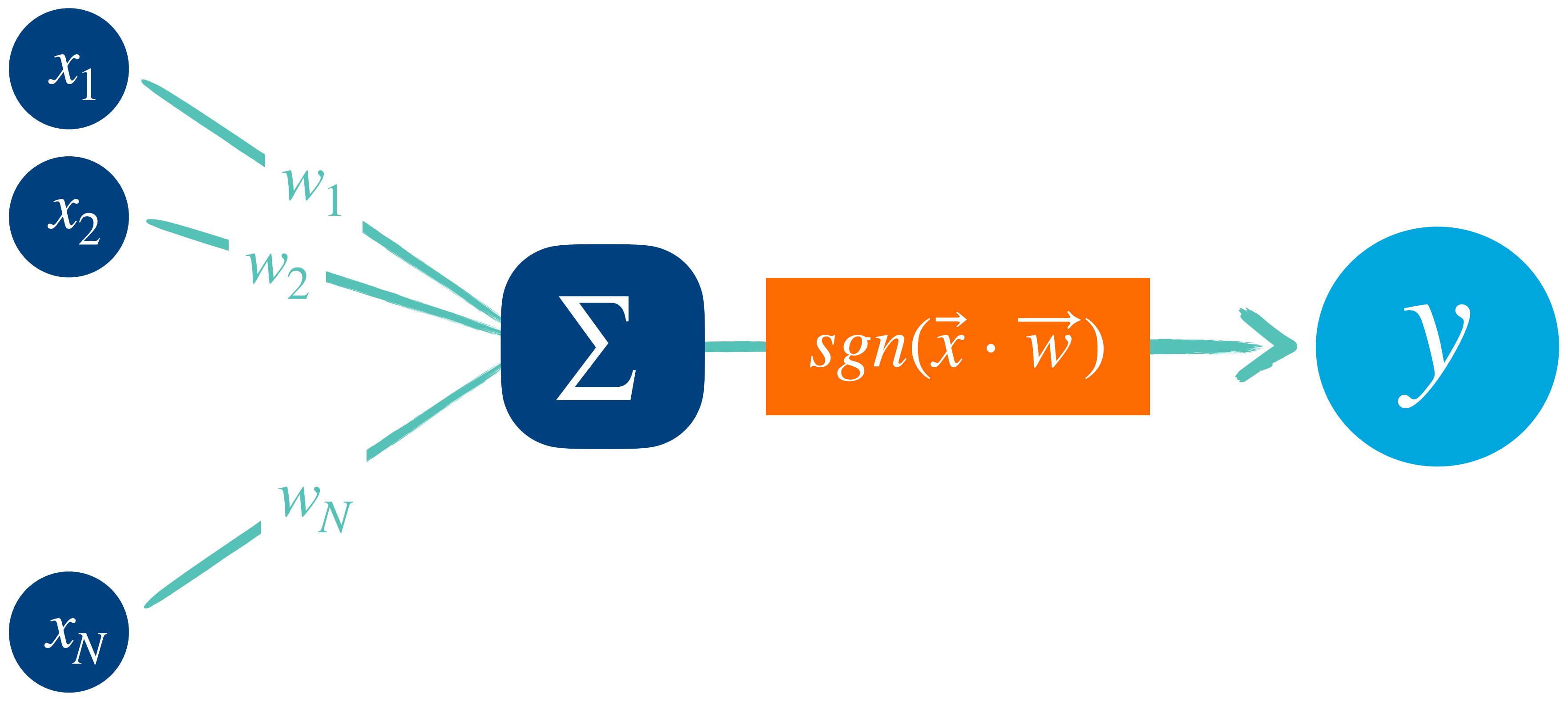
Weight vector w

$$[-1,1,-1\ \ldots,-1,-1,1]$$

Labels $\{y_i\}$

$$y_i = \text{sgn}\left(w\, x_i\right)$$

Perceptron



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$$E_w = \sum_i^P \Theta\left(-y_i \cdot \mathrm{sgn}\left(w\, x_i\right)\right)$$

Number of Errors

Entropy

$$\boxed{S(\overline{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \overline{E})\right)}$$

N small (< 25) **EASY**

N big (>30)

Inputs $\{x_i\}_1^P$

P

$[1,1,-1,\ldots,1,-1,-1]$

$[-1,1,1,\ \ldots,-1,1,-1]$

$\vdots$

$[-1,-1,1,\ \ldots,-1,1,1]$

N

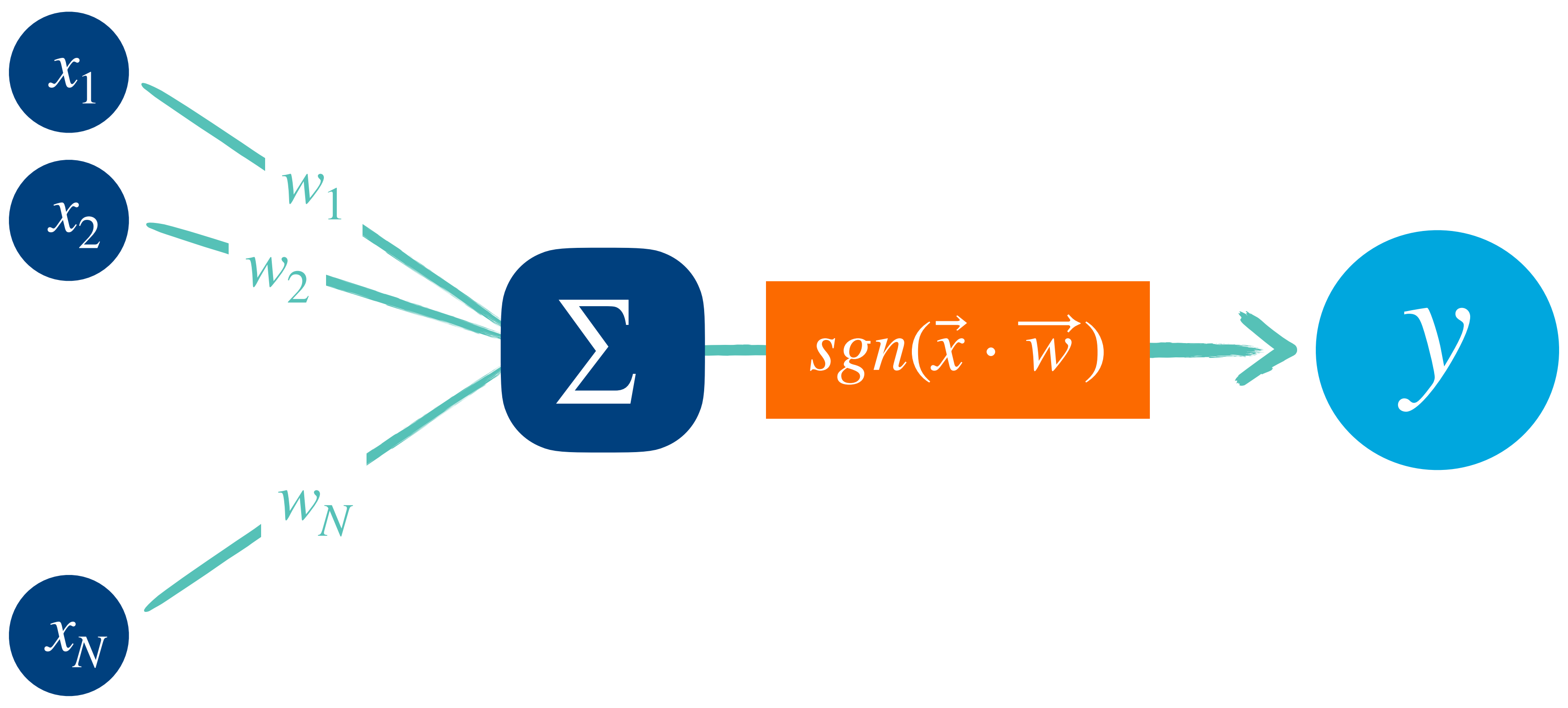
Weight vector w

$[-1,1,-1\ \ldots,-1,-1,1]$

Labels $\{y_i\}$

$$y_i = \mathrm{sgn}\left(w\, x_i\right)$$

Perceptron



Energy

$$E_w = \sum_i^P \Theta\left(-y_i \cdot \mathrm{sgn}\left(w\, x_i\right)\right)$$

Number of Errors

Entropy

$$S(\bar{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \bar{E})\right)$$

N small (< 25) → **EASY**

N big (>30) → **HARD**

Inputs $\{x_i\}_1^P$

$$\begin{array}{c} [1,1,-1,\ldots,1,-1,-1] \\ [-1,1,1,\ \ldots,-1,1,-1] \\ \vdots \\ [-1,-1,1,\ \ldots,-1,1,1] \end{array}$$

P

N

Weight vector w

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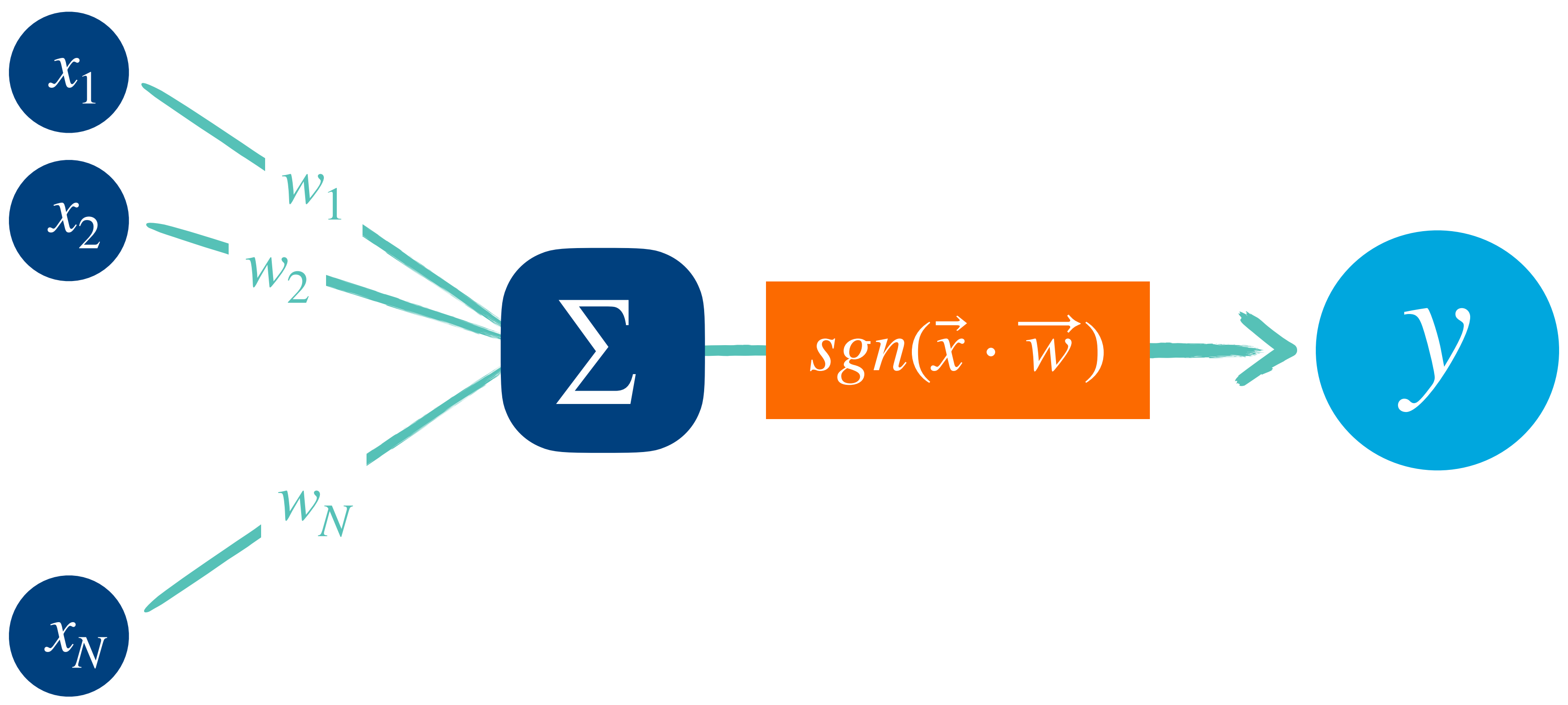

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Number of Errors

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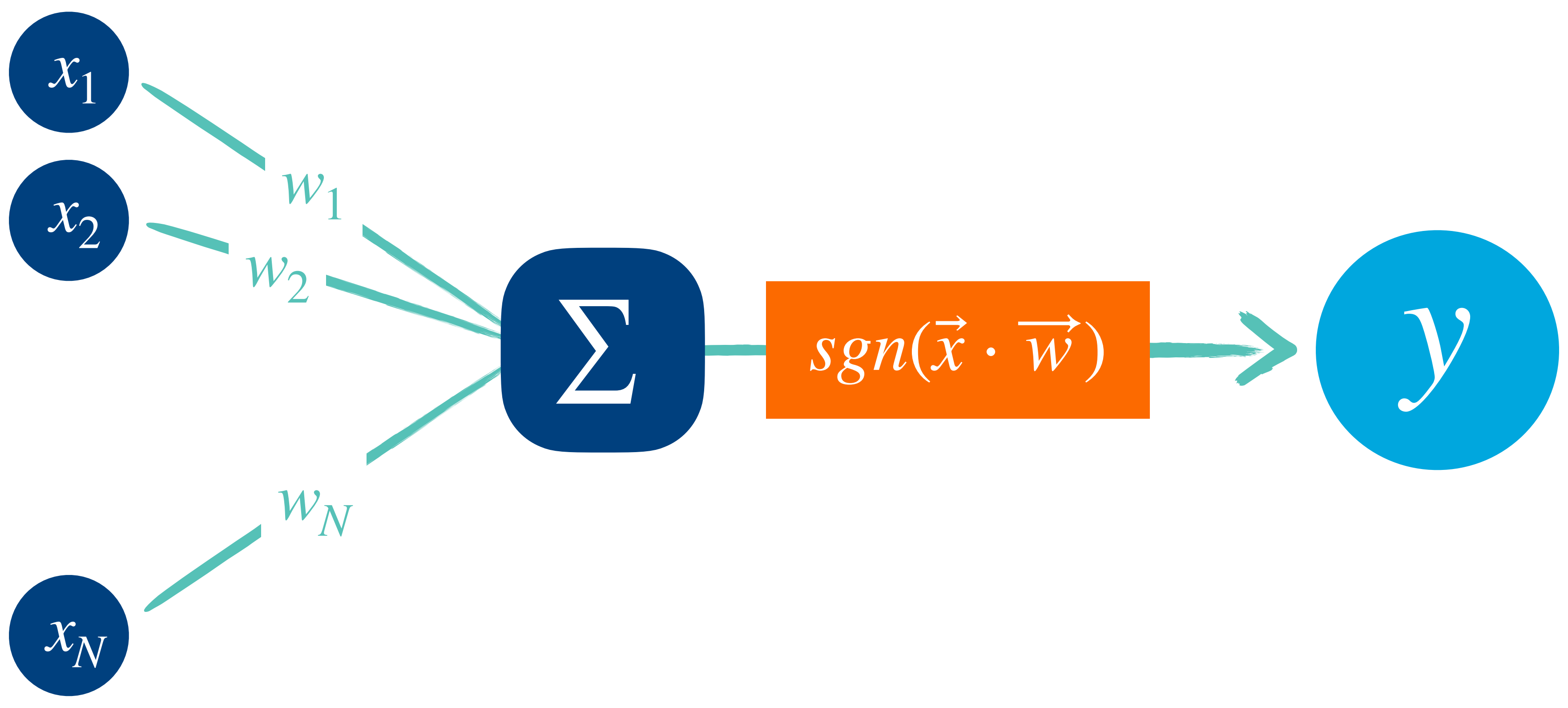
$$\boxed{S(\overline{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \overline{E})\right)}$$

N small (< 25) → **EASY**

N big (>30) → **HARD**

- Huge configurational space $2^{30} = 1073741824$

Perceptron



Inputs $\{x_i\}_1^P$

$$\begin{array}{c|c} & [1,1,-1,\ldots,1,-1,-1] \\ P & [-1,1,1,\ldots,-1,1,-1] \\ & \vdots \\ & [-1,-1,1,\ldots,-1,1,1] \end{array}$$

N

Weight vector w

$$[-1,1,-1 \ldots, -1,-1,1]$$

Labels $\{y_i\}$

$$y_i = \mathrm{sgn}\,(w\,x_i)$$

Energy

$$E_w = \sum_i^P \Theta\left(-y_i \cdot \mathrm{sgn}\,(w\,x_i)\right)$$

Number of Errors

Entropy

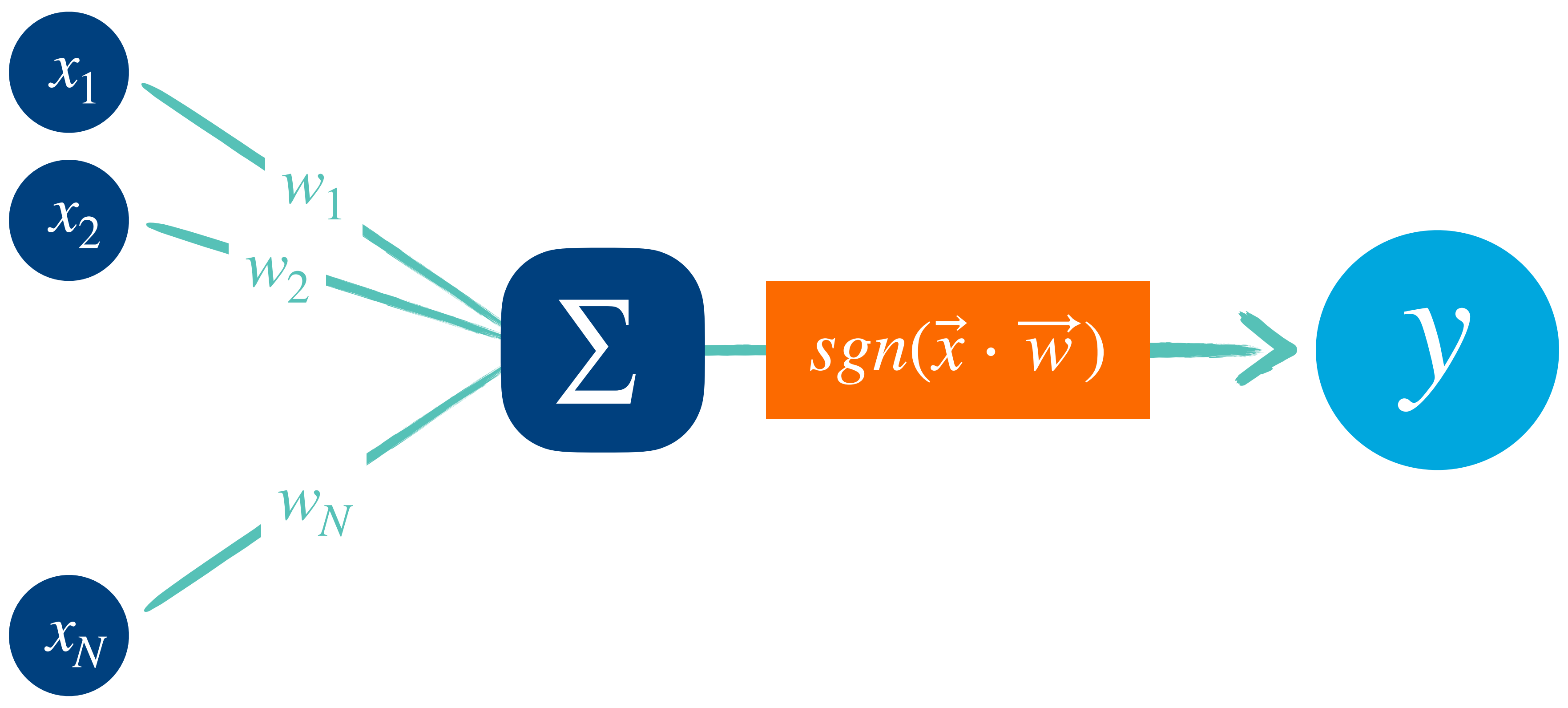
$$\boxed{S(\bar{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \bar{E})\right)}$$

N small (< 25) $\longrightarrow$ **EASY**

N big (>30) $\longrightarrow$ **HARD**

- Huge configurational space $2^{30} = 1073741824$
- Sampling algorithms get trapped in local minima

Perceptron



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$$E_w = \sum_i^P \Theta\left(-y_i \cdot \mathrm{sgn}\left(w\, x_i\right)\right)$$

Number of Errors

Entropy

$$\boxed{S(\overline{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \overline{E})\right)}$$

N small (< 25) → **EASY**

N big (>30) → **HARD**

Inputs $\{x_i\}_1^P$

$$\begin{array}{c} [1,1,-1,\ldots,1,-1,-1] \\ [-1,1,1,\ldots,-1,1,-1] \\ \vdots \\ [-1,-1,1,\ldots,-1,1,1] \end{array}$$

P (rows), N (columns)

Weight vector w

$$[-1,1,-1\ \ldots,-1,-1,1]$$

Labels $\{y_i\}$

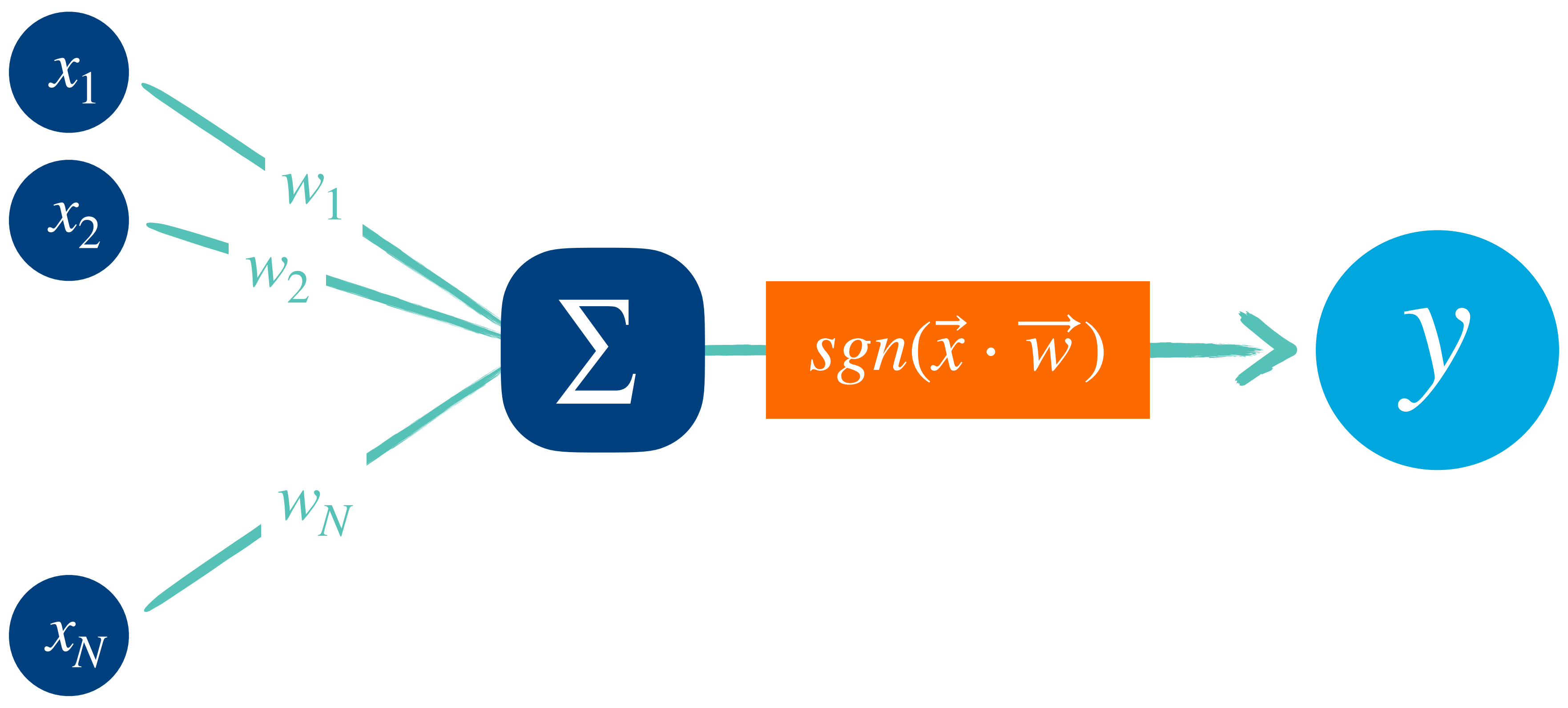
$$y_i = \mathrm{sgn}\left(w\, x_i\right)$$

- Huge configurational space $2^{30} = 1073741824$
- Sampling algorithms get trapped in local minima

→ **Self-consistent entropy estimation**

→ **Uniform exploration of the energy spectrum**

Perceptron



Energy

$$E_w = \sum_{i}^{P} \Theta\left(-y_i \cdot \operatorname{sgn}\left(w\, x_i\right)\right)$$

Number of Errors

Entropy

$$S(\overline{E}) = \log\left(\sum_{\{w\}} \delta(E_w - \overline{E})\right)$$

Inputs $\{x_i\}_1^P$

P

$[1,1,-1,\ldots,1,-1,-1]$

$[-1,1,1,\ \ldots,-1,1,-1]$

$\vdots$

$[-1,-1,1,\ \ldots,-1,1,1]$

N

Weight vector w

$[-1,1,-1\ \ldots,-1,-1,1]$

Labels $\{y_i\}$

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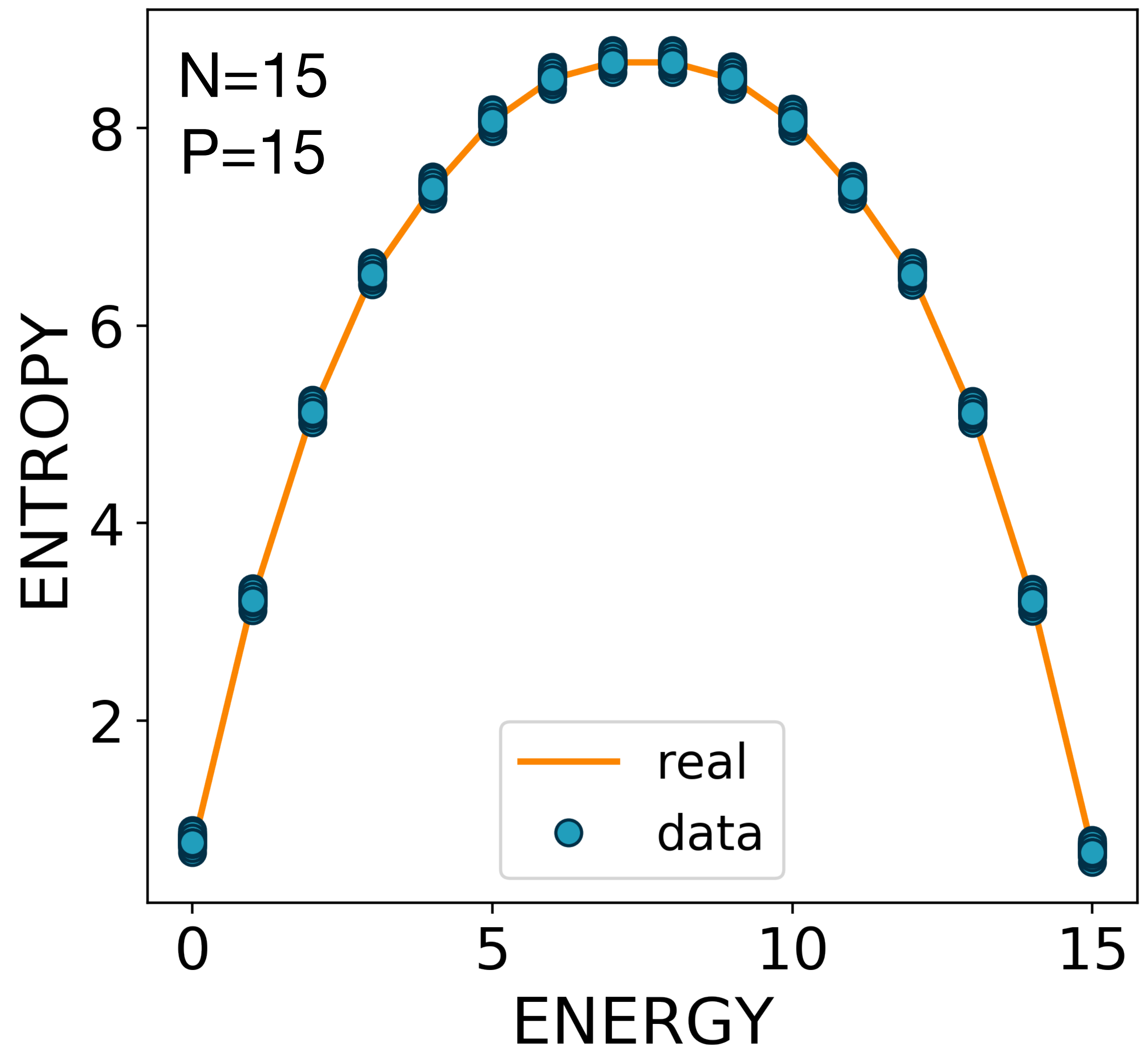
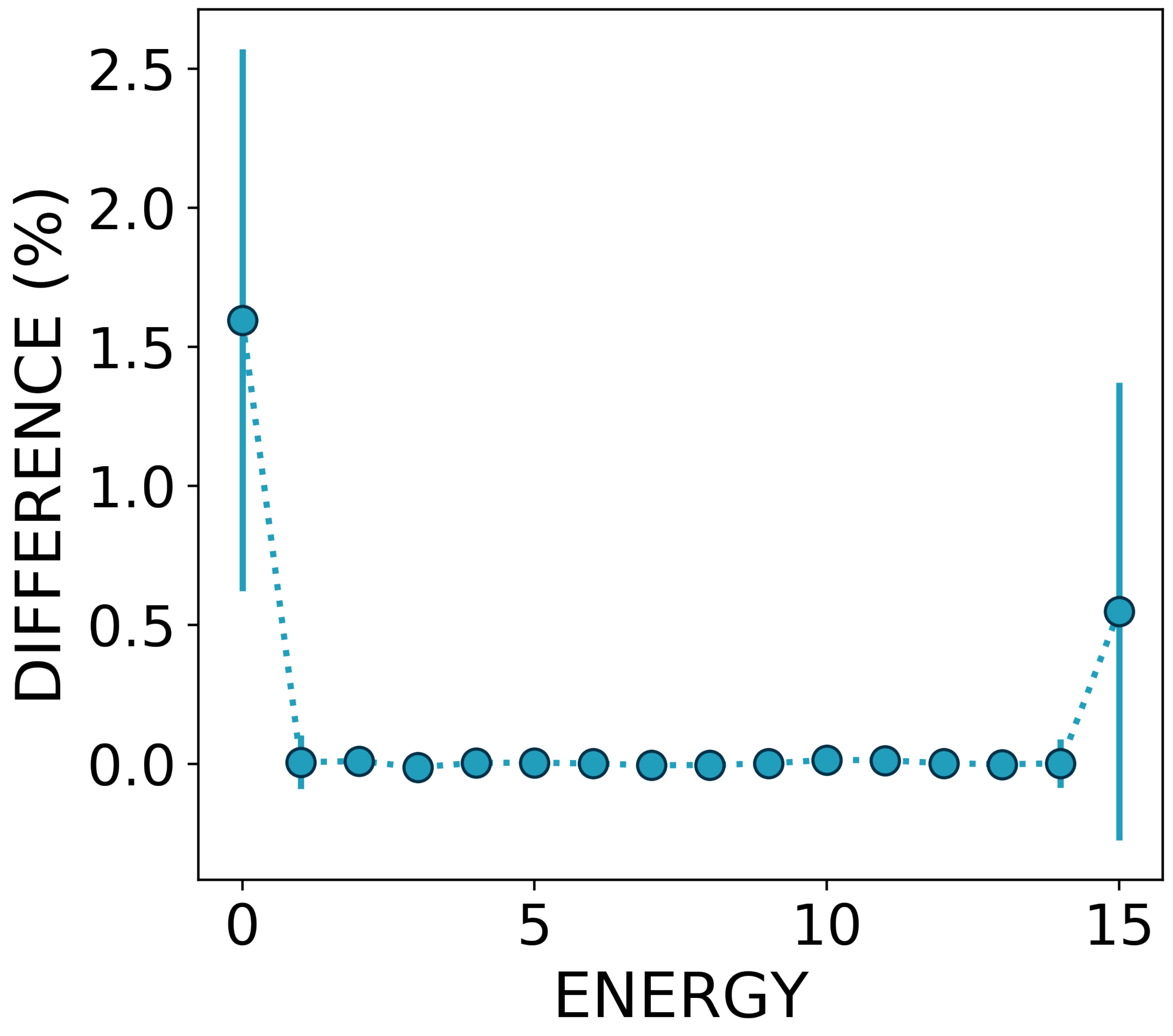
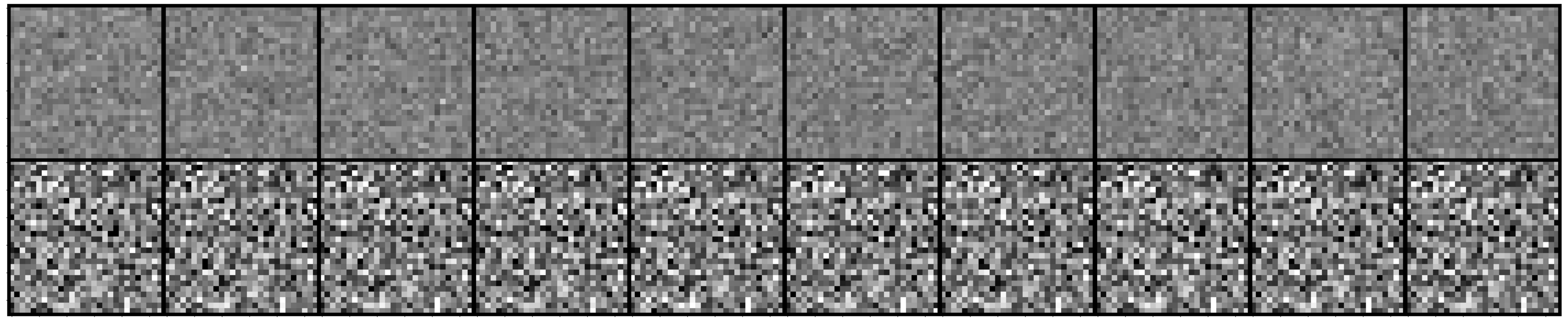
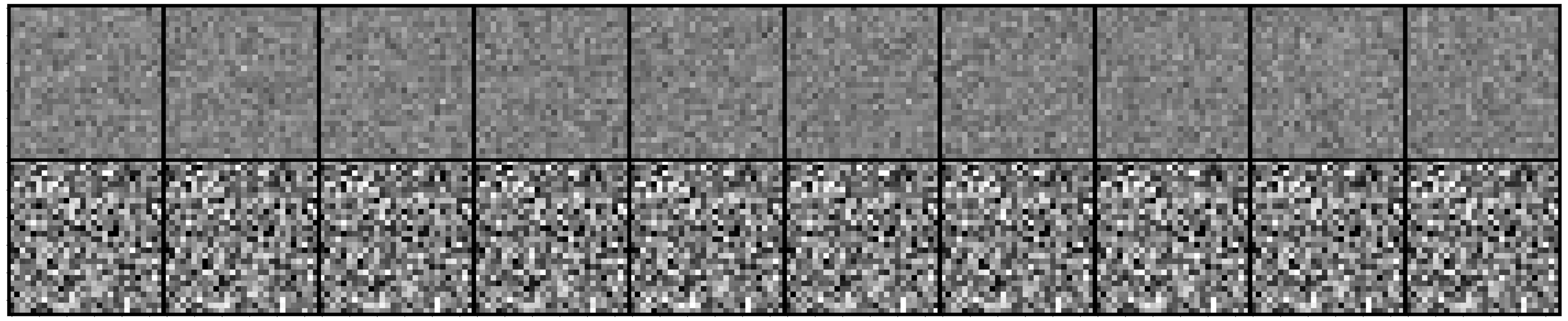


