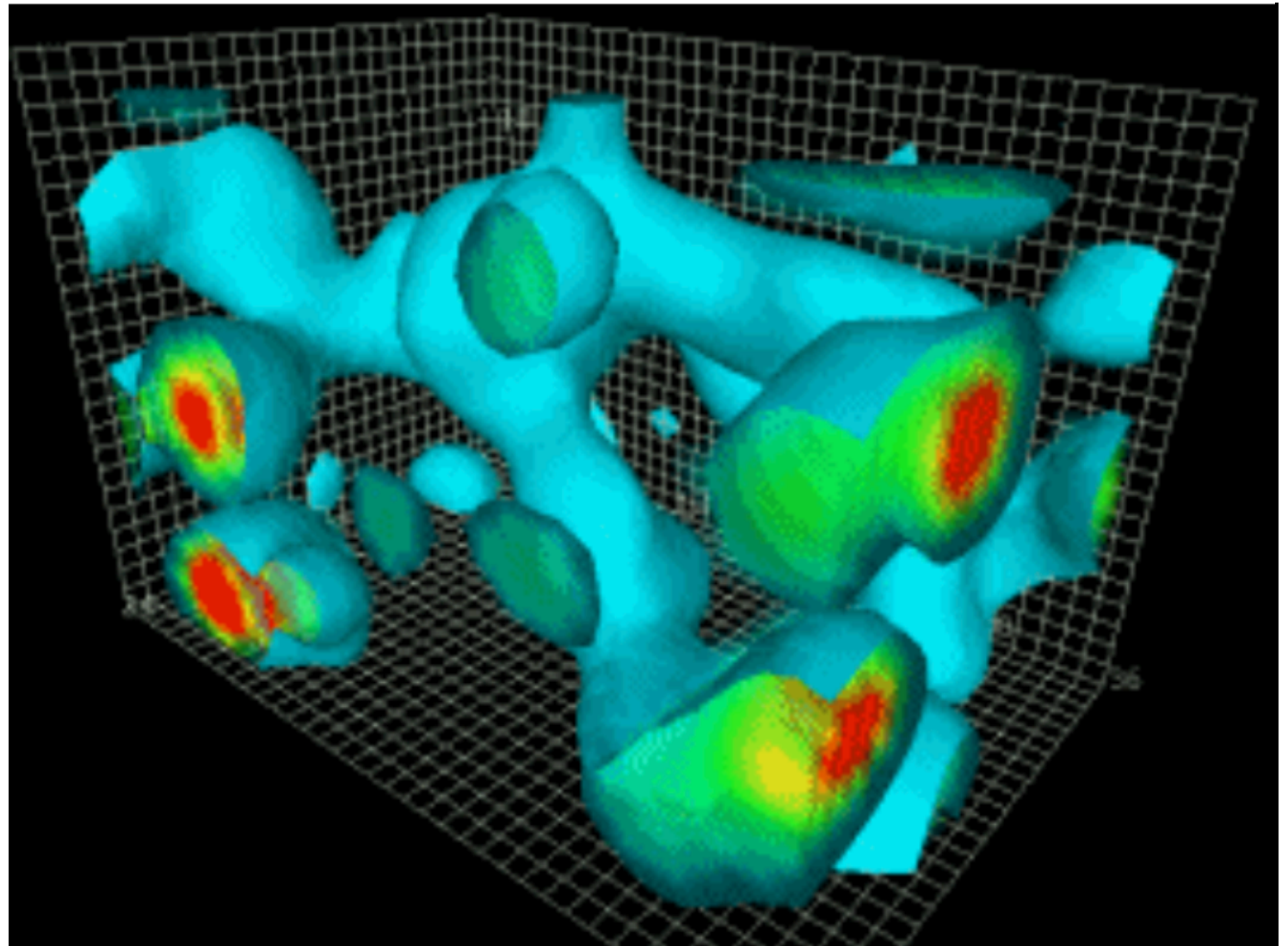
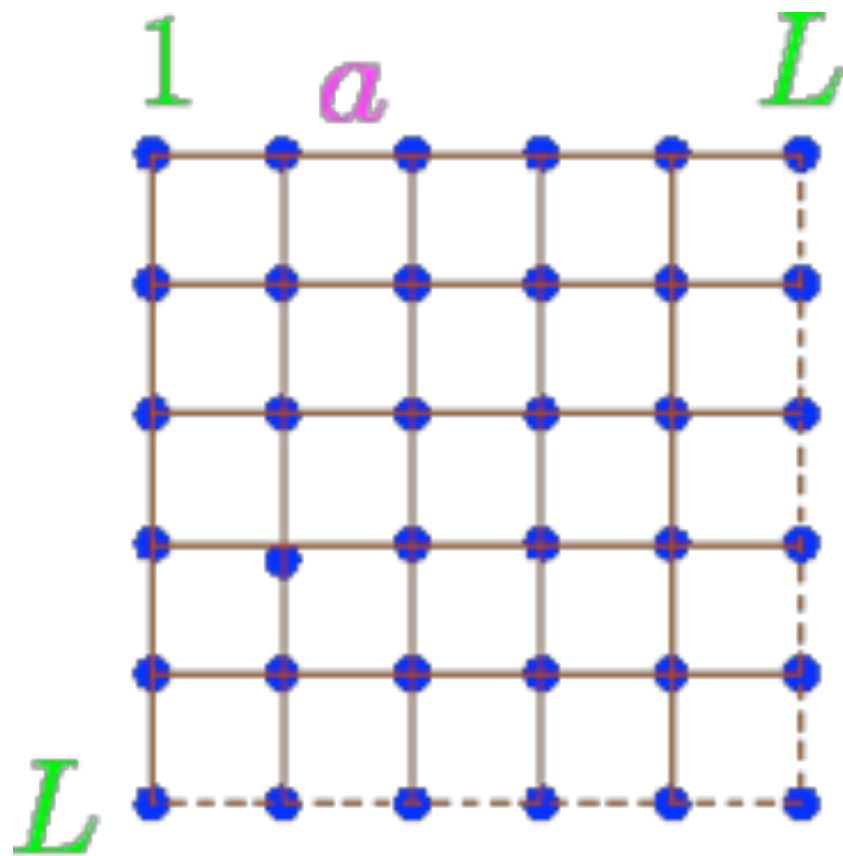
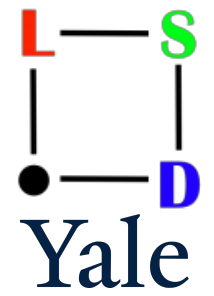


# Extracting Excited States from Lattice Correlation Functions

Kimmy Cushman & George Fleming

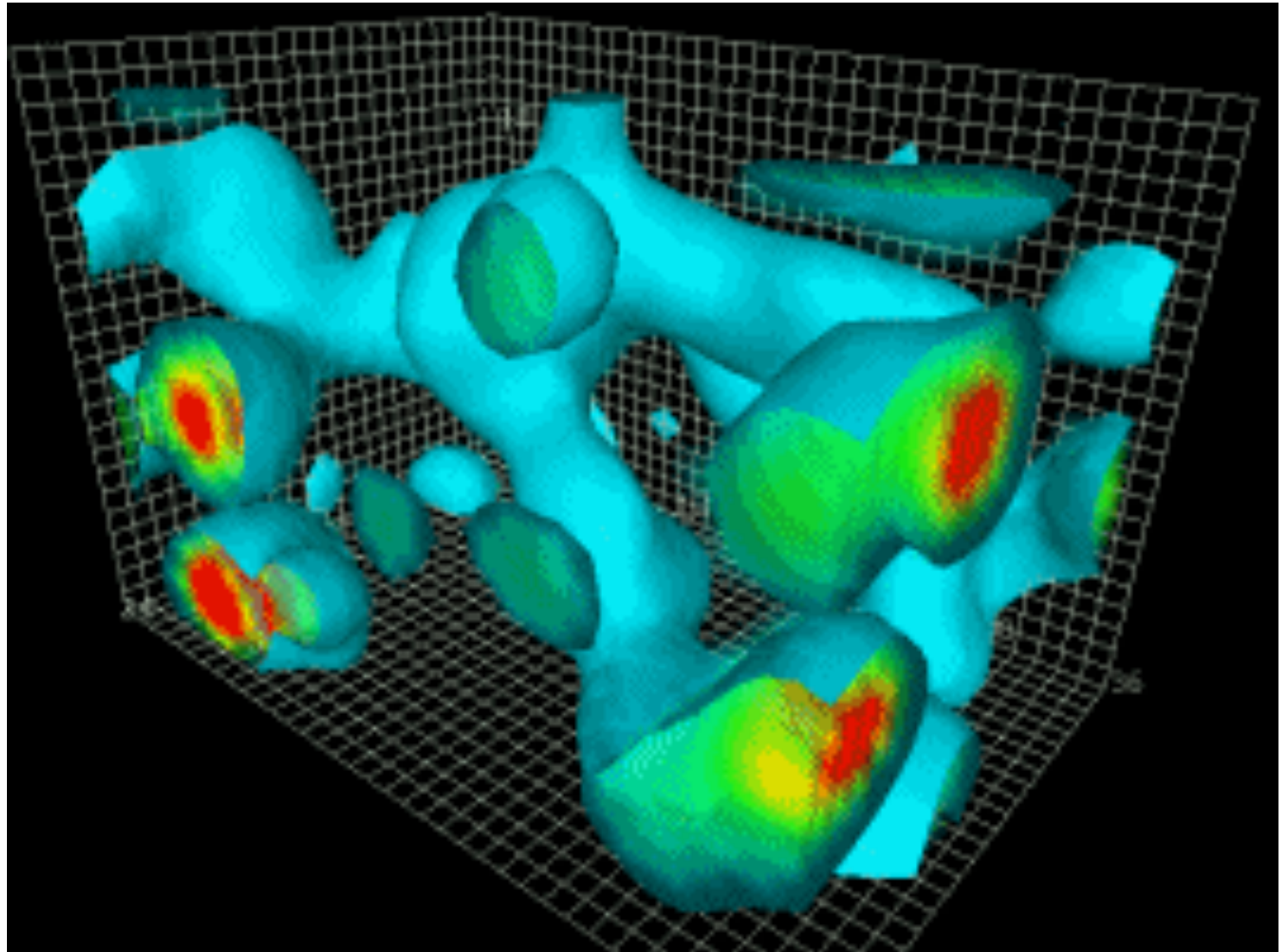


# Outline

- **Introduction and motivation**
- **Correlation functions**
- **Prony's method**
- **Bootstrapping and results**
- **Clustering**
- **Future work**

# Lattice QCD... what is it?

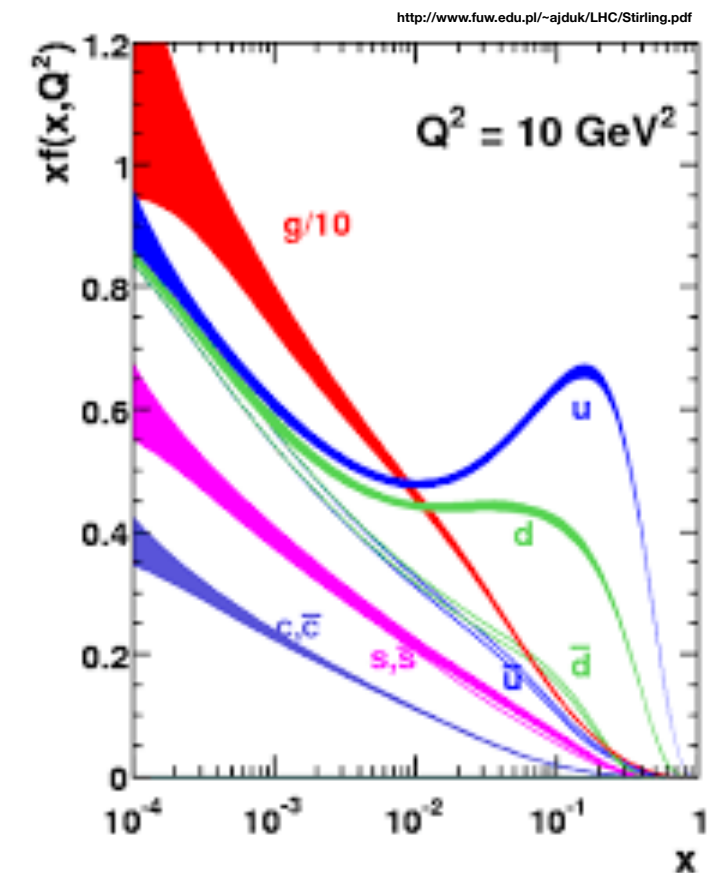
- Gauge field simulation from first principles
- Discretized space-time
- Finite volume with periodic conditions
- Volume  $\sim$  size of proton



<http://www.physics.adelaide.edu.au/cssm/lattice/>

# Motivation for QCD

- QCD strongly coupled at low energies
  - > not perturbative
  - jet fragmentation functions
  - parton distribution functions





# Motivation for QCD

- QCD strongly coupled at low energies
  - > not perturbative
  - jet fragmentation functions
  - parton distribution functions
- Increased computational power = competitive and supplementary to experiment!

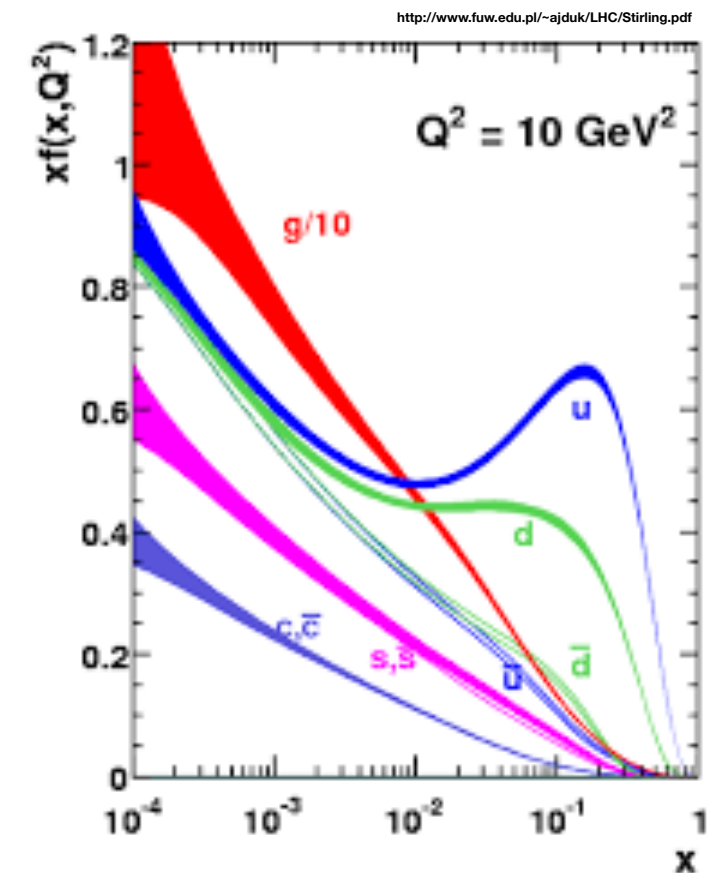
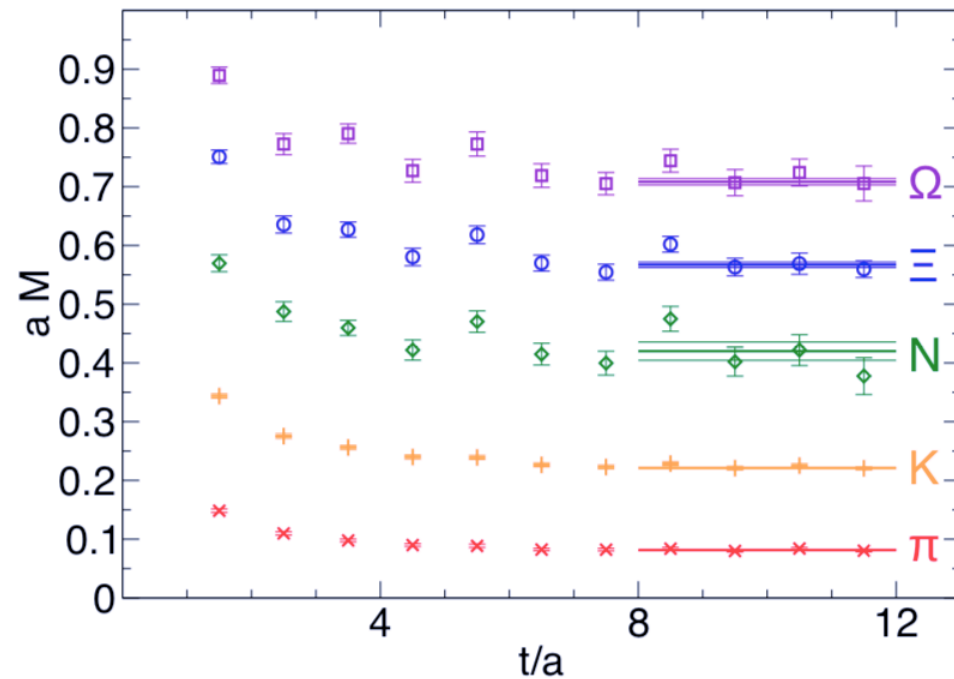


Image credit: Carlos Jones/ORNL

# Motivation for QCD

## 1) > 95% of mass of hadrons come from QCD dynamics



### Ab-initio Determination of Light Hadron Masses

S. Dürer<sup>1</sup>, Z. Fodor<sup>1,2,3</sup>, J. Frison<sup>4</sup>, C. Hoelbling<sup>2,3,4</sup>,  
R. Hoffmann<sup>2</sup>, S. D. Katz<sup>2,3</sup>, S. Krieg<sup>2</sup>, T. Kurth<sup>2</sup>,  
L. Lellouch<sup>4</sup>, T. Lippert<sup>2,5</sup>, K.K. Szabo<sup>2</sup>, G. Vulvert<sup>4</sup>

<sup>1</sup>NIC, DESY Zeuthen, D-15738 Zeuthen and FZ Jülich, D-52425 Jülich, Germany.