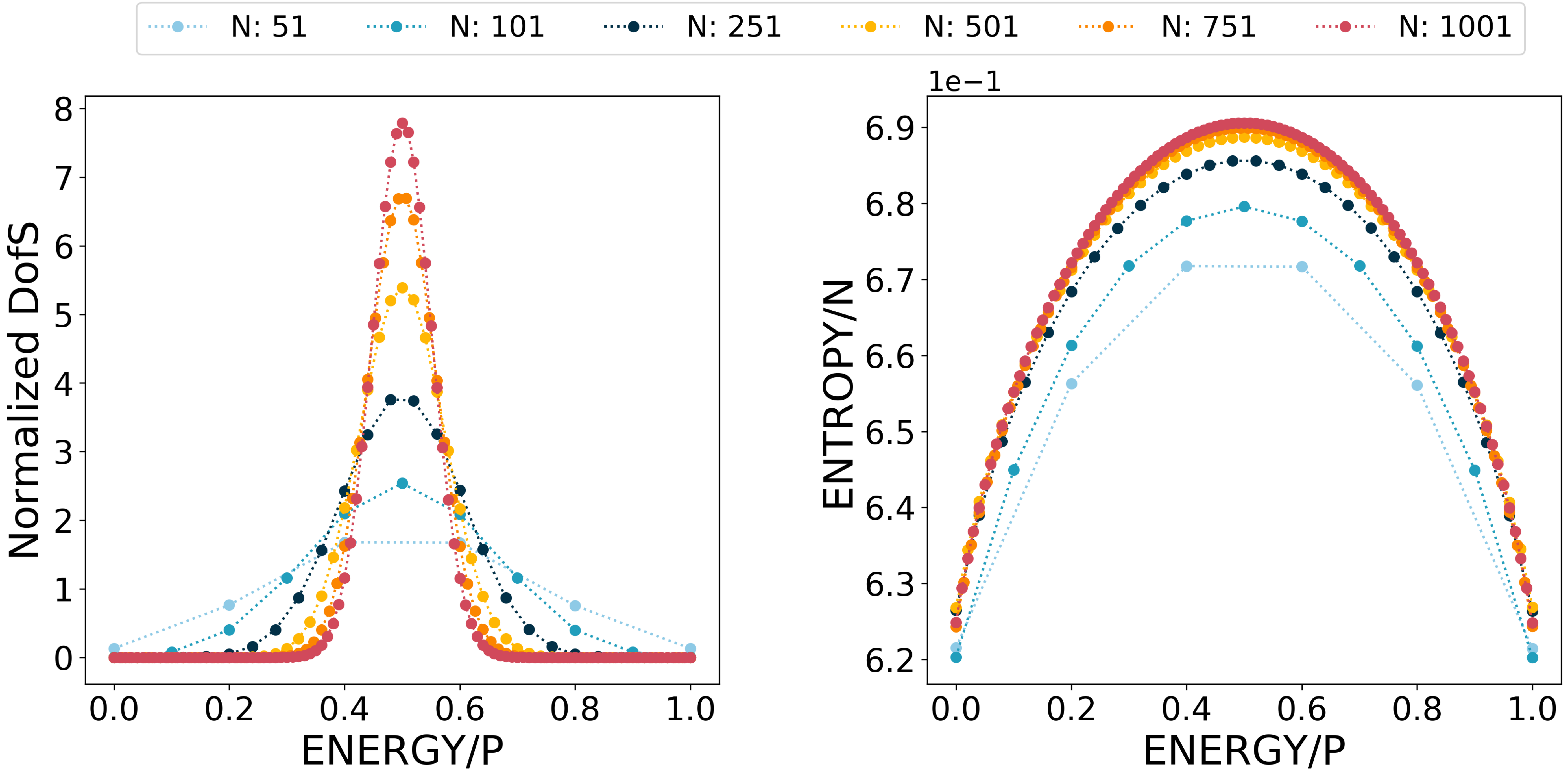


Random Data

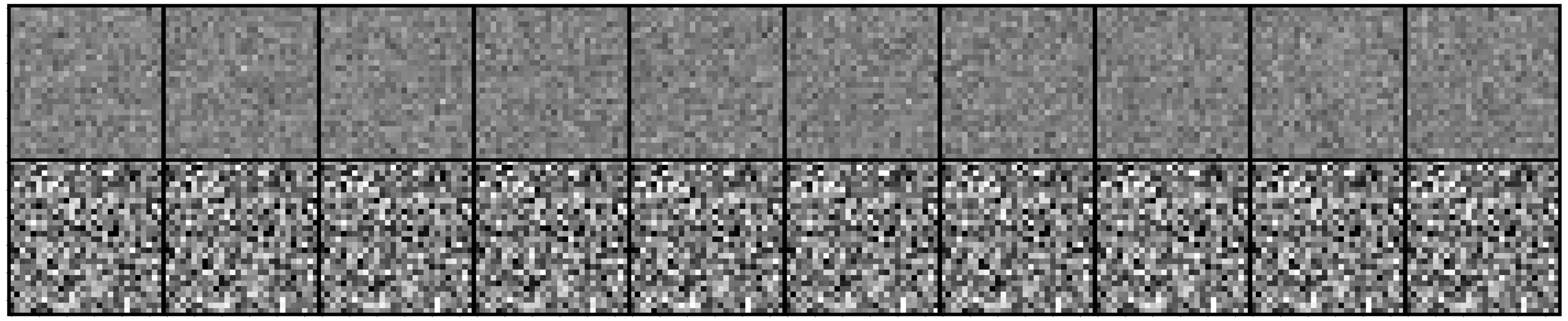


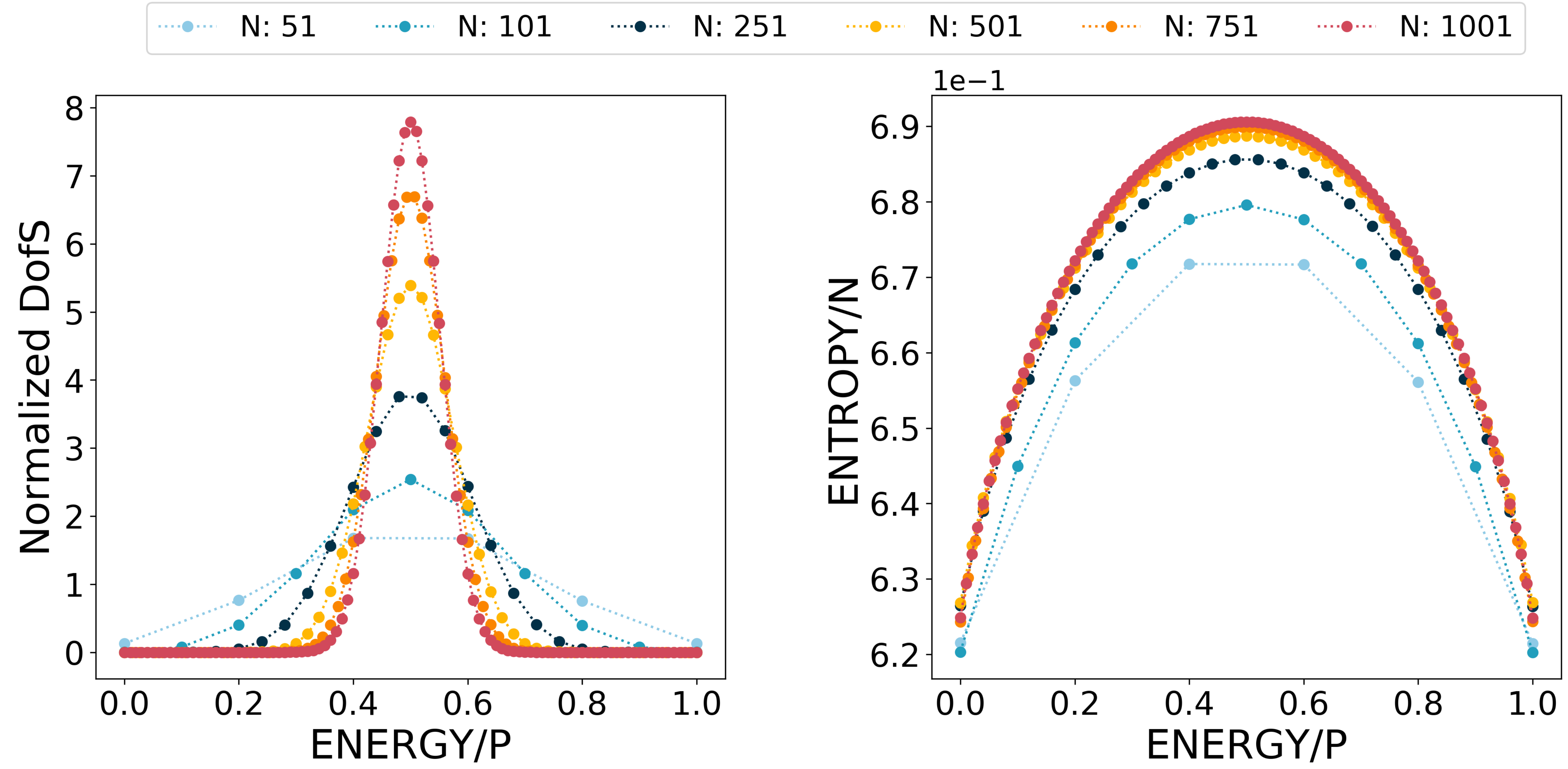
Random Data




N: 51
N: 101
N: 251
N: 501
N: 751
N: 1001
Normalized DofS
ENERGY/P
1e−1
ENTROPY/N
ENERGY/P

Random Data





N: 51
N: 101
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Normalized DofS
ENERGY/P
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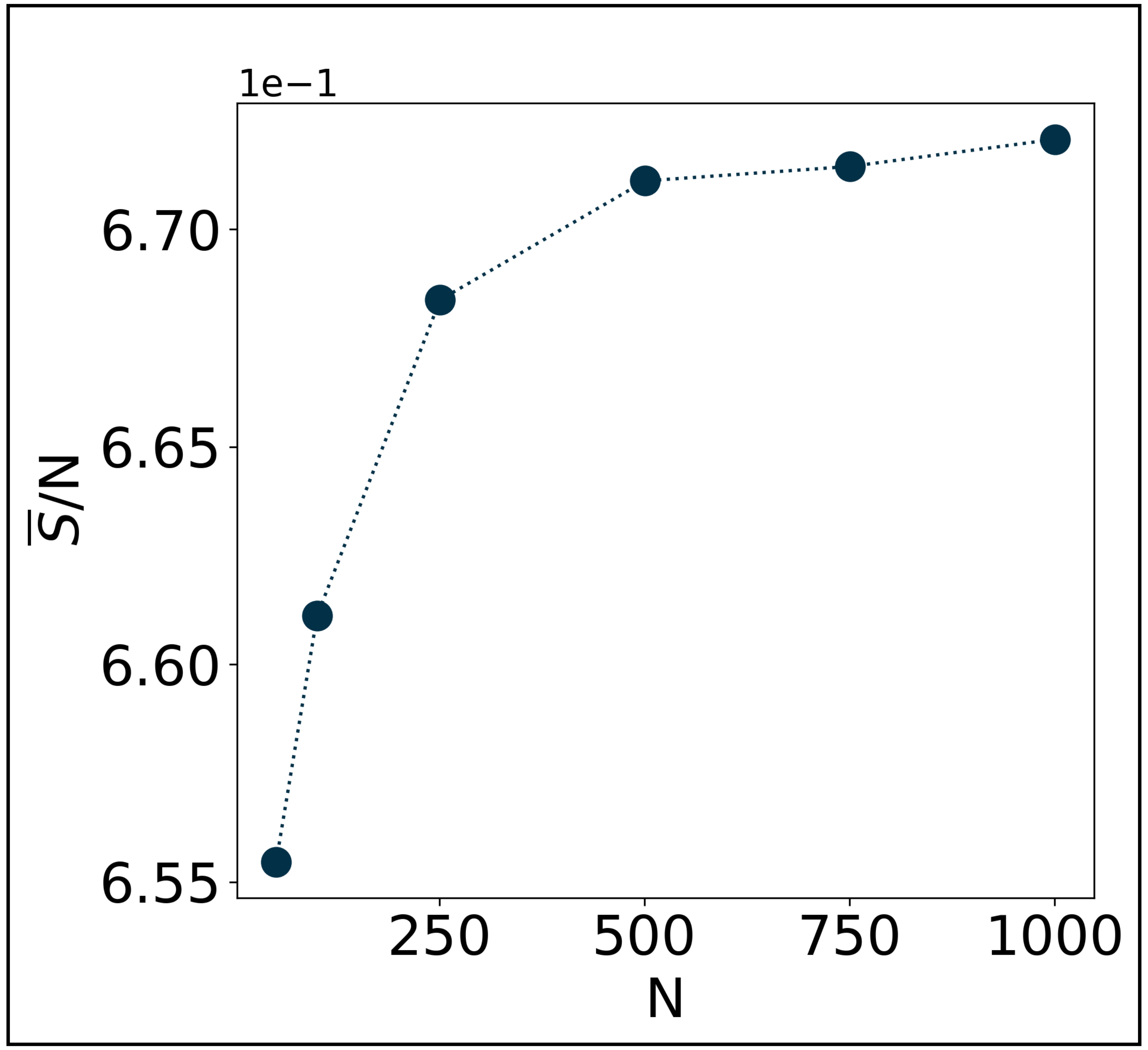
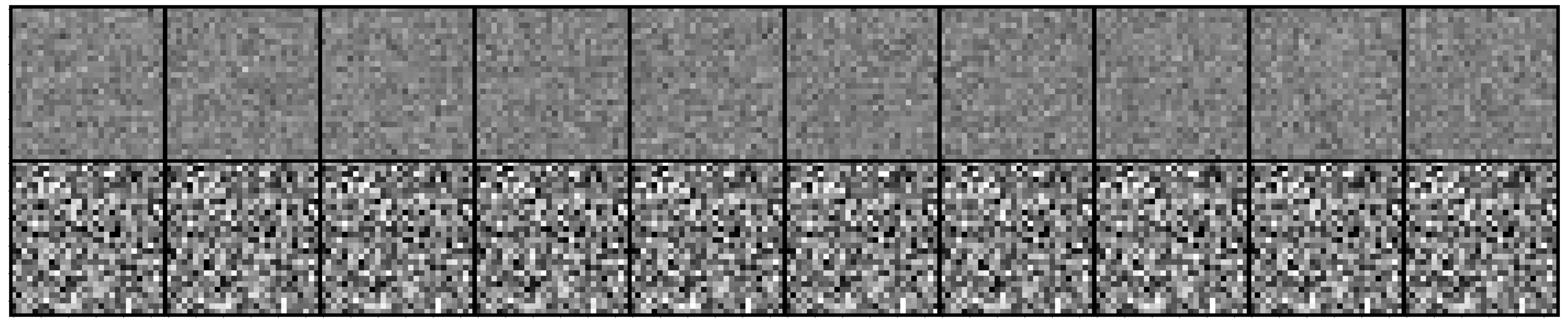
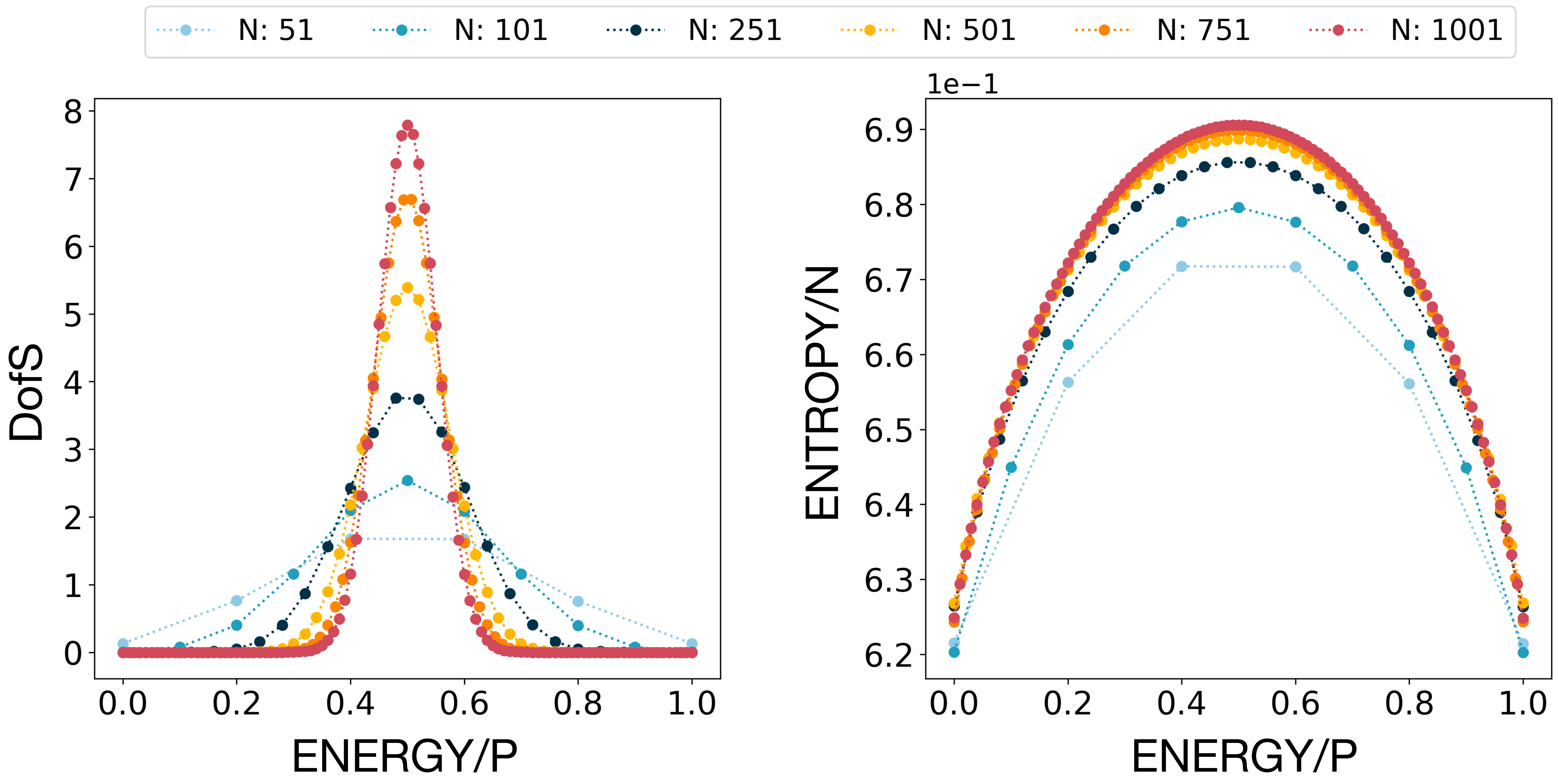


1e−1
$\overline{S}$/N
N

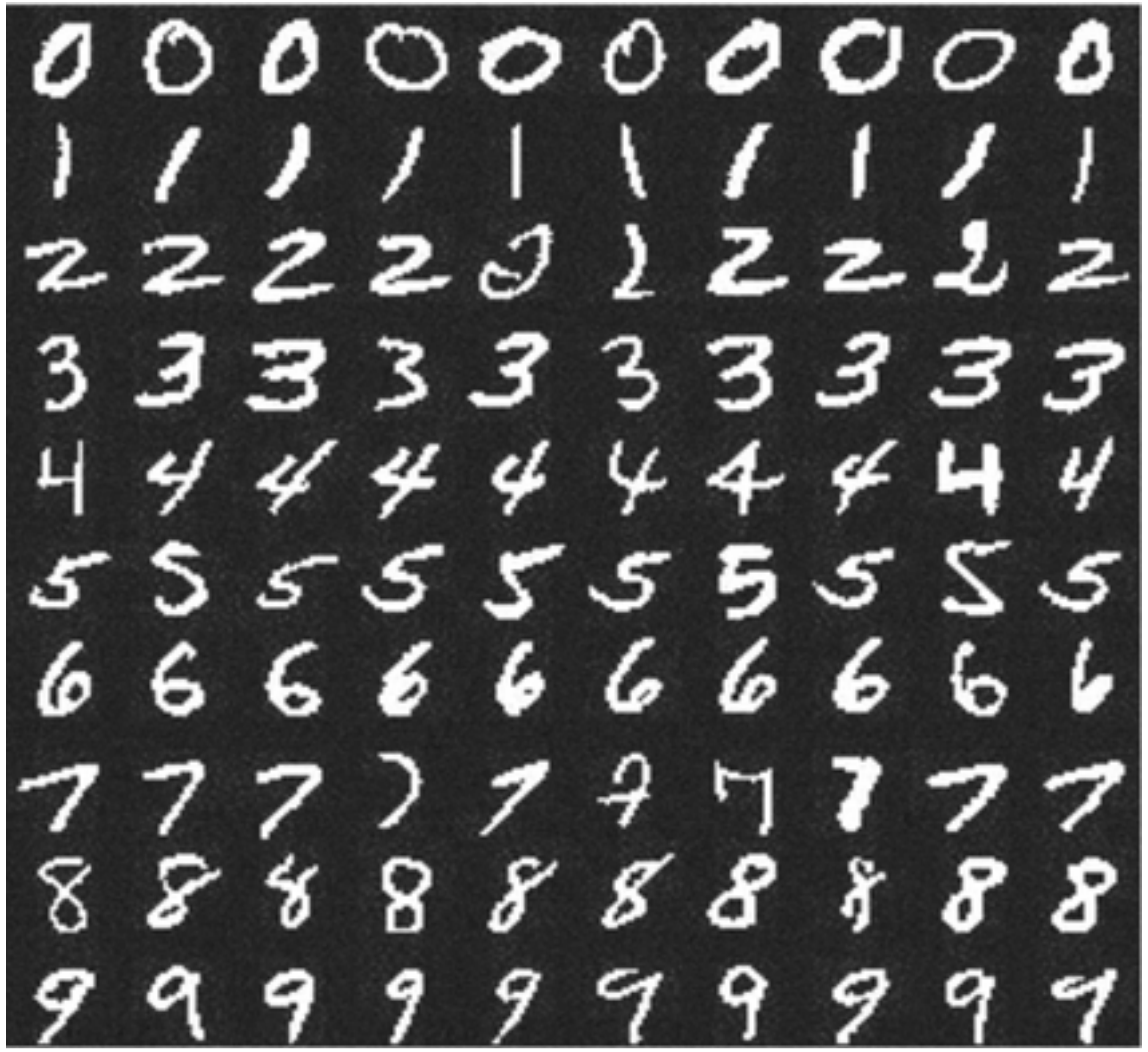
Random vs Real

Random



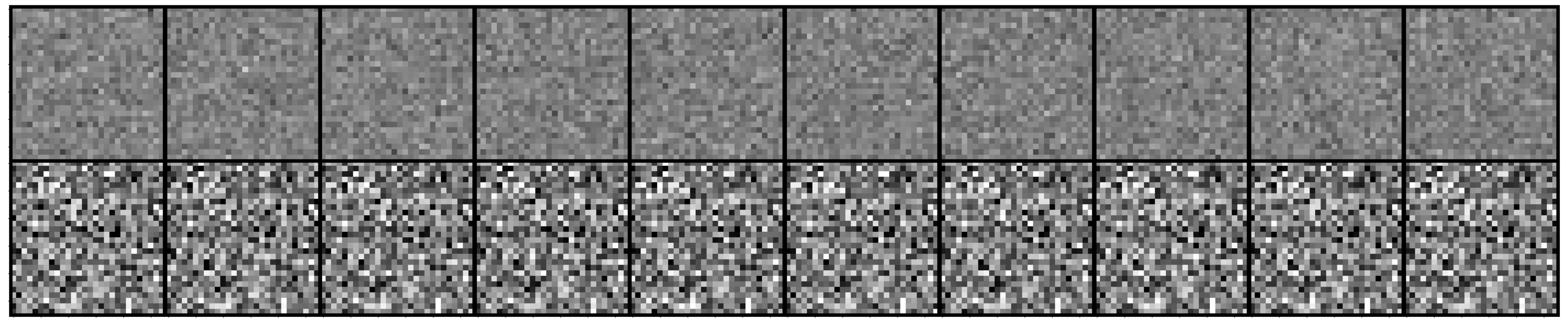


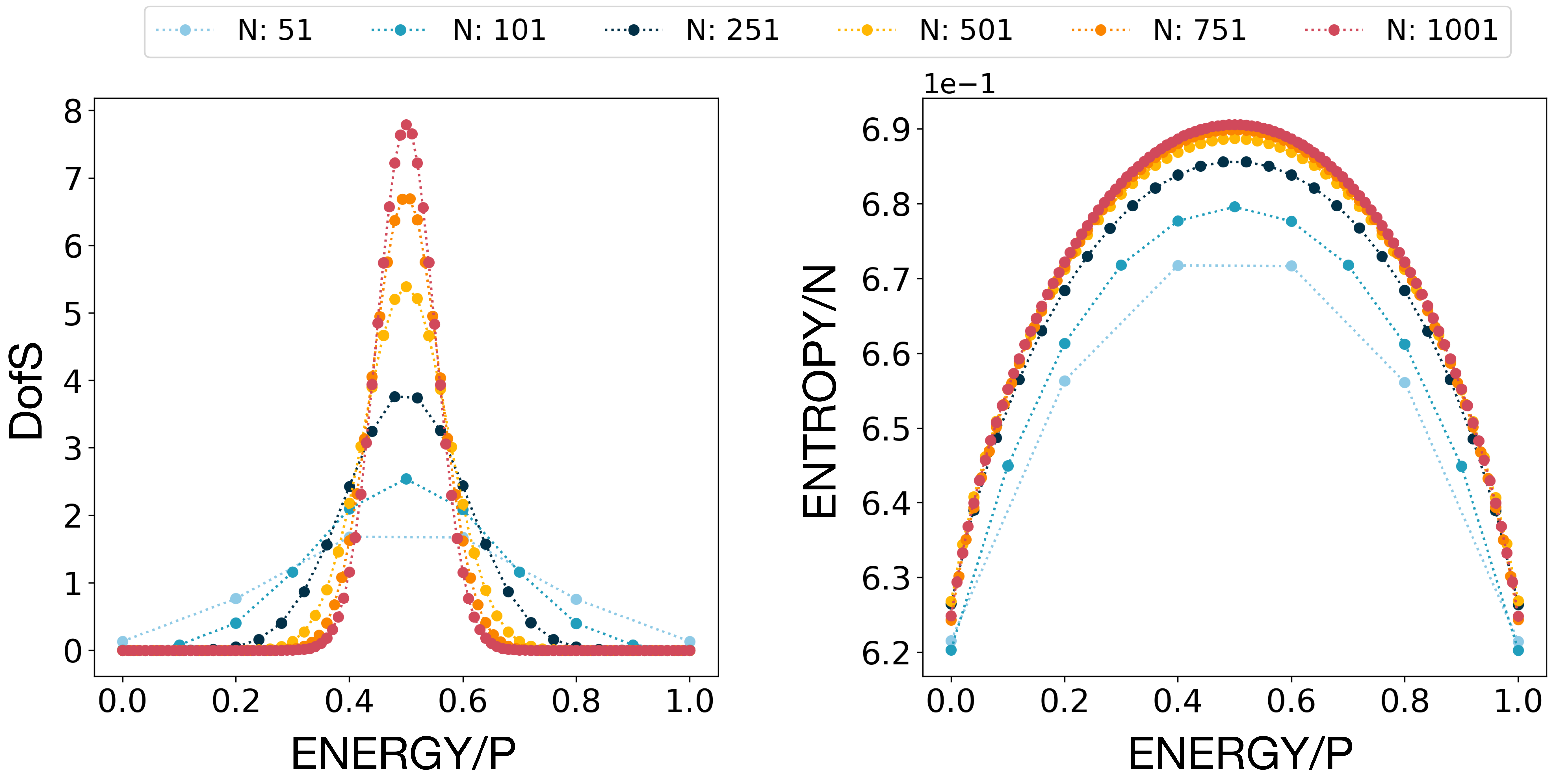
MNIST



Random vs Real

Random

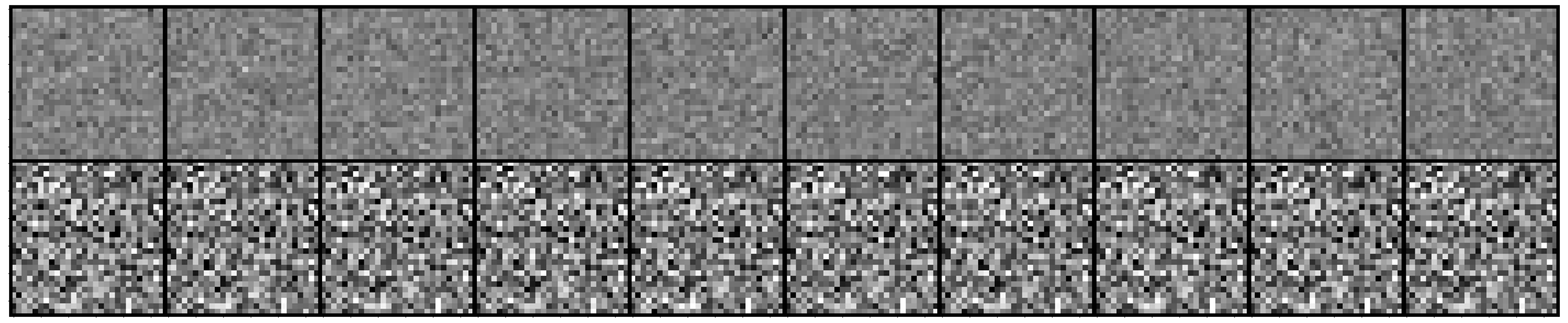


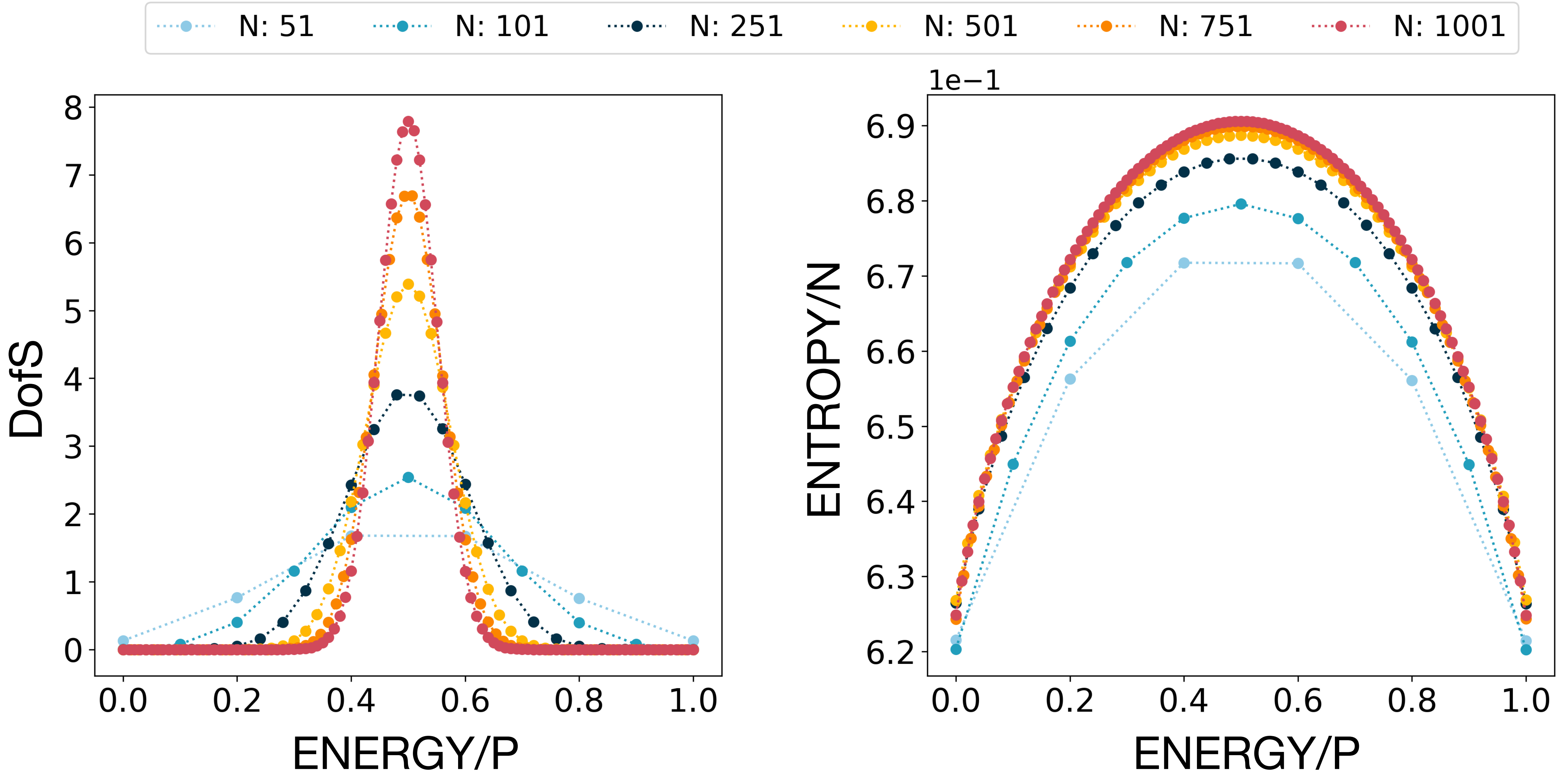


MNIST

Random vs Real

Random





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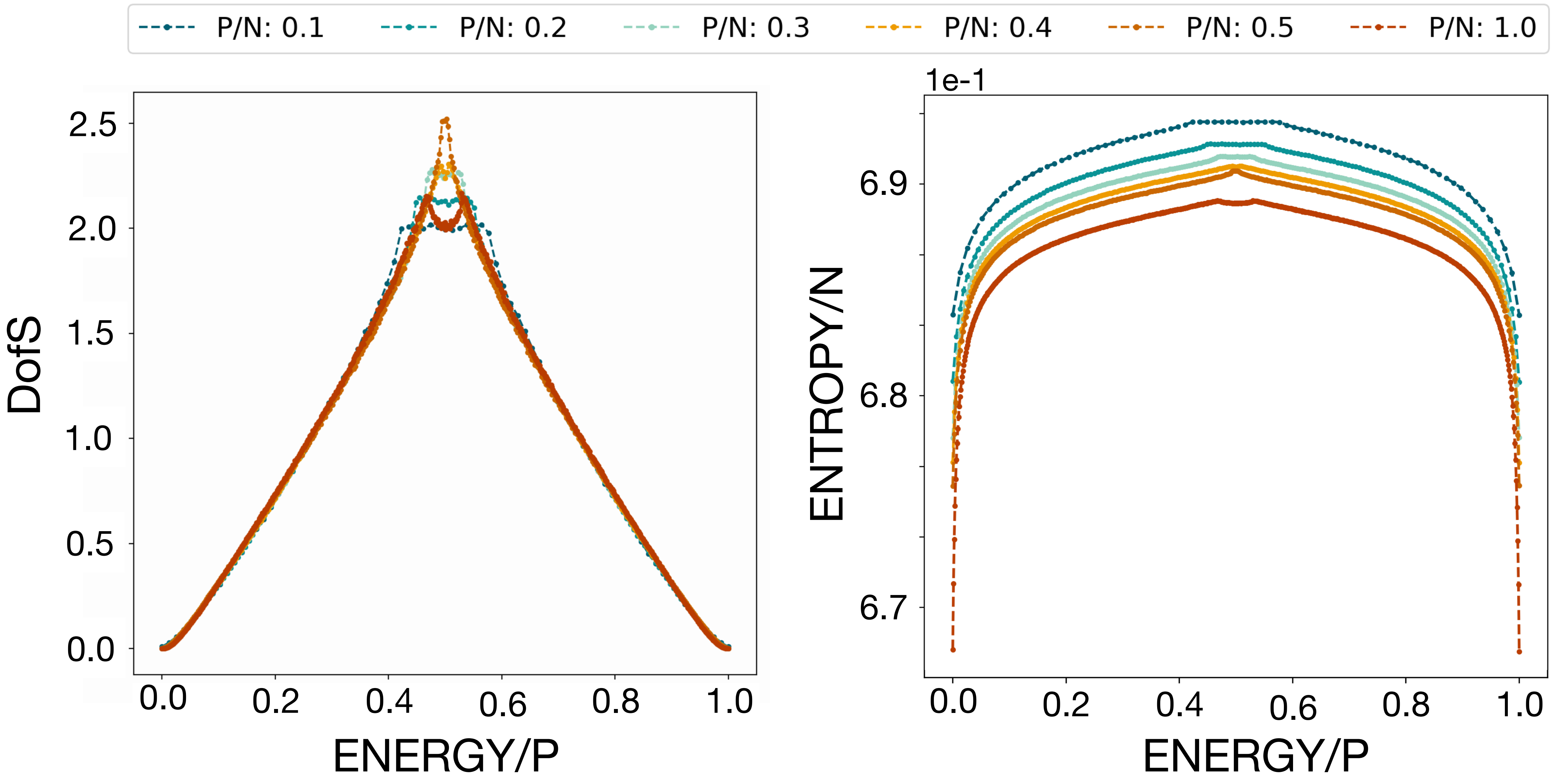
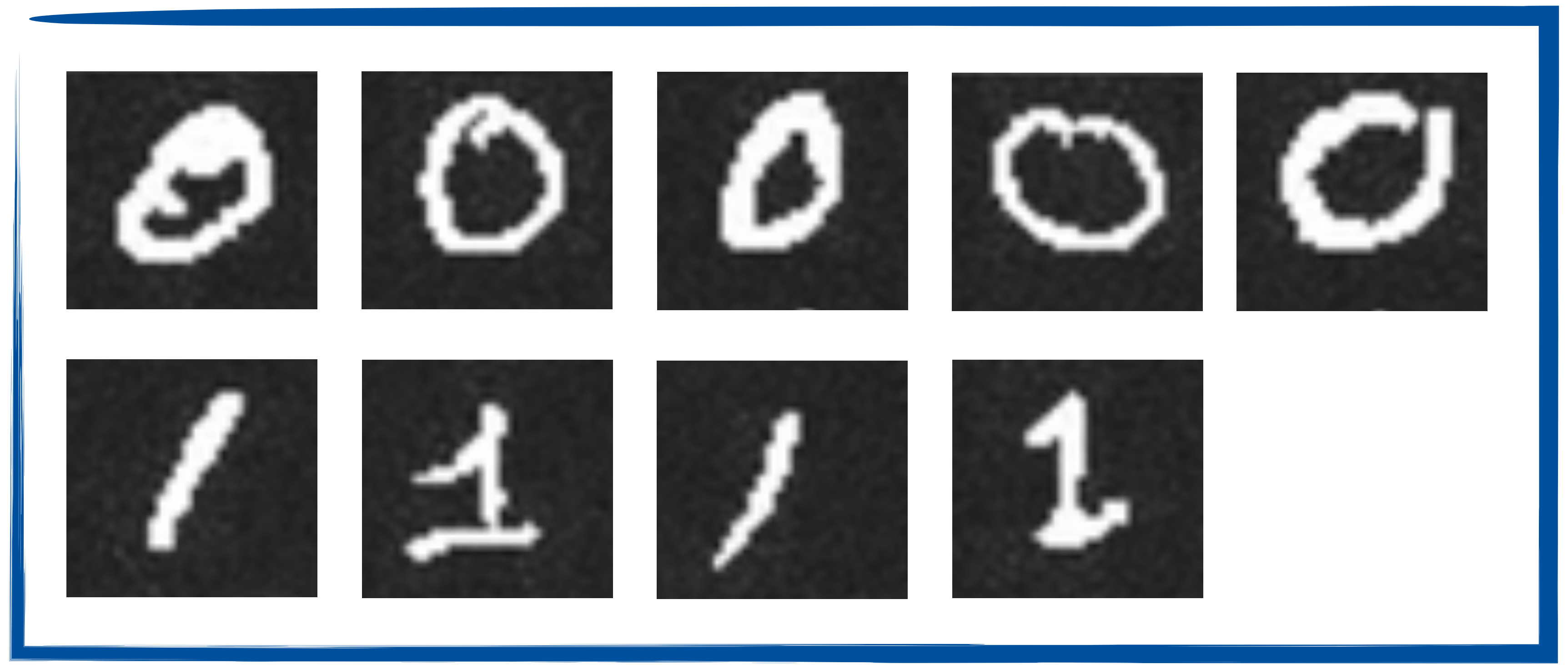


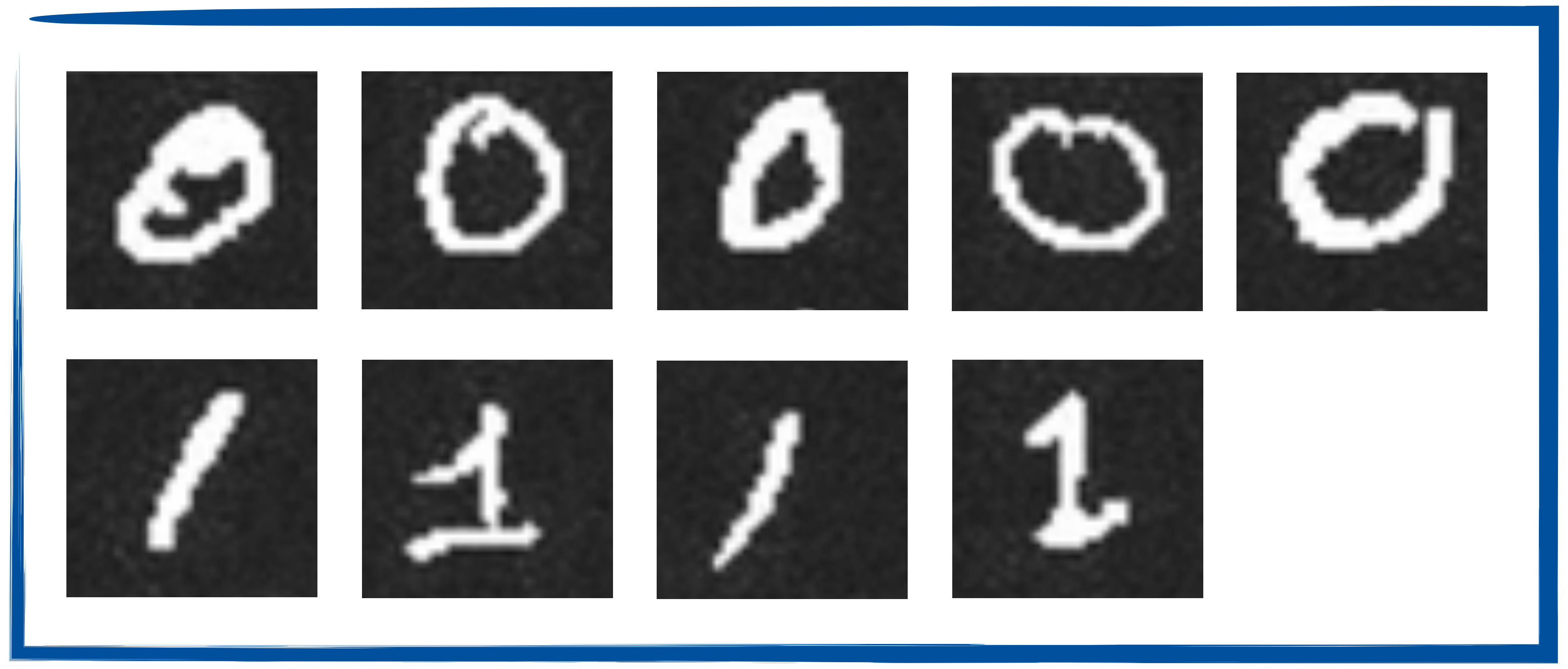
Class Unbalancing



$$P_0 \neq P_1$$

$$\frac{P_1}{P} \neq 0.5$$

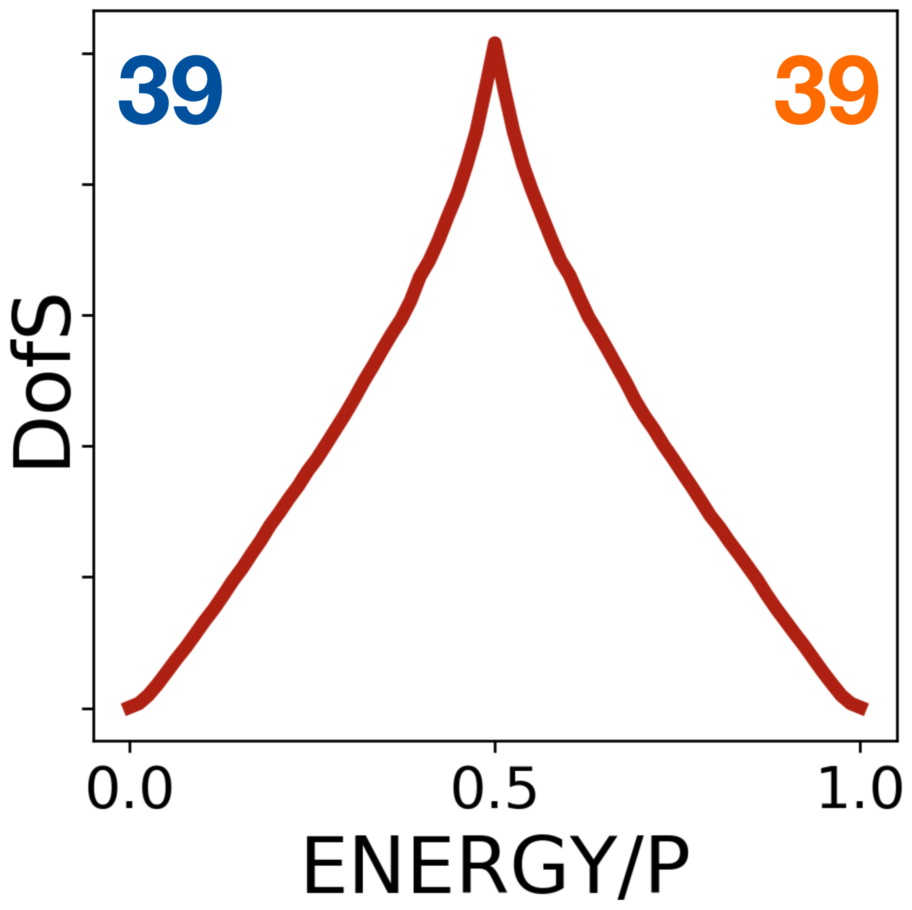
Class Unbalancing



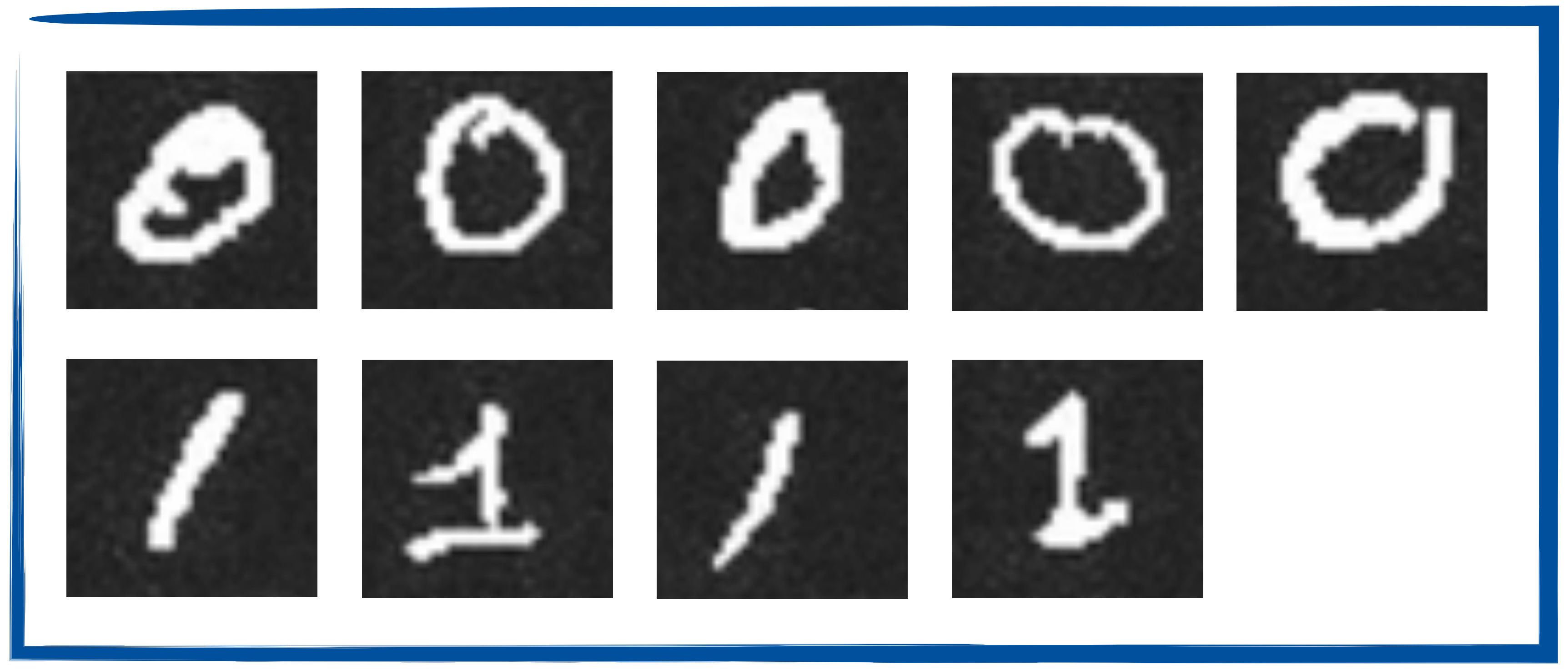
$$P_0 \neq P_1$$

$$\frac{P_1}{P} \neq 0.5$$

$$P_1 = P_0$$



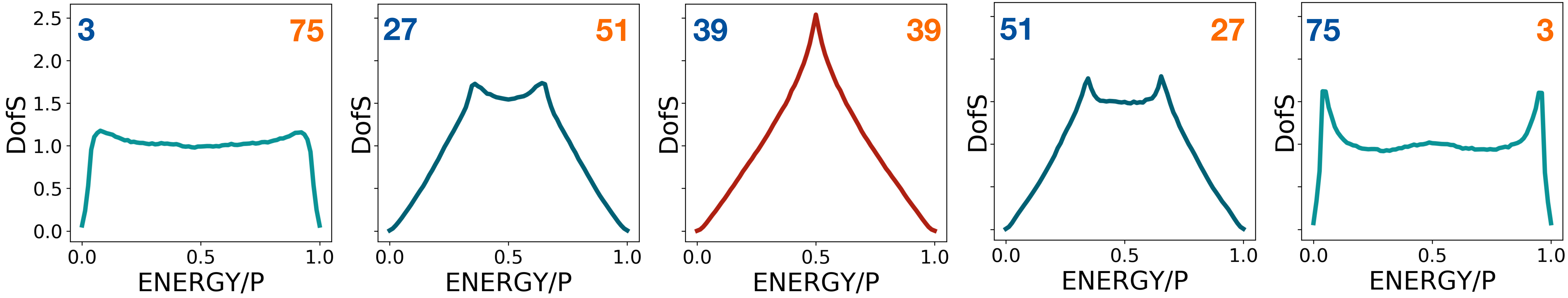
Class Unbalancing



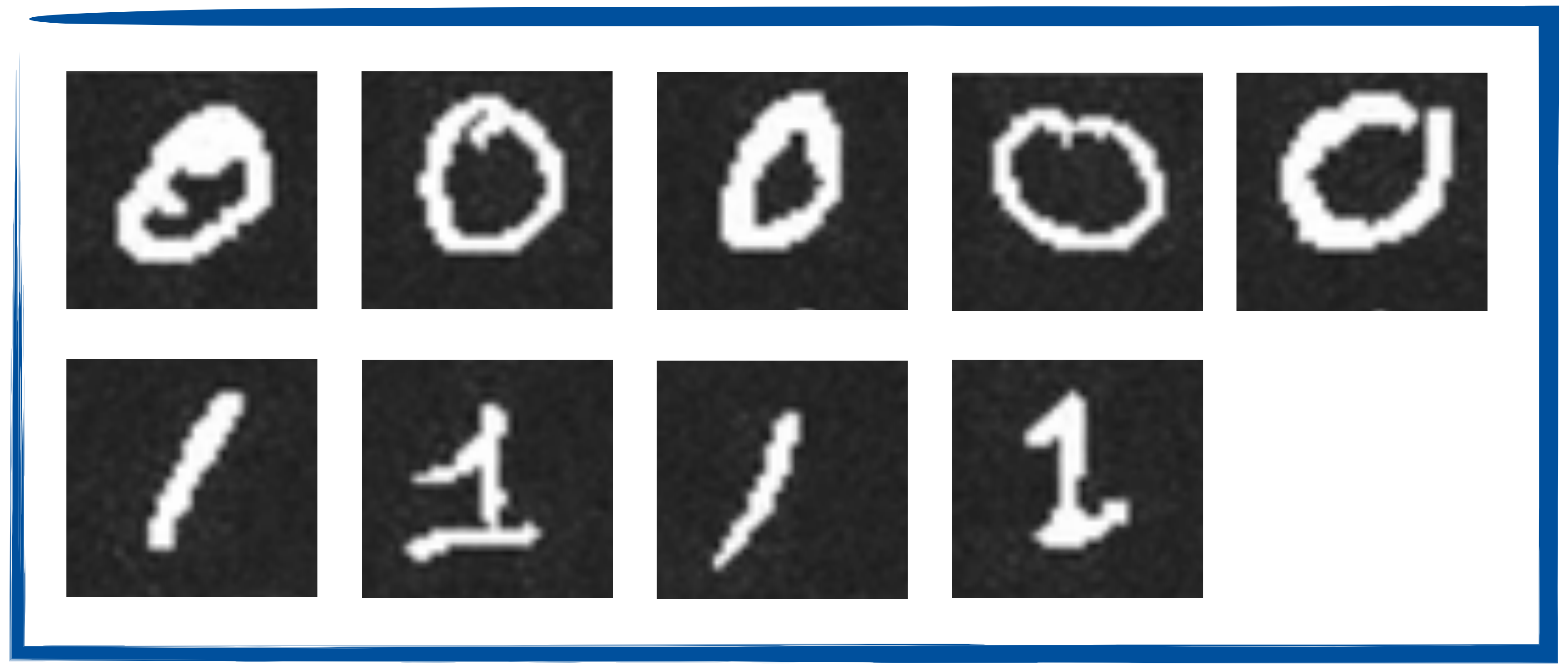
$$P_0 \neq P_1$$

$$\frac{P_1}{P} \neq 0.5$$

$P_1 \ll P_0$ | $P_1 = P_0$ | $P_1 \gg P_0$



Class Unbalancing



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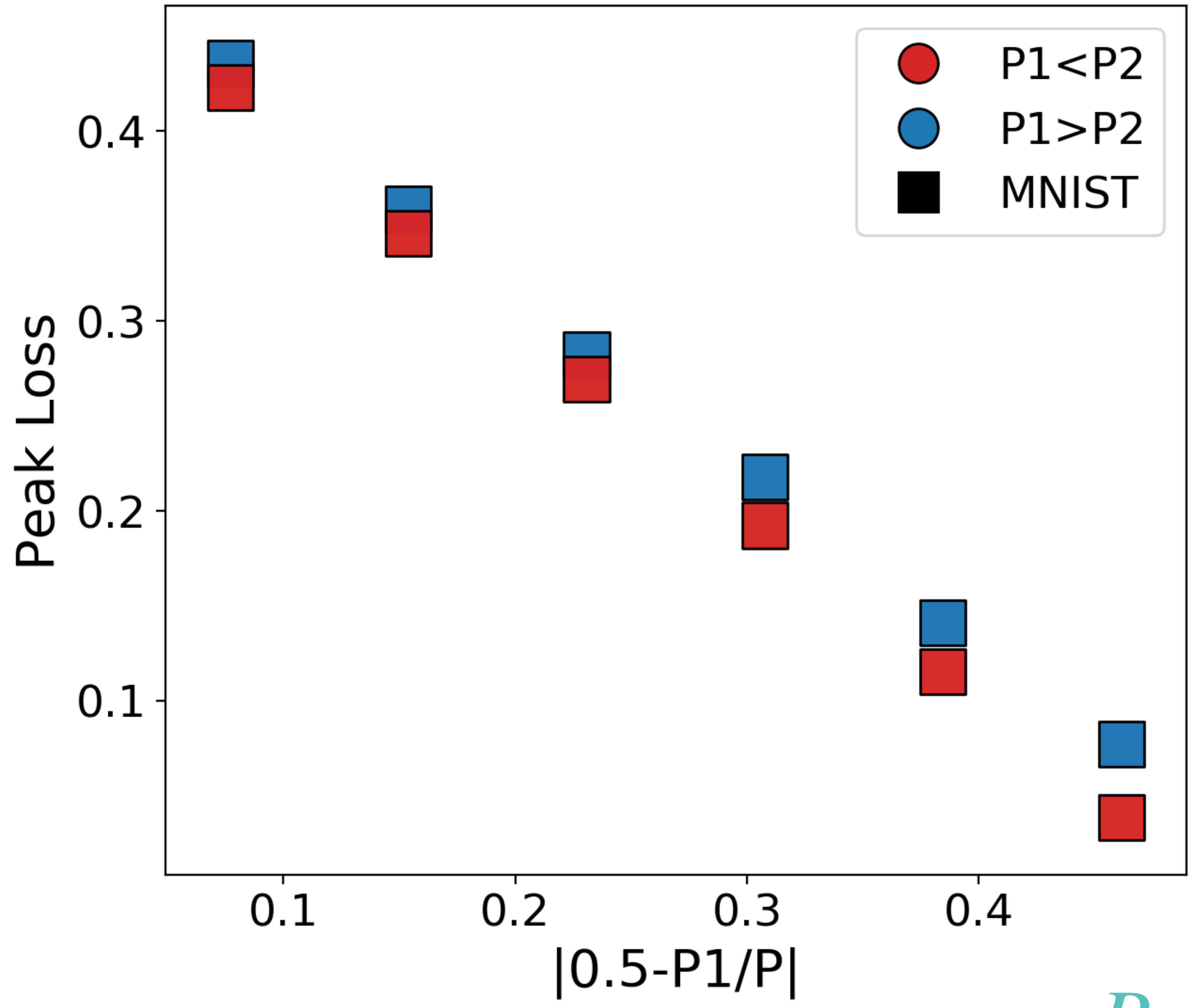
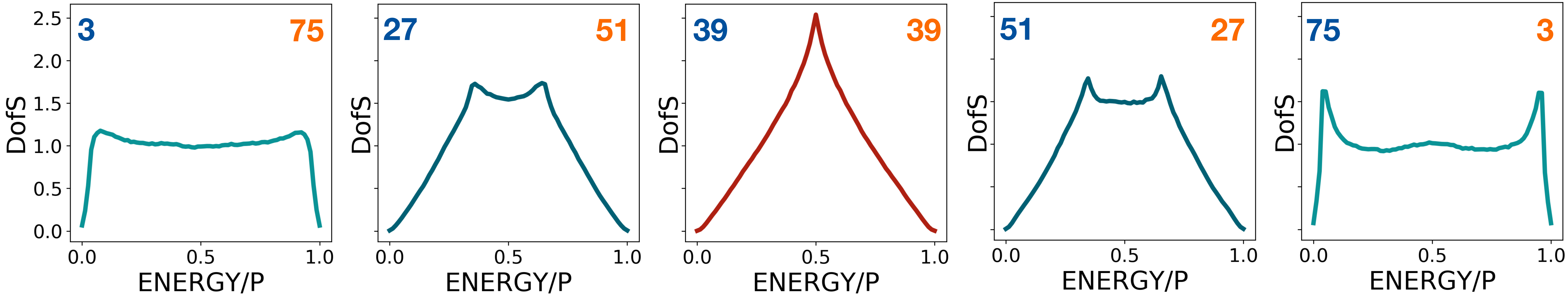


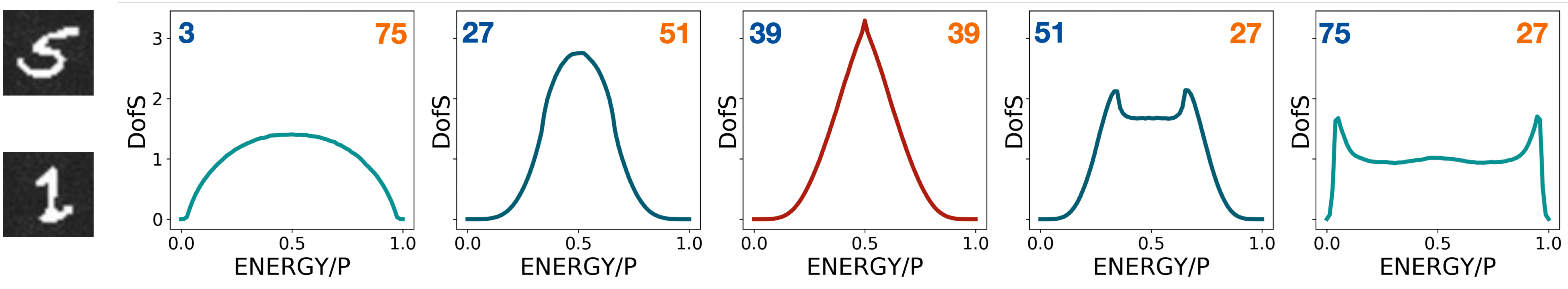
$P_1 \ll P_0$ $\quad P_1 = P_0$ $\quad P_1 \gg P_0$



Class Unbalancing

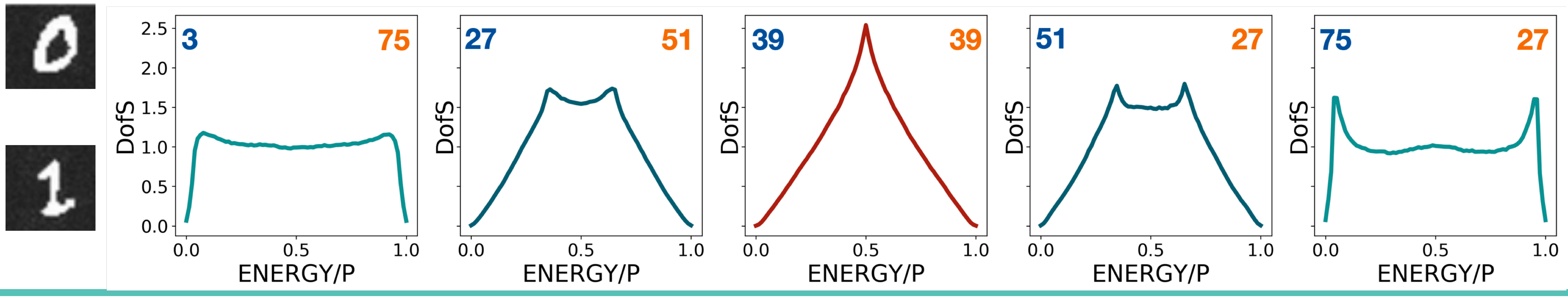
5 vs 1

$P_1 \ll P_5$ $P_1 \gg P_5$



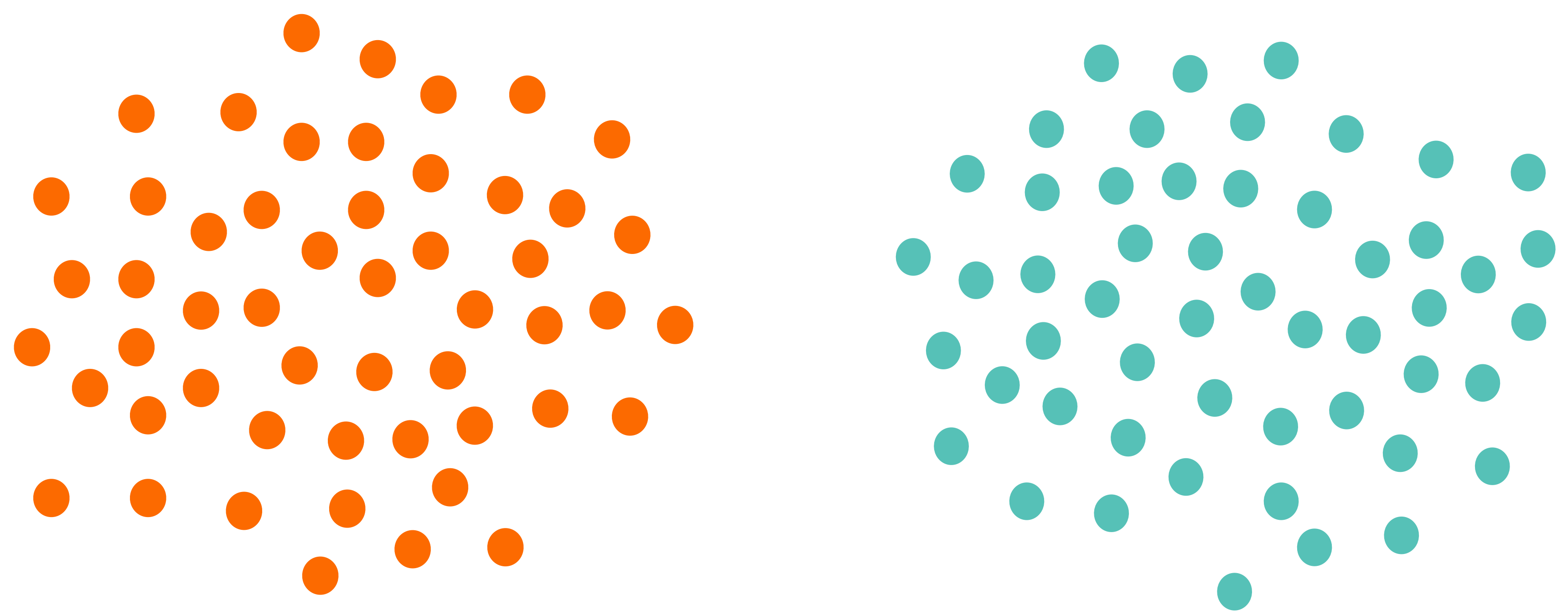
0 vs 1

$P_1 \ll P_0$ $P_1 \gg P_0$



Class Unbalancing

Back to random data



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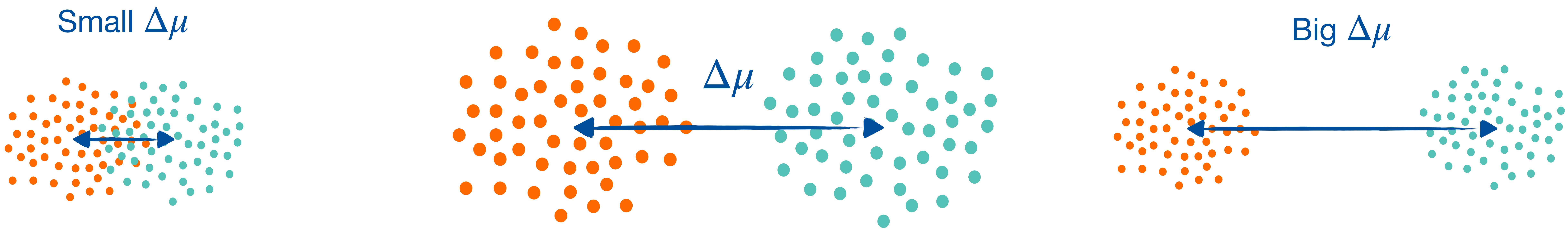

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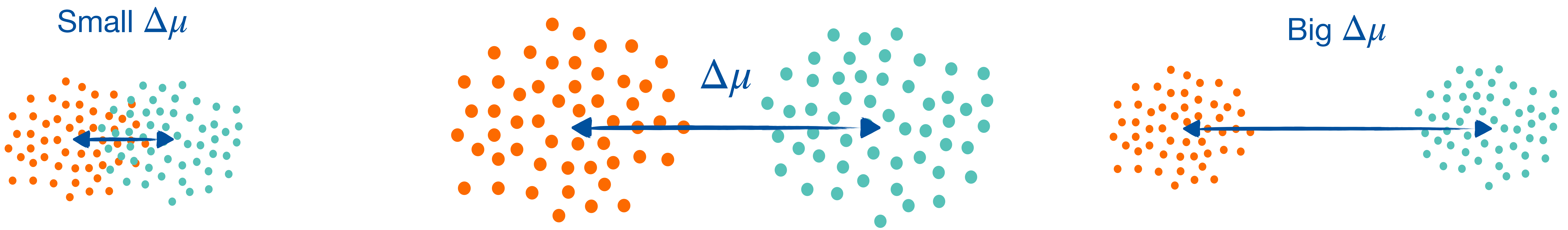

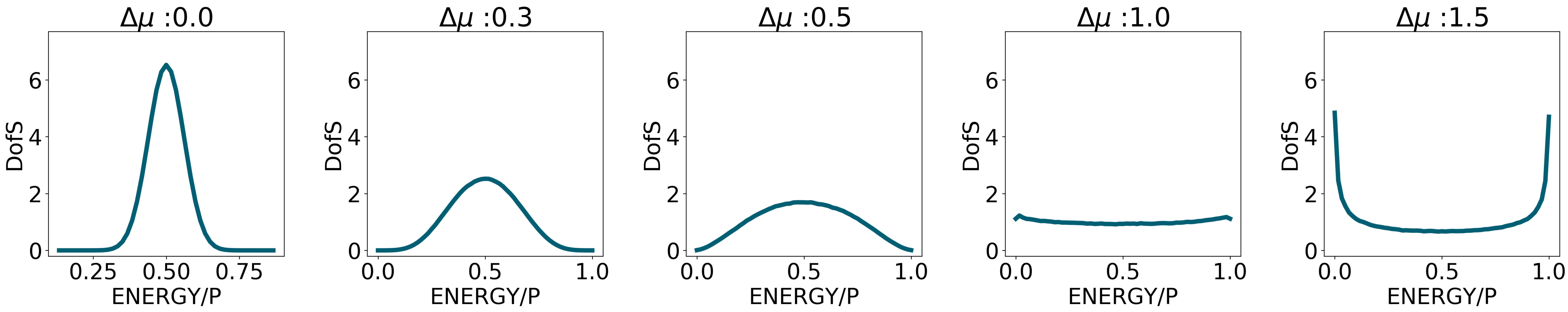

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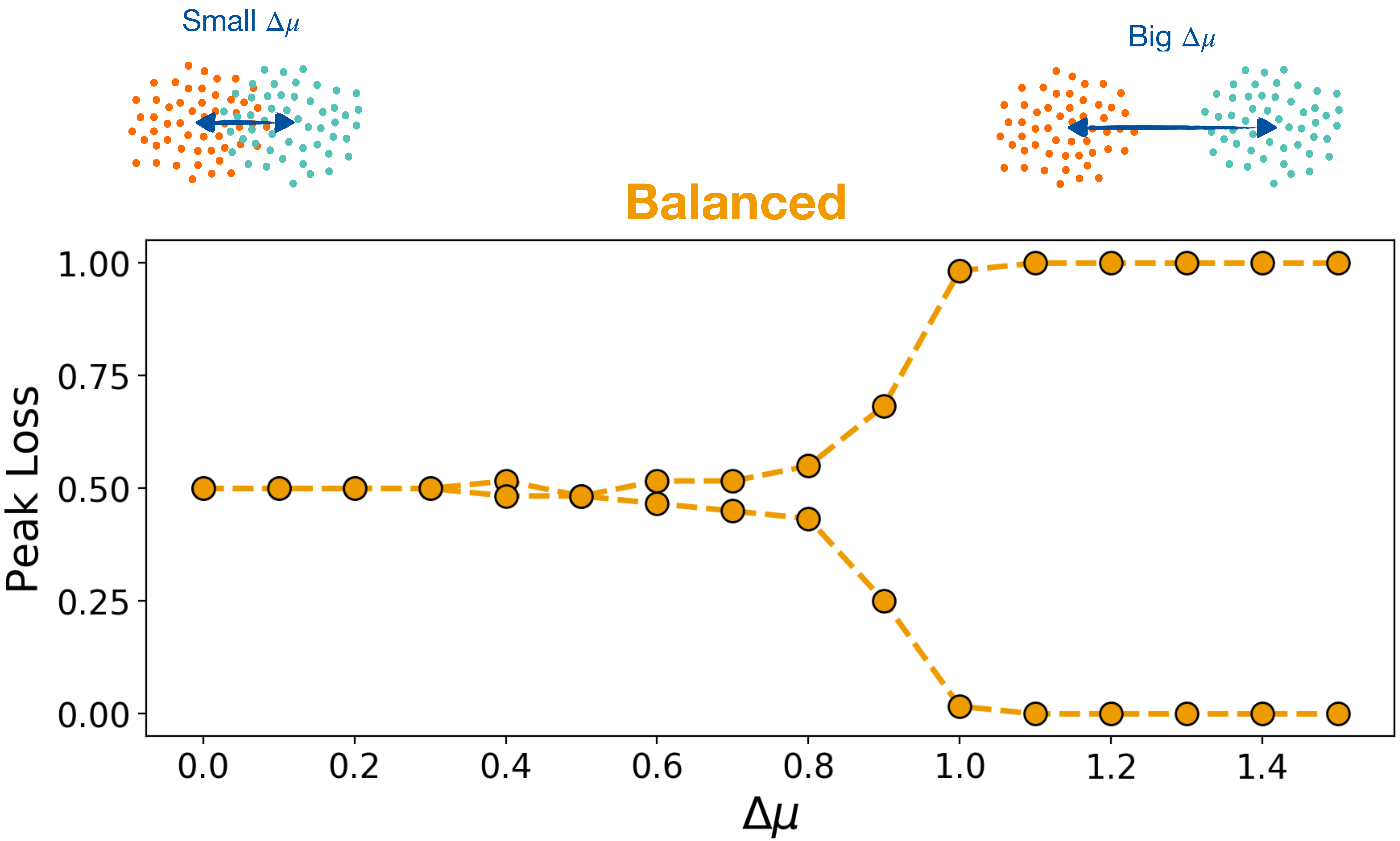

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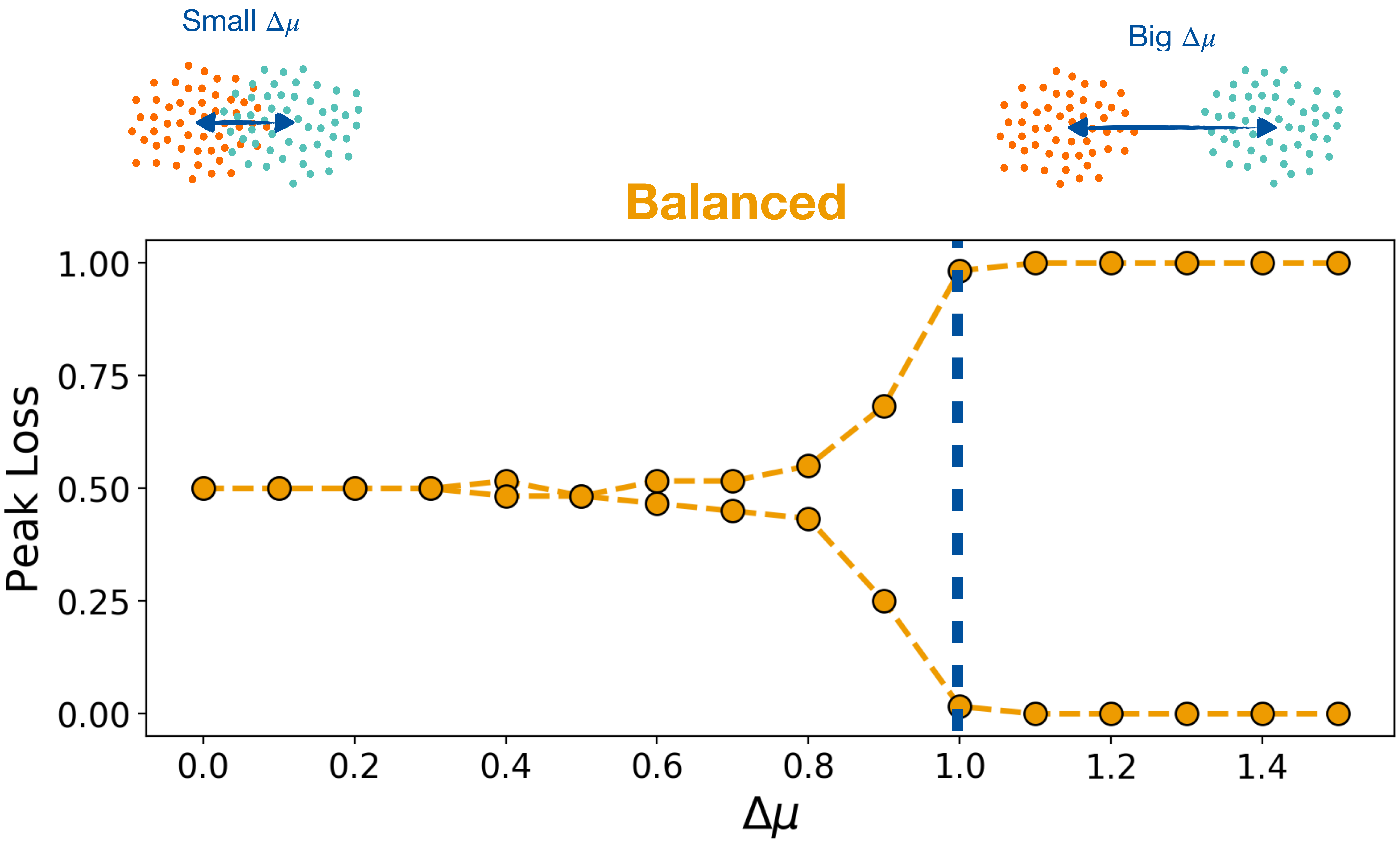