<sup>2</sup>Bergische Universität Wuppertal, Gausstr. 20, D-42119 Wuppertal, Germany.

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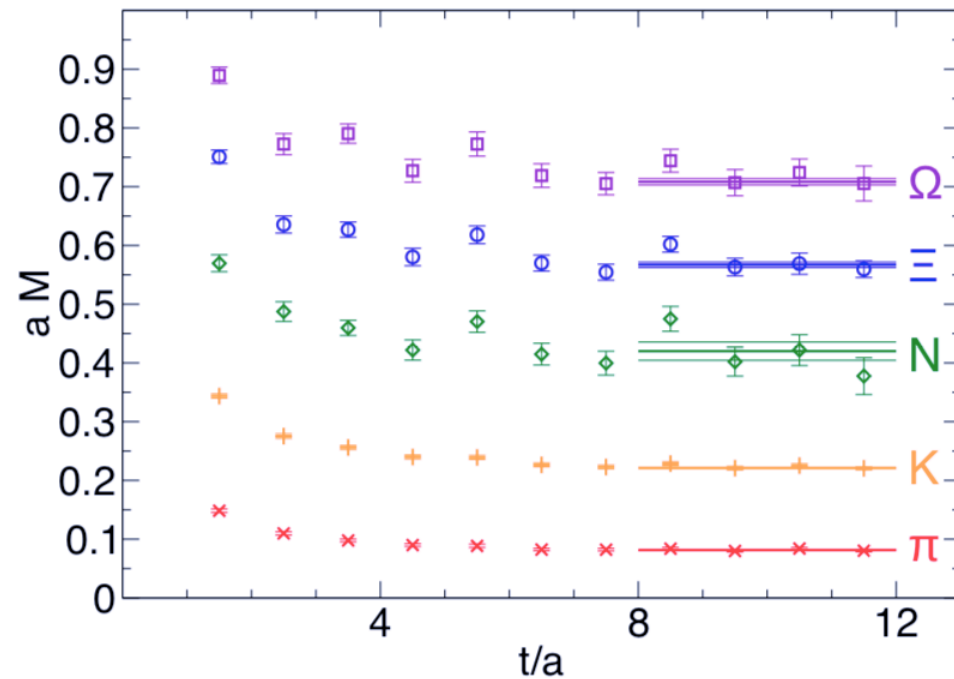
<sup>4</sup>Centre de Physique Théorique\*, Case 907, Campus de Luminy, F-13288 Marseille Cedex 9, France.

<sup>5</sup>Jülich Supercomputing Centre, FZ Jülich, D-52425 Jülich, Germany.

Budapest-Marseille-Wuppertal Collaboration

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## 2) Computation of matrix elements for weak flavor mixing

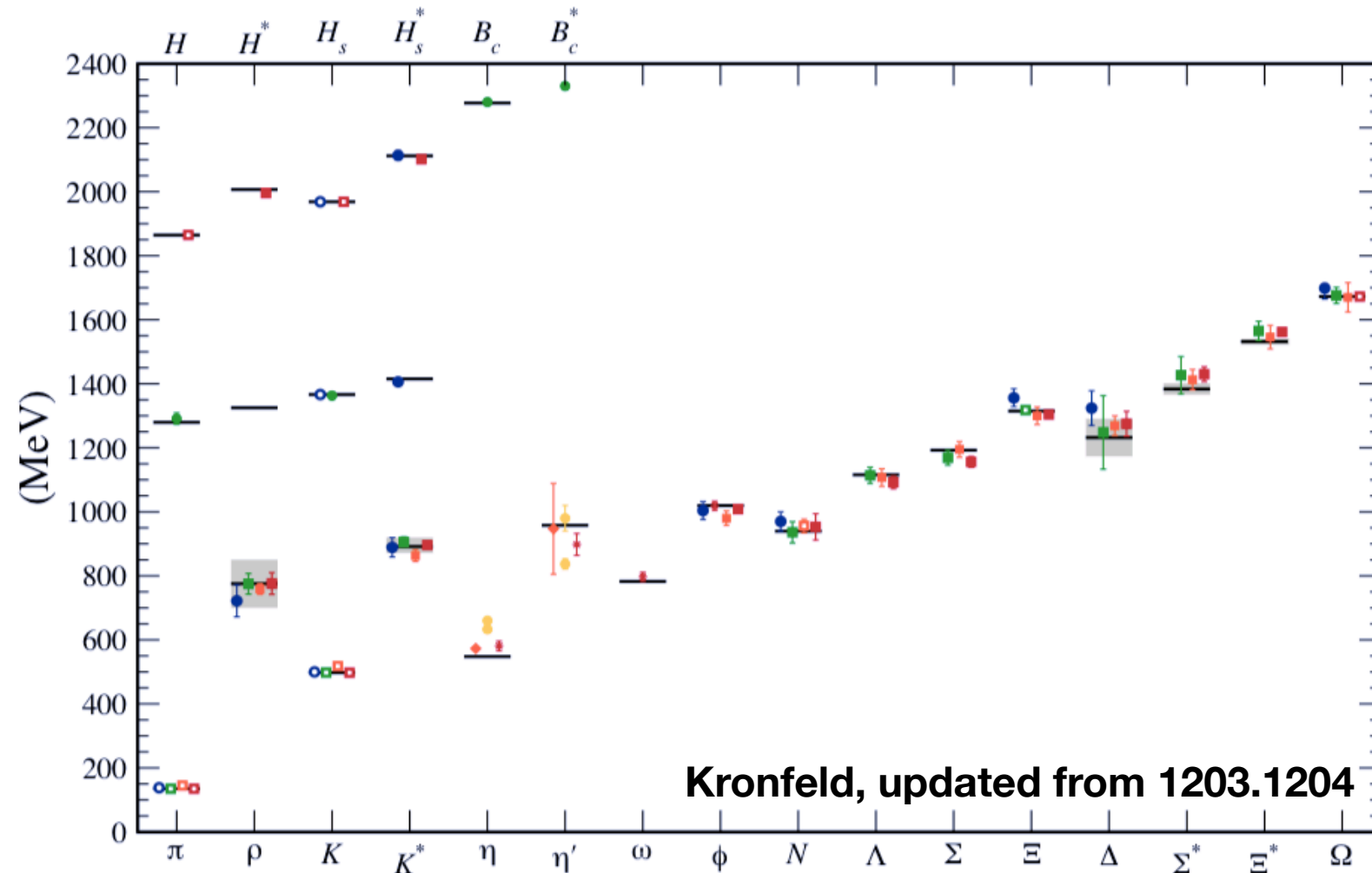
$$\Gamma(\pi \rightarrow l\nu) = \underbrace{\frac{G_F^2 |V_{ud}|^2 f_\pi^2}{8\pi} m_\pi m_l^2 \left(1 - \frac{m_l^2}{m_\pi^2}\right)^2}_{\text{Non-perturbative}}$$

↑
Perturbative

$$\begin{pmatrix} d' \\ s' \\ b' \end{pmatrix} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix}$$

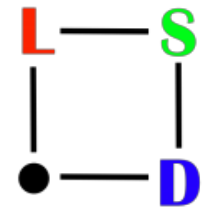
# Motivation for Beyond the Standard Model

- Predict spectrum of QCD  
baryons and mesons

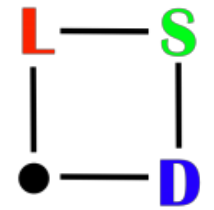




# Motivation for Beyond the Standard Model



# Motivation for Beyond the Standard Model



New gauge forces  
to explain...

- Higgs mechanism?

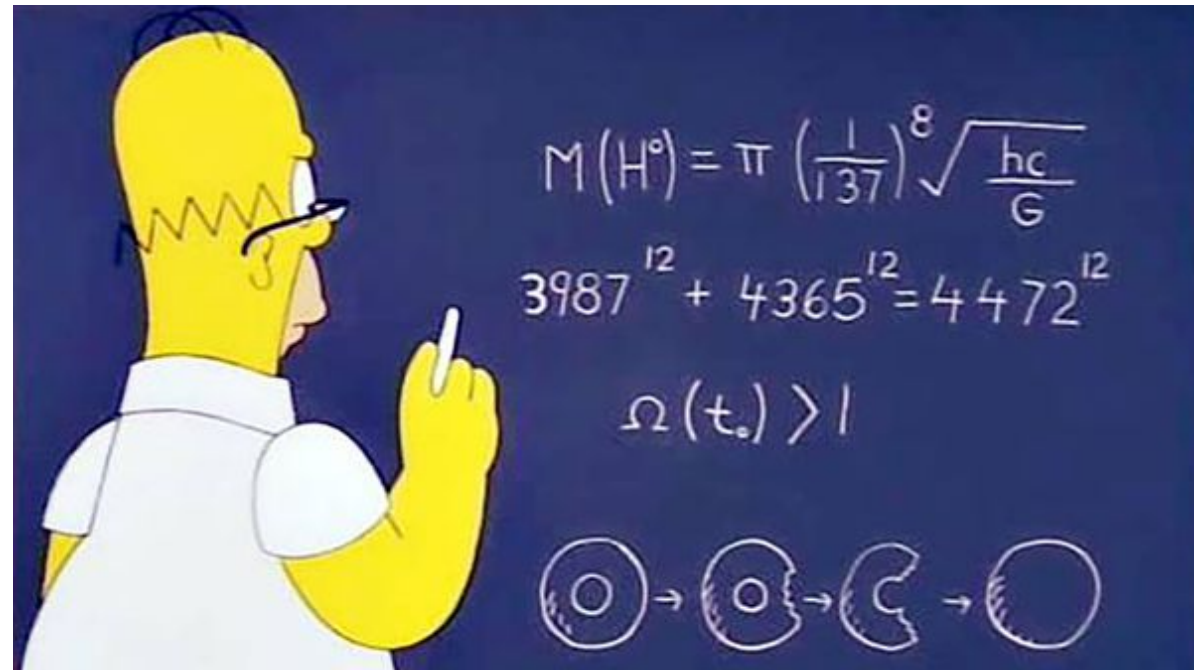


- Dark matter?



# Motivation for Beyond the Standard Model

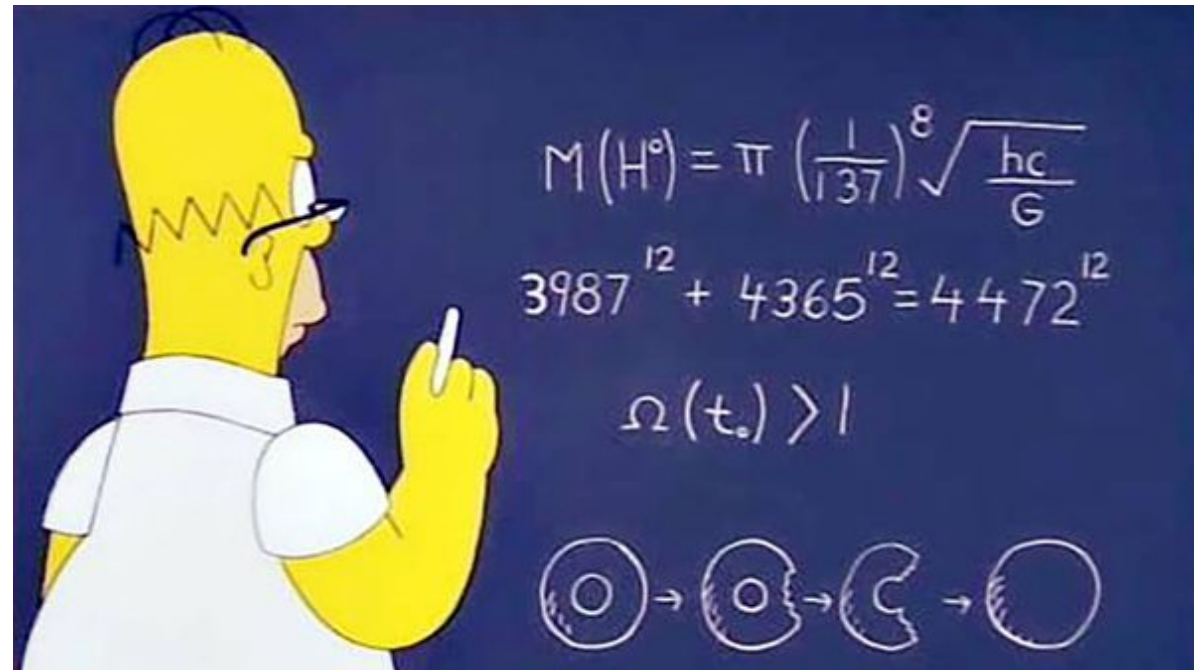
Why composite Higgs?



<https://motls.blogspot.com/2015/03/did-homer-simpson-calculate->

1) Hierarchy problem - no longer a *fundamental* scalar

# Motivation for Beyond the Standard Model



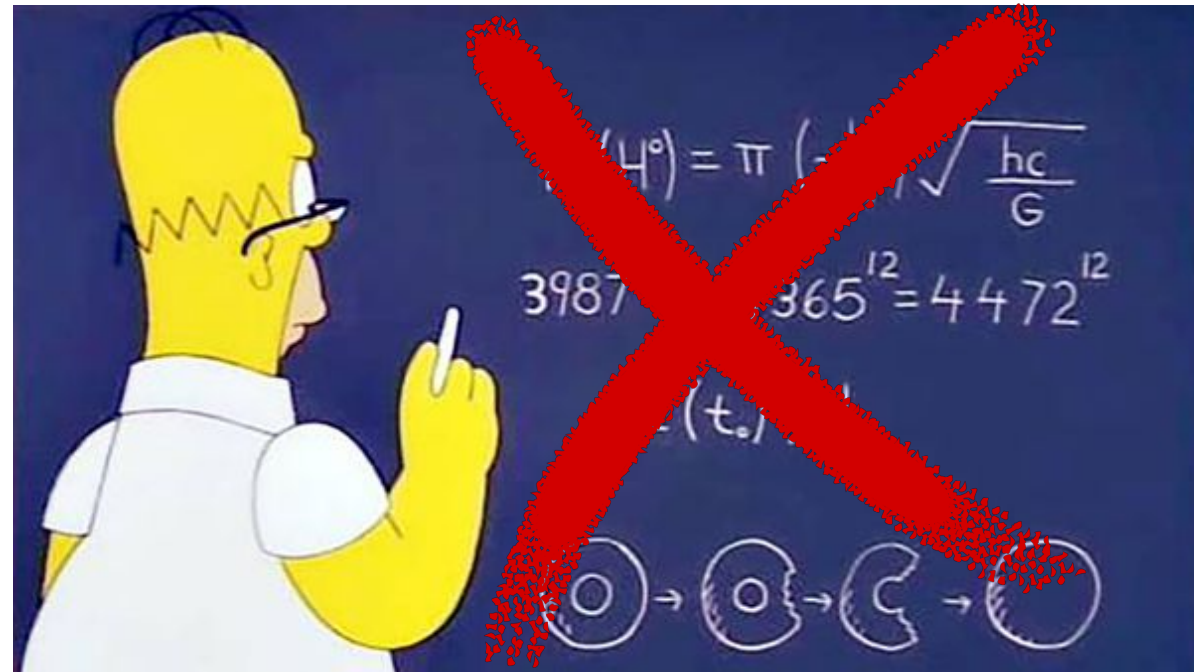
<https://motls.blogspot.com/2015/03/did-homer-simpson-calculate->

## Why composite Higgs?

- 1) Hierarchy problem - no longer a *fundamental* scalar  
- no fine tuning necessary if composite



# Motivation for Beyond the Standard Model

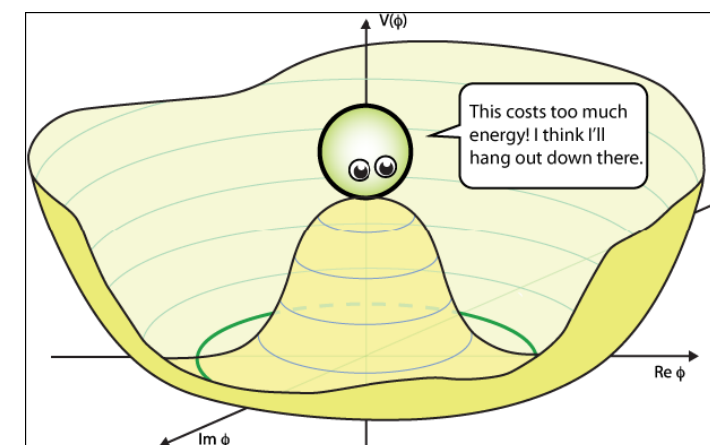


<https://motls.blogspot.com/2015/03/did-homer-simpson-calculate-correct.html>

## Why composite Higgs?

- 1) Hierarchy problem - no longer a *fundamental* scalar  
- no fine tuning necessary if composite
- 2) Dynamical symmetry breaking - Higgs model describes *effective* potential. Explains where potential comes from

??  $V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2$  ??