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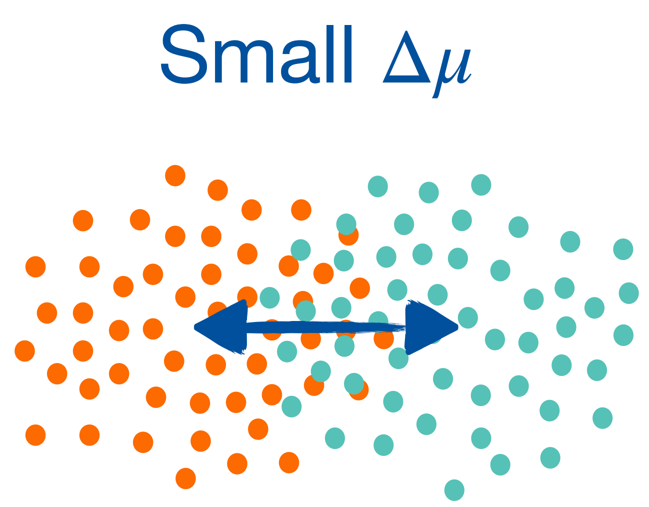

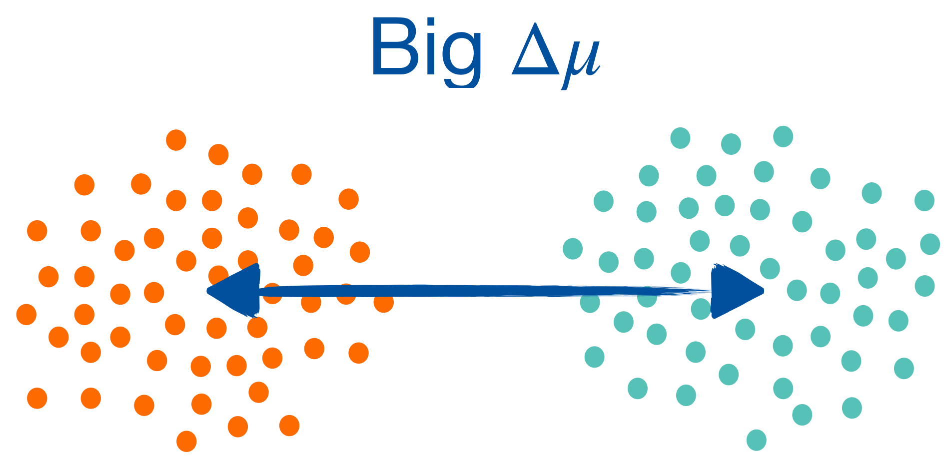

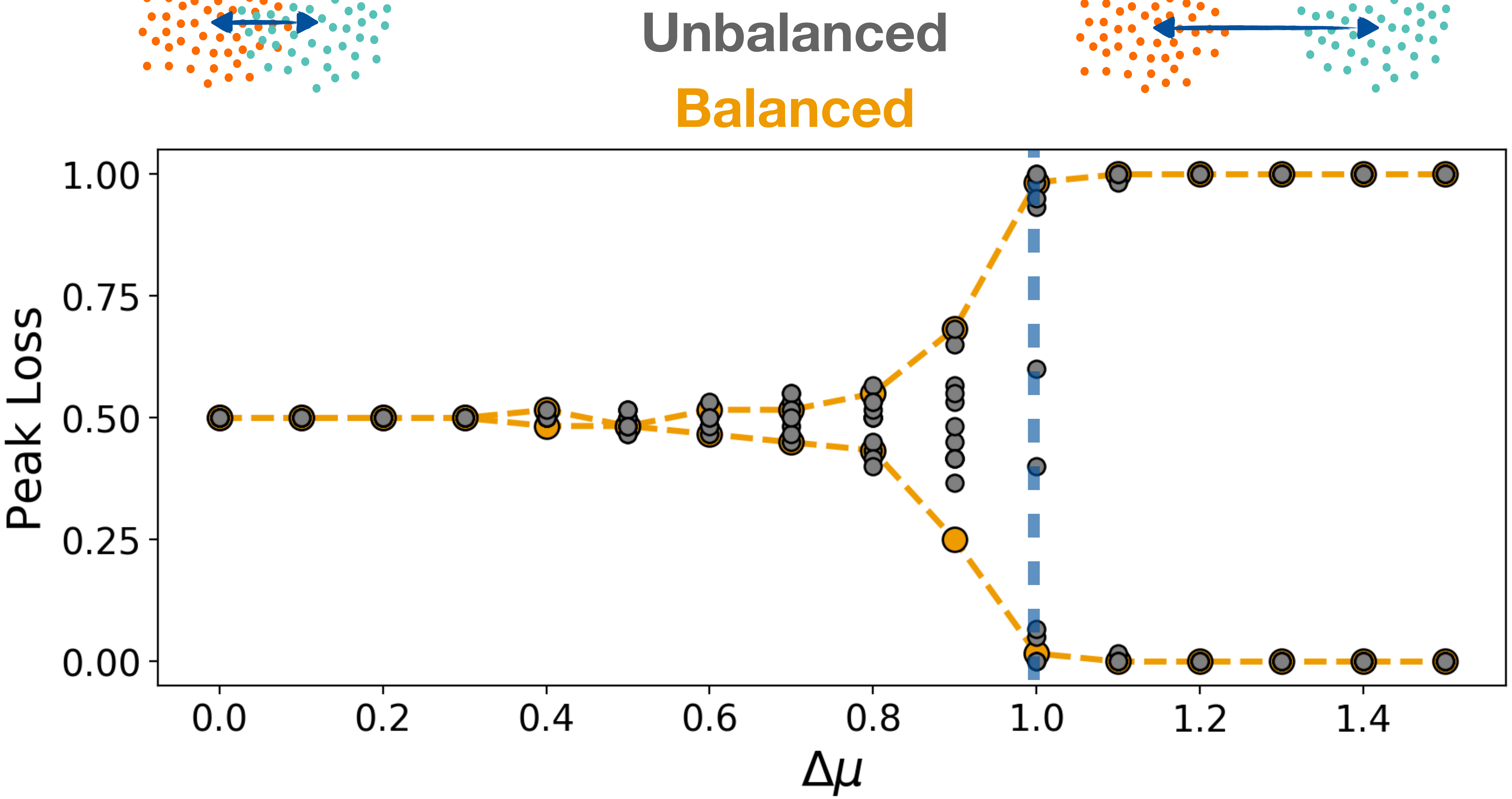

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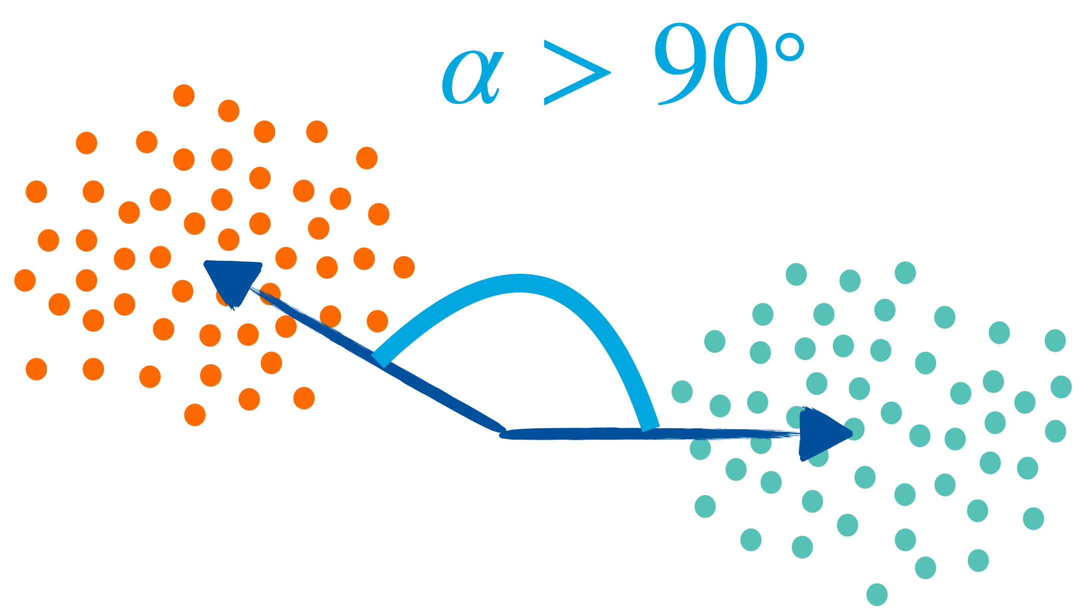
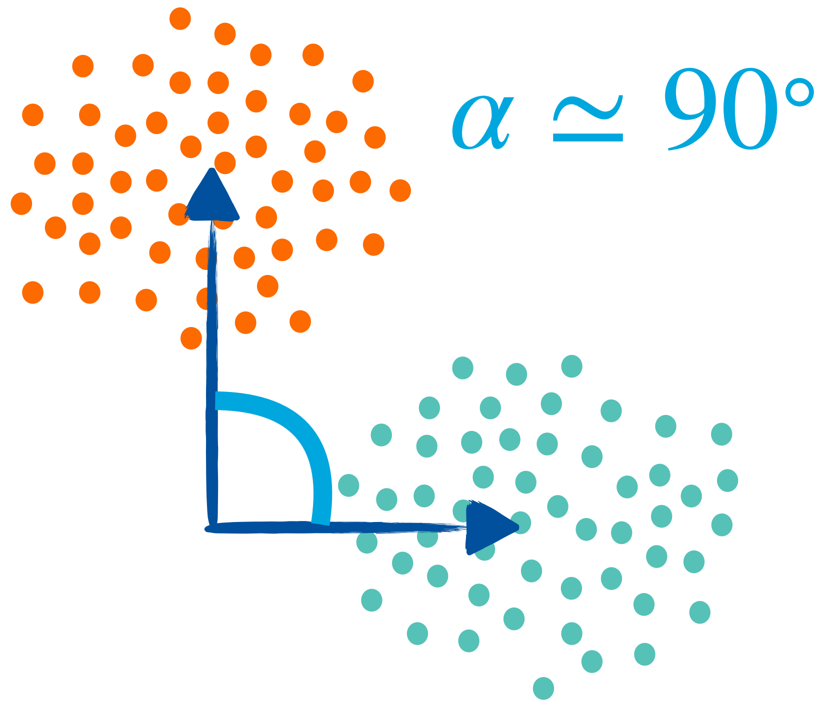
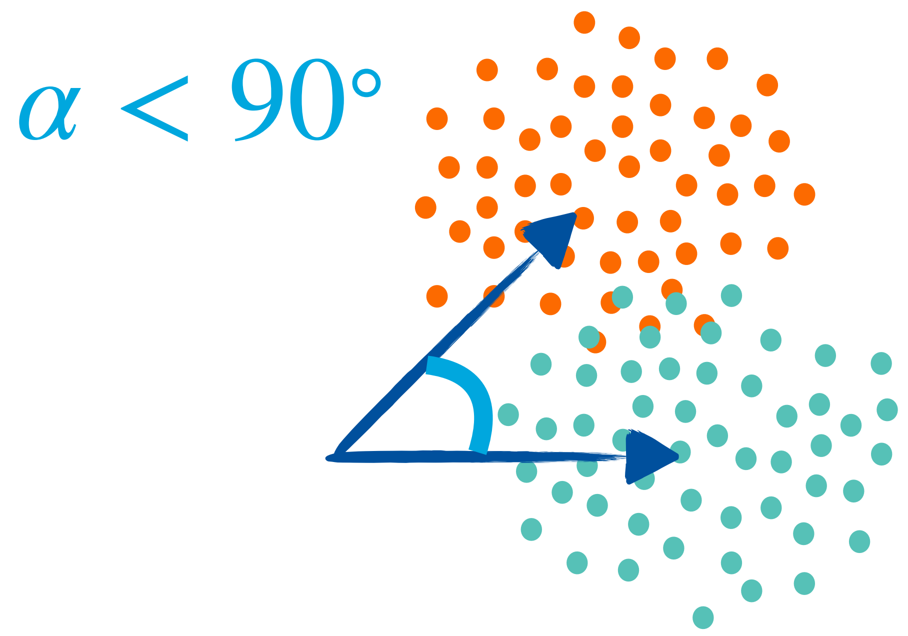
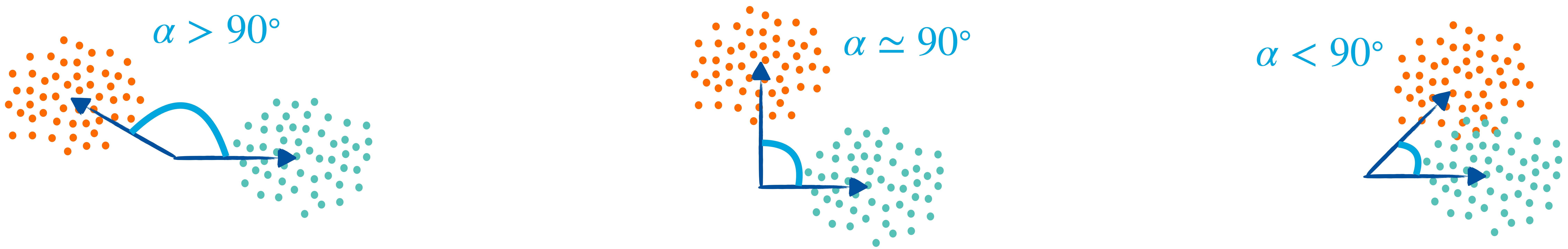


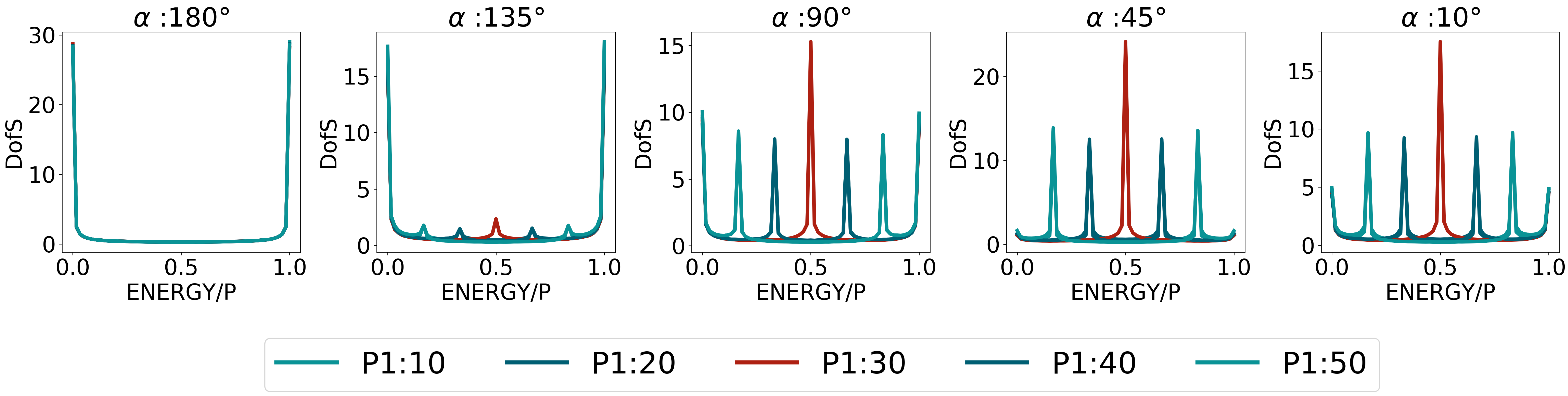




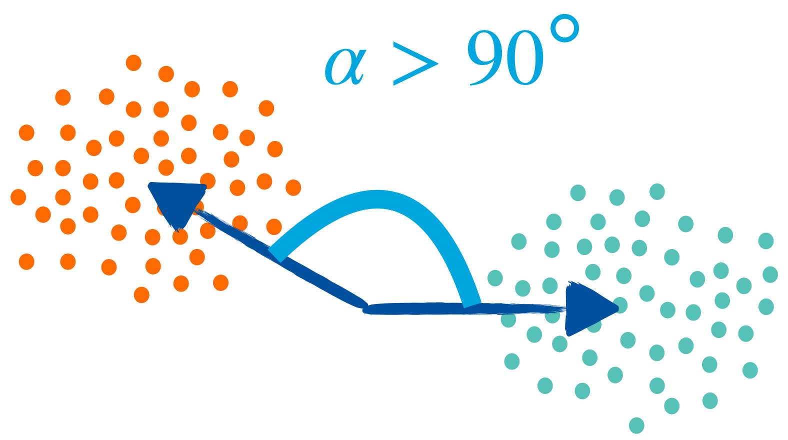
Back to random data

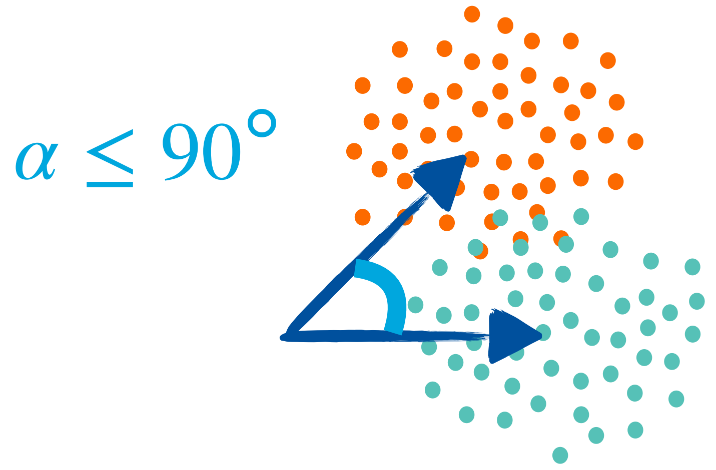


$\Delta\mu \gg 1$



Back to random data





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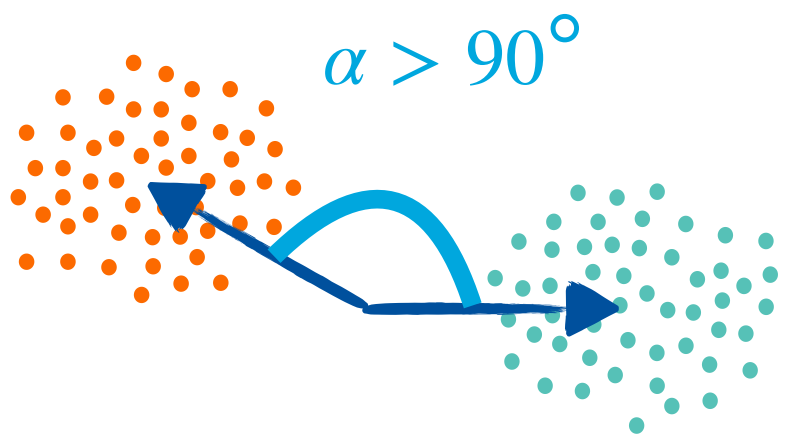

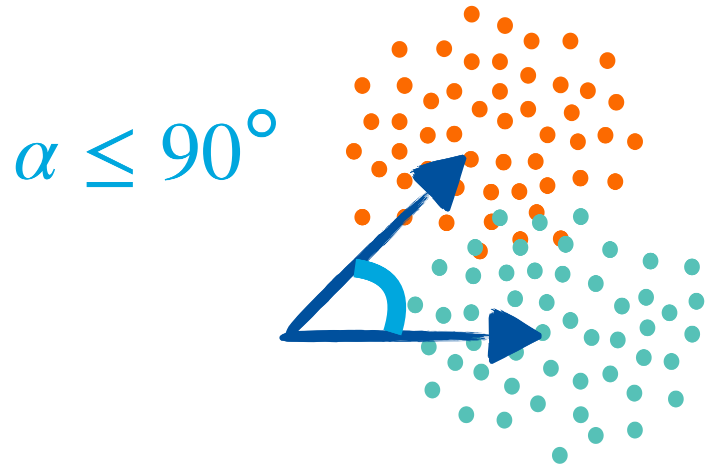

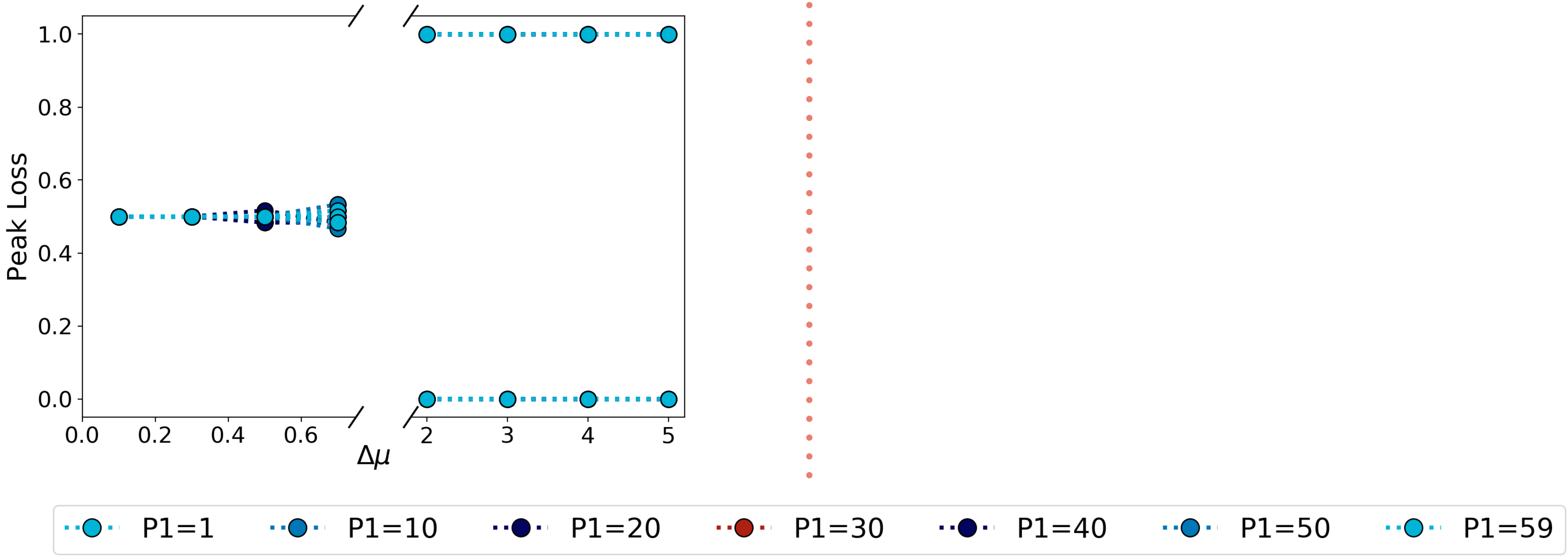

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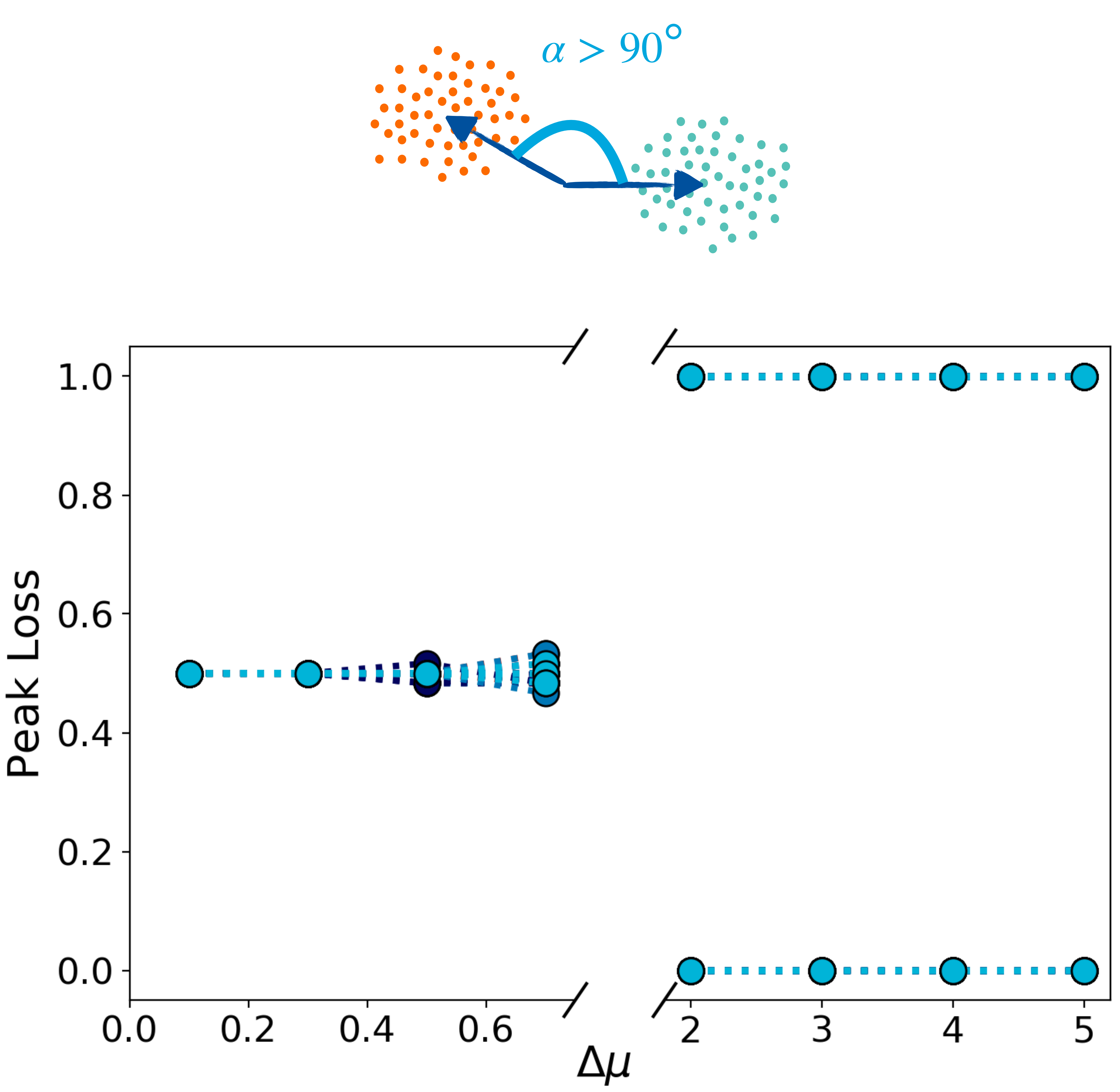
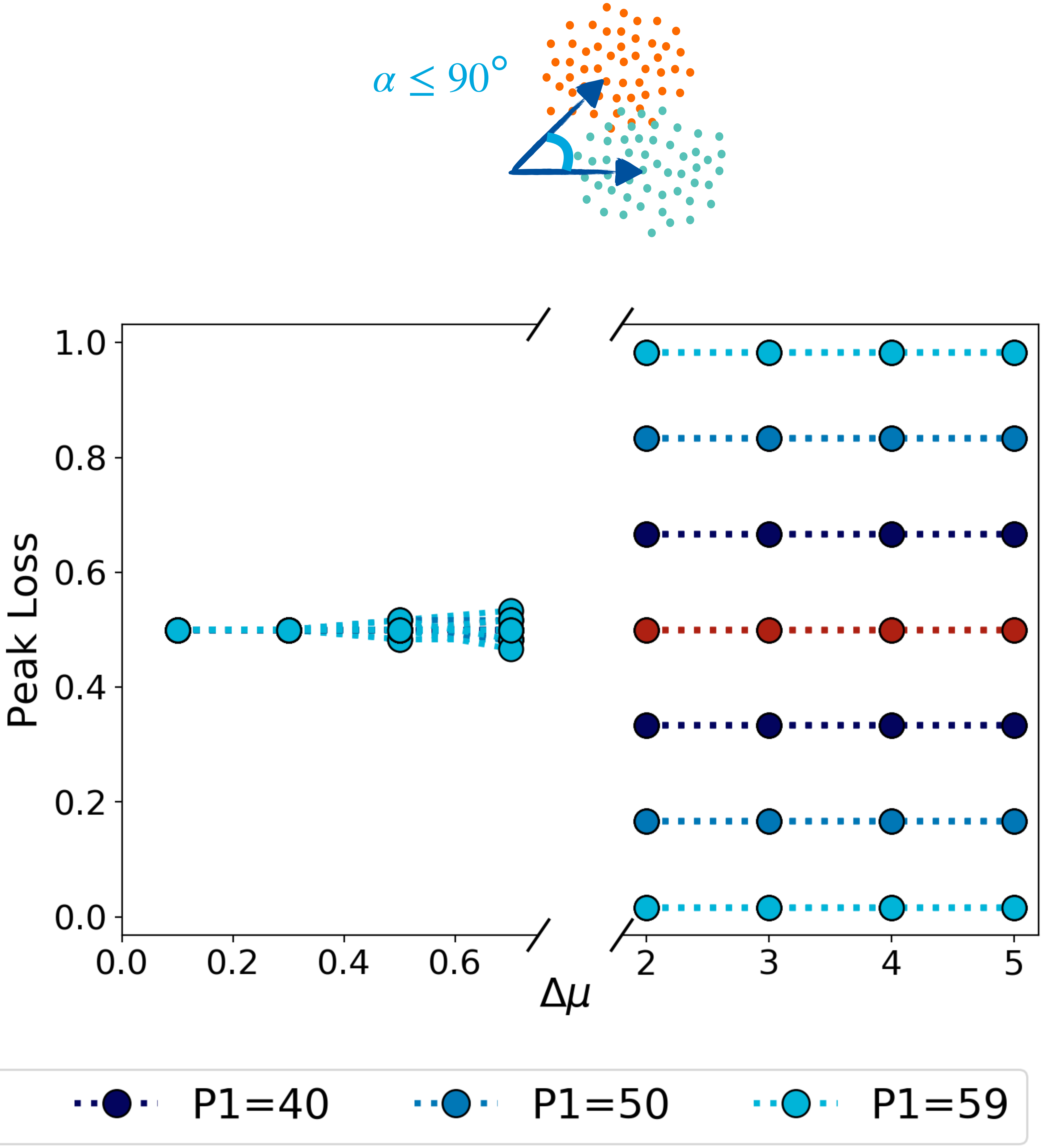
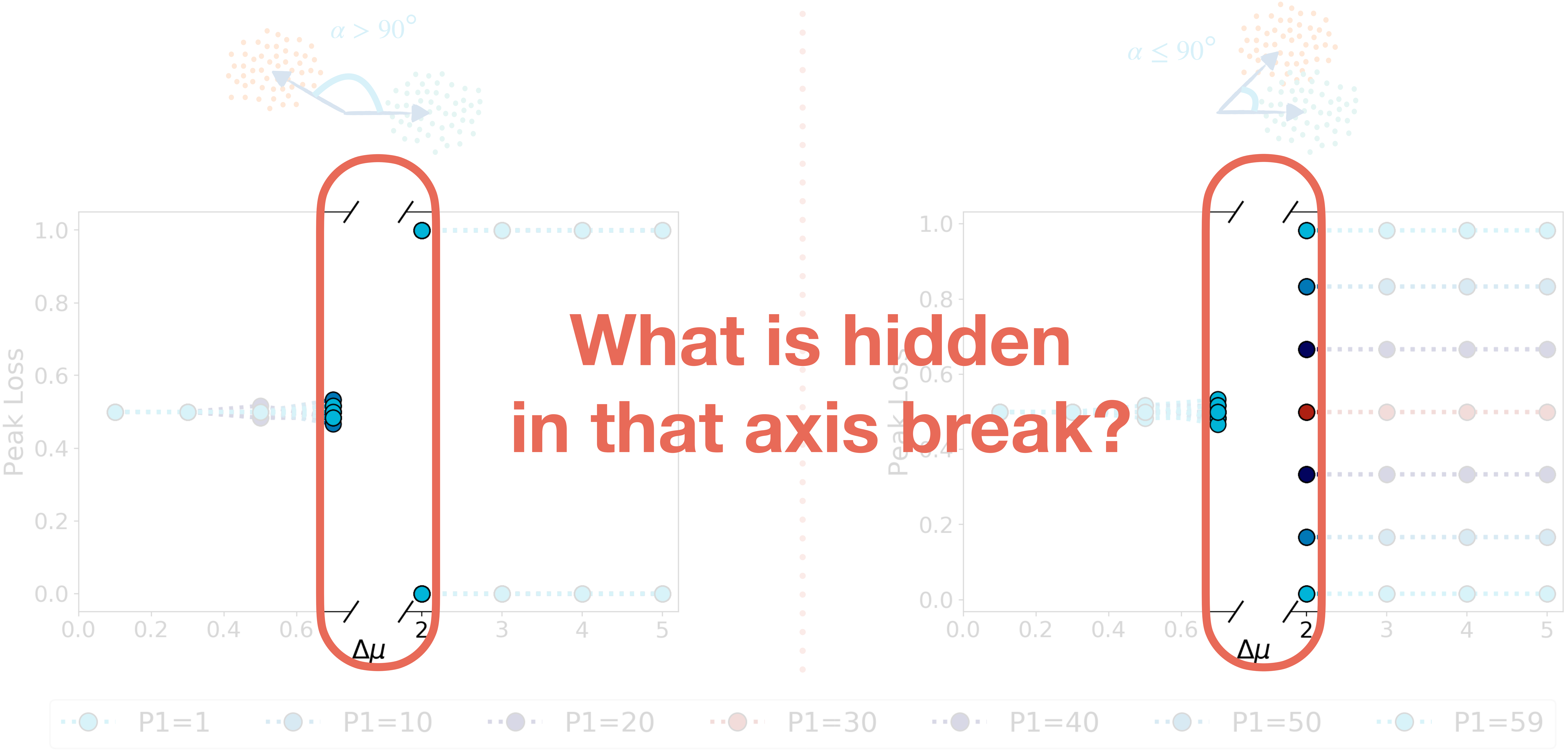


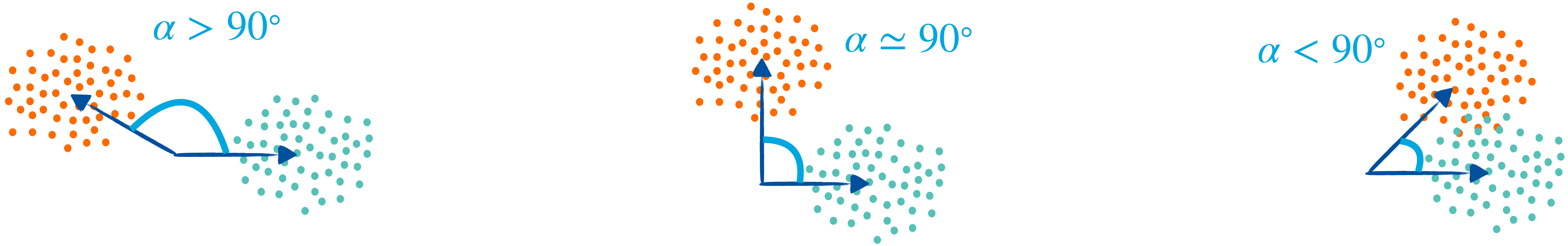


Back to random data

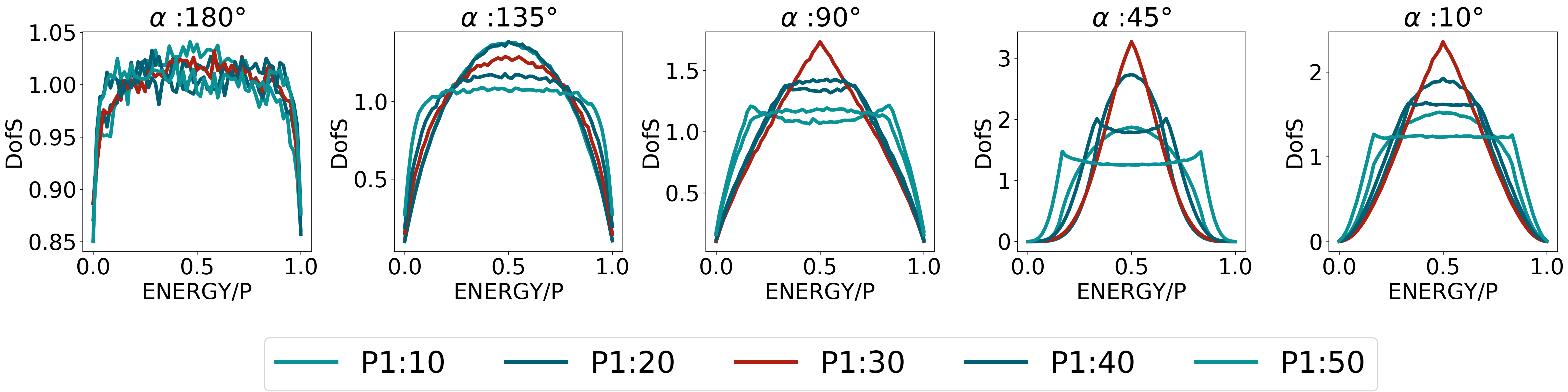


What is hidden in that axis break?

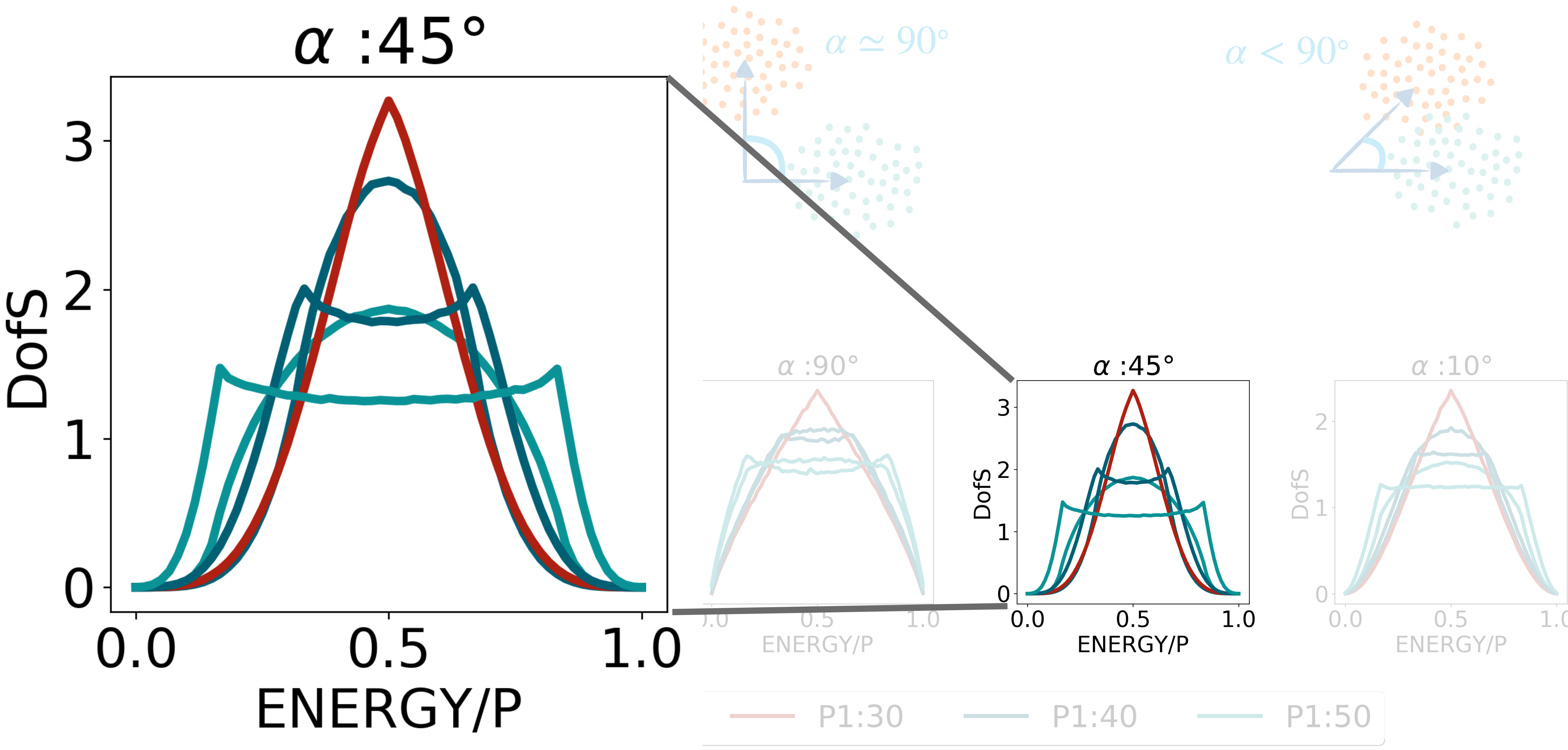
Back to random data



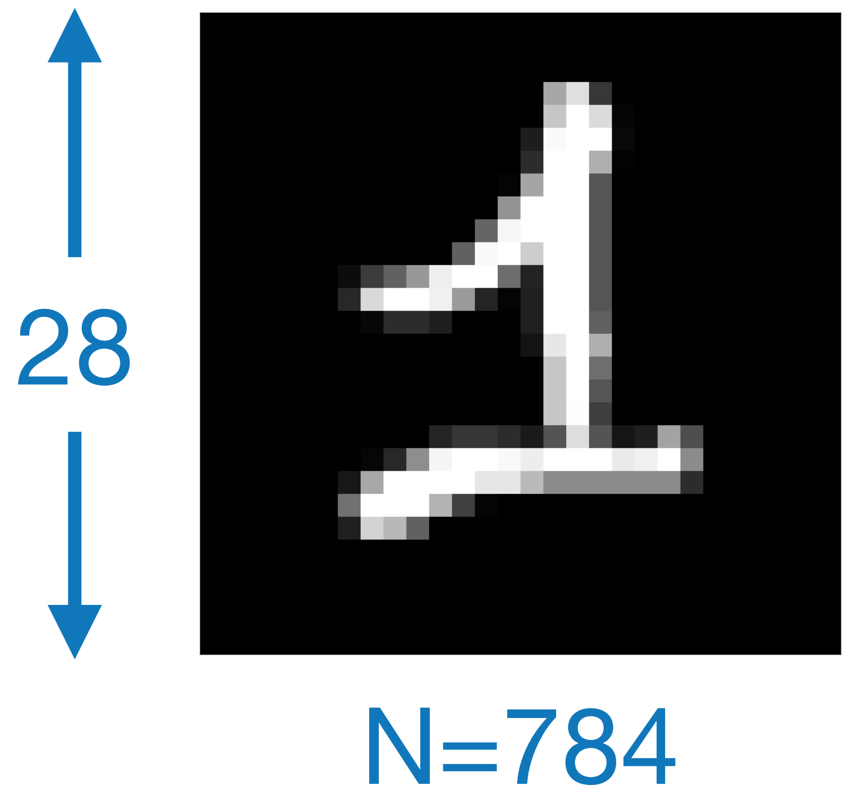
$\Delta\mu \simeq 1$



Back to random data

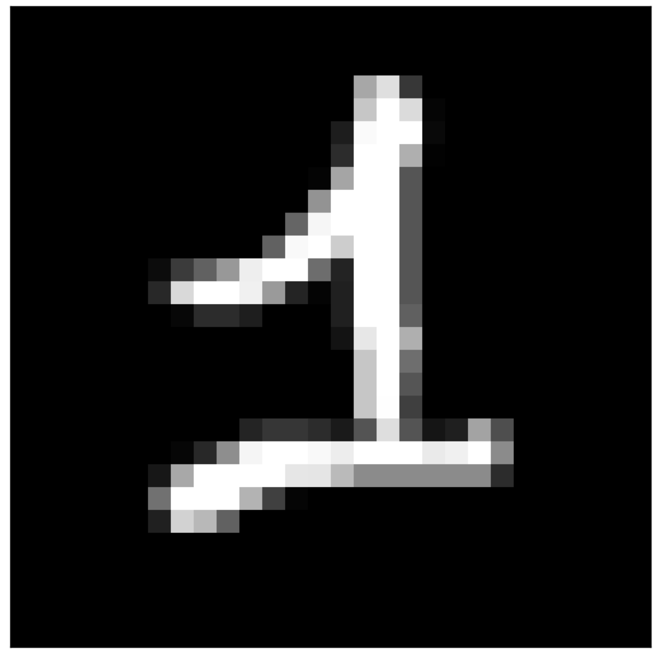


Back back to *realistic* data



Back back to *realistic* data

28

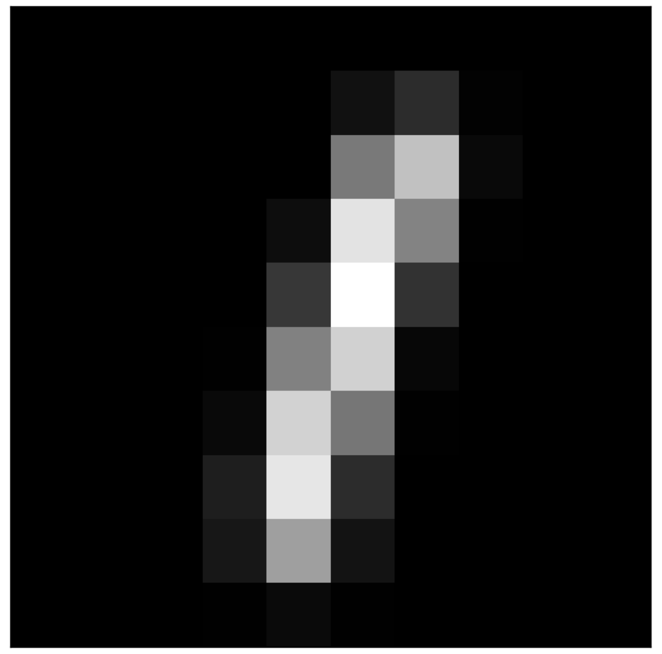


N=784

Reduce Dimensions

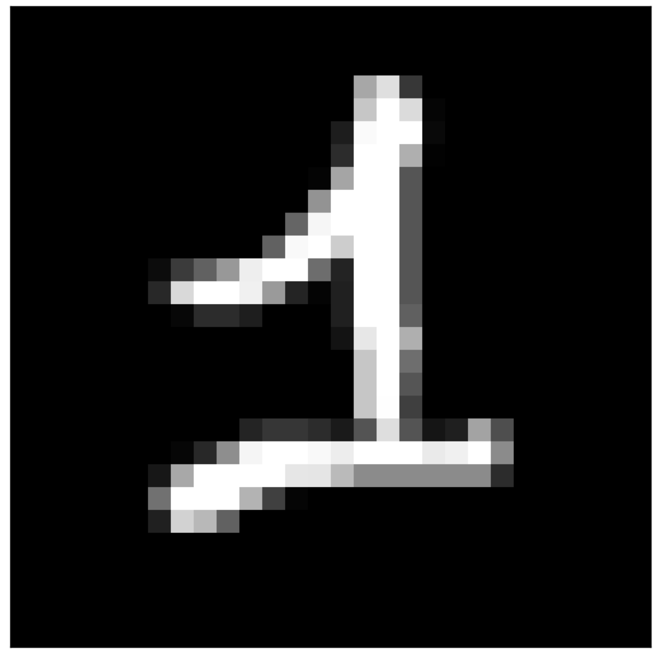
N=100

10



Back back to *realistic* data

28



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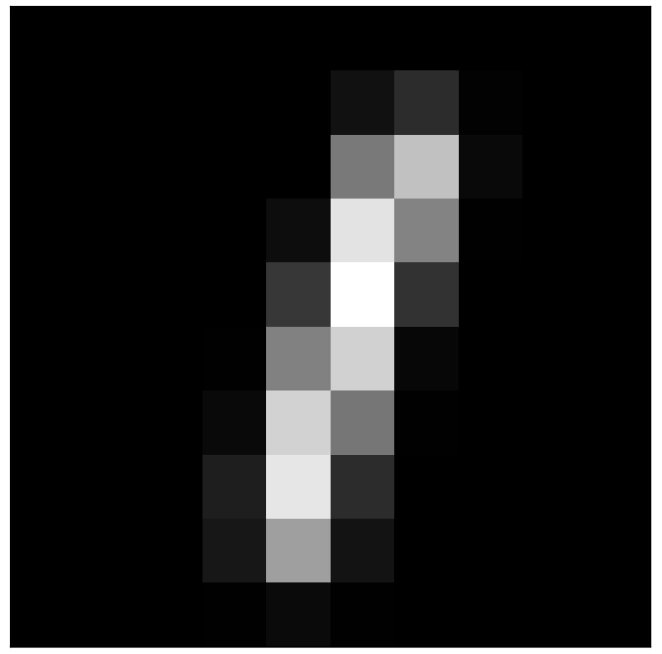
10



Gaussian Clones

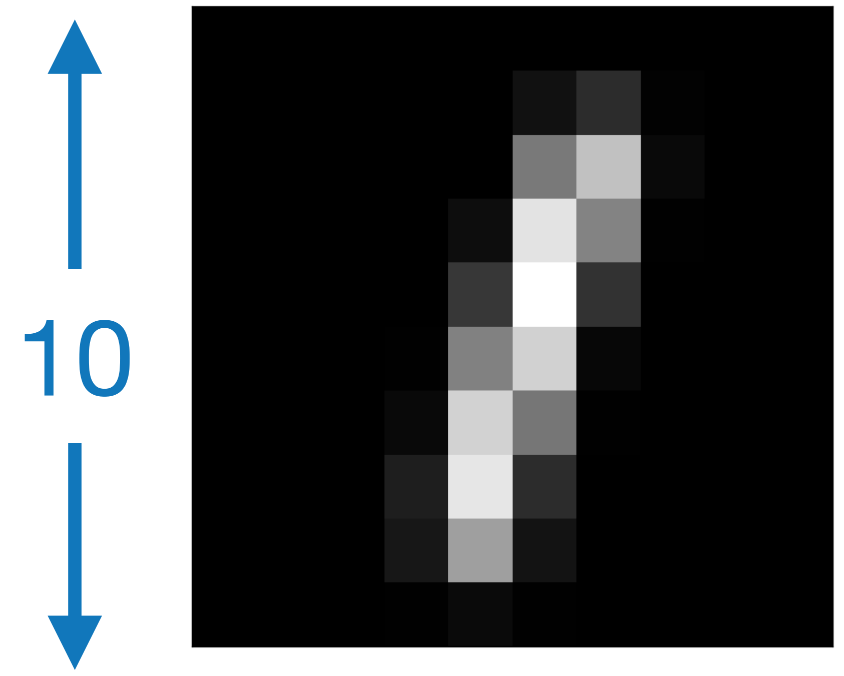
$$N(x, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^k \det \Sigma}} \exp\left(-\frac{1}{2}(x-\mu)^T\, \Sigma^{-1}\, (x-\mu)\right)$$

Back back to *realistic* data

N=784

Reduce Dimensions

N=100



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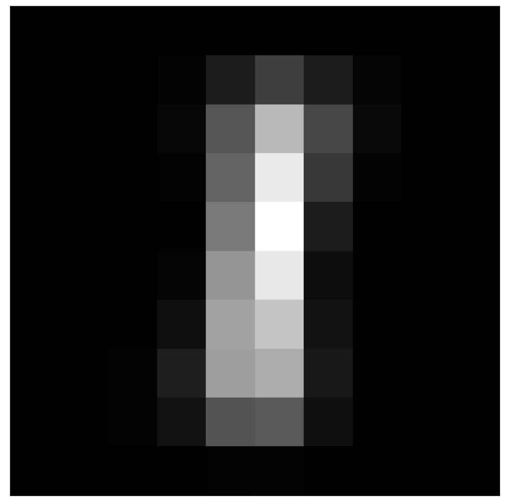
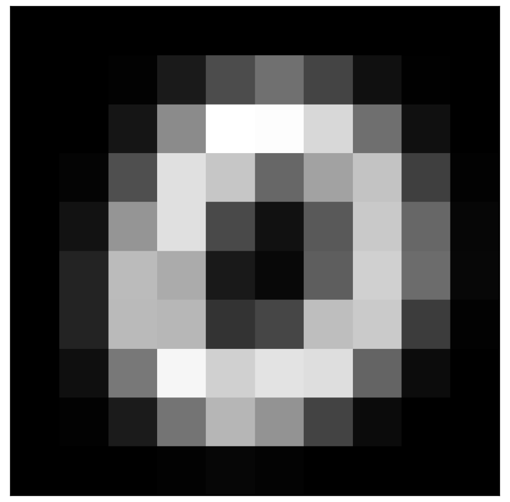
Mean - μ



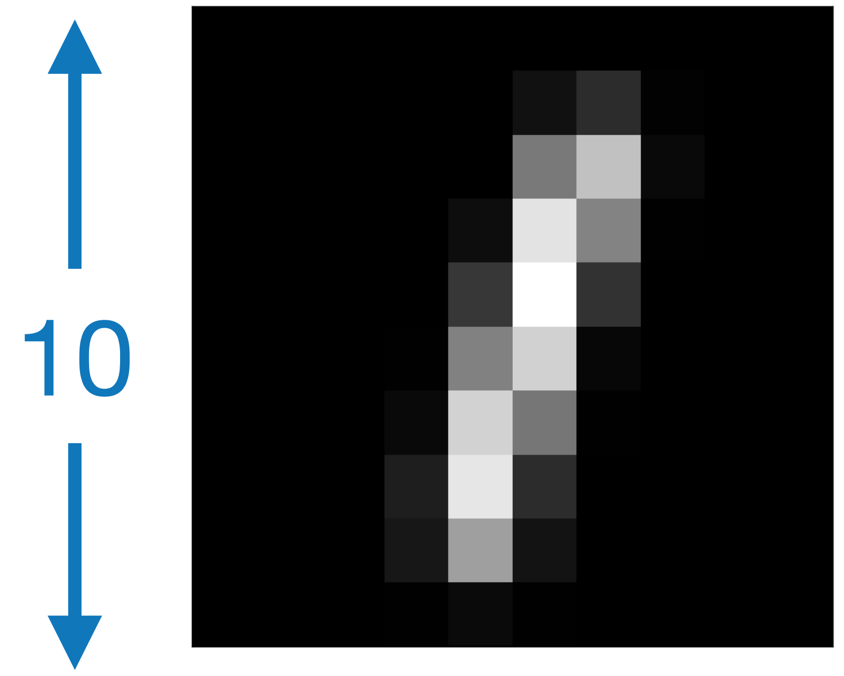


Back back to *realistic* data

N=784

Reduce Dimensions

N=100



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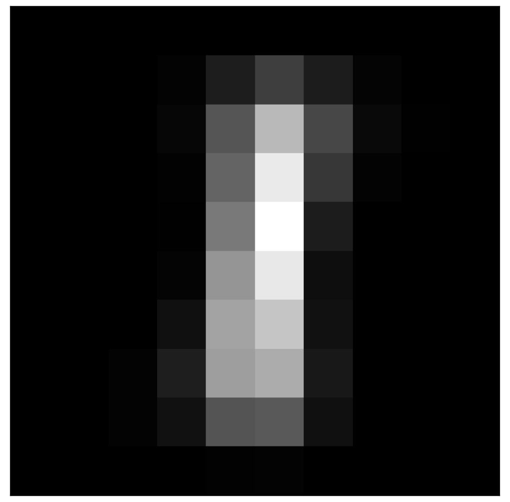
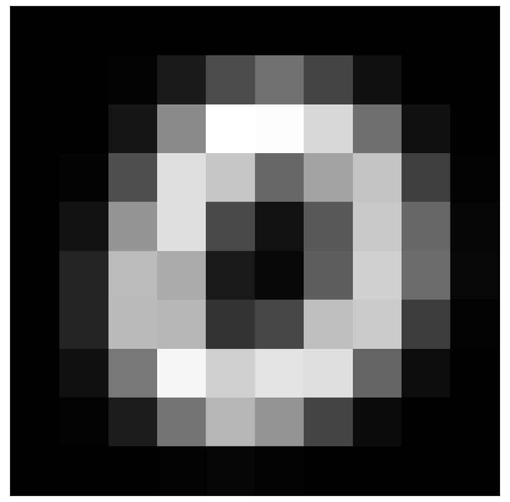


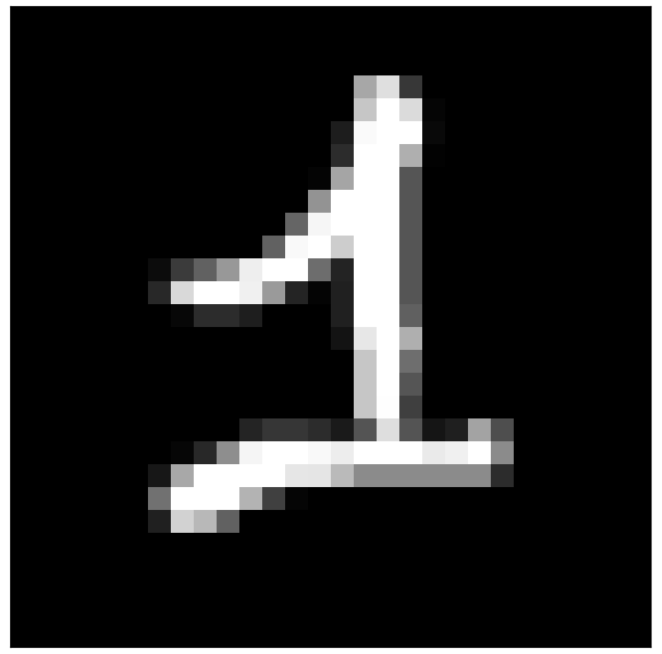


+

Covariance - Σ

Back back to *realistic* data

28

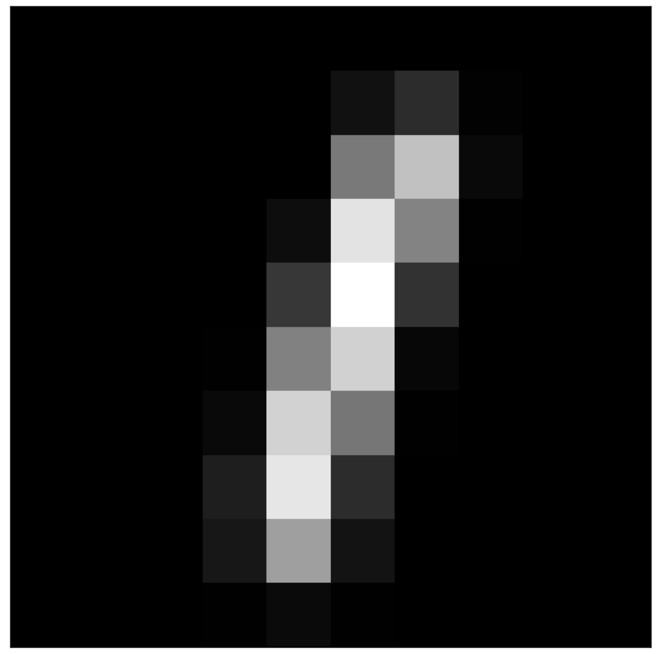


N=784

Reduce Dimensions

N=100

10



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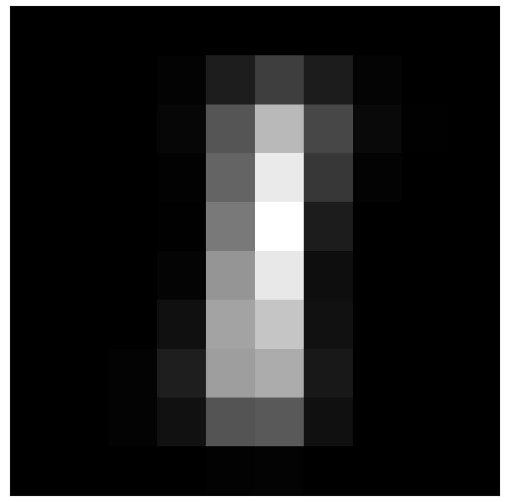
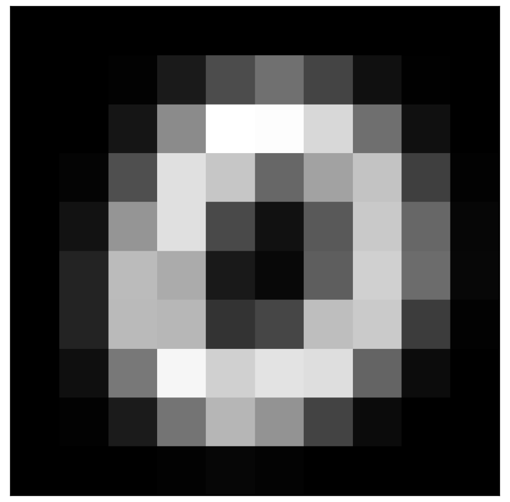
Mean - μ

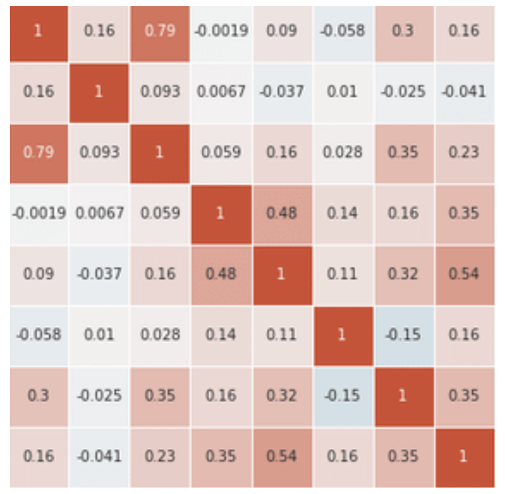


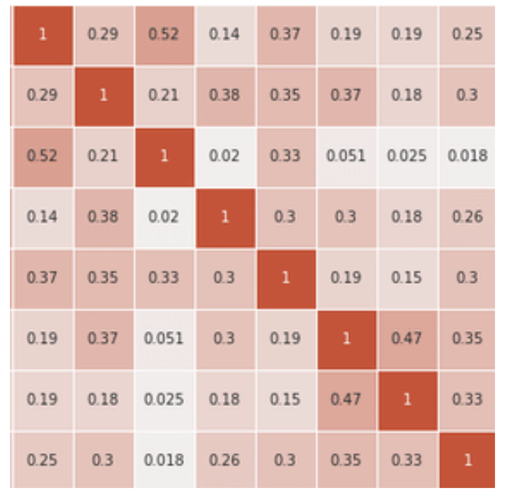


+

Covariance - Σ

GM

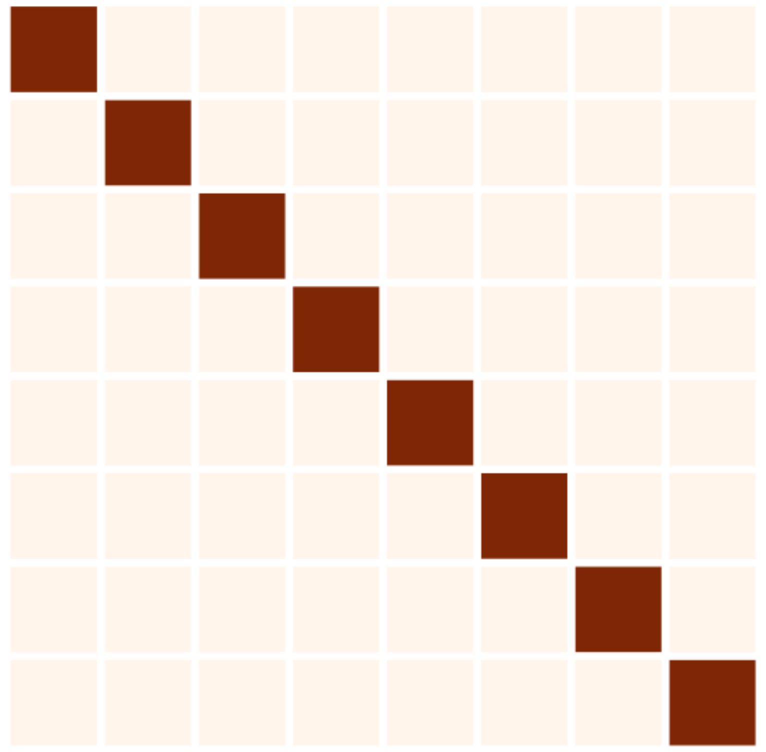




2ISO

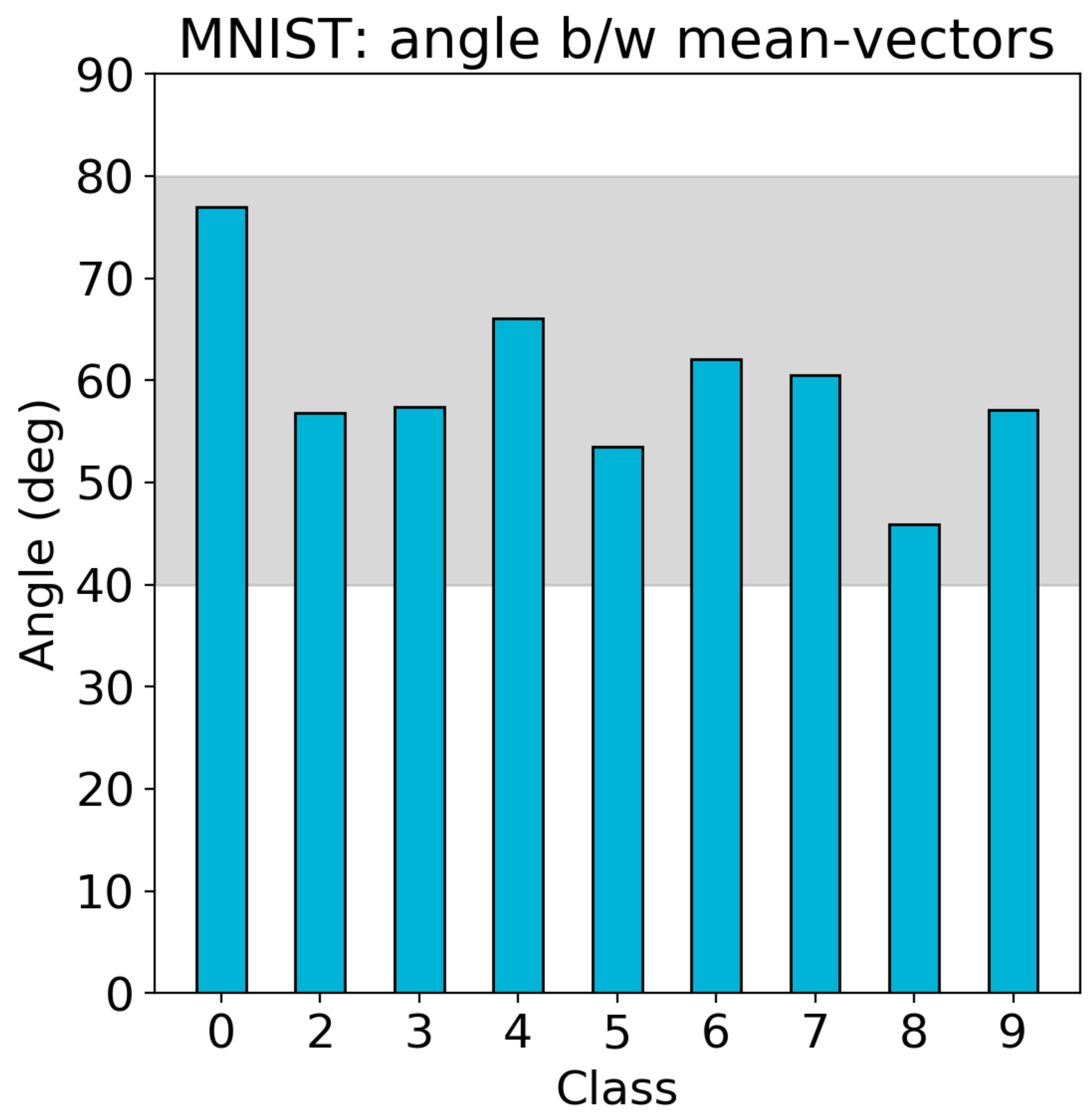
diagonal matrix

$v=\sqrt{v_1\cdot v_2}$



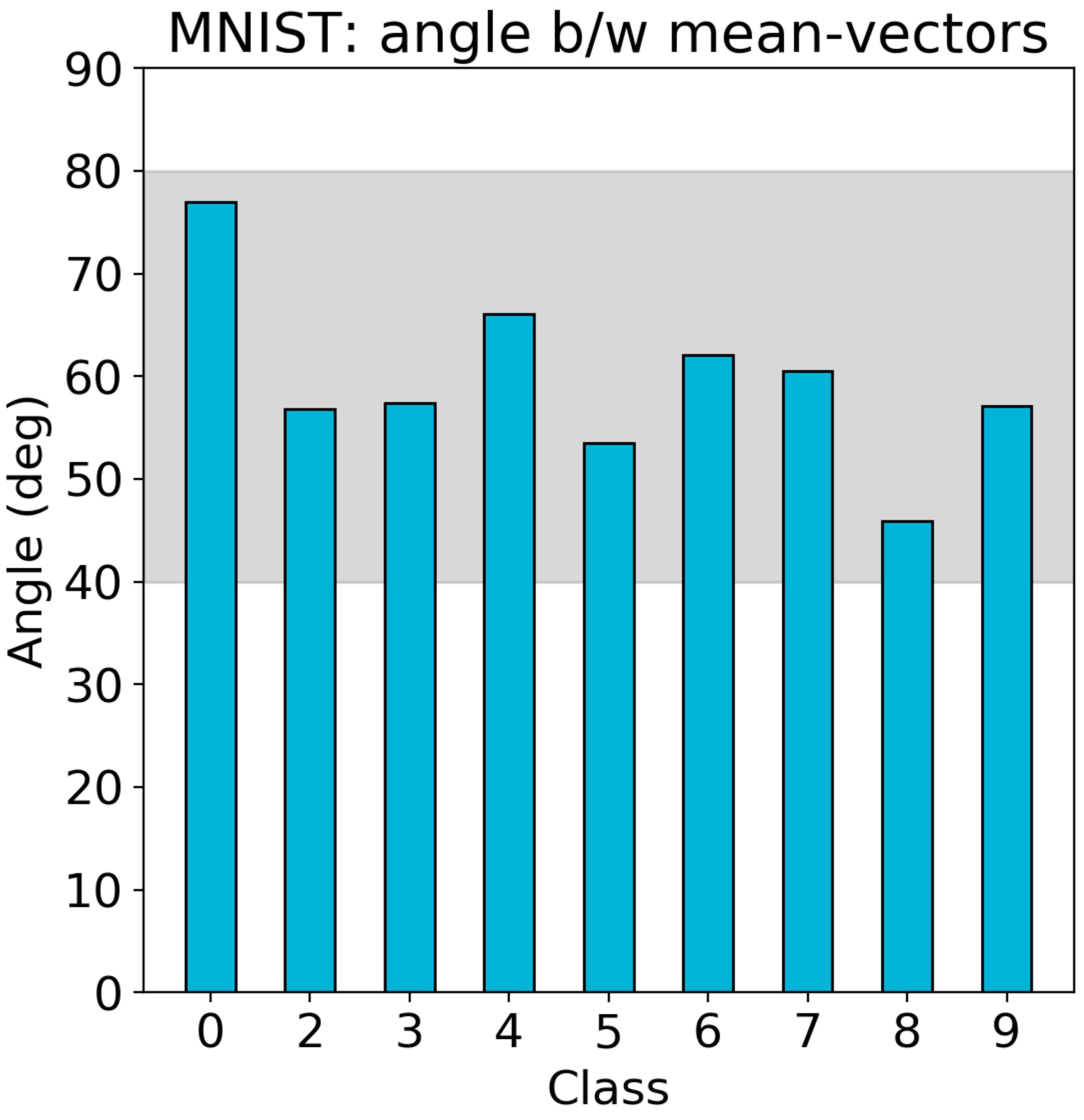
Back back to *realistic* data

1 vs ✱

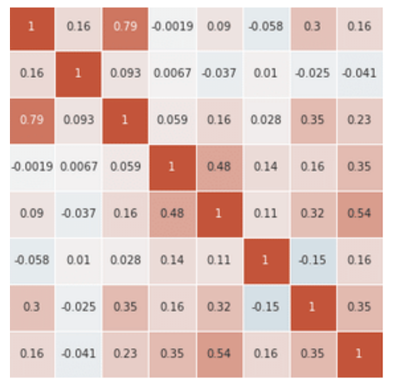


Back back to *realistic* data

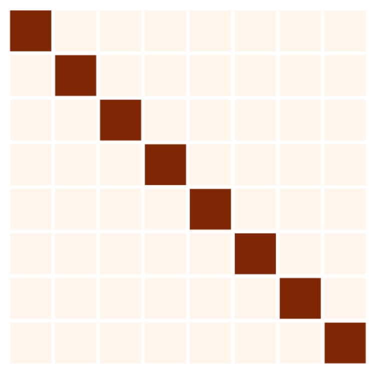
1 vs ✱

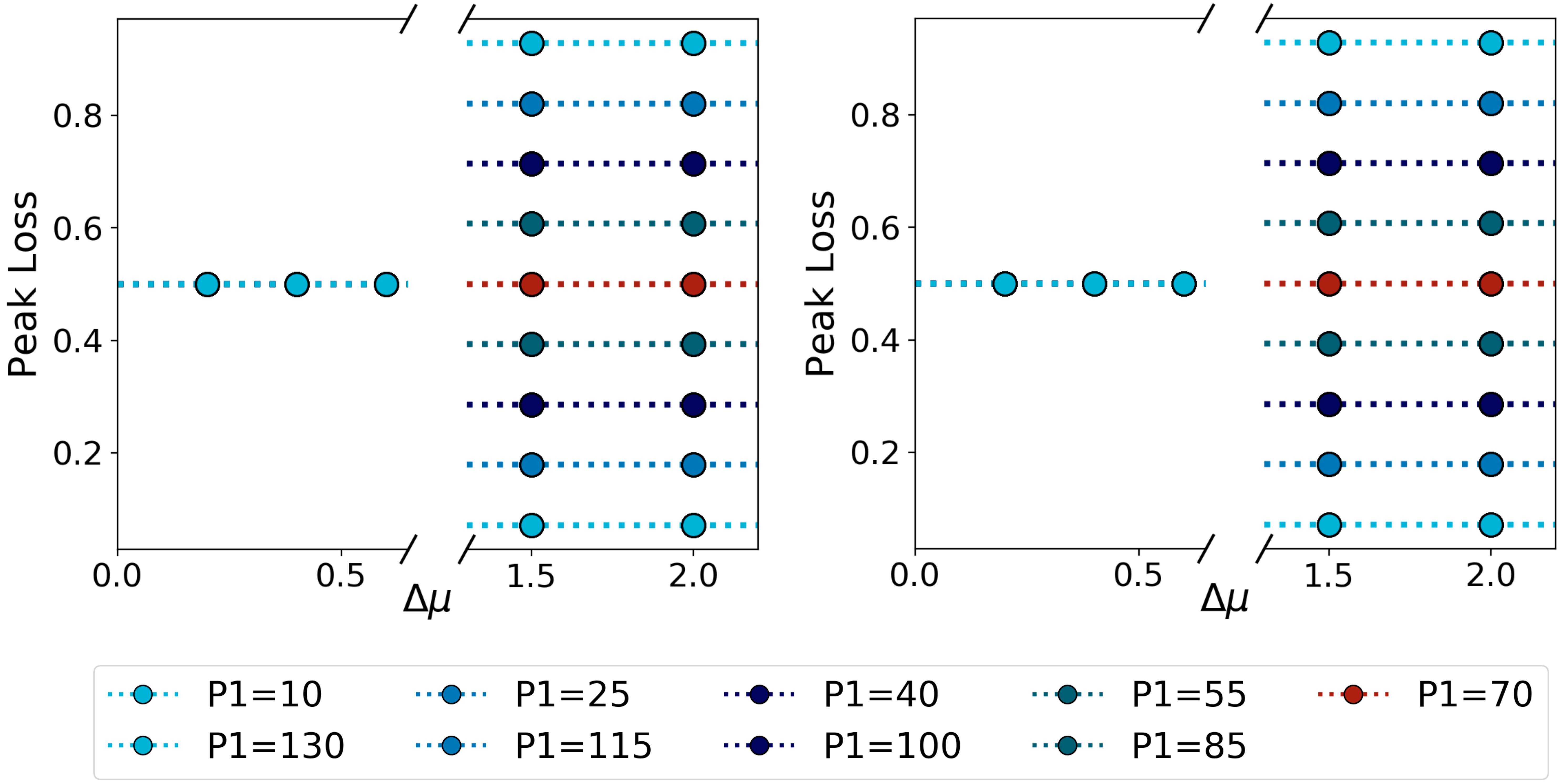


GM



2ISO





Are there other parameters to control the peaks?