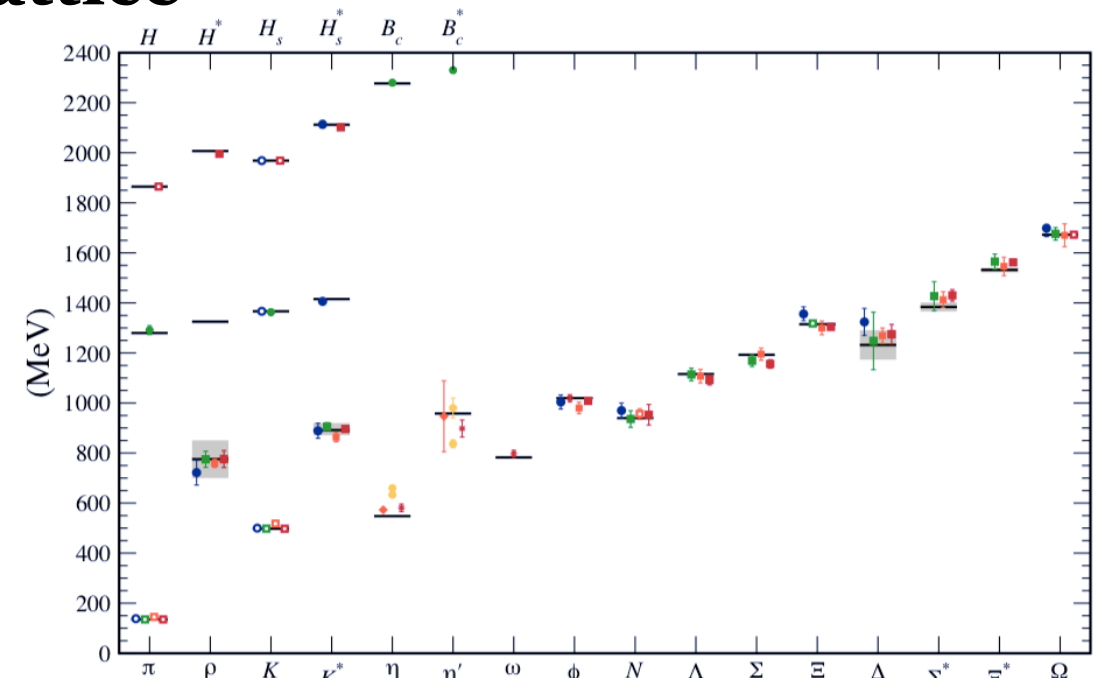
[http://www.tifr.res.in/TSN/news\\_detail.php?id=69](http://www.tifr.res.in/TSN/news_detail.php?id=69)



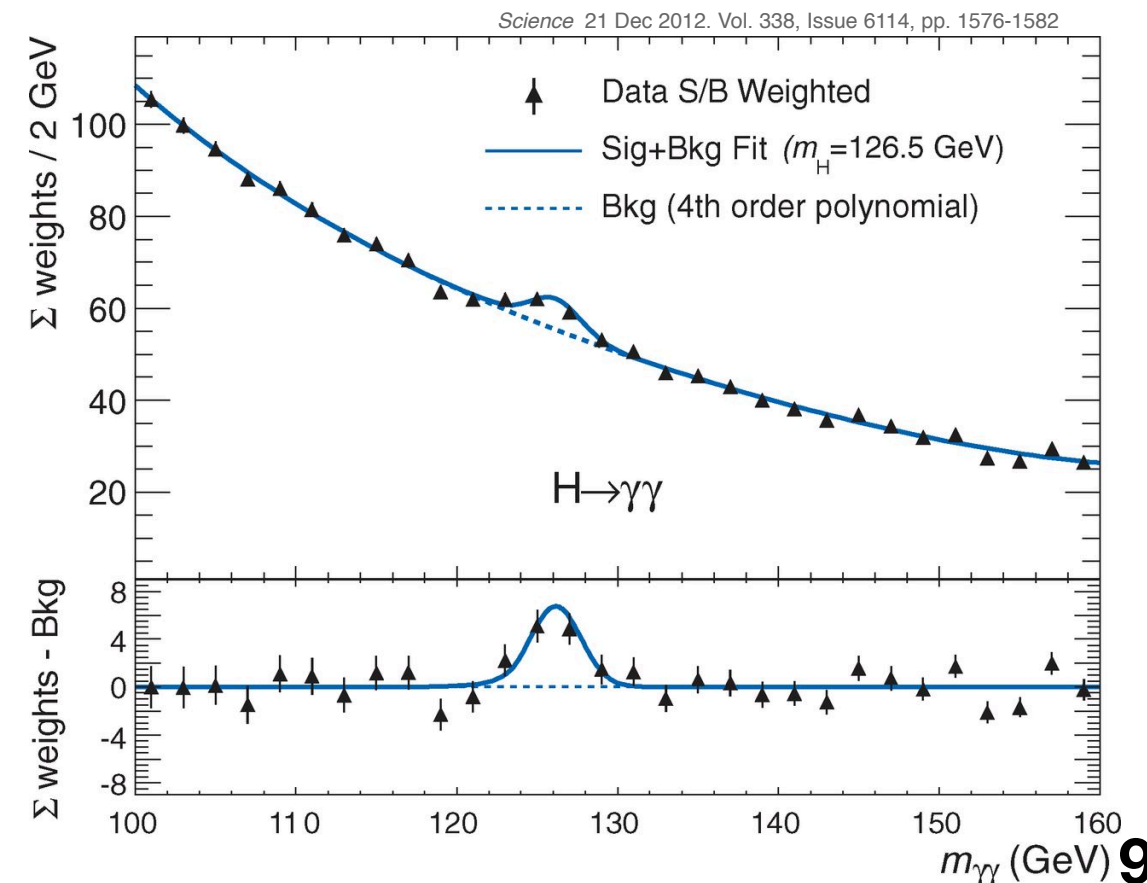
# Motivation for Beyond the Standard Model

- Every confining force has a spectrum of states
- New force of composite Higgs would have spectrum

## Lattice



## Experiment



# Feynman path integral trick

$$\langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle = C_{\pi}(t) = \mathcal{O}$$

# Feynman path integral trick

$$\langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle = C_{\pi}(t) = \mathcal{O}$$

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{D}} O[A] e^{-iS[A]}}{\int_{\mathcal{D}} e^{-iS[A]}}$$

# Feynman path integral trick

$$\langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle = C_{\pi}(t) = \mathcal{O}$$

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{D}} \mathcal{O}[A] e^{-iS[A]} \mathcal{D}A}{\int_{\mathcal{D}} e^{-iS[A]} \mathcal{D}A} \longrightarrow \langle \mathcal{O} \rangle = \frac{1}{Z} \sum_i e^{-\beta S} \mathcal{O}_i$$

# Feynman path integral trick

$$\langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle = C_{\pi}(t) = \mathcal{O}$$

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{D}} \mathcal{O}[A] e^{-iS[A]} dA}{\int_{\mathcal{D}} e^{-iS[A]} dA} \longrightarrow \langle \mathcal{O} \rangle = \frac{1}{Z} \sum_i e^{-\beta S} \mathcal{O}_i$$

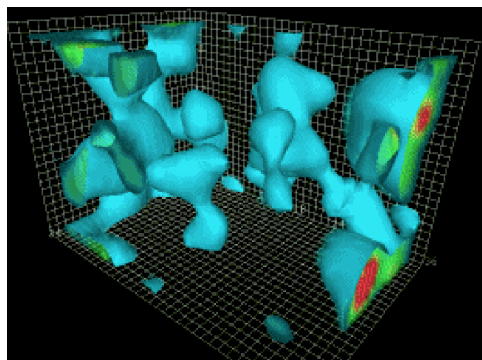
**Our only hope!**



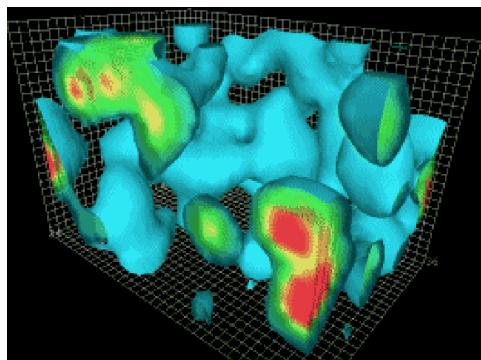
# Importance Sampling

$$\langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle = C_{\pi}(t) = \mathcal{O}$$

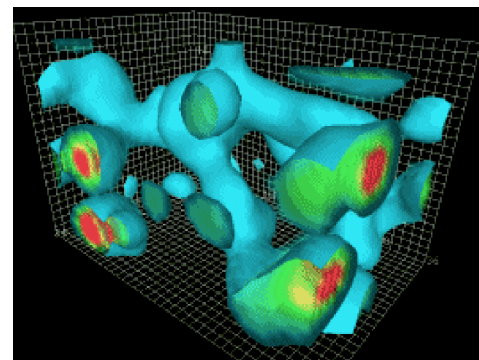
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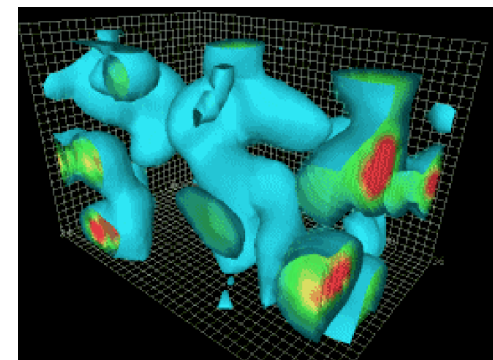
Configuration 1  $\mathcal{O}_1$



Configuration 2  $\mathcal{O}_2$



Configuration 3  $\mathcal{O}_3$



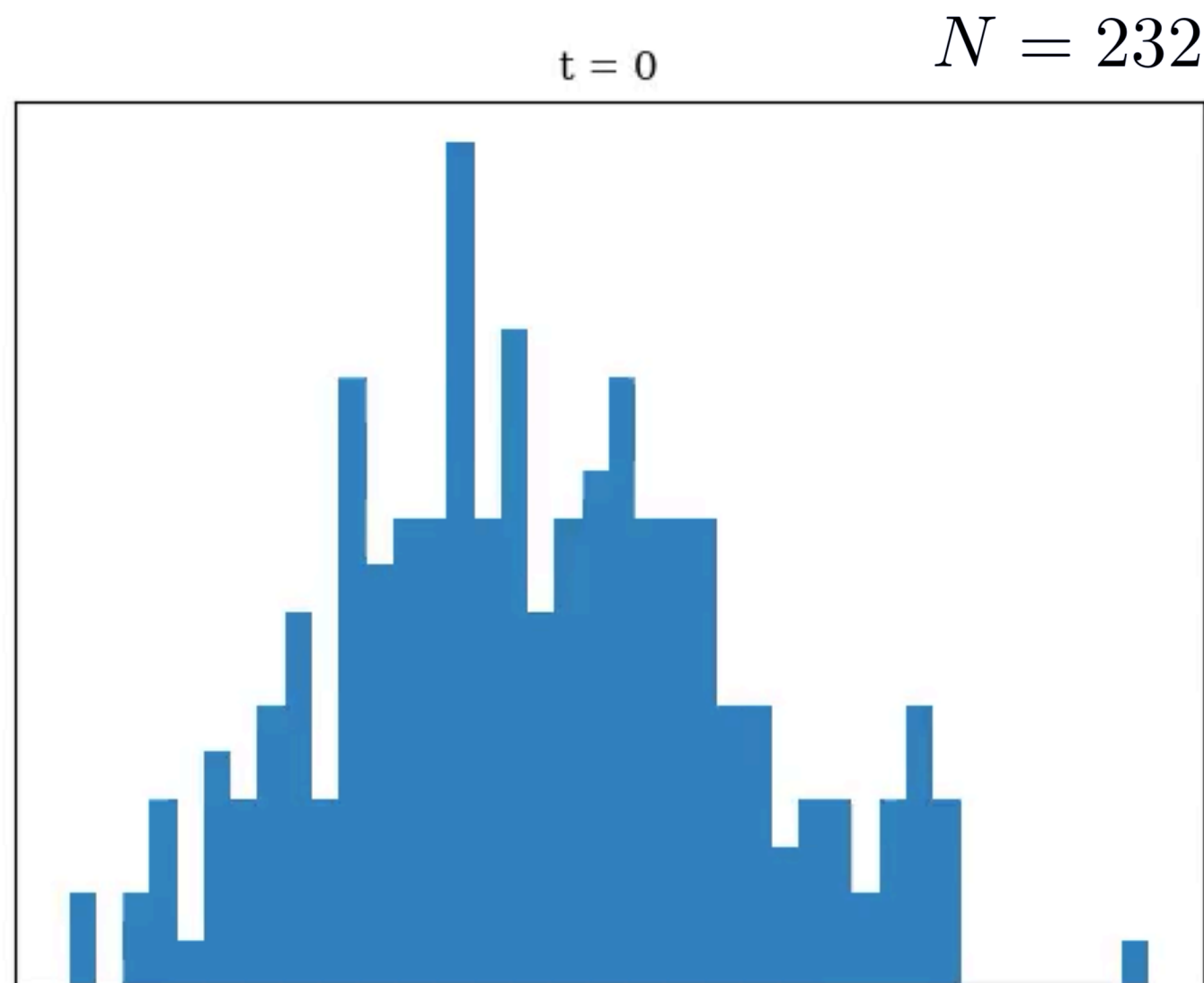
Configuration 4  $\mathcal{O}_4$

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N \mathcal{O}_i$$

# Importance Sampling

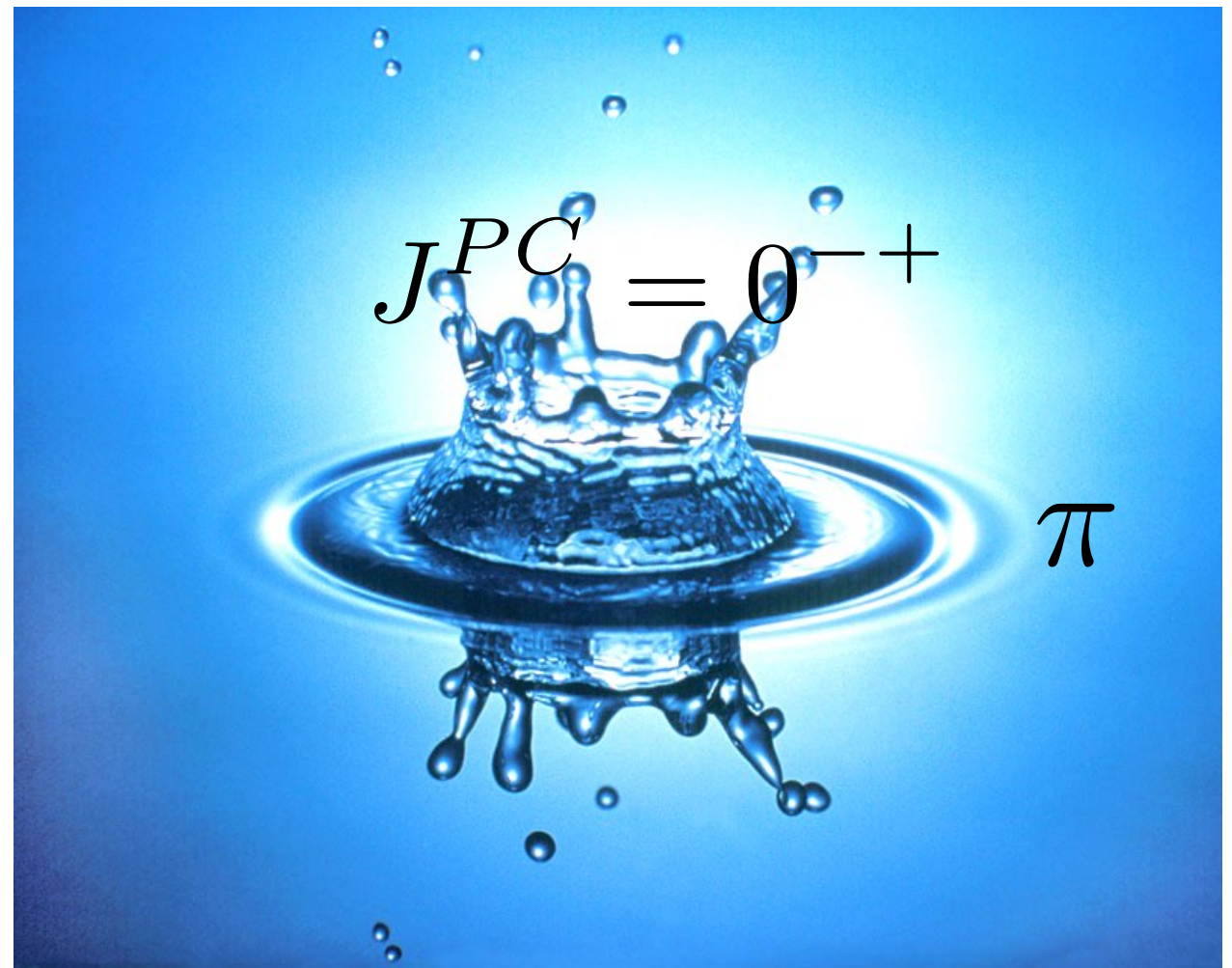
$$\langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle = C_{\pi}(t) = \mathcal{O}$$
$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N \mathcal{O}_i$$

- **SU(3)  $N_f = 8$**
- **$64^3 \times 128$**
- **$\beta = 4.8$**
- **$m_q = 0.00125$**