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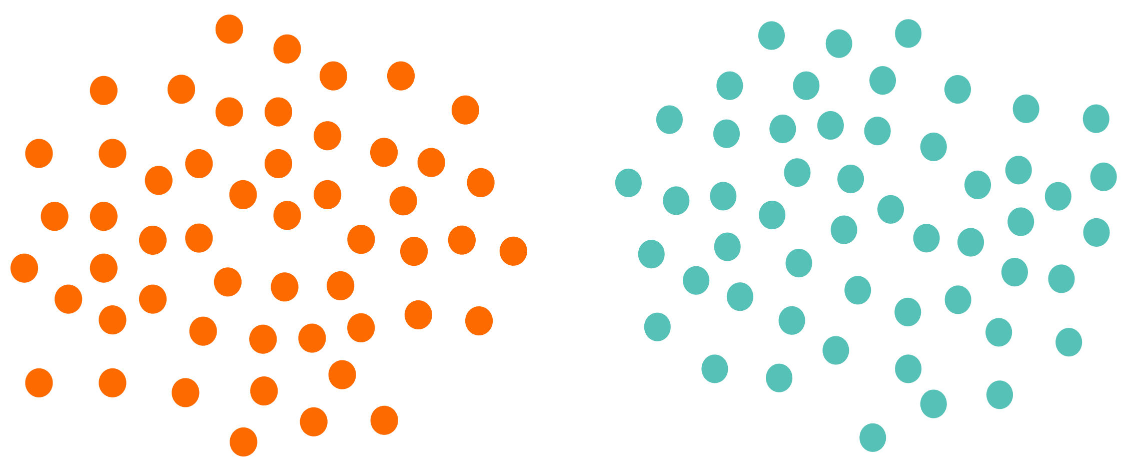
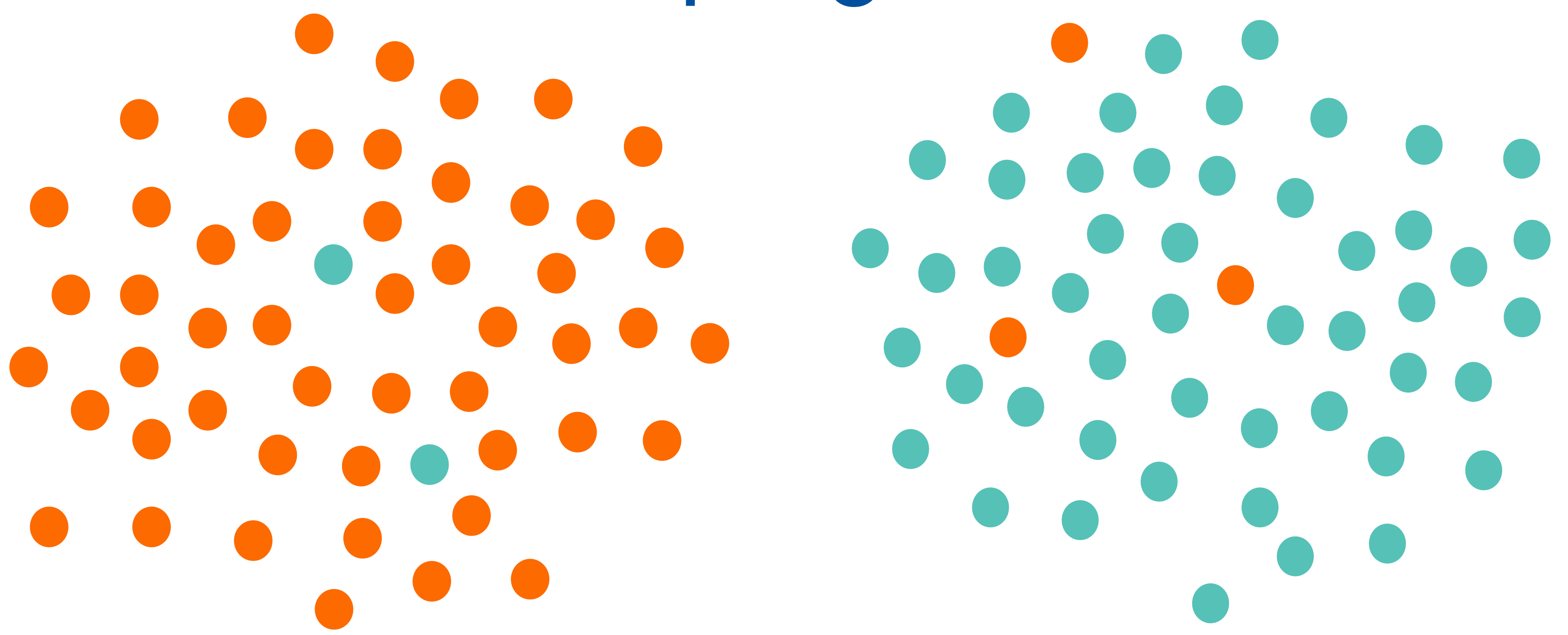
MISLABELLING

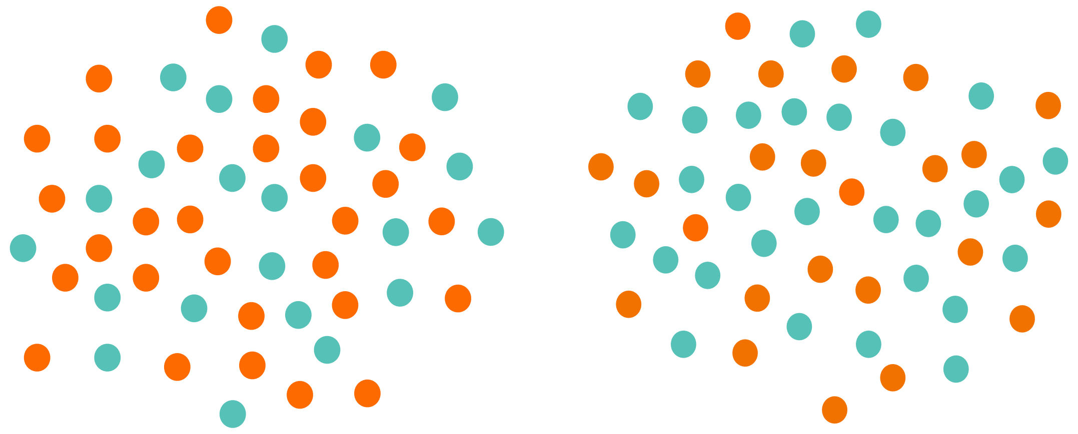
f = 0



f = 5



f = P/2



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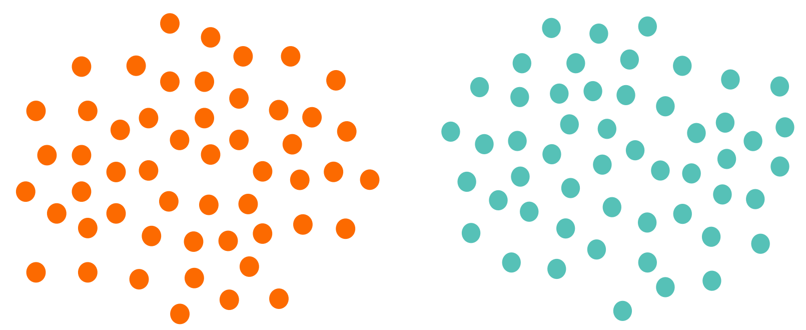
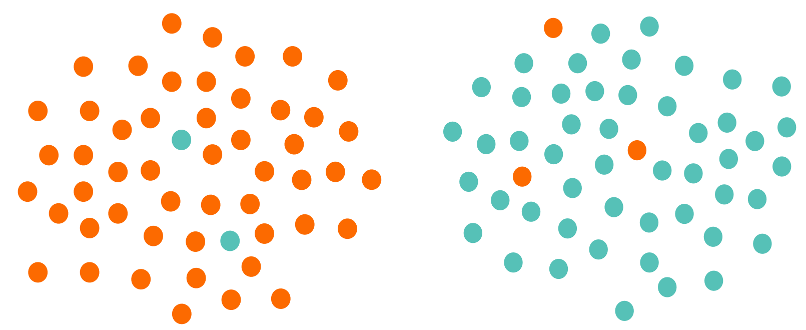


f = 5



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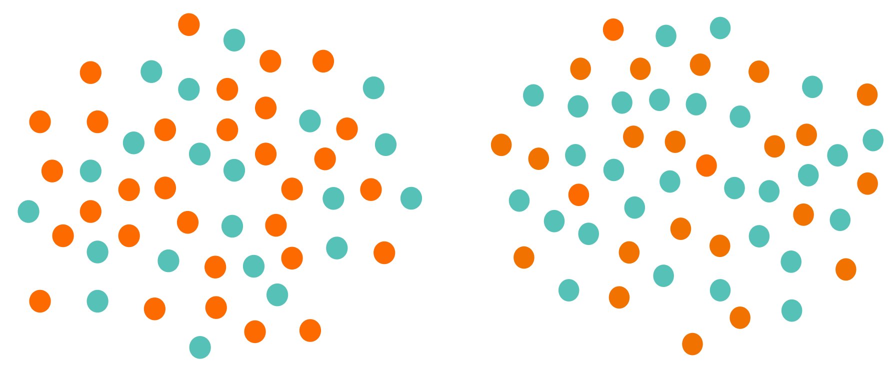
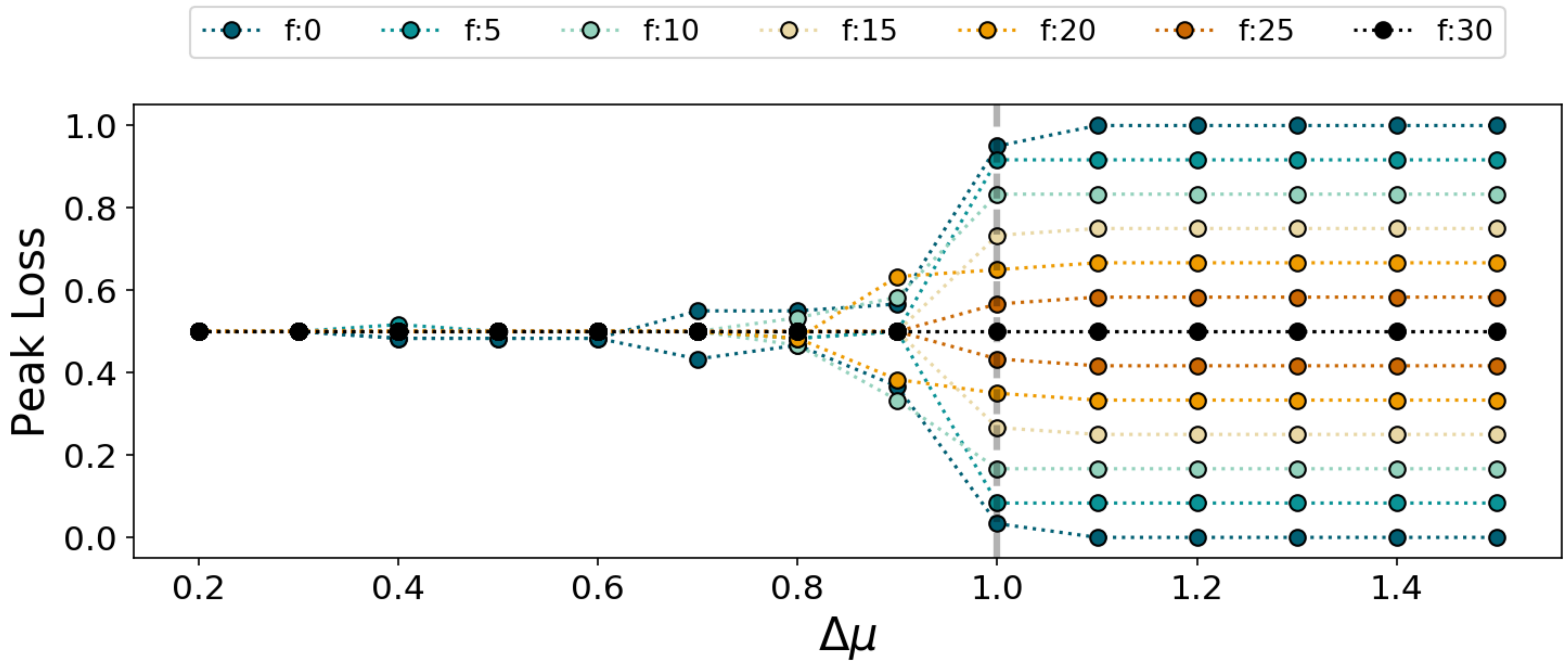
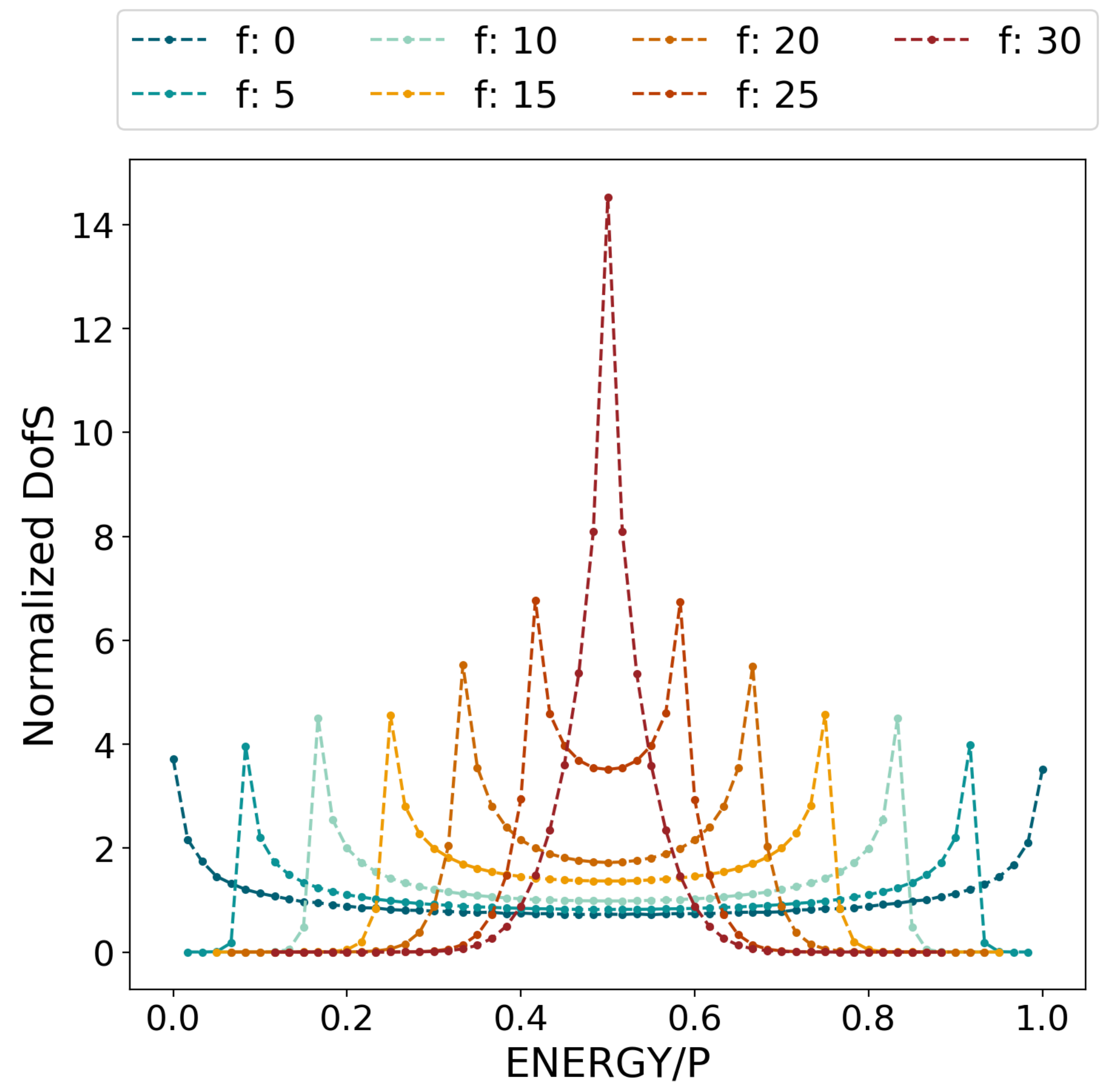






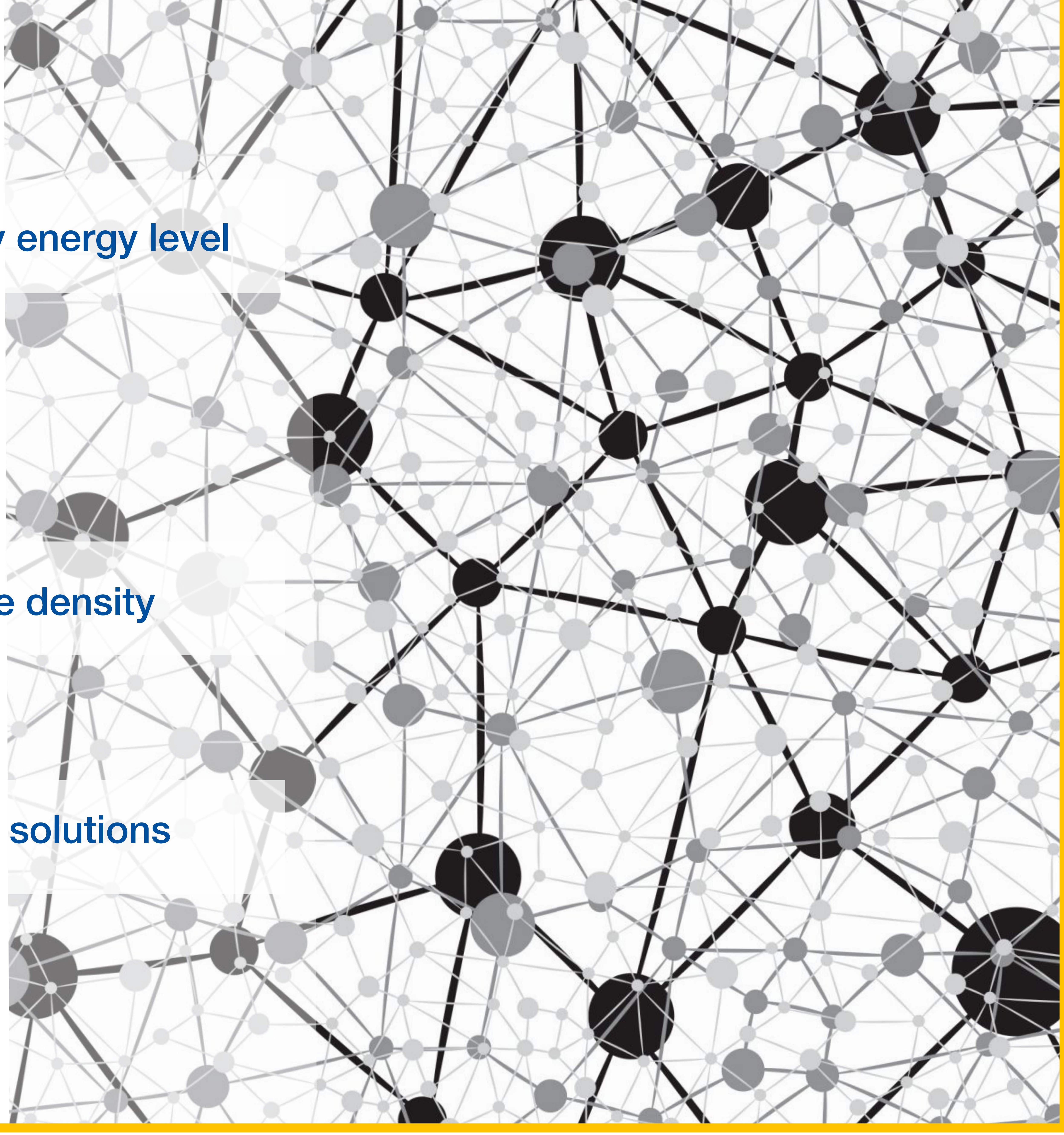
Conclusions

- Thermodynamic characterisation of the system at any energy level

- Possibility to study real learning problems

- Input-output correlation structure directly impacts the density of states of learning problems

- Insight into the learning process due to a large pull of solutions and higher energy states



Conclusions

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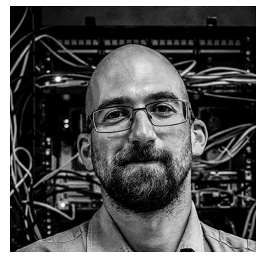
Statistical and Biological Physics group
University of Trento - TIFPA

Raffaello Potestio
University of Trento - TIFPA



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Istituto Nazionale di Fisica Nucleare
TIFPA
Trento Institute for Fundamental Physics and Applications

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The Abdus Salam International Centre for Theoretical Physics

FONDAZIONE CASSA RURALE DI TRENTO

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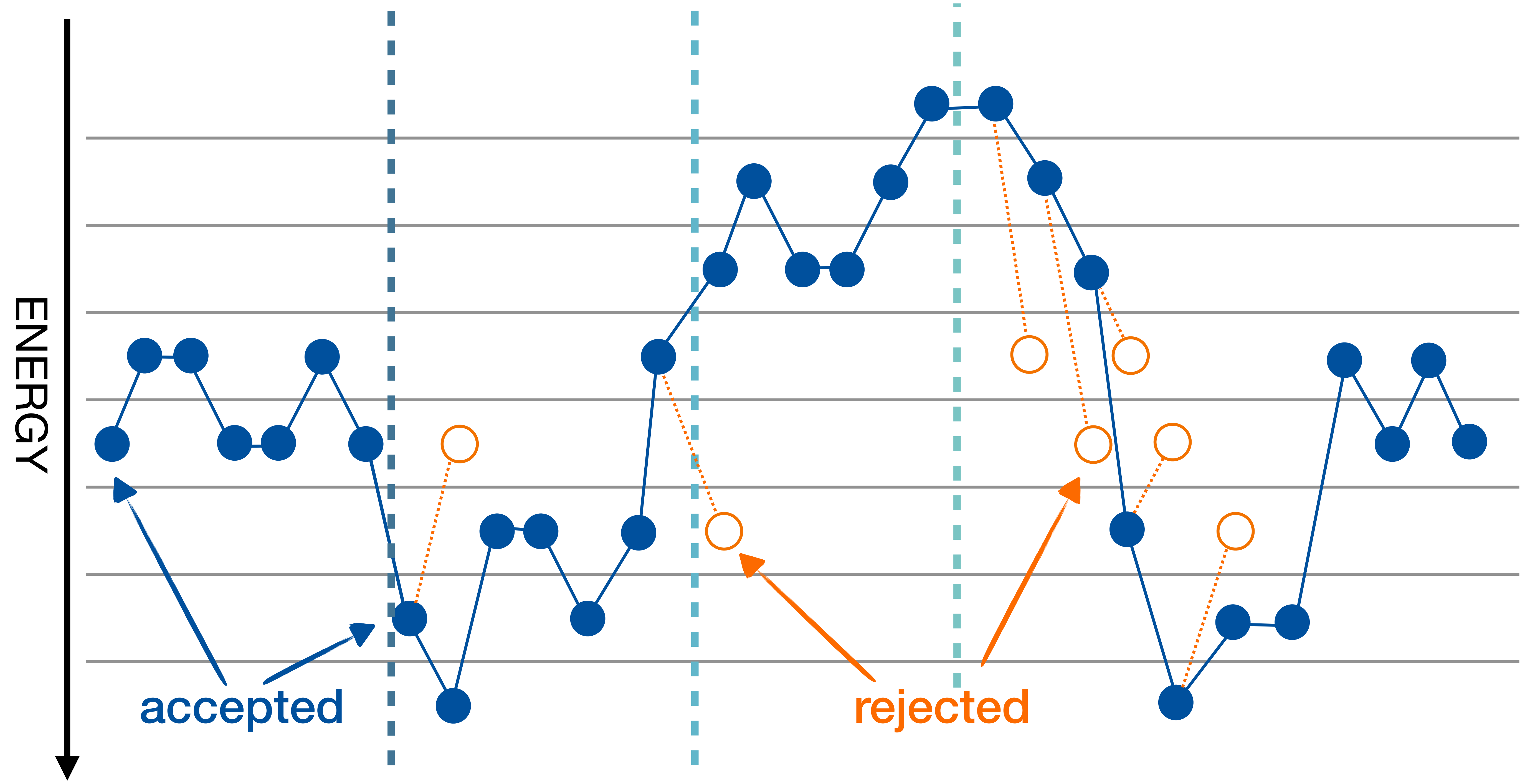
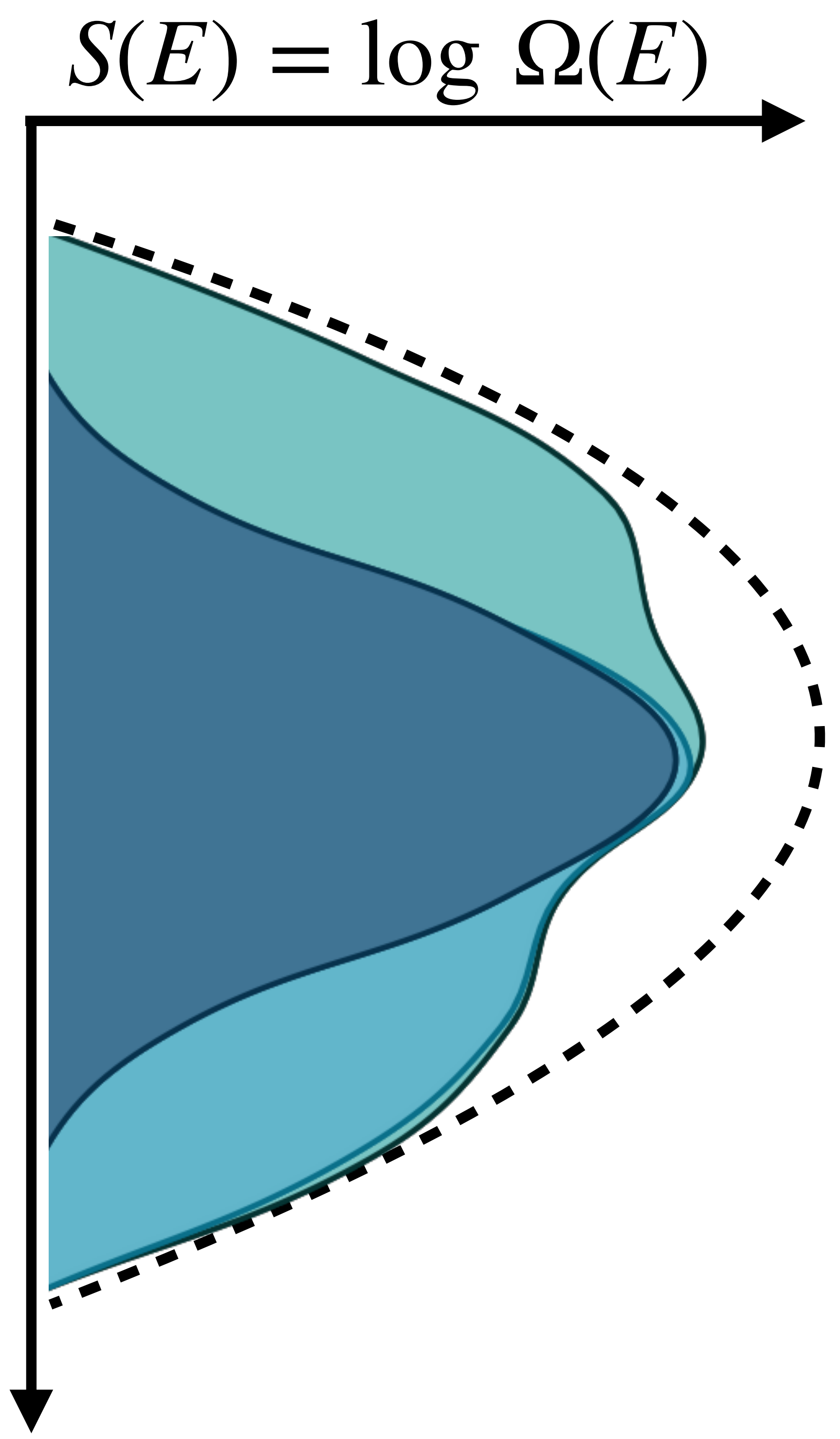
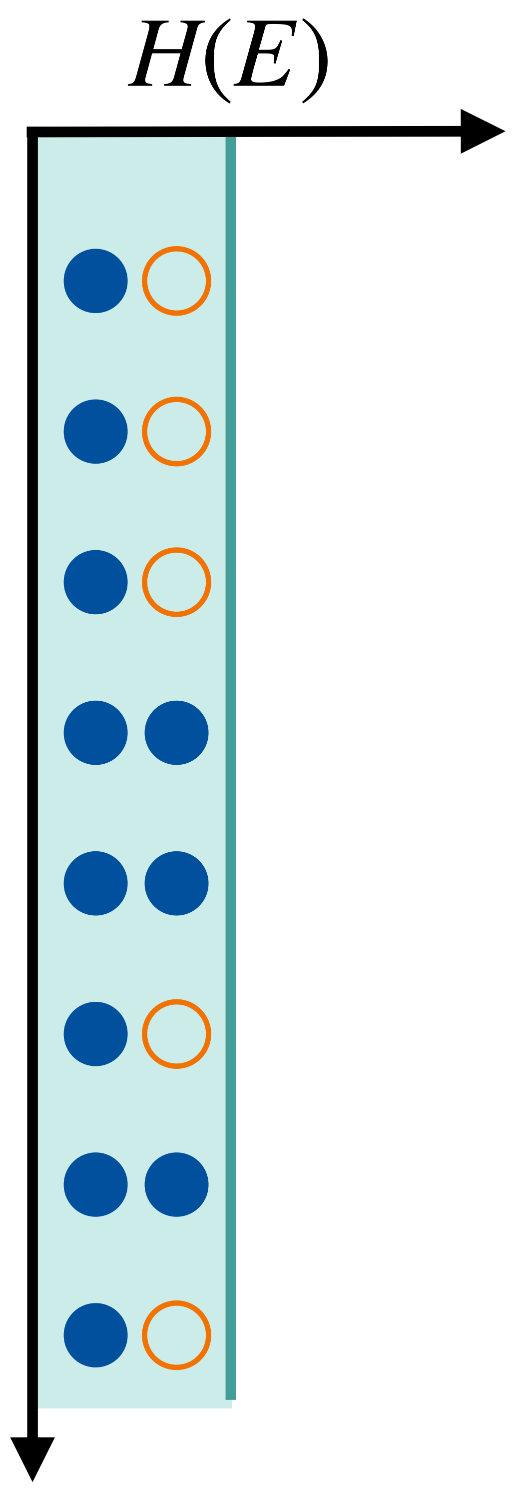
Wang-Landau algorithm







Proposal

$$g(w, \tilde{w})$$

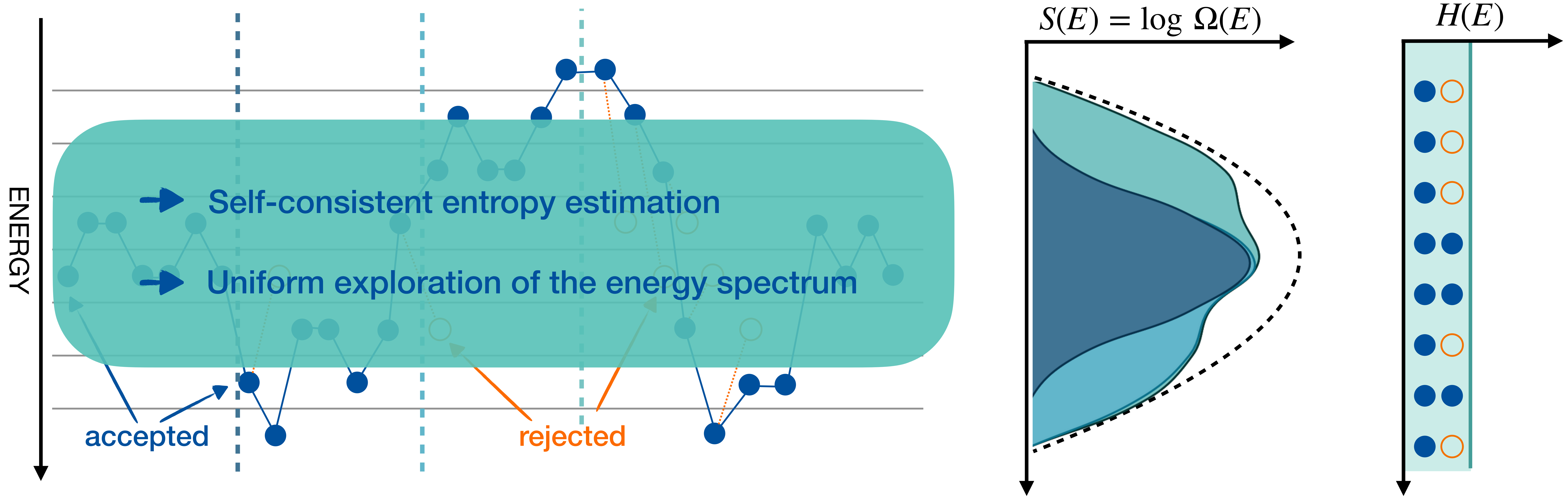
Acceptance

$$A(w,\tilde{w}) = \min\left\{1,\ e^{S_w - S_{\tilde{w}}}\frac{g(\tilde{w},w)}{g(w,\tilde{w})}\right\}$$

Updates

$$S_w \leftarrow S_w + f \qquad H_w \leftarrow H_w + 1$$

Wang-Landau algorithm



Proposal

$$g(w,\tilde{w})$$

Acceptance

$$A(w,\tilde{w}) = \min\left\{1,\ e^{S_w - S_{\tilde{w}}}\frac{g(\tilde{w},w)}{g(w,\tilde{w})}\right\}$$

Updates

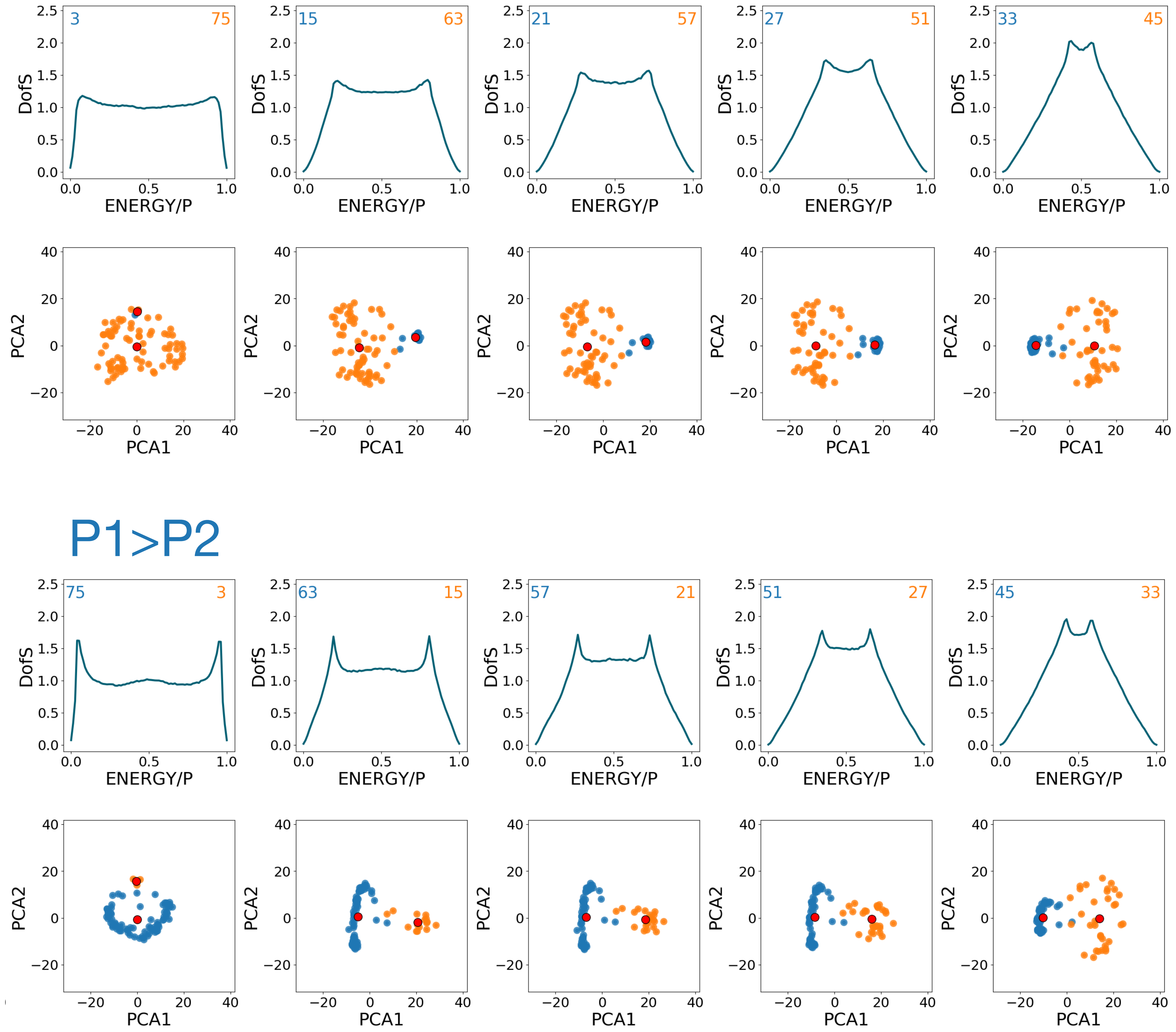
$$S_w \leftarrow S_w + f \qquad H_w \leftarrow H_w + 1$$