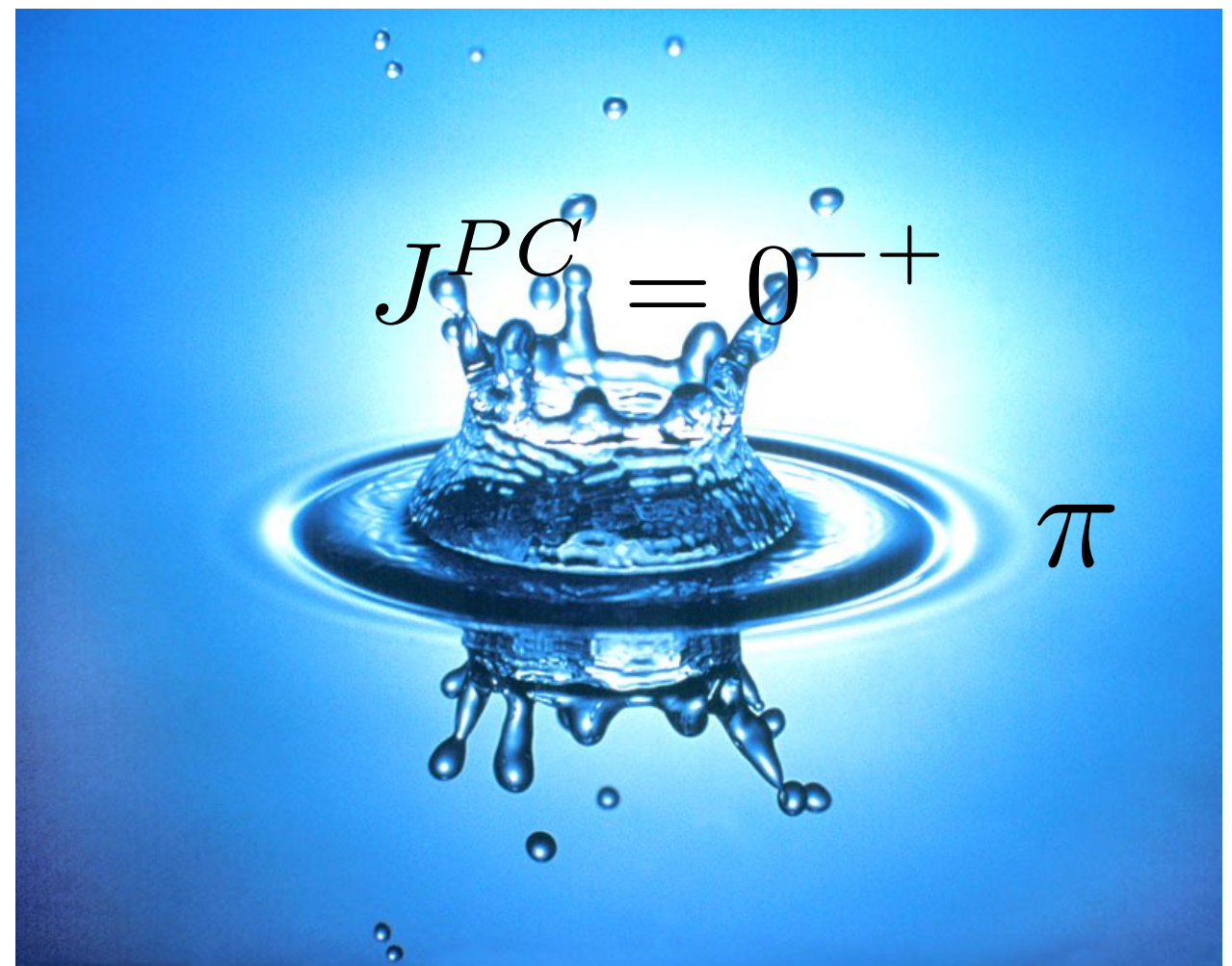
# Energy Spectrum + Matrix Elements

$$C(t) = \langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle$$



# Energy Spectrum + Matrix Elements

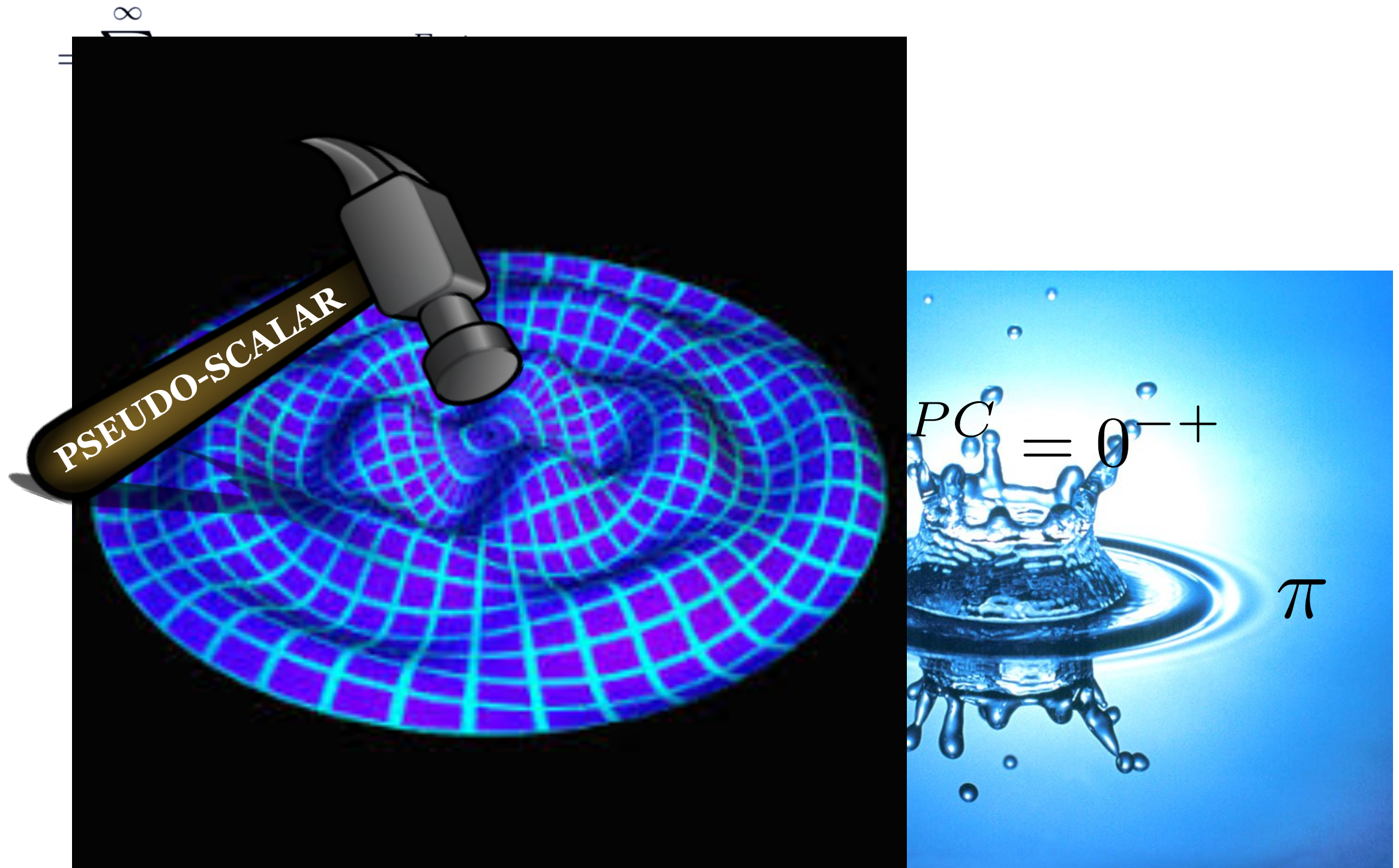
$$\begin{aligned} C(t) &= \langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle \\ &= \sum_m^{\infty} \langle 0 | \pi(0) | E_m \rangle e^{-E_m t} \langle E_m | \pi(0) | 0 \rangle \end{aligned}$$





# Energy Spectrum + Matrix Elements

$$C(t) = \langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle$$



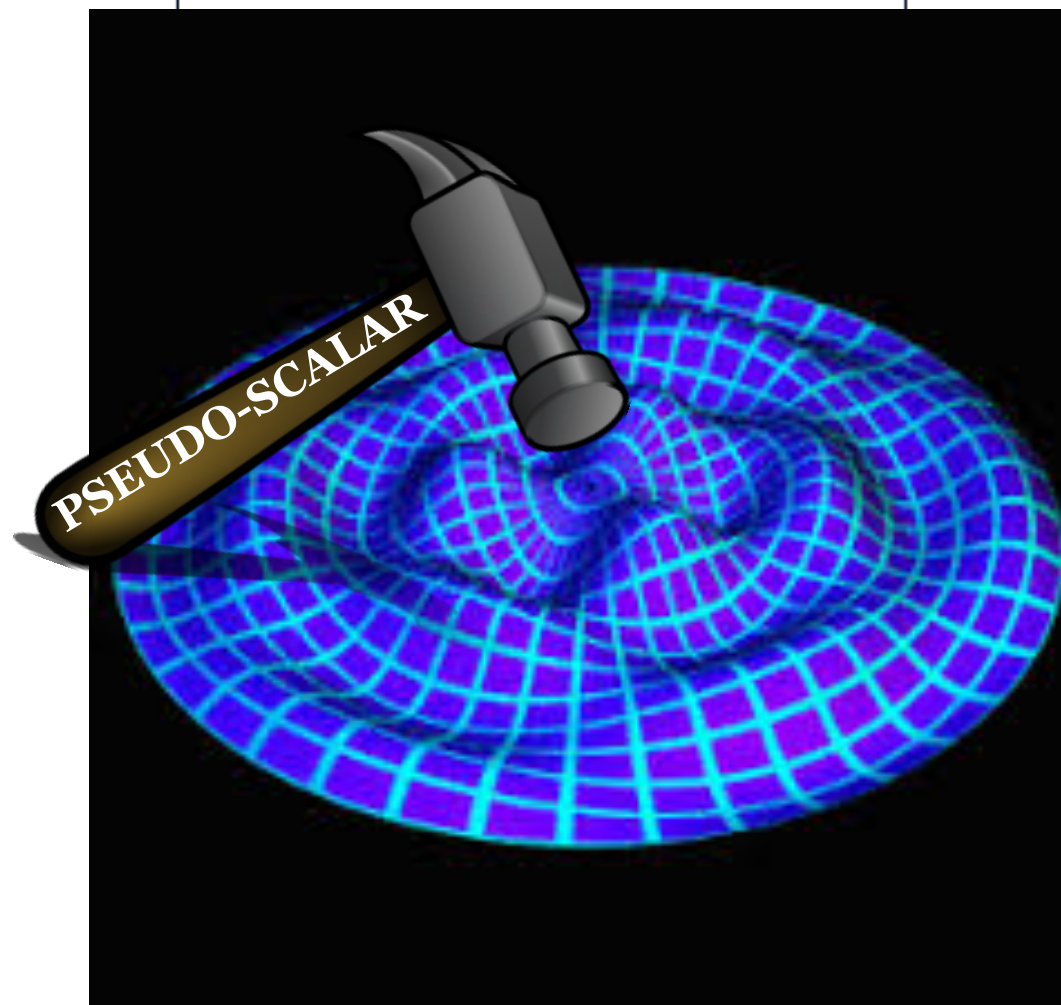
<http://watersoundimage.yolasite.com/what-is-a-w-s-image.php>



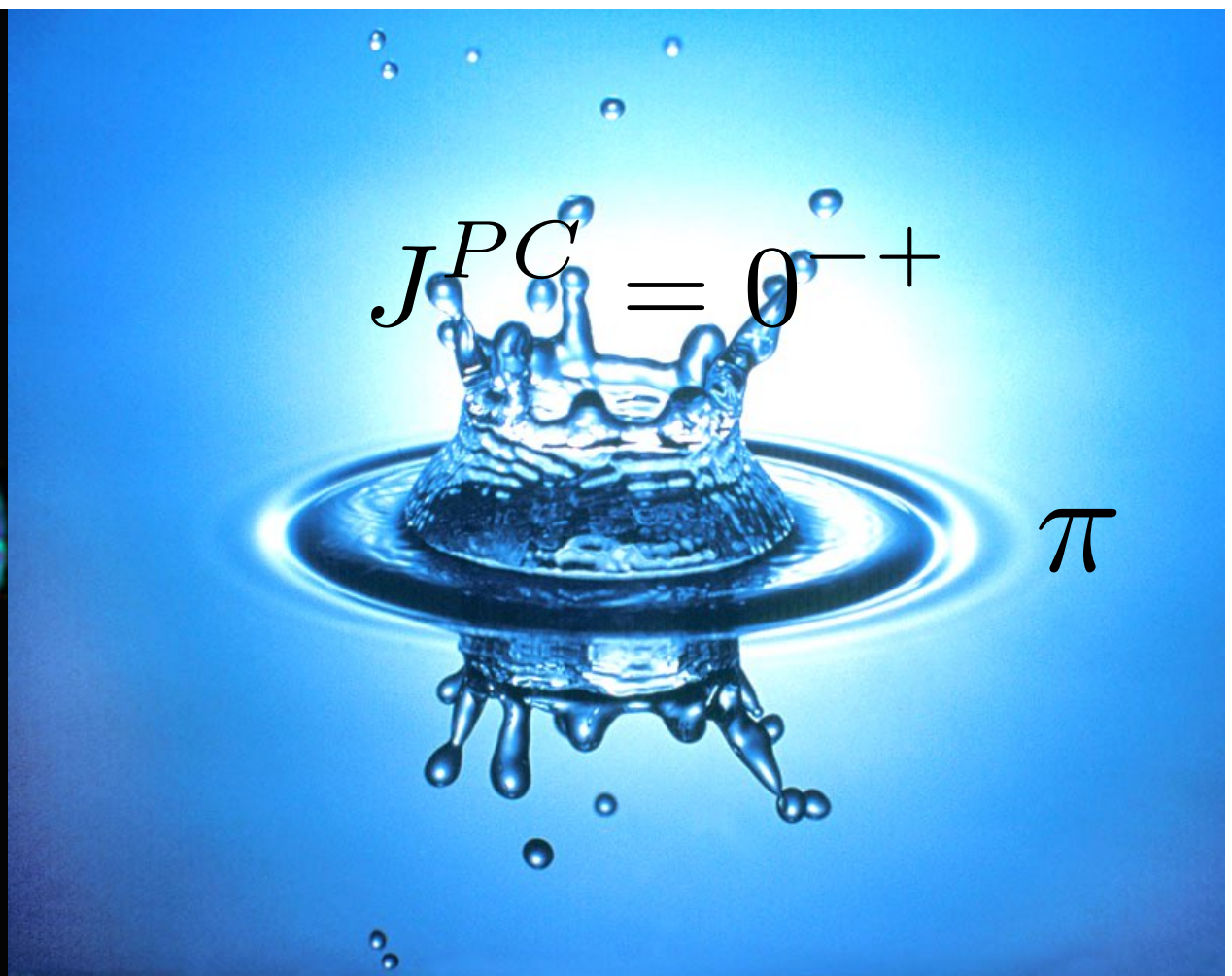
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$$= \sum_m^{\infty} \langle 0 | \pi(0) | E_m \rangle e^{-E_m t} \langle E_m | \pi(0) | 0 \rangle$$

$$\Rightarrow C(t) = \sum_m^{\infty} a_m e^{-E_m t}$$



<http://watersoundimage.yolasite.com/what-is-a-w-s-image.php>

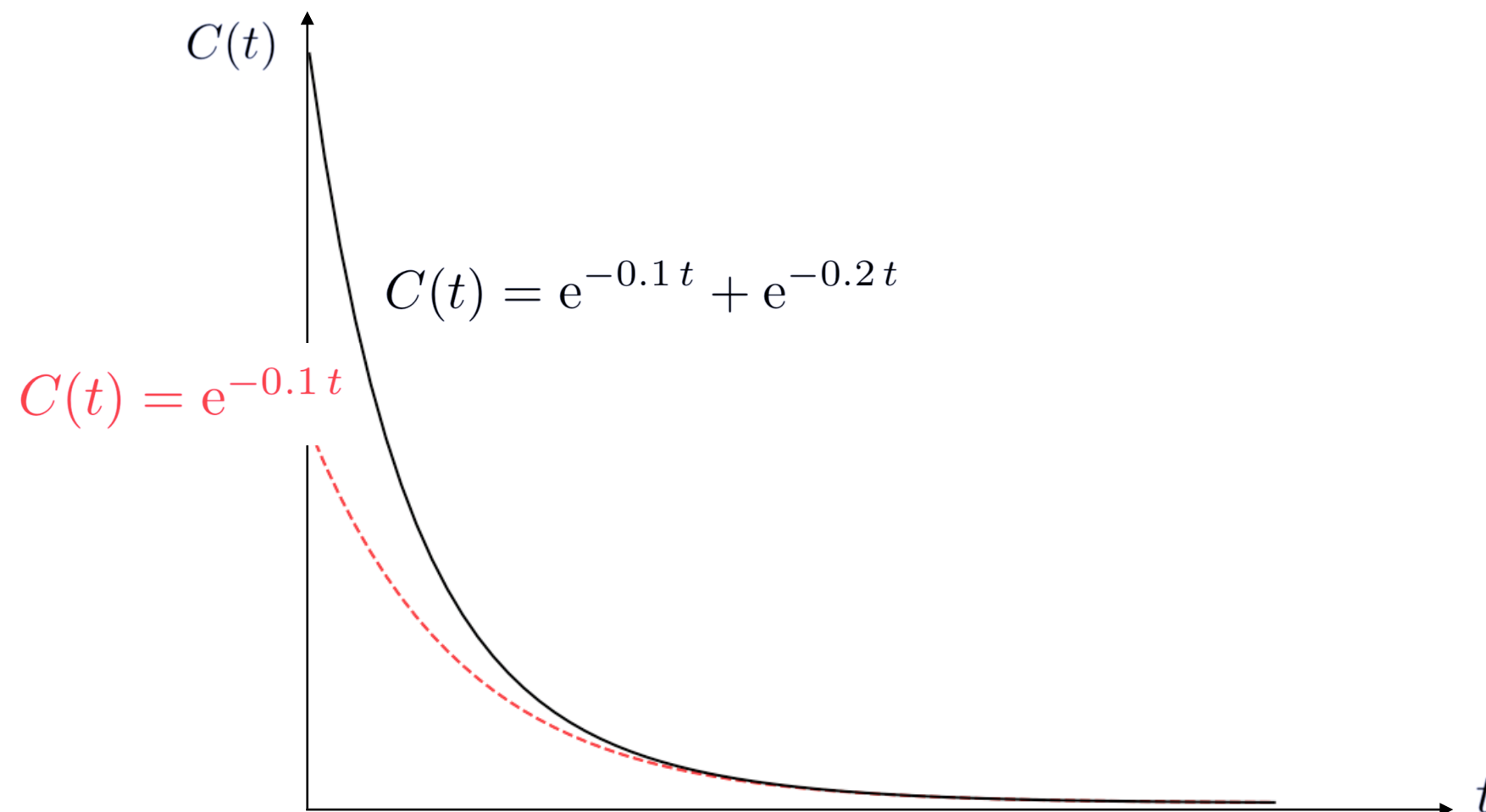


# Energy Spectrum + Matrix Elements

$$\begin{aligned} C(t) &= \langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle \\ &= \sum_m^{\infty} \langle 0 | \pi(0) | E_m \rangle e^{-E_m t} \langle E_m | \pi(0) | 0 \rangle \end{aligned}$$

$$\begin{aligned} C(t) &= a_0 e^{-E_0 t} + a_1 e^{-E_1 t} + \dots \\ &\approx a_0 e^{-E_0 t} \end{aligned}$$

$$\Rightarrow C(t) = \sum_m^{\infty} a_m e^{-E_m t}$$



# Energy Spectrum + Matrix Elements

$$C(t) = \langle 0 | \bar{\pi}(t) \pi(0) | 0 \rangle$$

$$= \sum_m^{\infty} \langle 0 | \pi(0) | E_m \rangle e^{-E_m t} \langle E_m | \pi(0) | 0 \rangle$$