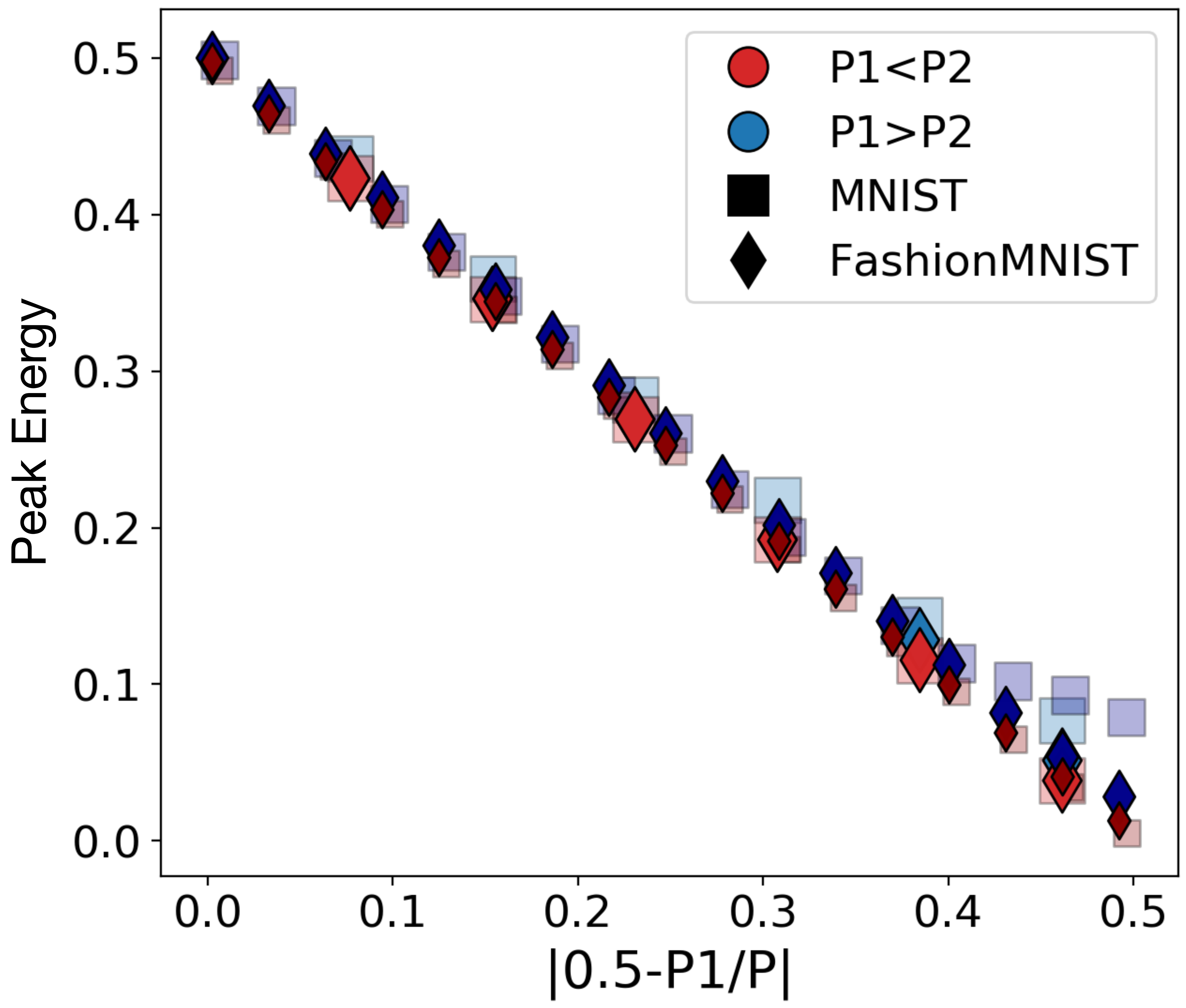
MNIST & FashionMNIST

MNIST (P/N=0.1)

P1<P2

P1>P2



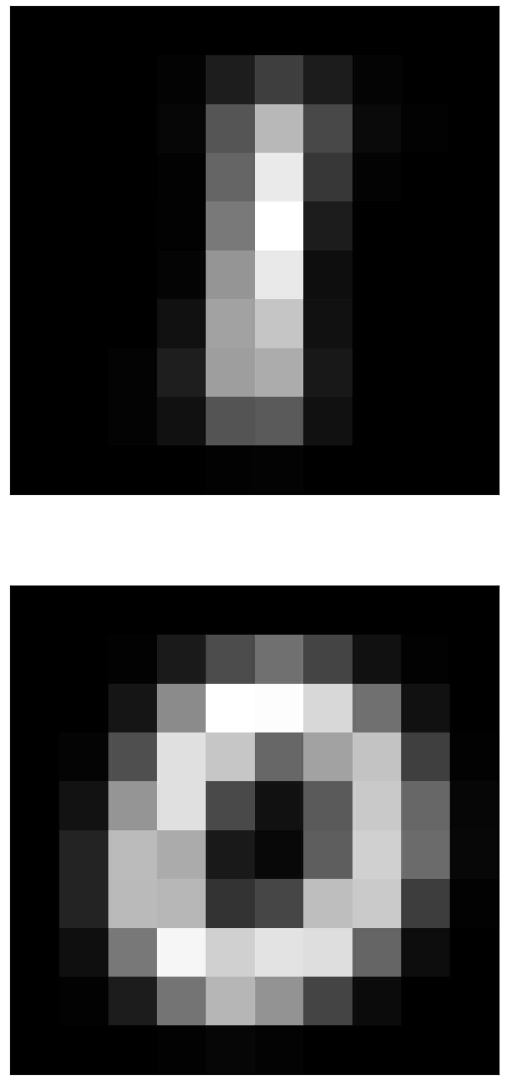


Back back to *realistic* data

Gaussian Clones

$$N(x, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^k \det \Sigma}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\right)$$

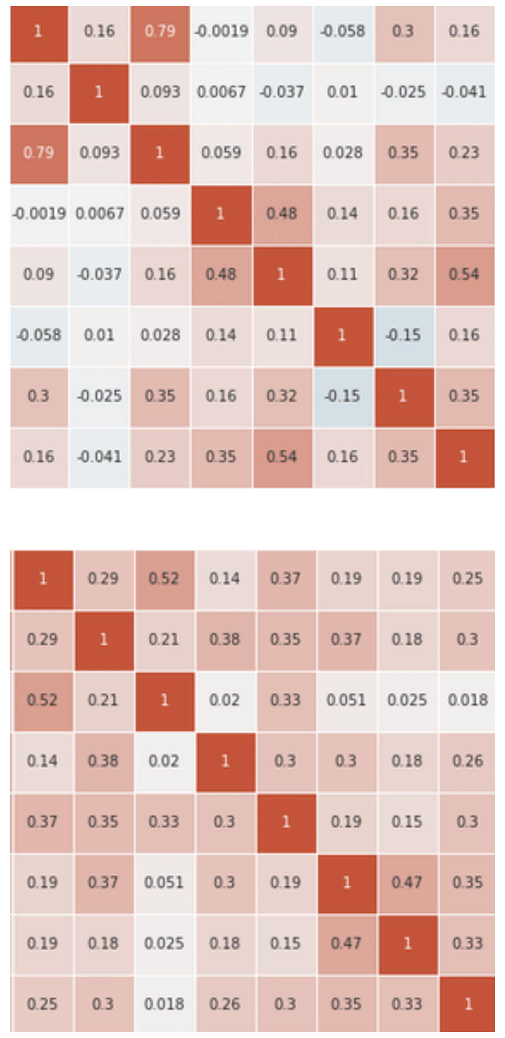
Mean - μ



+

Covariance - Σ

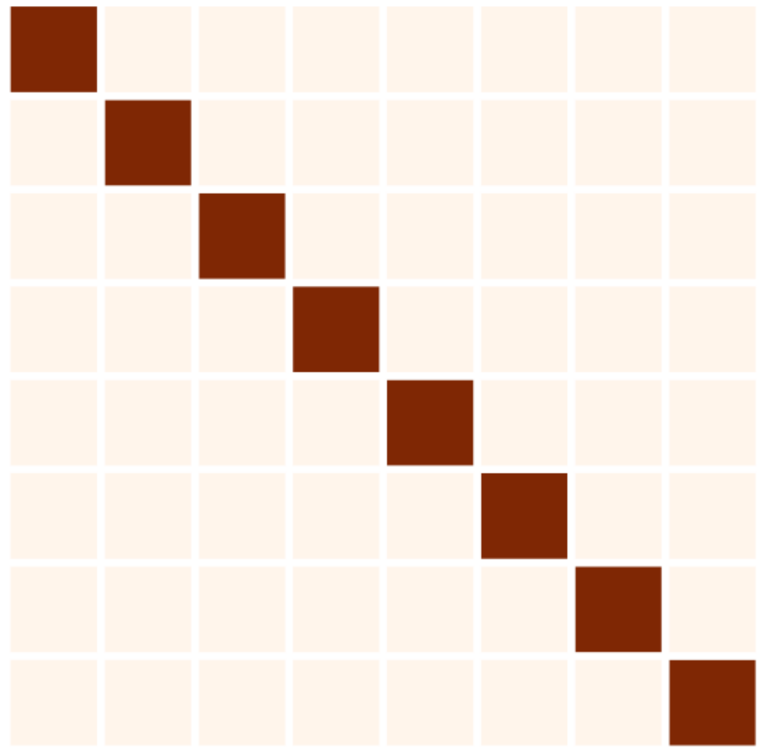
GM



2ISO

diagonal matrix

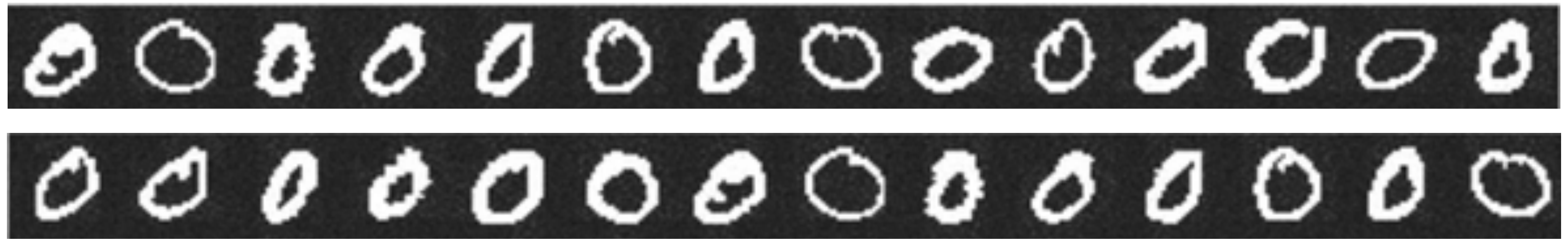
$$v = \sqrt{v_1 \cdot v_2}$$

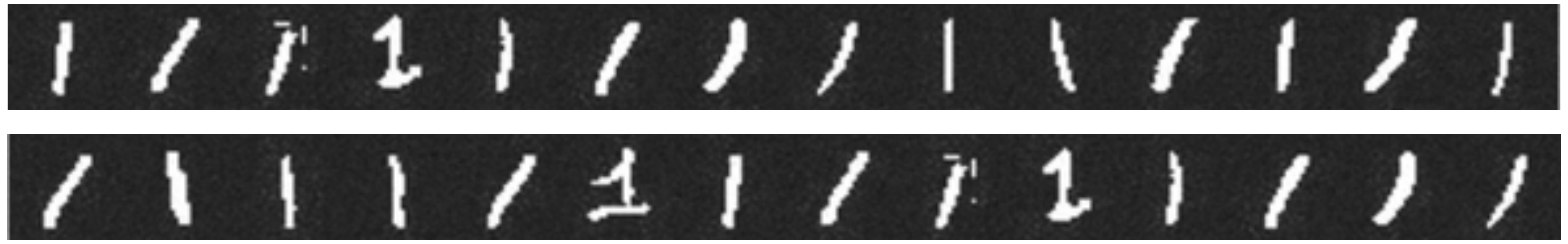


Gaussian Clones

Multivariate Normal Distribution

$$N(x, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^k \det \Sigma}} \exp\left(-\frac{1}{2}(x-\mu)^T \, \Sigma^{-1} \, (x-\mu)\right)$$





Gaussian Clones

Multivariate Normal Distribution

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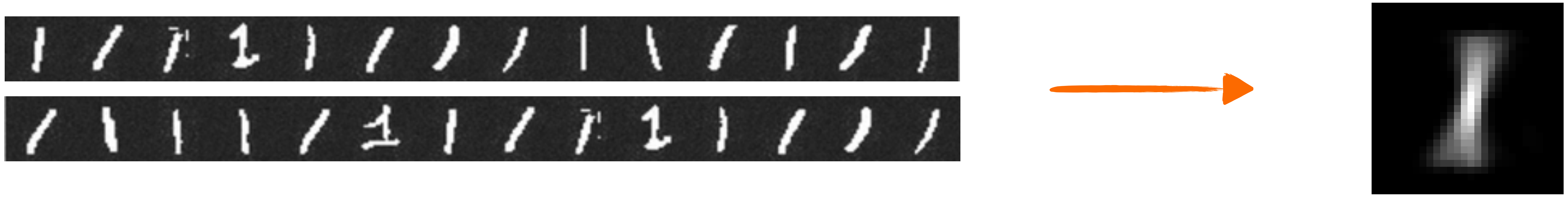

Gaussian Clones

Multivariate Normal Distribution

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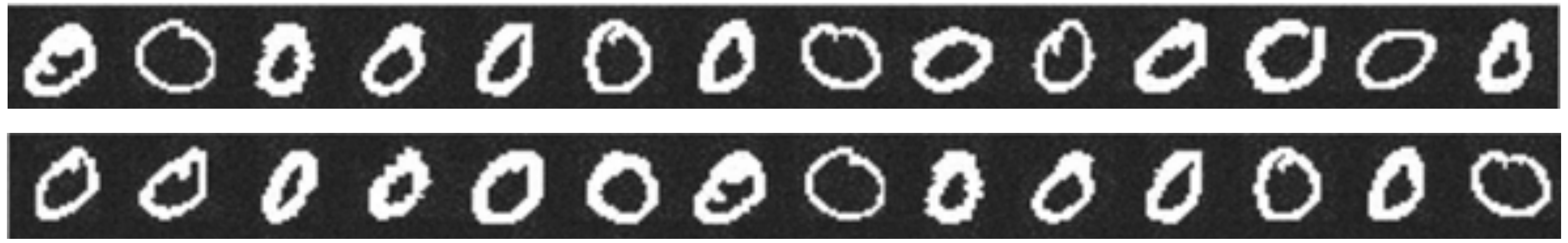
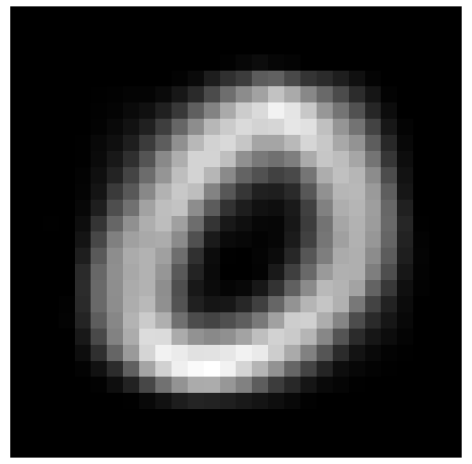
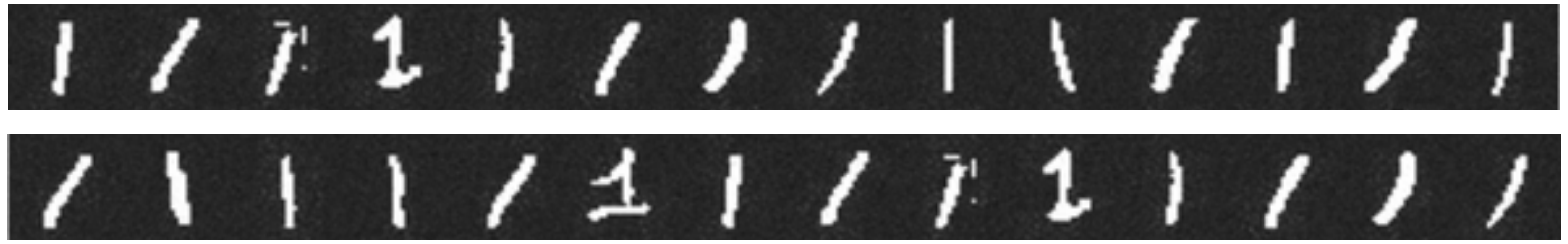
Mean - μ

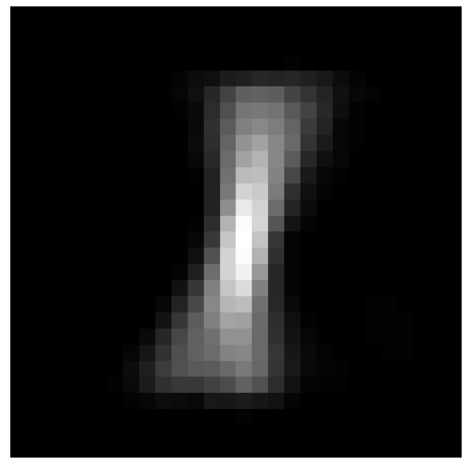
Covariance - Σ





1	0.16	0.79	-0.0019	0.09	-0.058	0.3	0.16
0.16	1	0.093	0.0067	-0.037	0.01	-0.025	-0.041
0.79	0.093	1	0.059	0.16	0.028	0.35	0.23
-0.0019	0.0067	0.059	1	0.48	0.14	0.16	0.35
0.09	-0.037	0.16	0.48	1	0.11	0.32	0.54
-0.058	0.01	0.028	0.14	0.11	1	-0.15	0.16
0.3	-0.025	0.35	0.16	0.32	-0.15	1	0.35
0.16	-0.041	0.23	0.35	0.54	0.16	0.35	1





1	0.02	0.33	0.051	0.025	0.018	0.0074	0.086
0.02	1	0.3	0.3	0.18	0.26	0.3	0.27
0.33	0.3	1	0.19	0.15	0.3	0.19	0.33
0.051	0.3	0.19	1	0.47	0.35	0.88	0.53
0.025	0.18	0.15	0.47	1	0.33	0.33	0.75
0.018	0.26	0.3	0.35	0.33	1	0.28	0.76
0.0074	0.3	0.19	0.88	0.33	0.28	1	0.4
0.086	0.27	0.33	0.53	0.75	0.76	0.4	1

Gaussian Clones

Multivariate Normal Distribution

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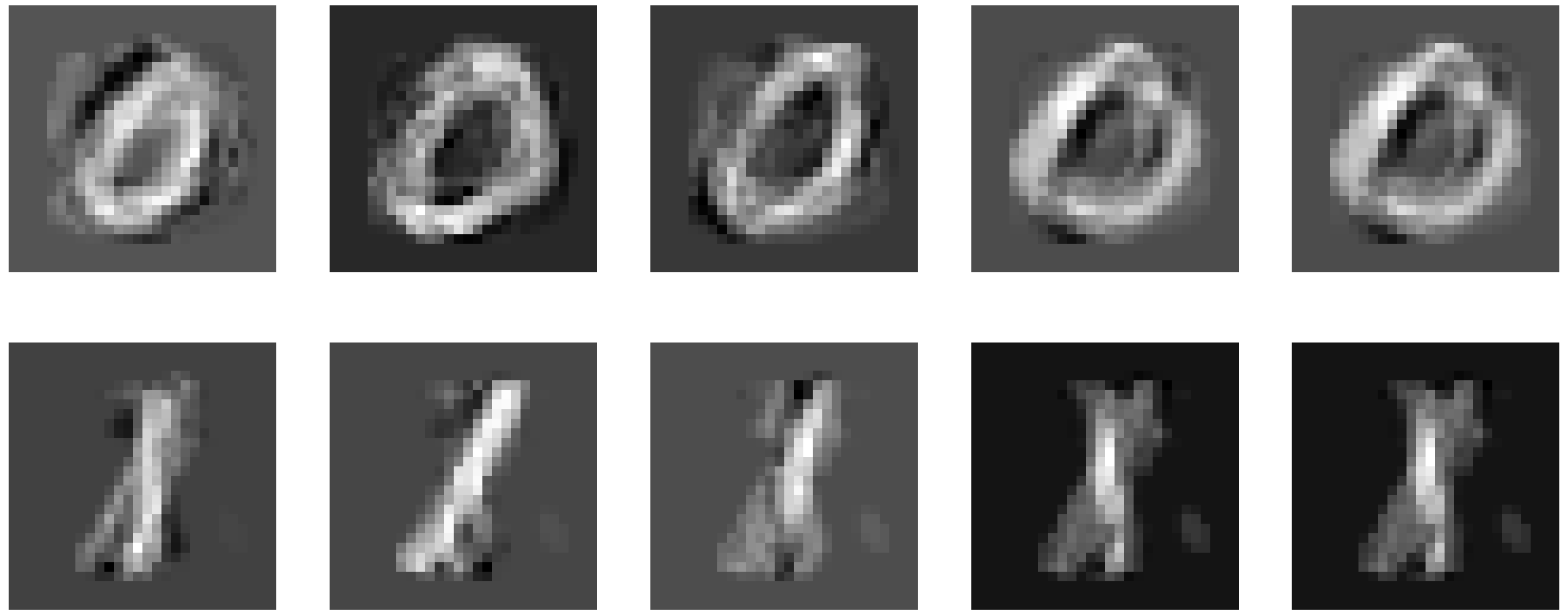
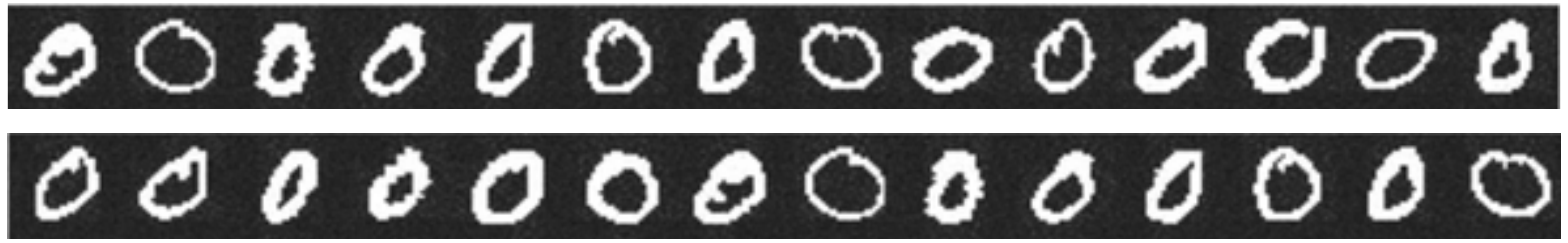
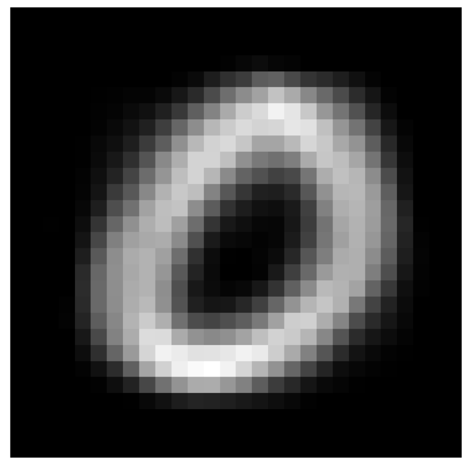


Mean - μ

Covariance - Σ





1	0.16	0.79	-0.0019	0.09	-0.058	0.3	0.16
0.16	1	0.093	0.0067	-0.037	0.01	-0.025	-0.041
0.79	0.093	1	0.059	0.16	0.028	0.35	0.23
-0.0019	0.0067	0.059	1	0.48	0.14	0.16	0.35
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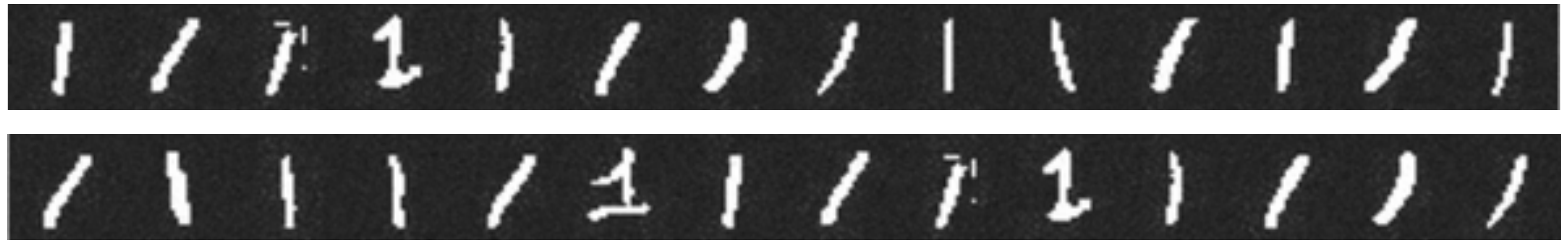
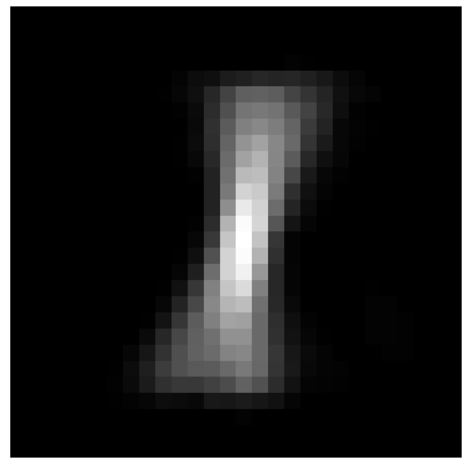
0.3	-0.025	0.35	0.16	0.32	-0.15	1	0.35
0.16	-0.041	0.23	0.35	0.54	0.16	0.35	1





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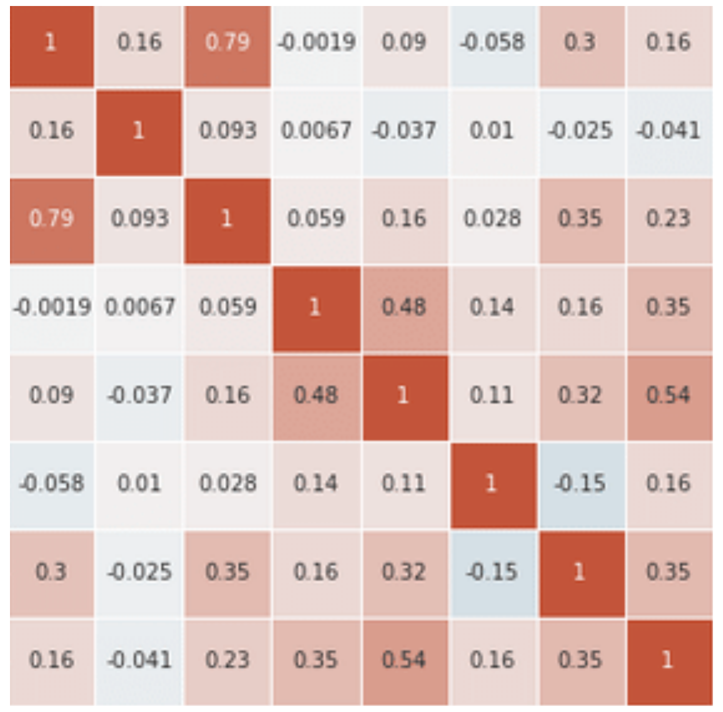
0.086	0.27	0.33	0.53	0.75	0.76	0.4	1

Gaussian Clones

Multivariate Normal Distribution

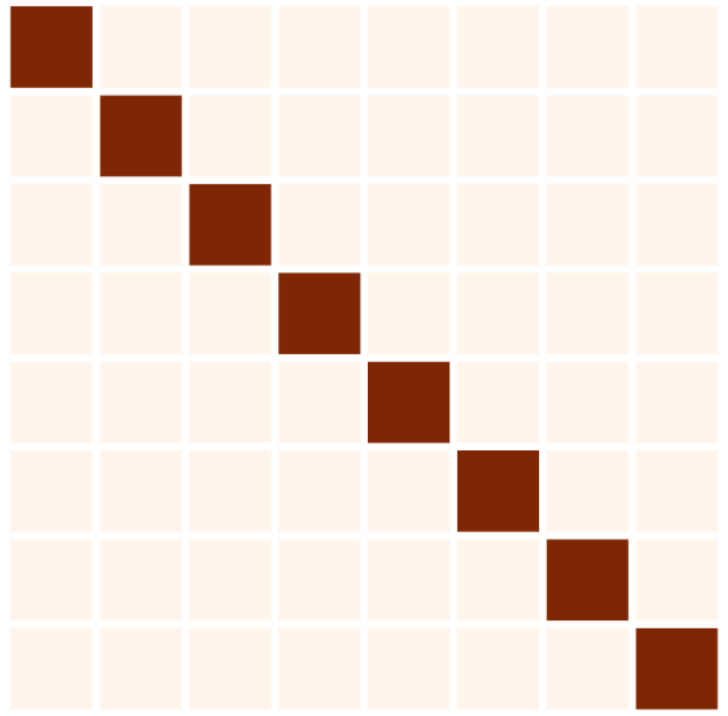
$$N(x, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^k \det \Sigma}} \exp\left(-\frac{1}{2}(x-\mu)^T \, \Sigma^{-1} \, (x-\mu) \right)$$

GM clone



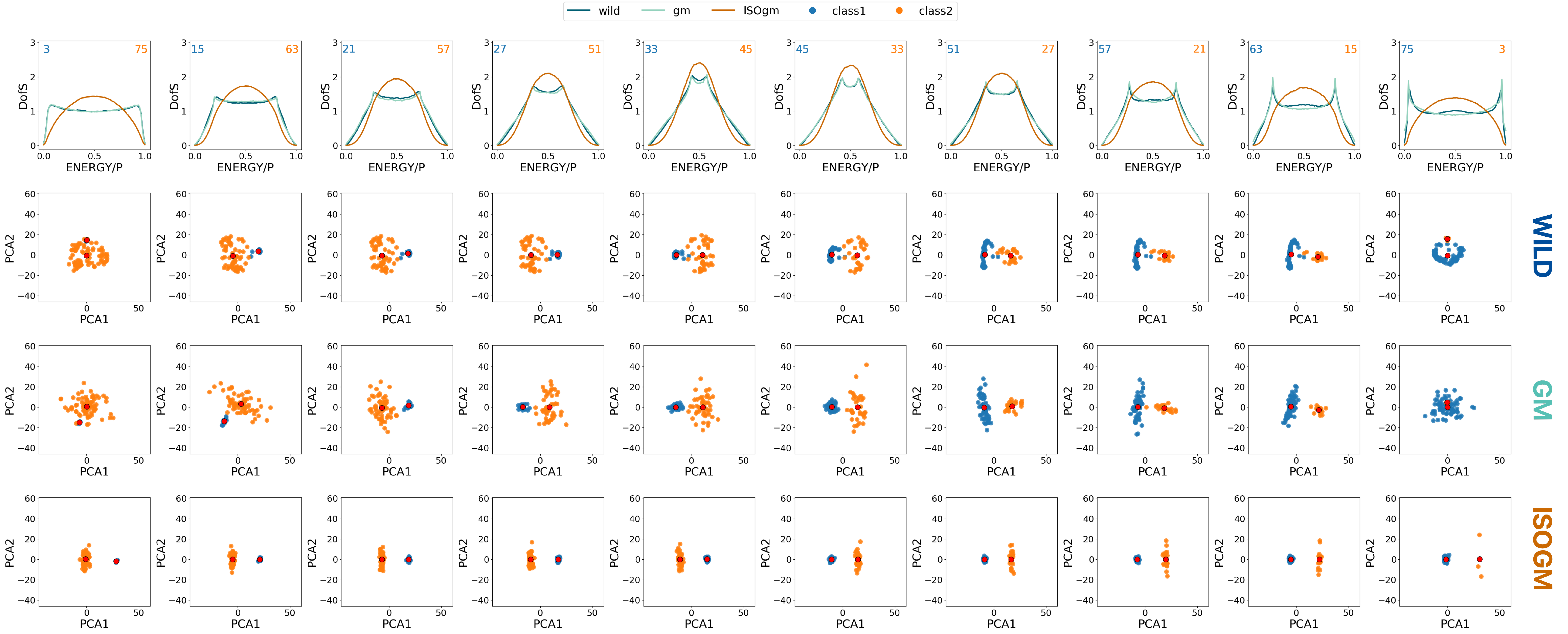
- **Mean vector**
- **Covariance matrix**

ISOGM clone

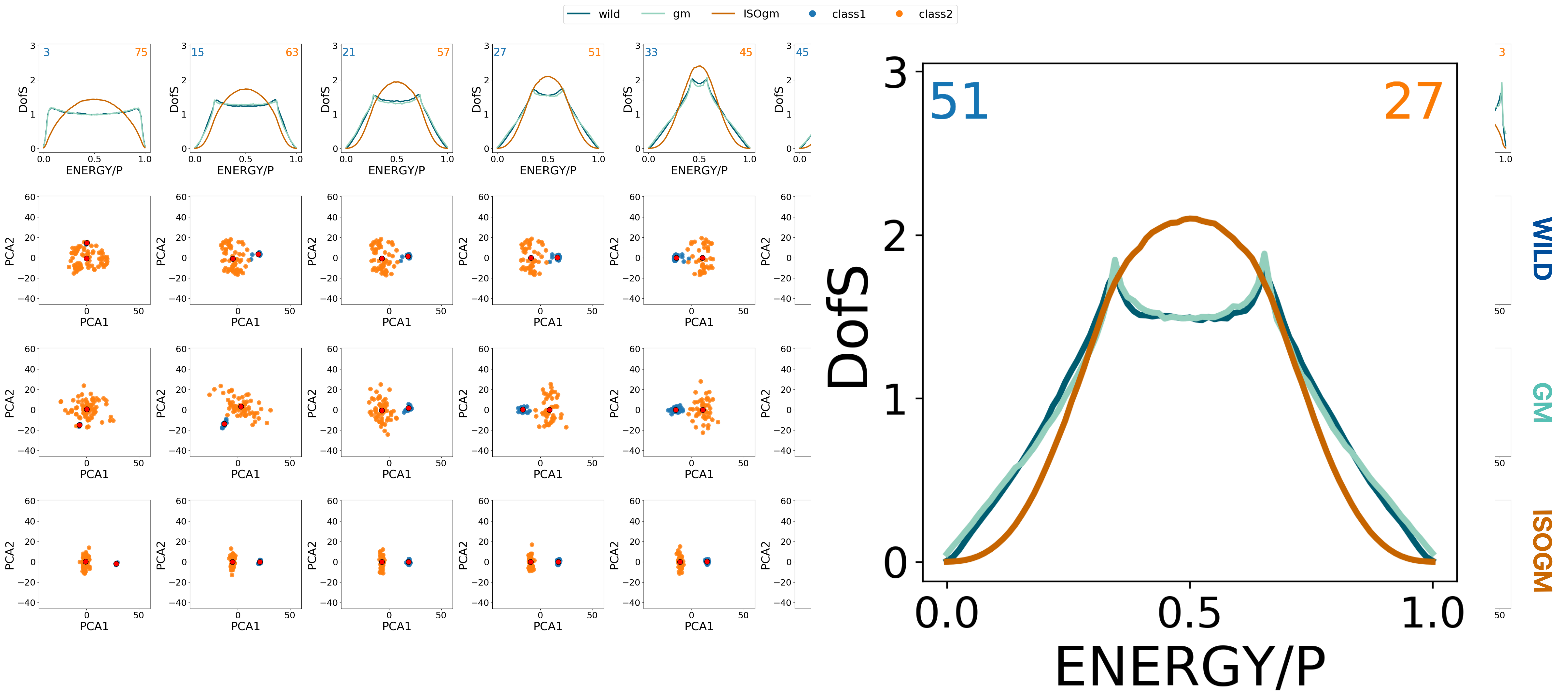


- **Mean vector**
- **Variance : diagonal matrix**

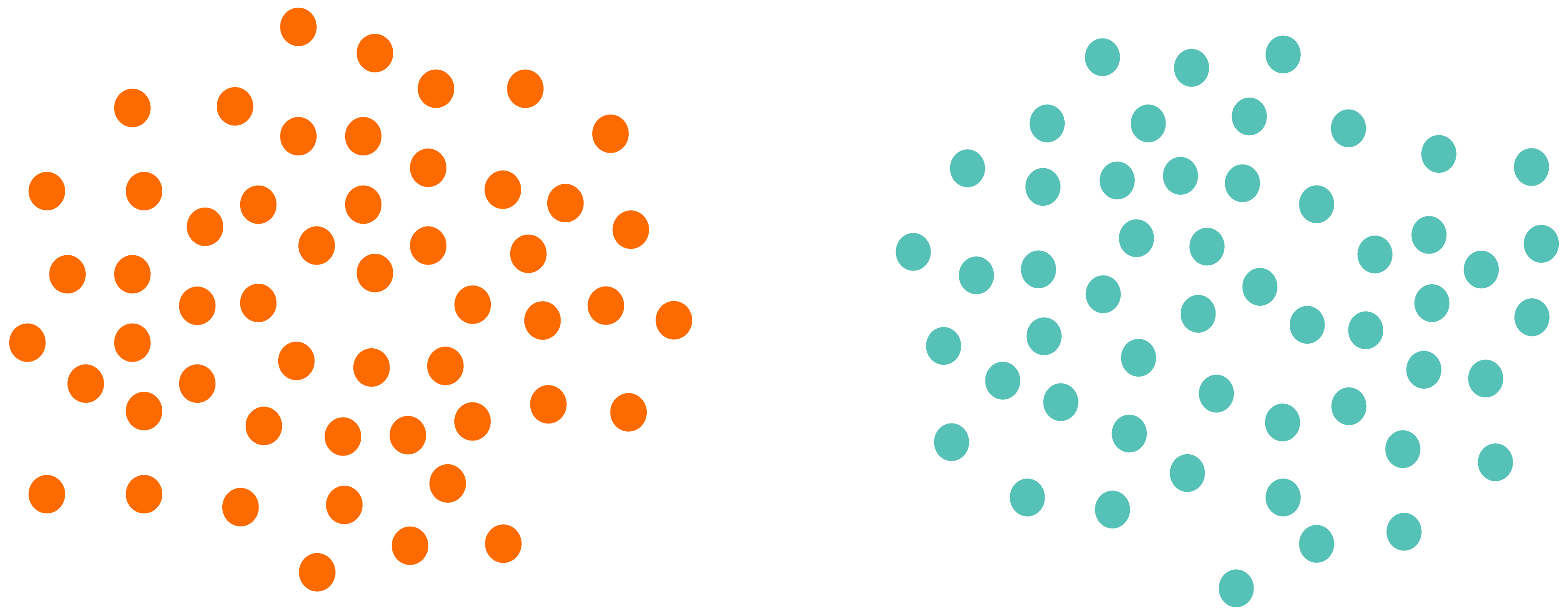
Gaussian Clones - MNIST (P/N=0.1)