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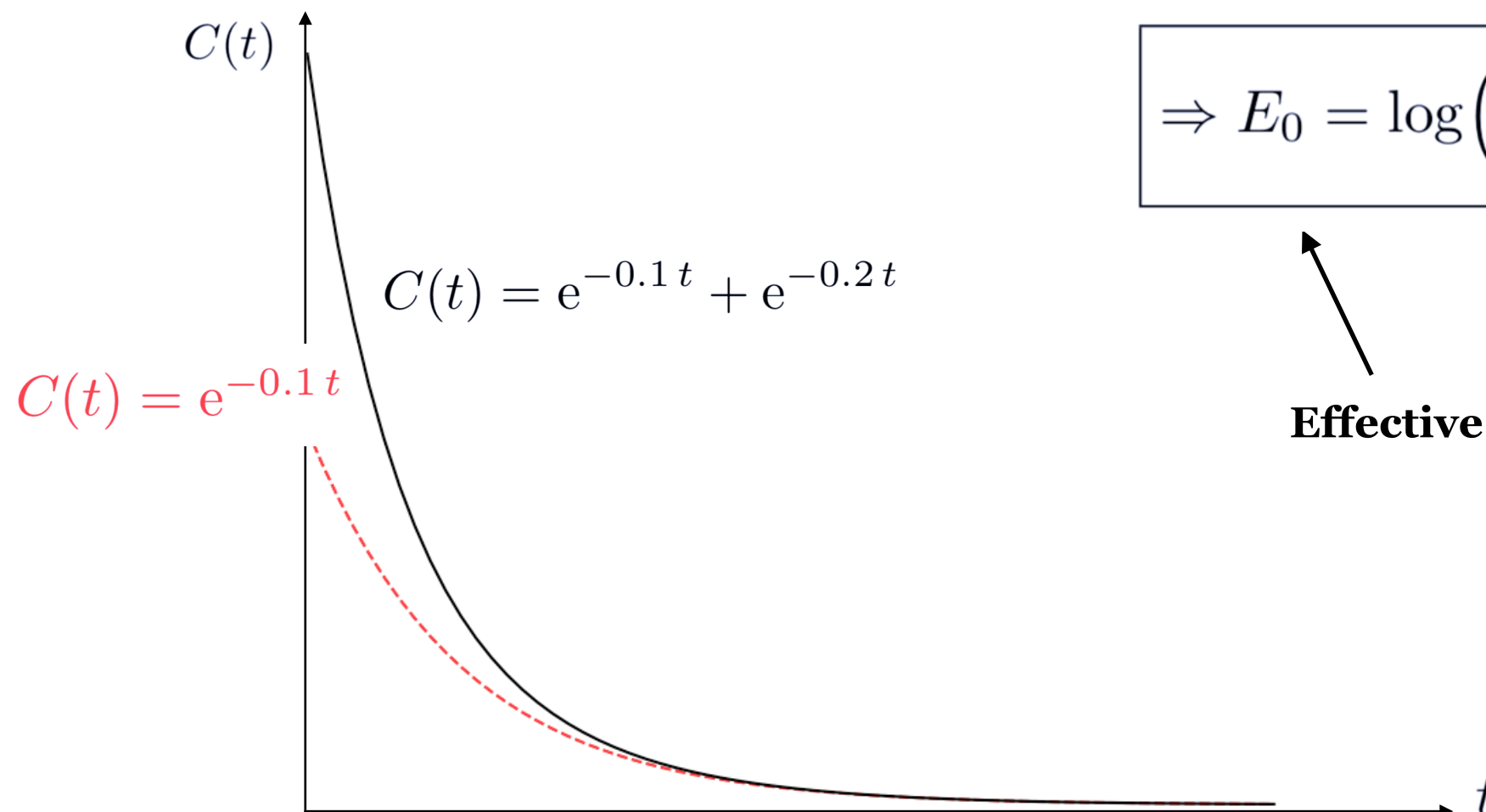
$$\approx a_0 e^{-E_0 t}$$

$$\frac{C(t+1)}{C(t)} \approx \frac{a_1 e^{-E_0(t+1)}}{a_1 e^{-E_0 t}}$$

$$= e^{-E_0}$$

$$\Rightarrow E_0 = \log \left( \frac{C(t)}{C(t+1)} \right)$$

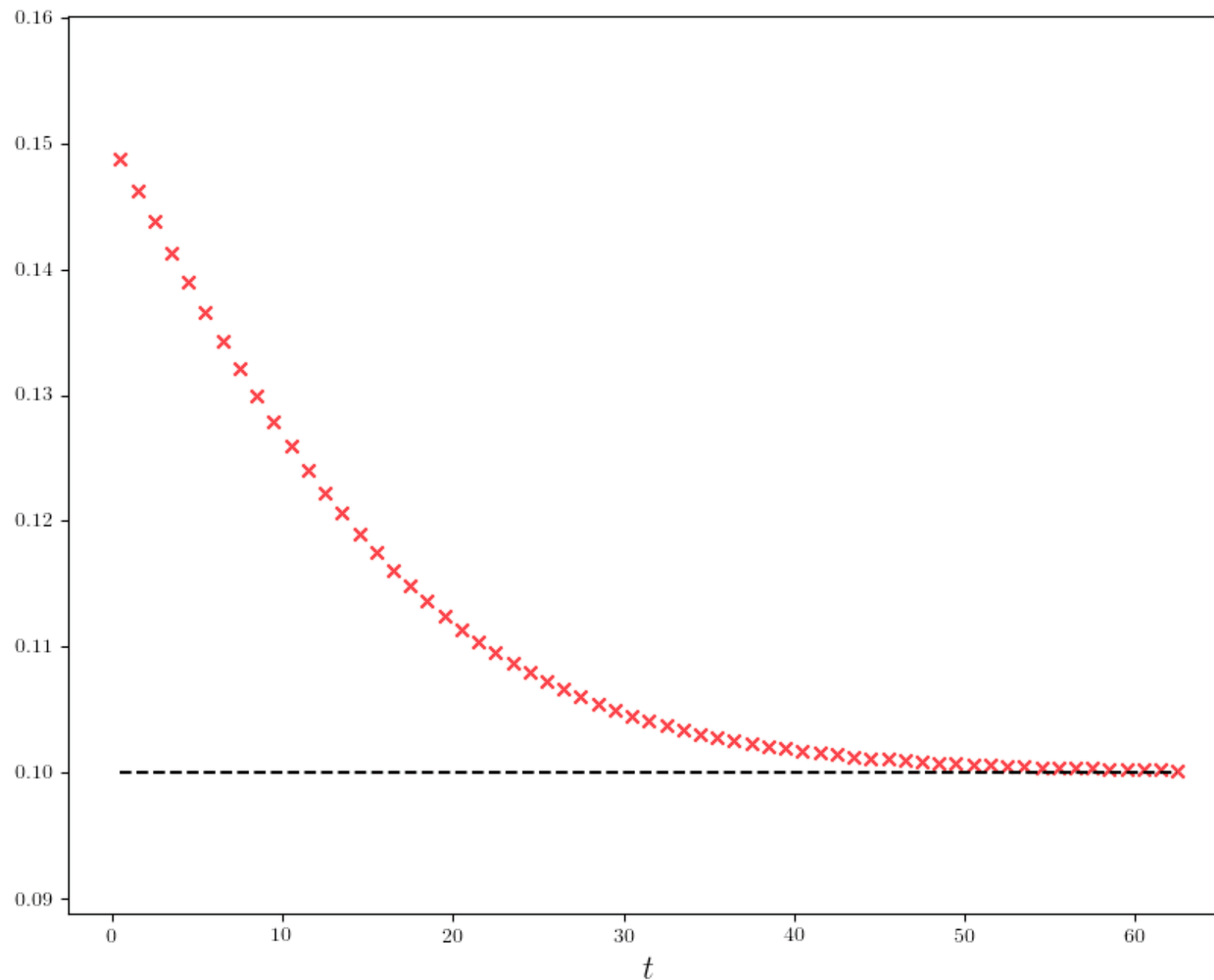
Effective mass



# Pion Effective Mass

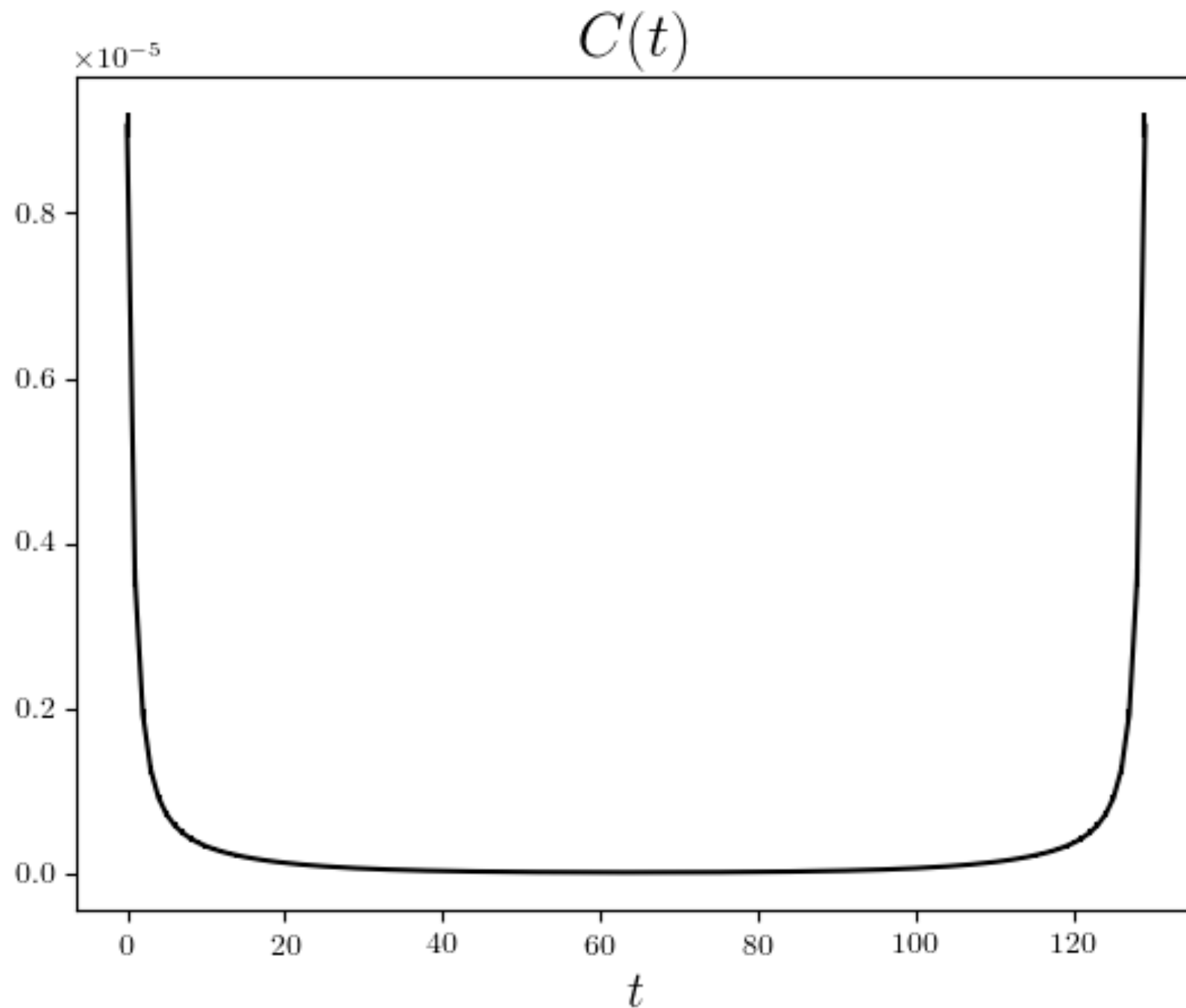
$$\Rightarrow E_1 = \log\left(\frac{C(t)}{C(t+1)}\right)$$

Effective Mass



# Pion Effective Mass

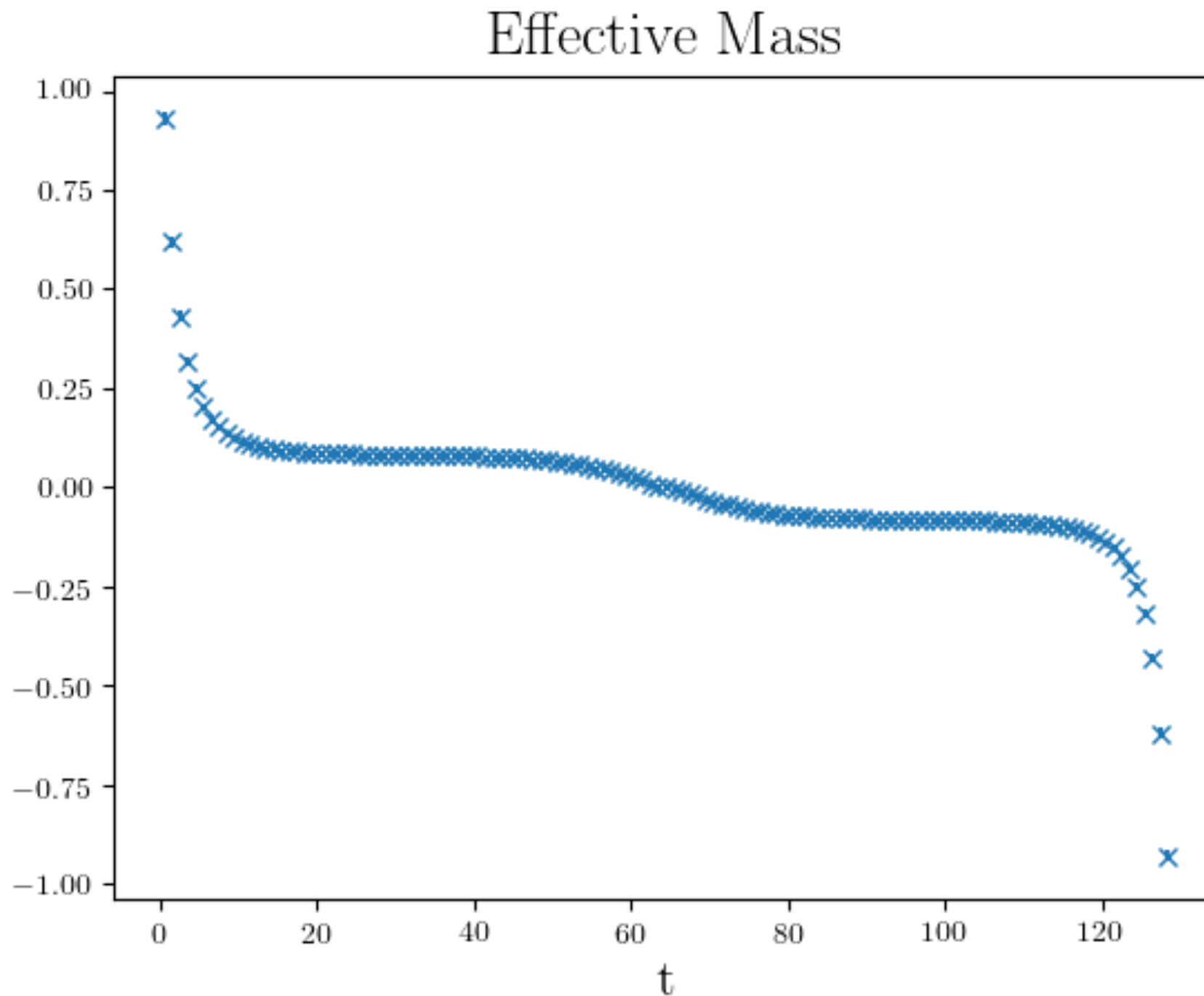
$$\Rightarrow E_1 = \log\left(\frac{C(t)}{C(t+1)}\right)$$





# Pion Effective Mass

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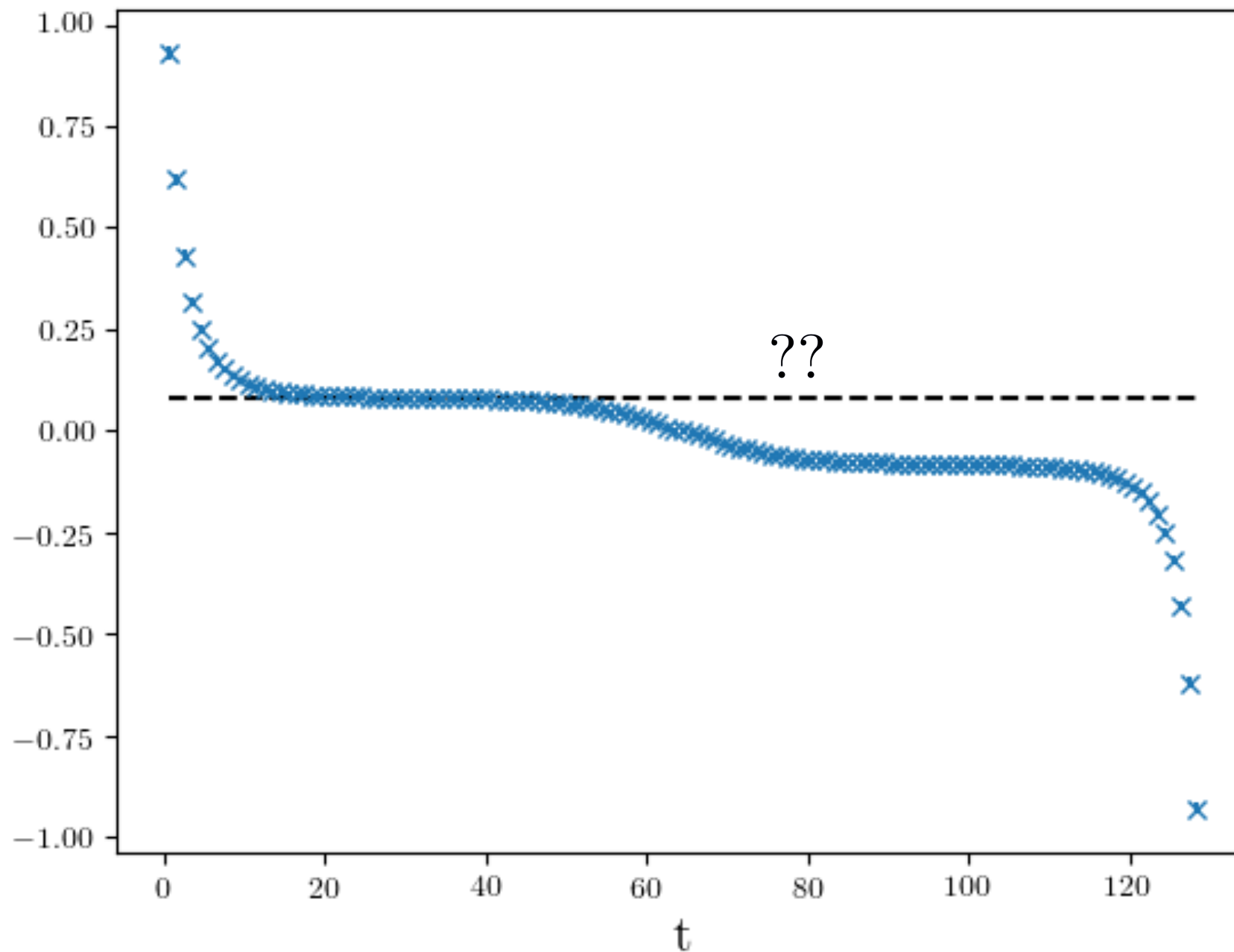


# Pion Effective Mass

$$\Rightarrow E_1 = \log\left(\frac{C(t)}{C(t+1)}\right)$$

$$\Rightarrow C(t) = \sum_m^{\infty} a_m e^{-E_m t}$$

Effective Mass

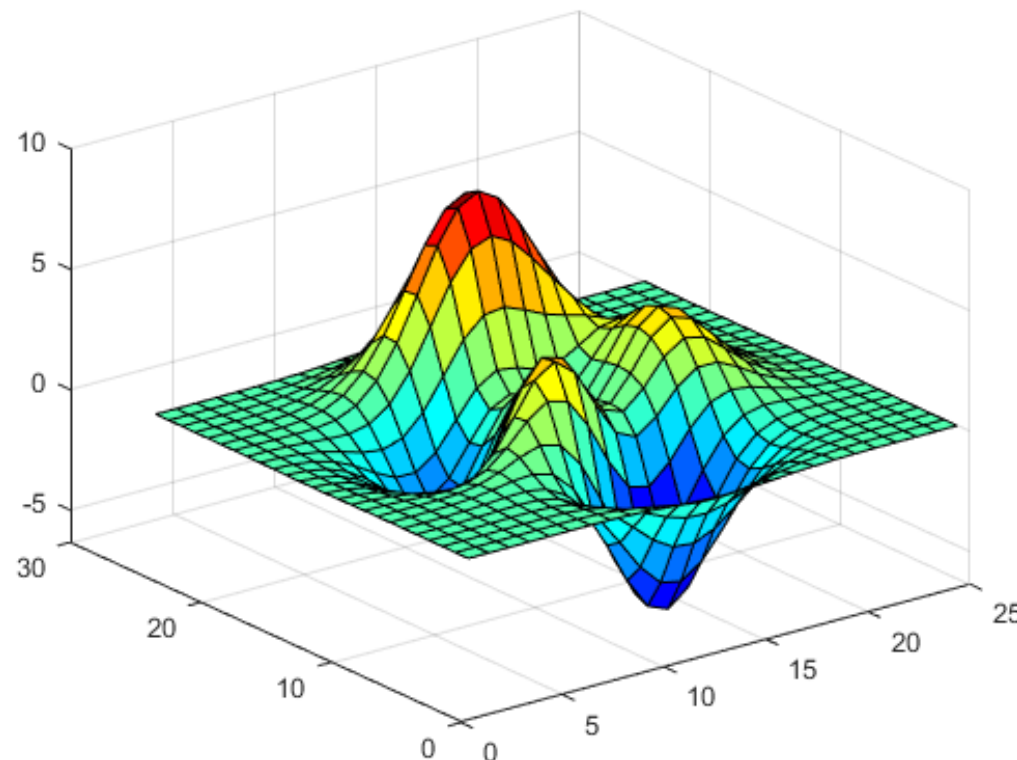


# Standard Method for Excited States

Fit more exponentials! .... but

$$\Rightarrow C(t) = \sum_m^{\infty} a_m e^{-E_m t}$$

- Difficult/time consuming with decaying exponentials
- Finding global minimum - best  $a_m, E_m$  is hard
- $2M$  dimensional parameter space
- Prone to user bias - choosing initial values



# **Algebraic Approach - Prony 1700's**

Prony, G. R. B. "J. de Lh Ecole Polytechnique." Paris 1 (1795): 24.

# Algebraic Approach - Prony 1700's

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$$\begin{aligned}
 y_n(t) &\equiv C(t+n) \\
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 &= \sum_m^M a_m e^{-E_m t} e^{-E_m n}
 \end{aligned}$$

$$\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{2M-1} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_M \\ z_1^2 & z_2^2 & \cdots & z_M^2 \\ \vdots & \vdots & \ddots & \vdots \\ z_1^{2M-1} & z_2^{2M-1} & \cdots & z_M^{2M-1} \end{pmatrix}}_{\text{Vandermode matrix}} \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_M \end{pmatrix}$$

$$\Rightarrow y_n(t) = \sum_m^M A_m(t) z_m^n$$

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**Non-linear**

**linear**



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**Non-linear**

**linear**

$$0 = \begin{vmatrix} y_0 & y_1 & \cdots & y_{M-2} & y_{M-1} & 1 \\ y_1 & y_2 & \cdots & y_{M-1} & y_M & z \\ y_2 & y_3 & \cdots & y_M & y_{M+1} & z^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ y_M & y_{M+1} & \cdots & y_{2M-2} & y_{2M-1} & z^M \end{vmatrix}$$

Hankel matrix

**We can do this!!**

G. Fleming, S. Cohen, H. Lin, V. Pereyra (2009)

# Prony's Method for $M=3$

$M=3$  means 6 y's

$$0 = \begin{vmatrix} y_0 & y_1 & y_2 & 1 \\ y_1 & y_2 & y_3 & z \\ y_2 & y_3 & y_4 & z^2 \\ y_3 & y_4 & y_5 & z^3 \end{vmatrix}$$

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Need to solve  $M^{\text{th}}$  order polynomial

$$0 = p_0 + p_1 z + p_2 z^2 + p_3 z^3$$

$$z_m = e^{-E_m}$$

# **Prony's Method, Linear Prediction, Matrix Prony**

E. Berkowitz, A. Nicholson, C. Chang et al. (2017)

S. Beane, W. Detmold, T. Luu et al. (2009)

# Prony's Method, Linear Prediction, Matrix Prony

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$$C(t) \rightarrow \begin{pmatrix} C_{11}(t) & C_{12}(t) \\ C_{21}(t) & C_{22}(t) \end{pmatrix}$$

$$C_{ij}(t) = \langle 0 | \mathcal{O}_i(t) \mathcal{O}_j(0) | 0 \rangle$$



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E. Berkowitz, A. Nicholson, C. Chang et al. (2017)

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$$C_{ij}(t) = \langle 0 | \mathcal{O}_i(t) \mathcal{O}_j(0) | 0 \rangle$$

**Effective mass becomes generalized eigenvalue problem**

$$0 = C(t+1) - zC(t)$$

$$e^{-E_0} = \frac{C(t+1)}{C(t)}$$

# Prony's Method, Linear Prediction, Matrix Prony

E. Berkowitz, A. Nicholson, C. Chang et al. (2017)

S. Beane, W. Detmold, T. Luu et al. (2009)

$$C(t) \rightarrow \begin{pmatrix} C_{11}(t) & C_{12}(t) \\ C_{21}(t) & C_{22}(t) \end{pmatrix}$$

$$C_{ij}(t) = \langle 0 | \mathcal{O}_i(t) \mathcal{O}_j(0) | 0 \rangle$$

**Effective mass becomes generalized eigenvalue problem**

$$0 = C(t+1) - zC(t) \qquad e^{-E_0} = \frac{C(t+1)}{C(t)}$$

$$C(t+1)v = \lambda C(t)v \qquad \lambda = e^{-E}$$

# Prony's Method, Linear Prediction, Matrix Prony

Effective mass becomes generalized eigenvalue problem

$$\lambda = e^{-E}$$

$$C(t+1)v = \lambda C(t)v$$

$$C(t+1)v_0 = e^{-E_0} C(t)v_0$$

$$C(t+1)v_1 = e^{-E_1} C(t)v_1$$

# Prony's Method, Linear Prediction, Matrix Prony

Effective mass becomes generalized eigenvalue problem

$$\lambda = e^{-E}$$

$$C(t+1)v = \lambda C(t)v$$

**maximal overlap**

$$C(t+1)v_0 = e^{-E_0} C(t)v_0 \longleftarrow \text{with ground state}$$

$$C(t+1)v_1 = e^{-E_1} C(t)v_1 \longleftarrow \text{with first excited state}$$

# Prony's Method, Linear Prediction, Matrix Prony

Effective mass becomes generalized eigenvalue problem

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**Ground state matrix equation**

$$\begin{pmatrix} C_{11}(t+1) & C_{12}(t+1) \\ C_{21}(t+1) & C_{22}(t+1) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = e^{-E_0} \begin{pmatrix} C_{11}(t) & C_{12}(t) \\ C_{21}(t) & C_{22}(t) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$



# Prony's Method, Linear Prediction, Matrix Prony

Effective mass becomes generalized eigenvalue problem

$$\lambda = e^{-E}$$

$$C(t+1)v = \lambda C(t)v$$

**maximal overlap**

$$C(t+1)v_0 = e^{-E_0} C(t)v_0 \longleftarrow \text{with ground state}$$

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**Ground state matrix equation**

$$\begin{pmatrix} C_{11}(t+1) & C_{12}(t+1) \\ C_{21}(t+1) & C_{22}(t+1) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = e^{-E_0} \begin{pmatrix} C_{11}(t) & C_{12}(t) \\ C_{21}(t) & C_{22}(t) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

$$e^{-E_0(t+1)} \begin{pmatrix} \langle 0 | \mathcal{O}_1 (b_1 \mathcal{O}_1 + b_2 \mathcal{O}_2) | 0 \rangle \\ \langle 0 | \mathcal{O}_2 (b_1 \mathcal{O}_1 + b_2 \mathcal{O}_2) | 0 \rangle \end{pmatrix} = e^{-E_0} e^{-E_0 t} \begin{pmatrix} \langle 0 | \mathcal{O}_1 (b_1 \mathcal{O}_1 + b_2 \mathcal{O}_2) | 0 \rangle \\ \langle 0 | \mathcal{O}_2 (b_1 \mathcal{O}_1 + b_2 \mathcal{O}_2) | 0 \rangle \end{pmatrix}$$

# Prony's Method, Linear Prediction, Matrix Prony

**Hankel Matrix determinant  
specifies eigenvalue problem**

$$0 = \begin{vmatrix} y_0 & y_1 & y_2 & 1 \\ y_1 & y_2 & y_3 & z \\ y_2 & y_3 & y_4 & z^2 \\ y_3 & y_4 & y_5 & z^3 \end{vmatrix}$$

**$M$  solutions**

$$0 = p_0 + p_1 z + p_2 z^2 + p_3 z^3 \quad z_m = e^{-E_m}$$

**Scalar  
equation**

# Prony's Method, Linear Prediction, Matrix Prony

**Hankel Matrix determinant specifies eigenvalue problem**

$$0 = \begin{vmatrix} y_0 & y_1 & y_2 & 1 \\ y_1 & y_2 & y_3 & z \\ y_2 & y_3 & y_4 & z^2 \\ y_3 & y_4 & y_5 & z^3 \end{vmatrix}$$

**$M$  solutions**

$$0 = p_0 + p_1 z + p_2 z^2 + p_3 z^3 \quad z_m = e^{-E_m}$$

**Scalar equation**



**$M \times N$  solutions**

$$0 = P_0 + \lambda P_1 + \lambda^2 P_2 + \lambda^3 P_3 \quad \lambda_m = e^{-E_m}$$

**Matrix equation**

# Prony's Method, Linear Prediction, Matrix Prony

**Hankel Matrix determinant  
specifies eigenvalue problem**

$$0 = \begin{vmatrix} y_0 & y_1 & y_2 & 1 \\ y_1 & y_2 & y_3 & z \\ y_2 & y_3 & y_4 & z^2 \\ y_3 & y_4 & y_5 & z^3 \end{vmatrix}$$

**$M$  solutions**

$$0 = p_0 + p_1 z + p_2 z^2 + p_3 z^3 \quad z_m = e^{-E_m}$$

**Scalar  
equation**

**Focus on labeling problem**

**$M \times N$  solutions**

$$0 = P_0 + \lambda P_1 + \lambda^2 P_2 + \lambda^3 P_3 \quad \lambda_m = e^{-E_m}$$

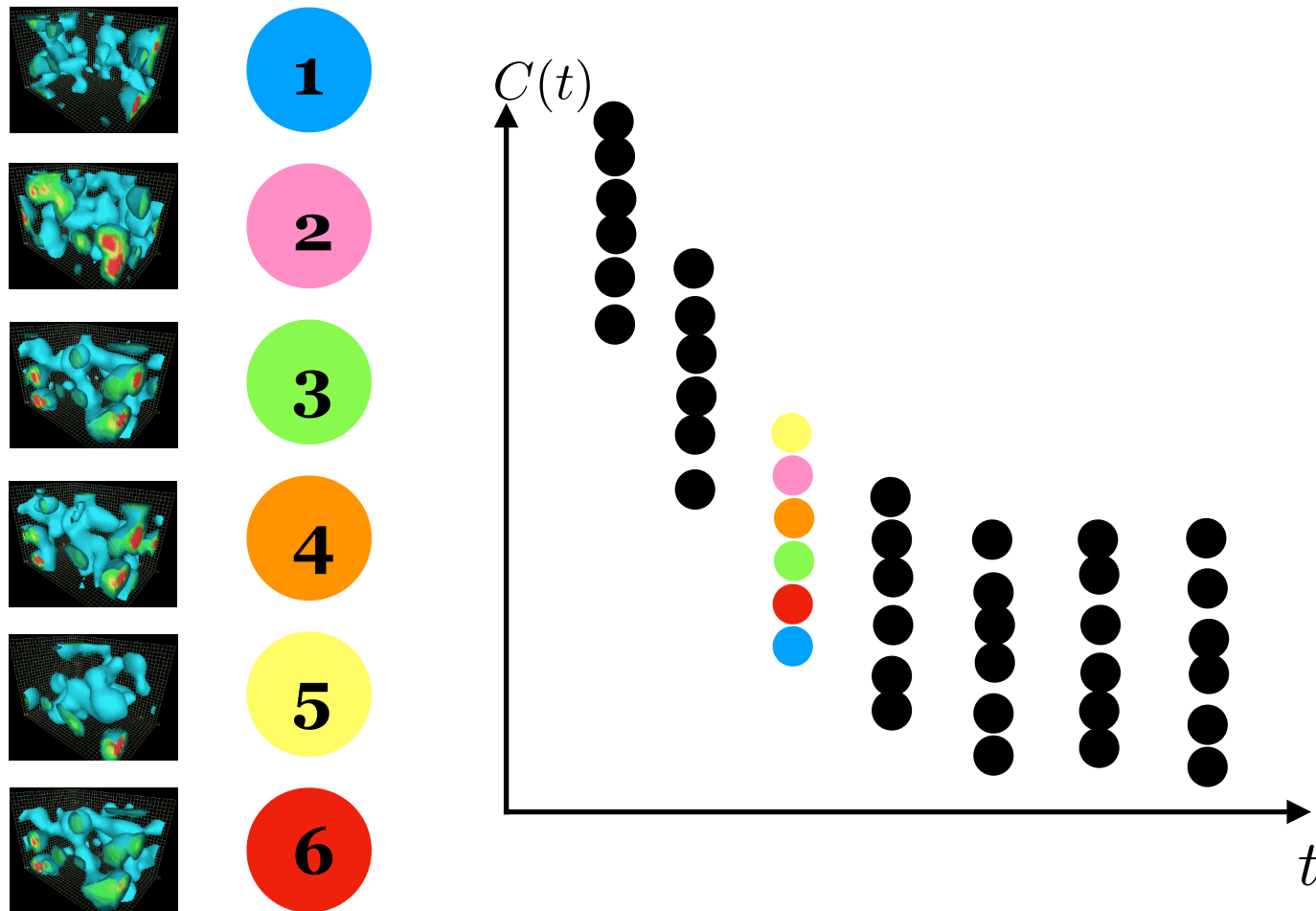
**Matrix  
equation**

# **From theory to practice: the bootstrap**



# From theory to practice: the bootstrap

6 data points  $C(t=t_0)$  for



# From theory to practice: the bootstrap

6 data points  $C(t=t_0)$  for

1

2

3

4

5

6

**Bootstrap**

$$\frac{1}{6} (\text{1} + \text{1} + \text{2} + \text{3} + \text{5} + \text{5}) = C_1(t=t_0)$$

$$\frac{1}{6} (\text{1} + \text{2} + \text{2} + \text{3} + \text{4} + \text{6}) = C_2(t=t_0)$$

$$\frac{1}{6} (\text{2} + \text{3} + \text{3} + \text{3} + \text{4} + \text{5}) = C_3(t=t_0)$$

$$\frac{1}{6} (\text{1} + \text{1} + \text{2} + \text{5} + \text{6} + \text{6}) = C_4(t=t_0)$$

$$\frac{1}{6} (\text{1} + \text{2} + \text{3} + \text{4} + \text{4} + \text{5}) = C_5(t=t_0)$$

$$\frac{1}{6} (\text{1} + \text{2} + \text{3} + \text{5} + \text{5} + \text{6}) = C_6(t=t_0)$$

$$\frac{1}{6} (\text{2} + \text{3} + \text{3} + \text{4} + \text{6} + \text{6}) = C_7(t=t_0)$$

$$\frac{1}{6} (\text{1} + \text{1} + \text{2} + \text{3} + \text{5} + \text{5}) = C_8(t=t_0)$$