Gaussian Clones - MNIST (P/N=0.1)

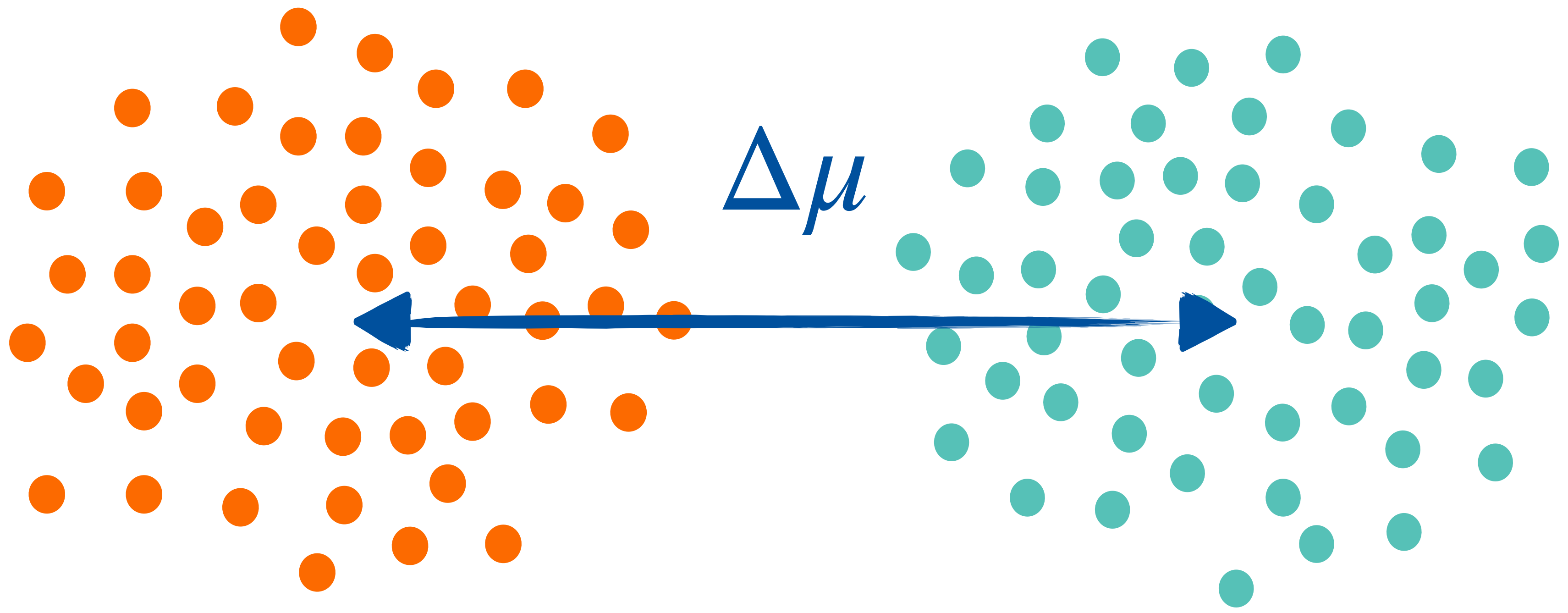


Silico dataset



Silico dataset

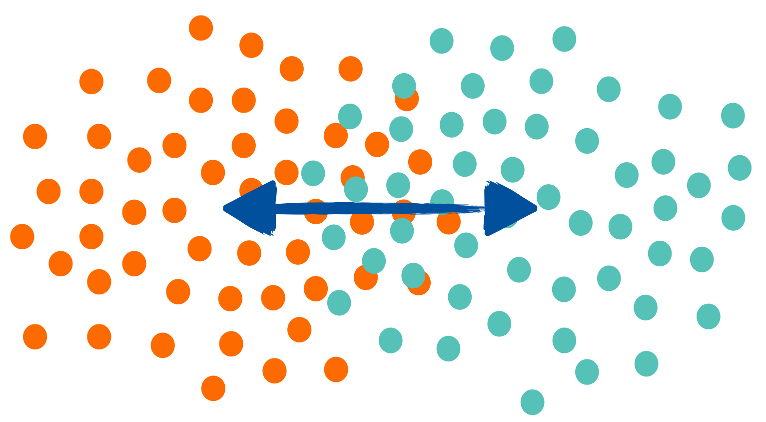
Class separation

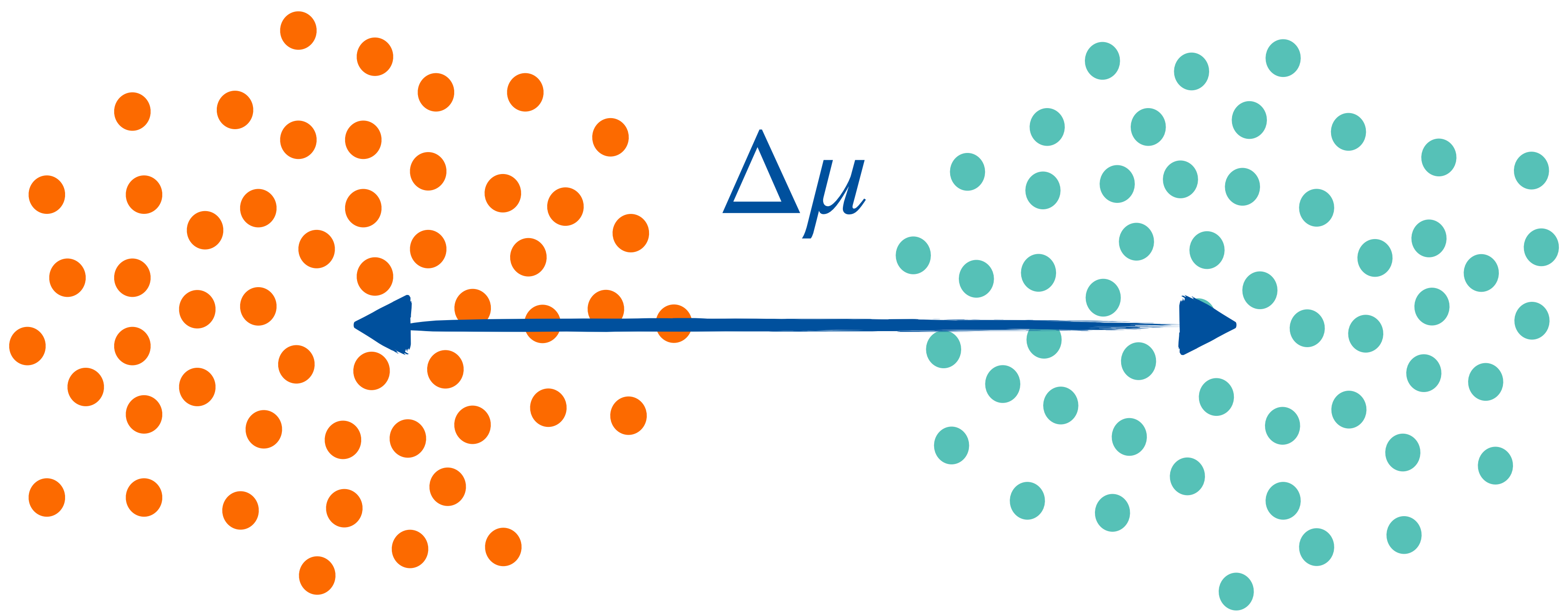


Silico dataset

Class separation

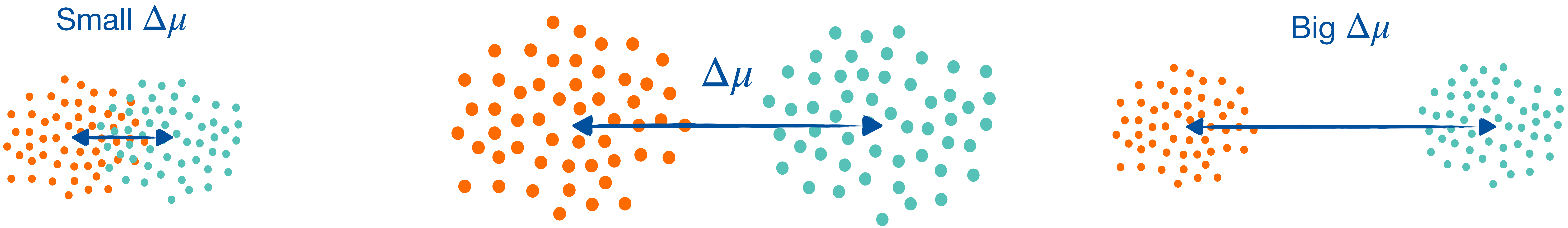
Small $\Delta\mu$





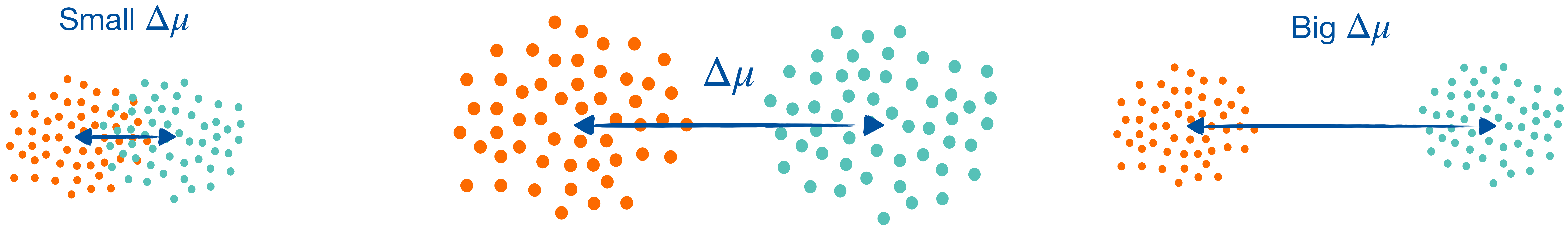
Silico dataset

Class separation

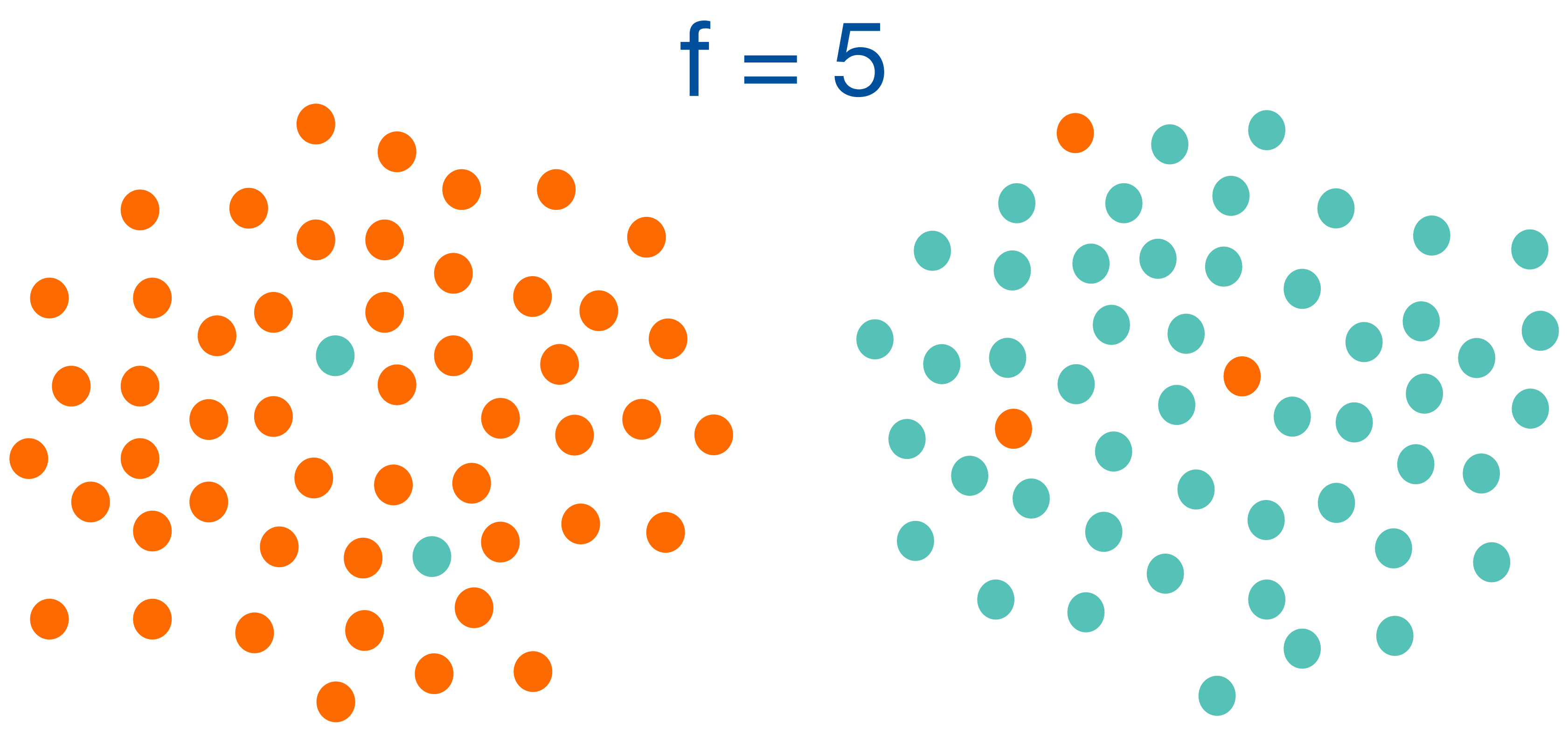


Silico dataset

Class separation

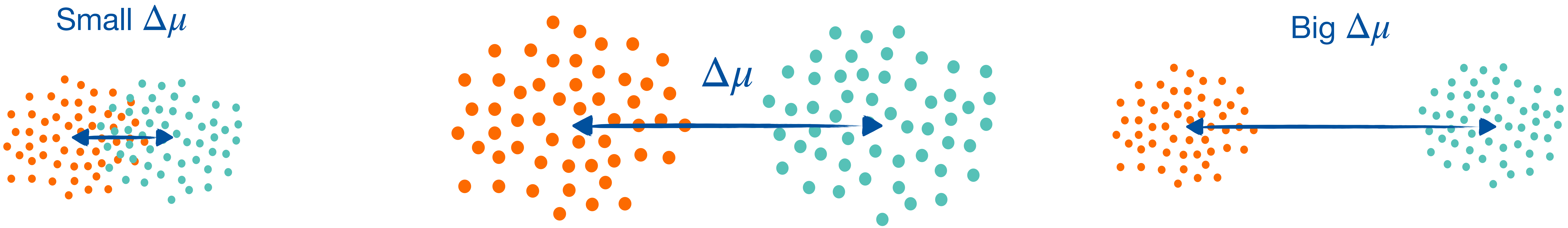


Misclassification

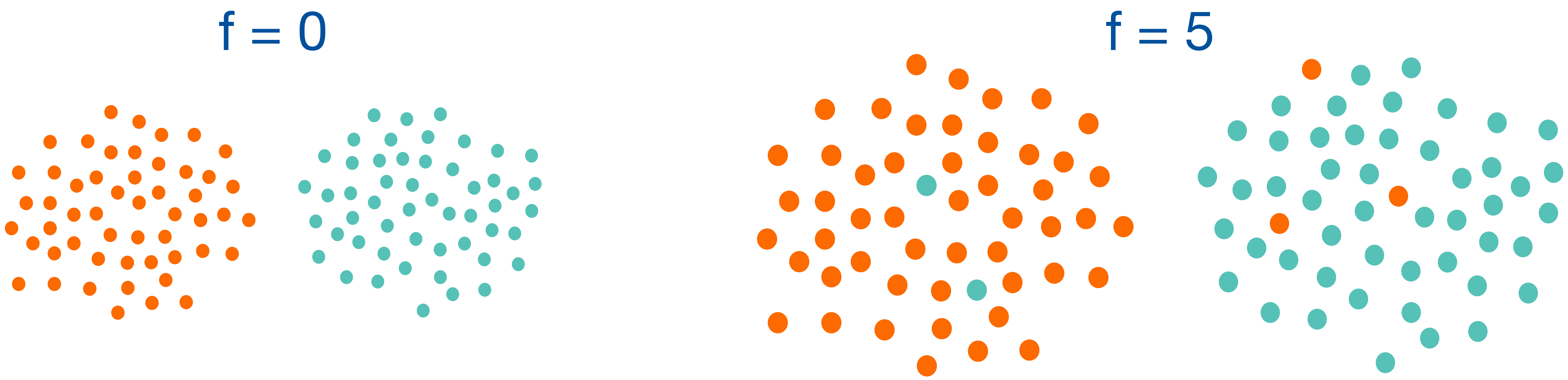


Silico dataset

Class separation

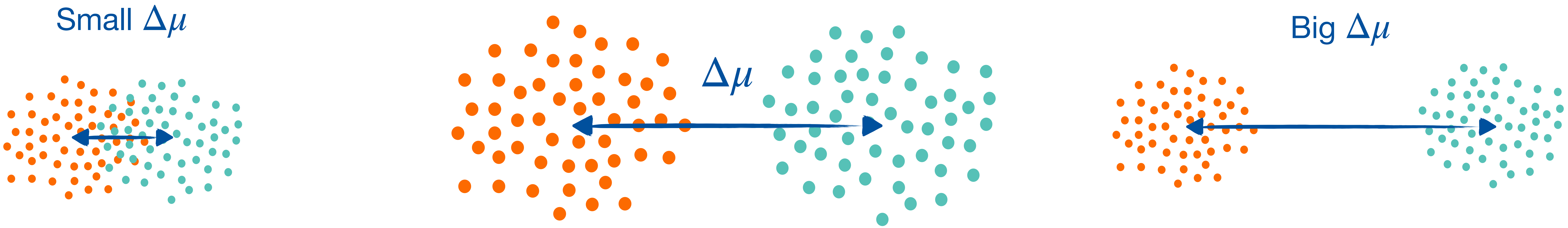


Misclassification

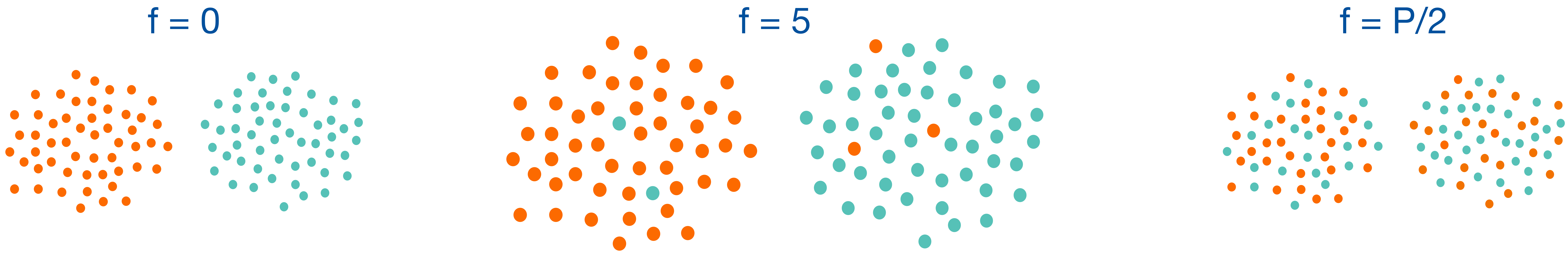


Silico dataset

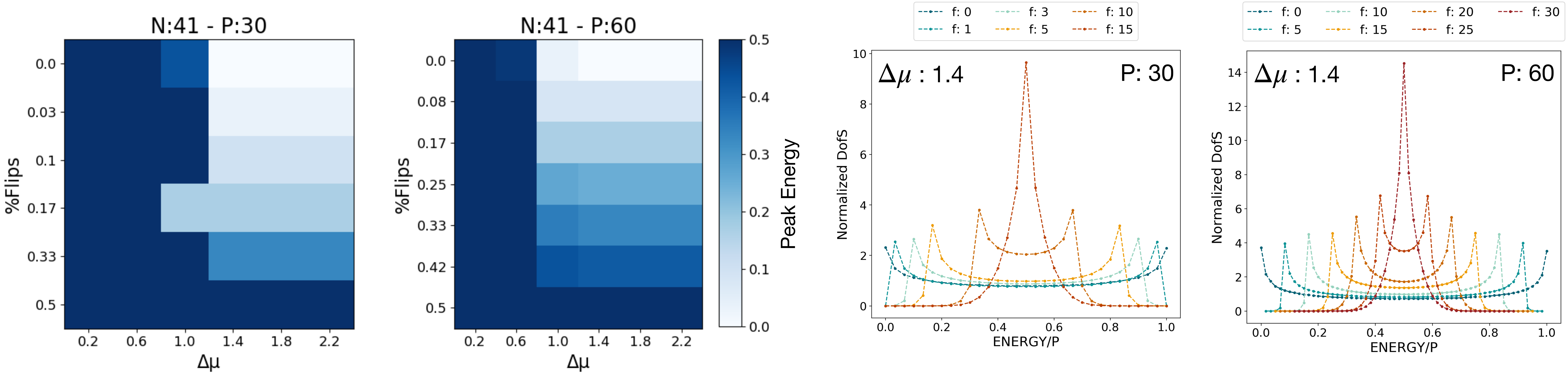
Class separation



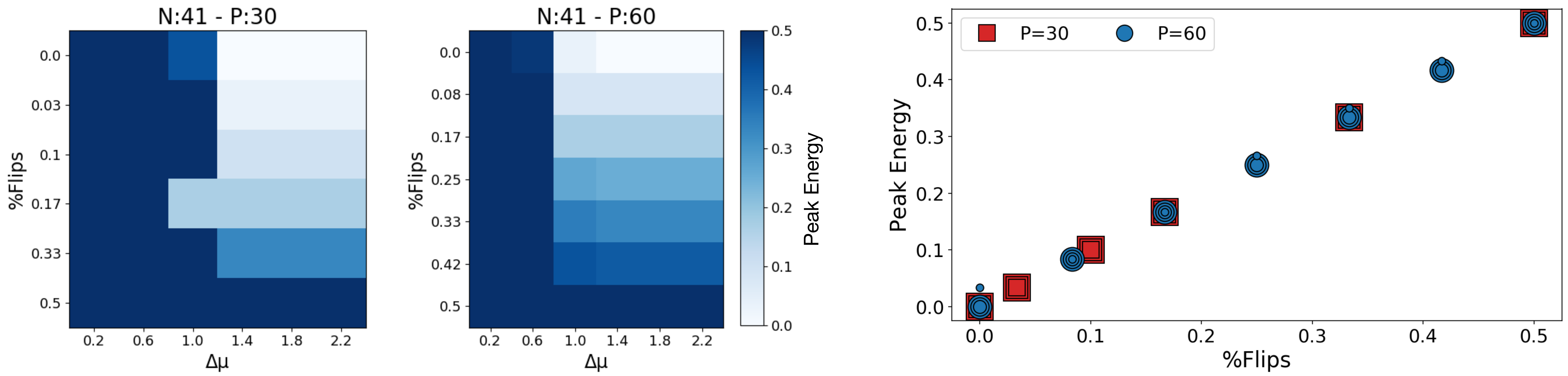
Misclassification



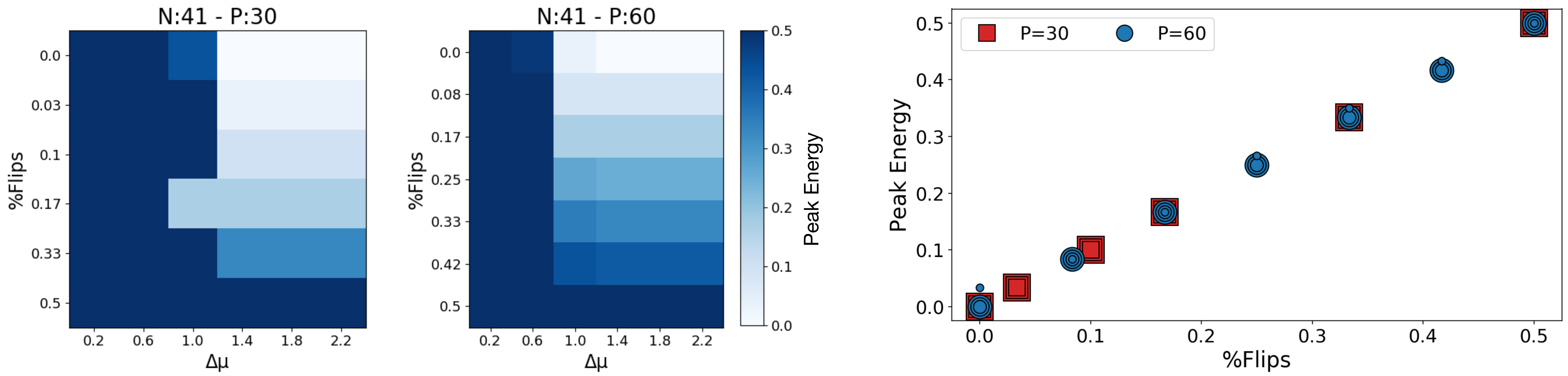
Silico dataset



Silico dataset



Silico dataset



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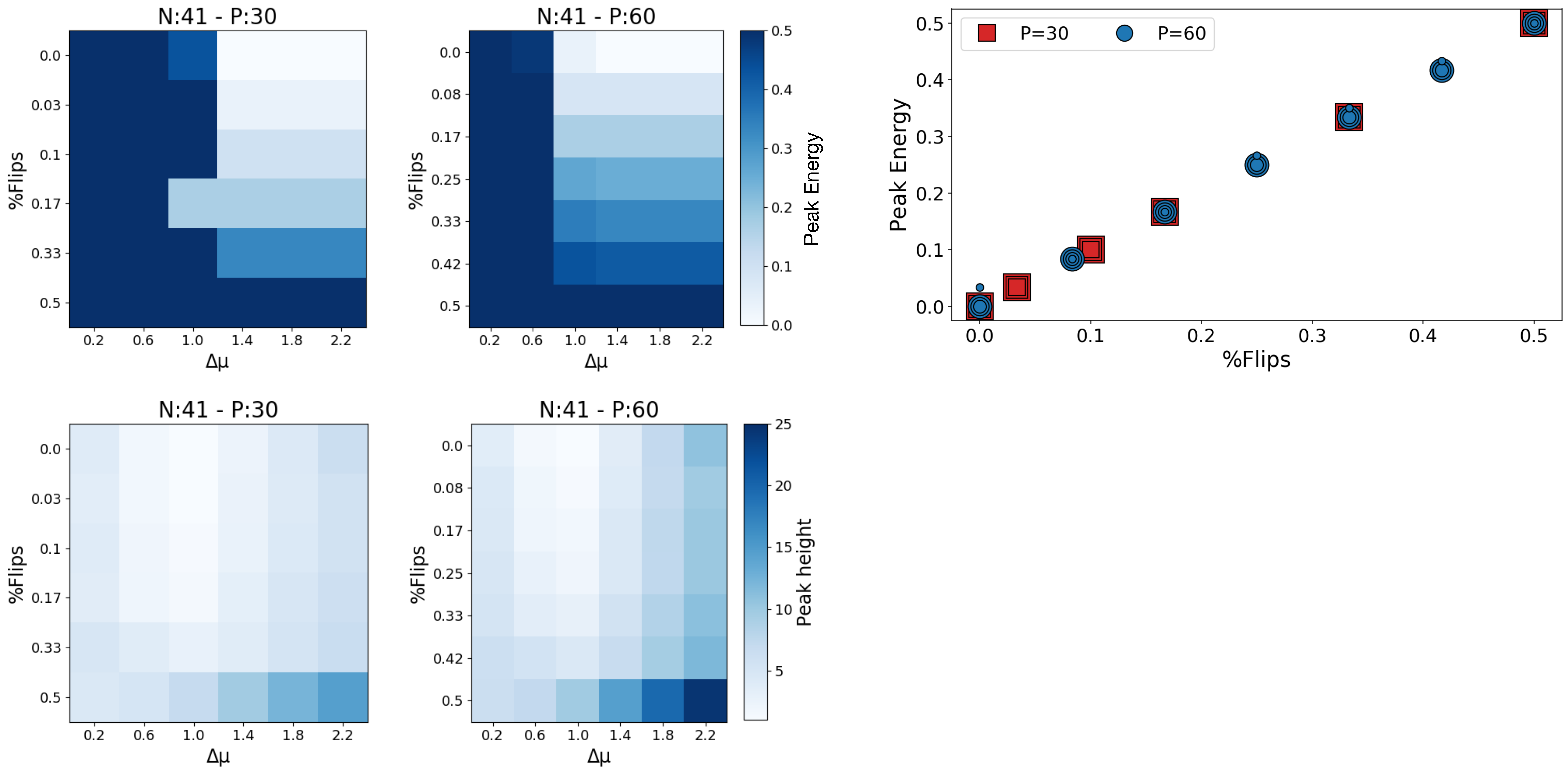

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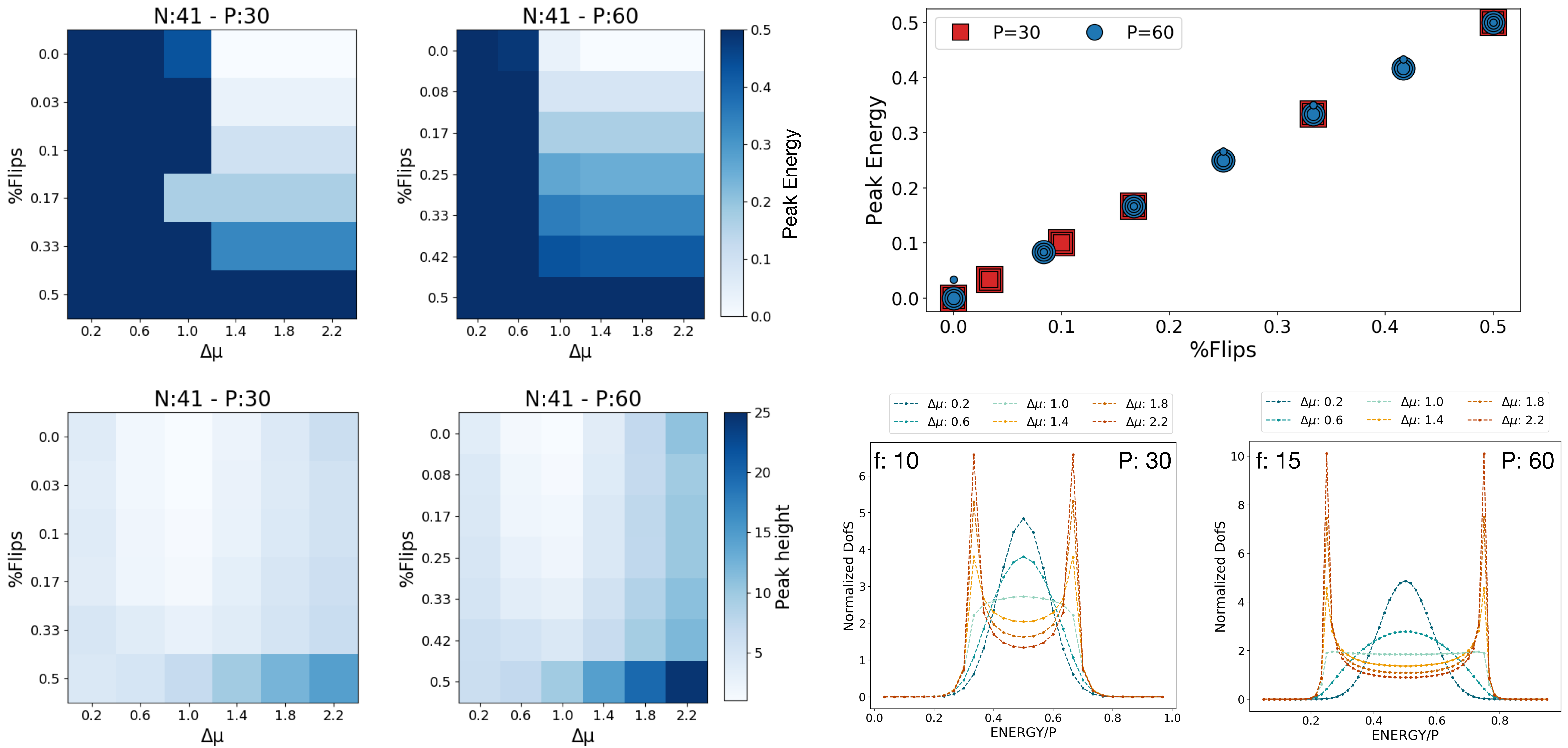
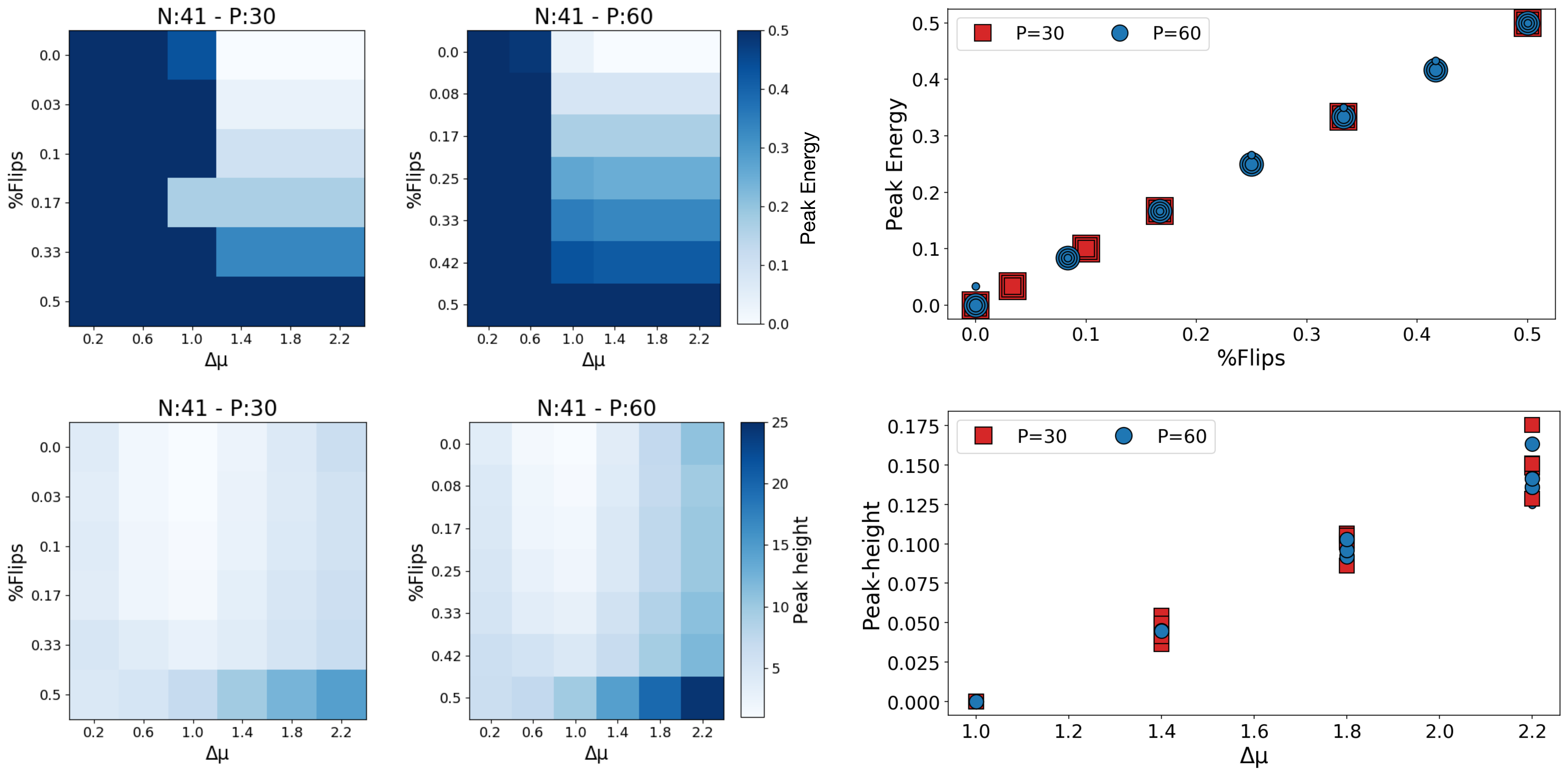


Silico dataset



Convergence time