# From theory to practice: the bootstrap

$$\frac{1}{6} (\textcolor{blue}{1} + \textcolor{blue}{1} + \textcolor{pink}{2} + \textcolor{green}{3} + \textcolor{yellow}{5} + \textcolor{yellow}{5}) = C_1(t=t_0)$$

**Repeat for all times to obtain  $C_1(0)$ ,  $C_1(1)$ ,  $C_1(2)$ ,  $C_1(3)$ , ...  $C_1(T)$**

# From theory to practice: the bootstrap

$$\frac{1}{6} (\textcolor{blue}{1} + \textcolor{blue}{1} + \textcolor{pink}{2} + \textcolor{green}{3} + \textcolor{yellow}{5} + \textcolor{yellow}{5}) = C_1(t=t_0)$$

Repeat for all times to obtain  $C_1(0), C_1(1), C_1(2), C_1(3), \dots C_1(T)$

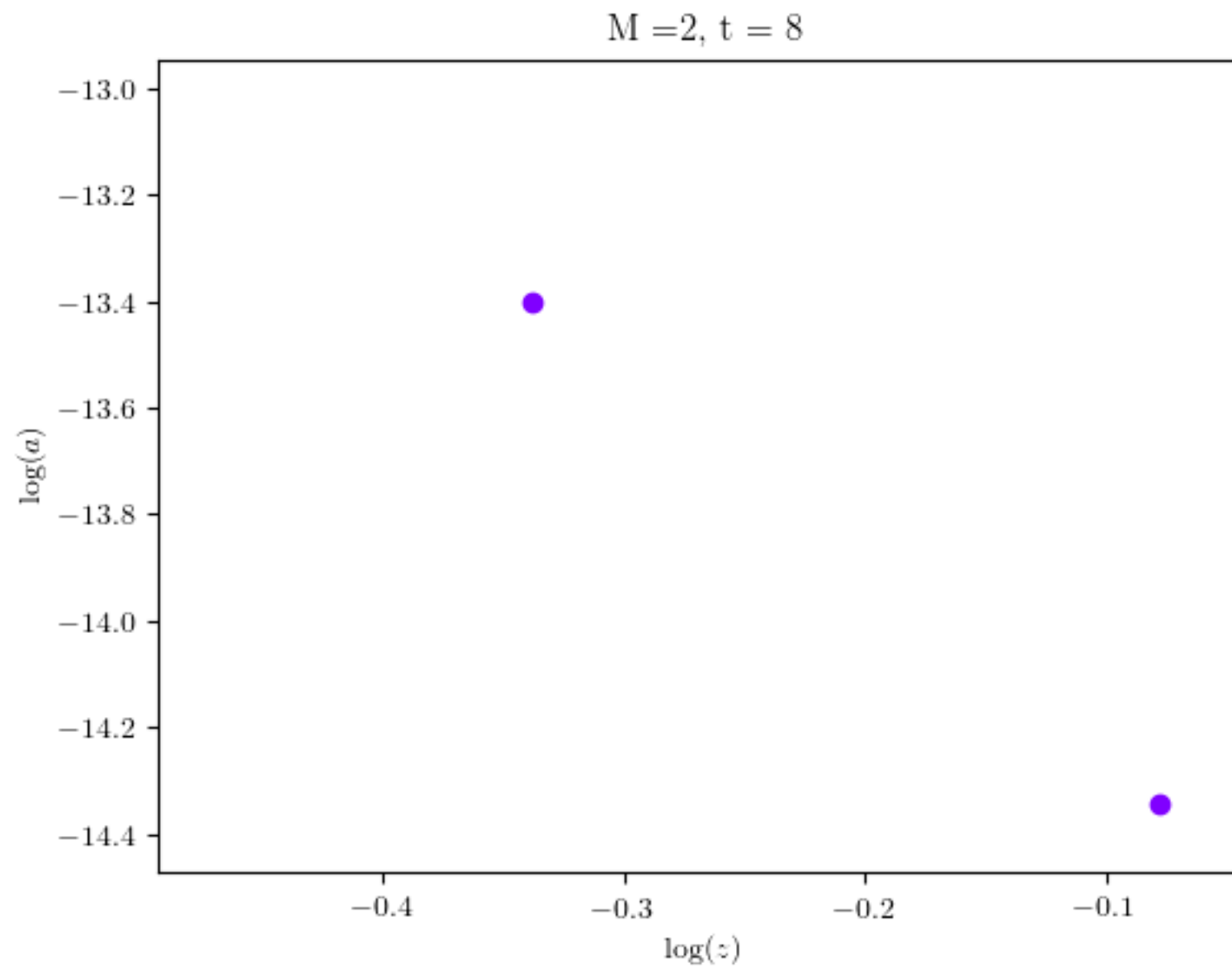
$$y_n(t) = C(t + n)$$

$$\begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ z_1 & z_2 \\ z_1^2 & z_2^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \quad 0 = \begin{vmatrix} y_0 & y_1 & 1 \\ y_1 & y_2 & z \\ y_2 & y_3 & z^2 \end{vmatrix}$$

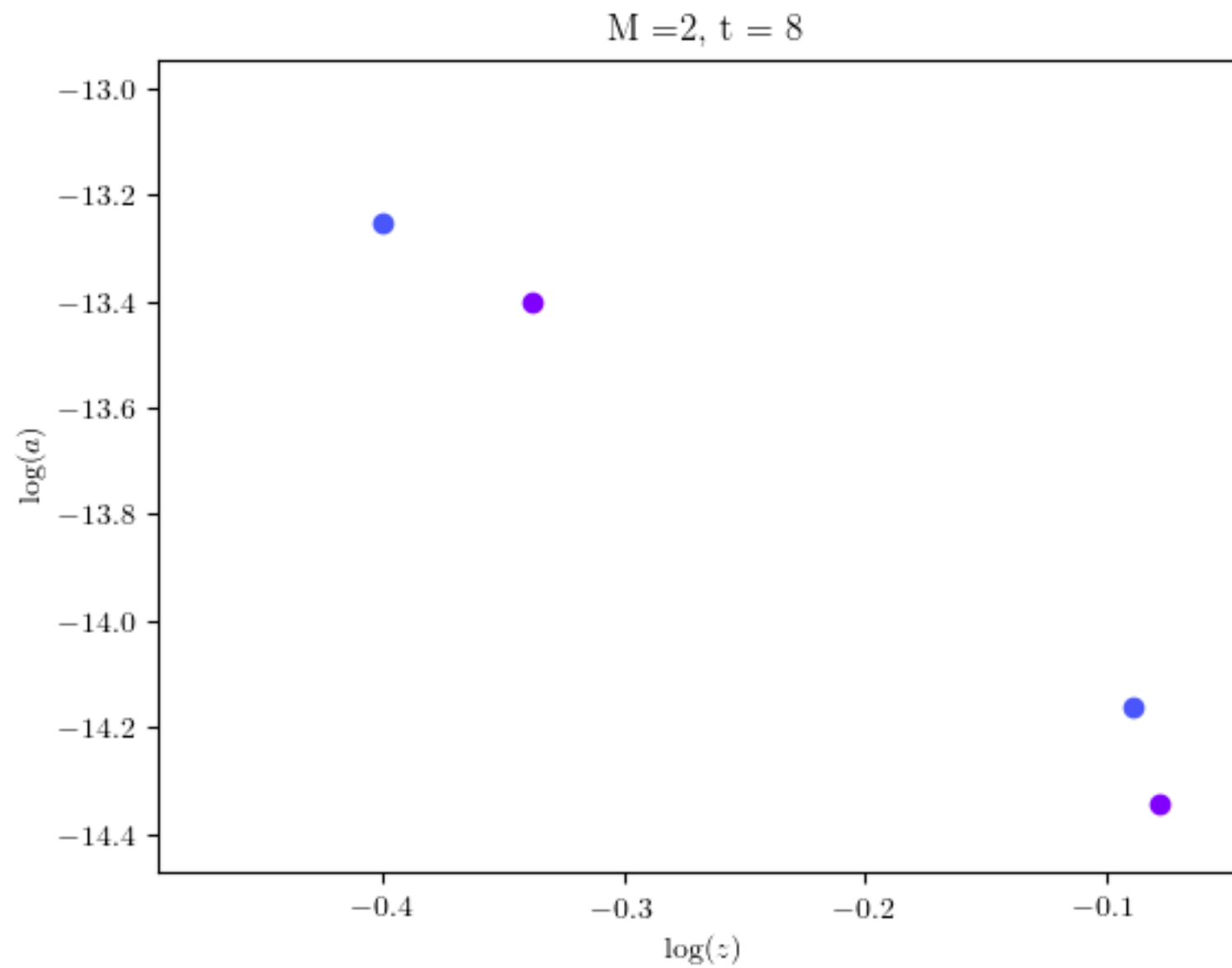
$$C_1(t) \Rightarrow \{ (z_1, a_1), (z_2, a_2) \}$$

# From theory to practice: the bootstrap

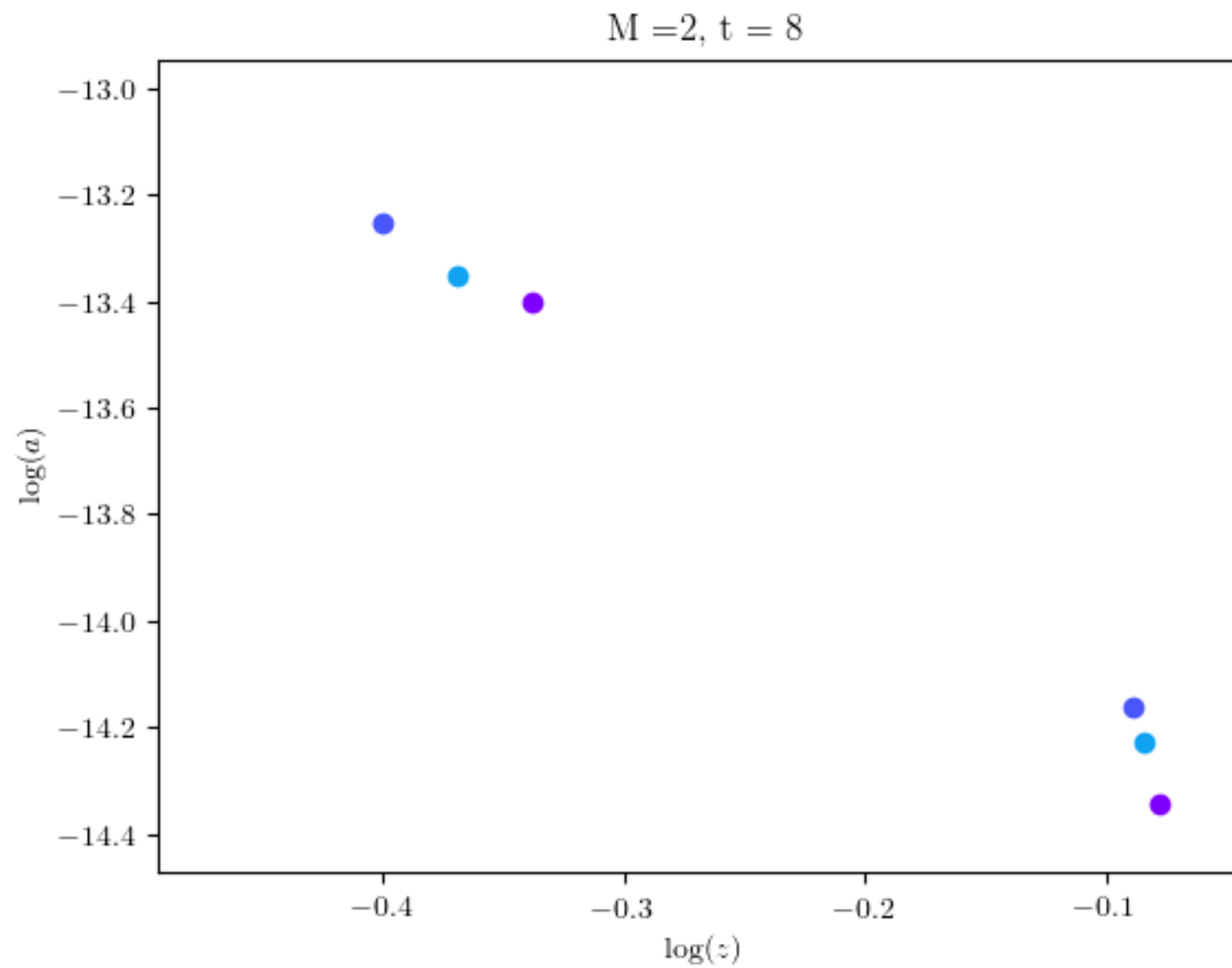
$$a_m = |\langle 0 | \pi | E_m \rangle|^2 \quad z_m = e^{-E_m}$$



# From theory to practice: the bootstrap

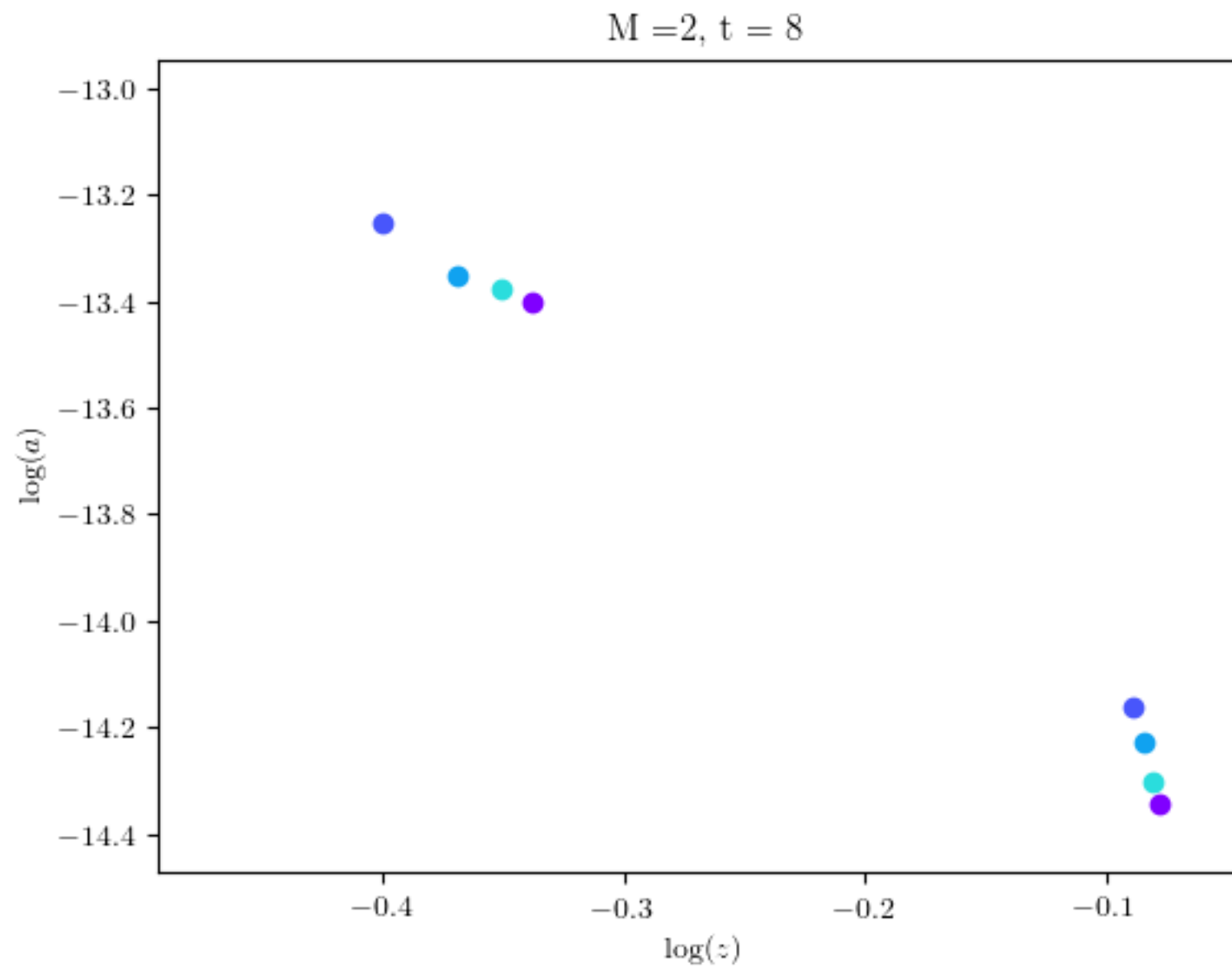


# From theory to practice: the bootstrap

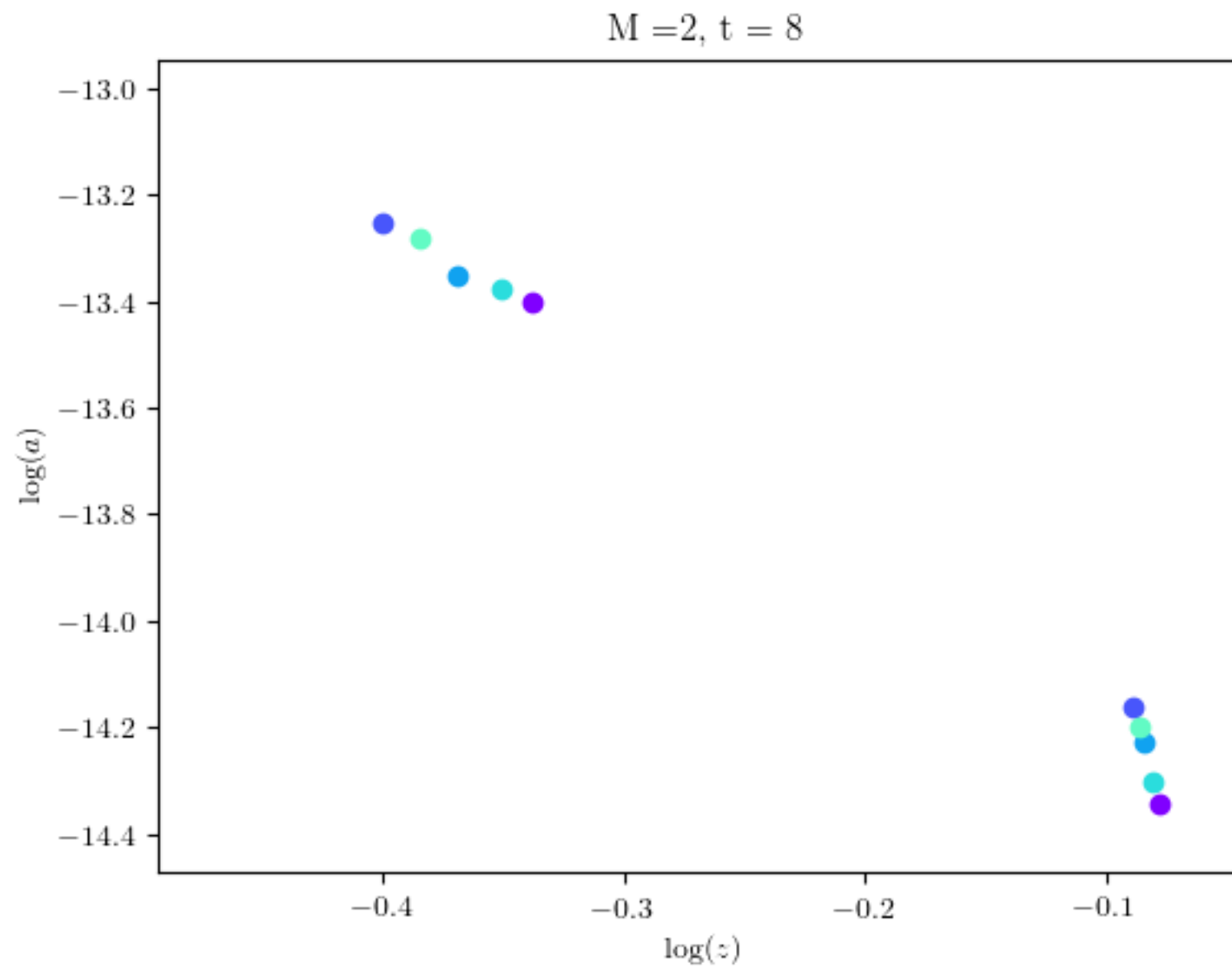




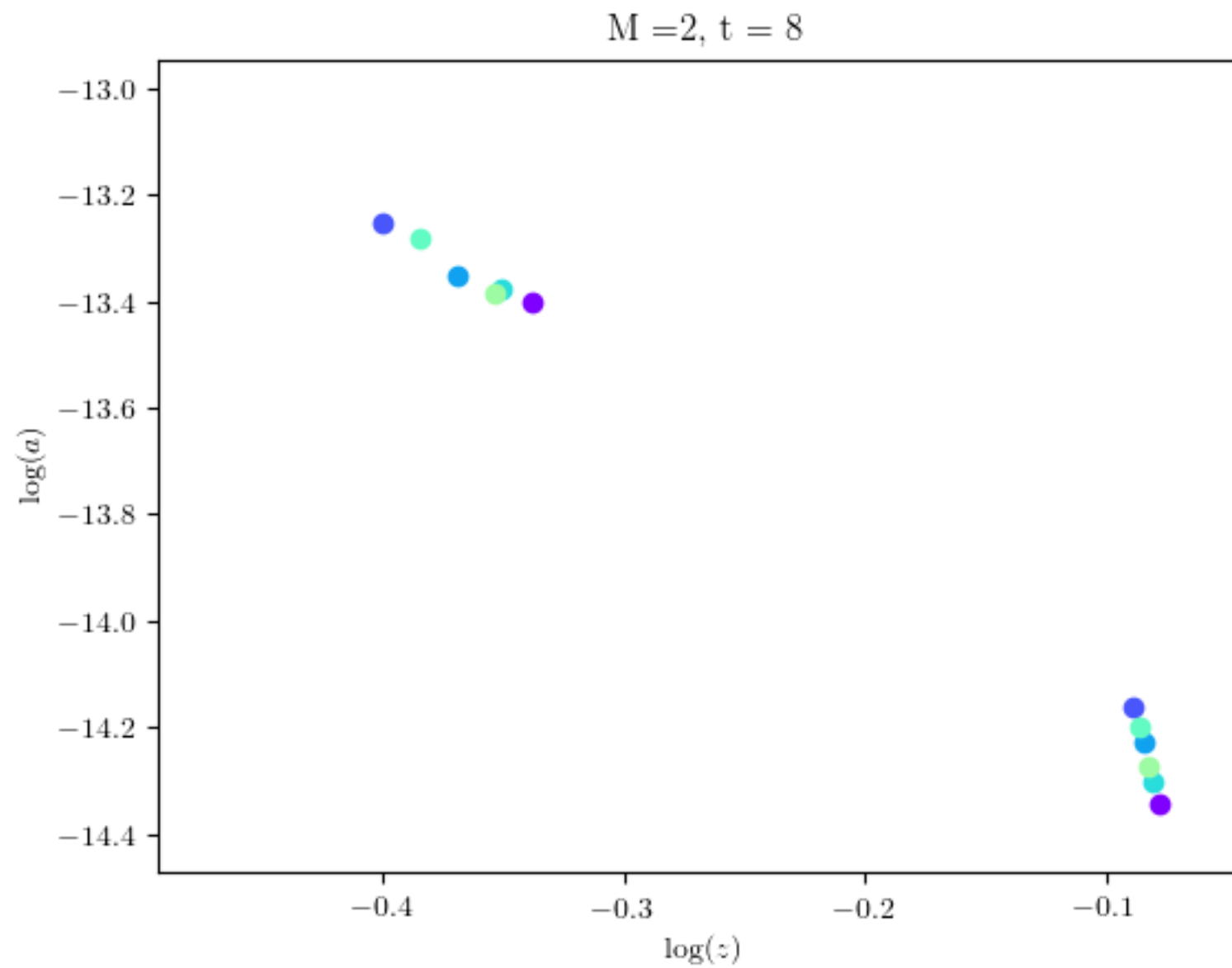
# From theory to practice: the bootstrap



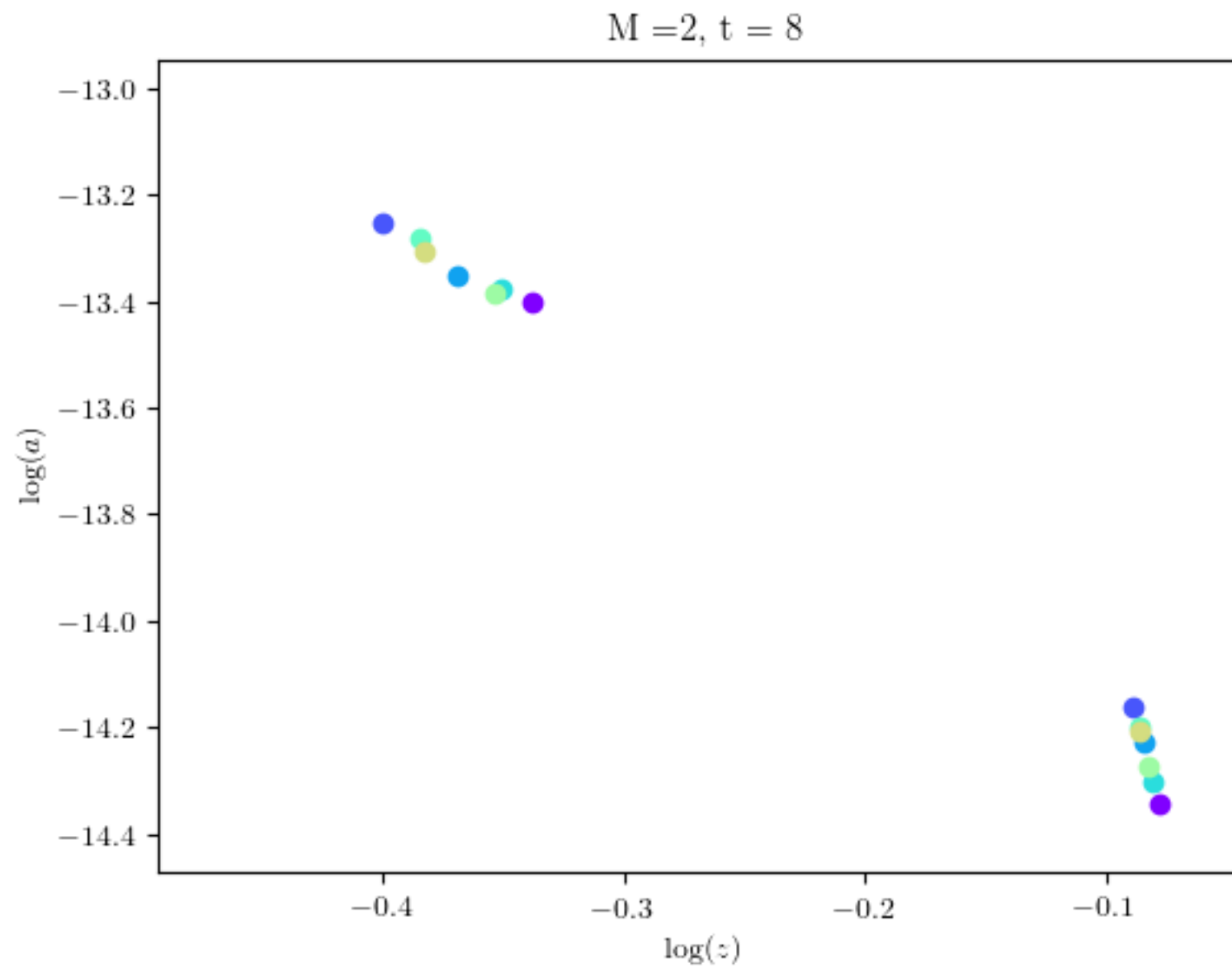
# From theory to practice: the bootstrap



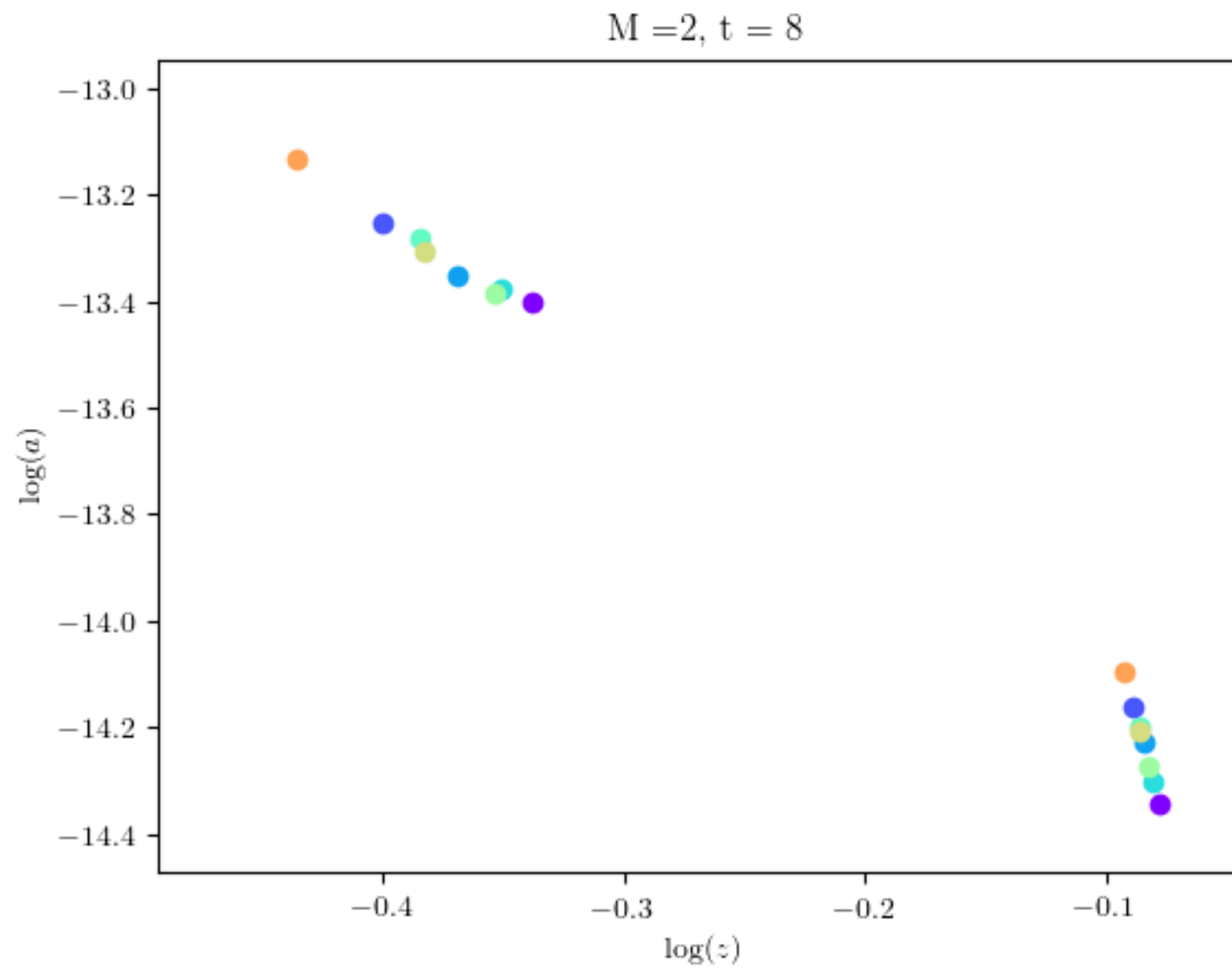
# From theory to practice: the bootstrap



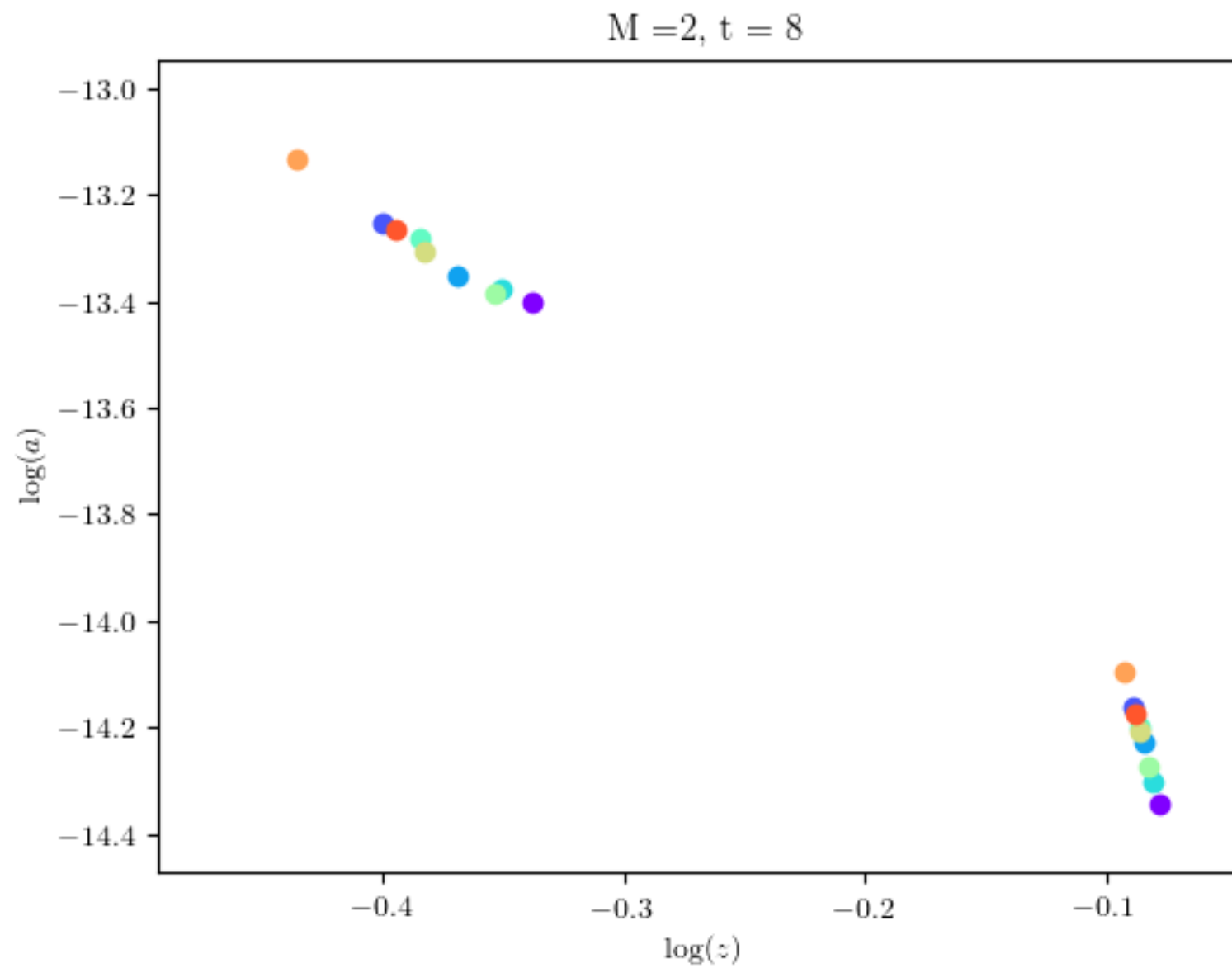
# From theory to practice: the bootstrap



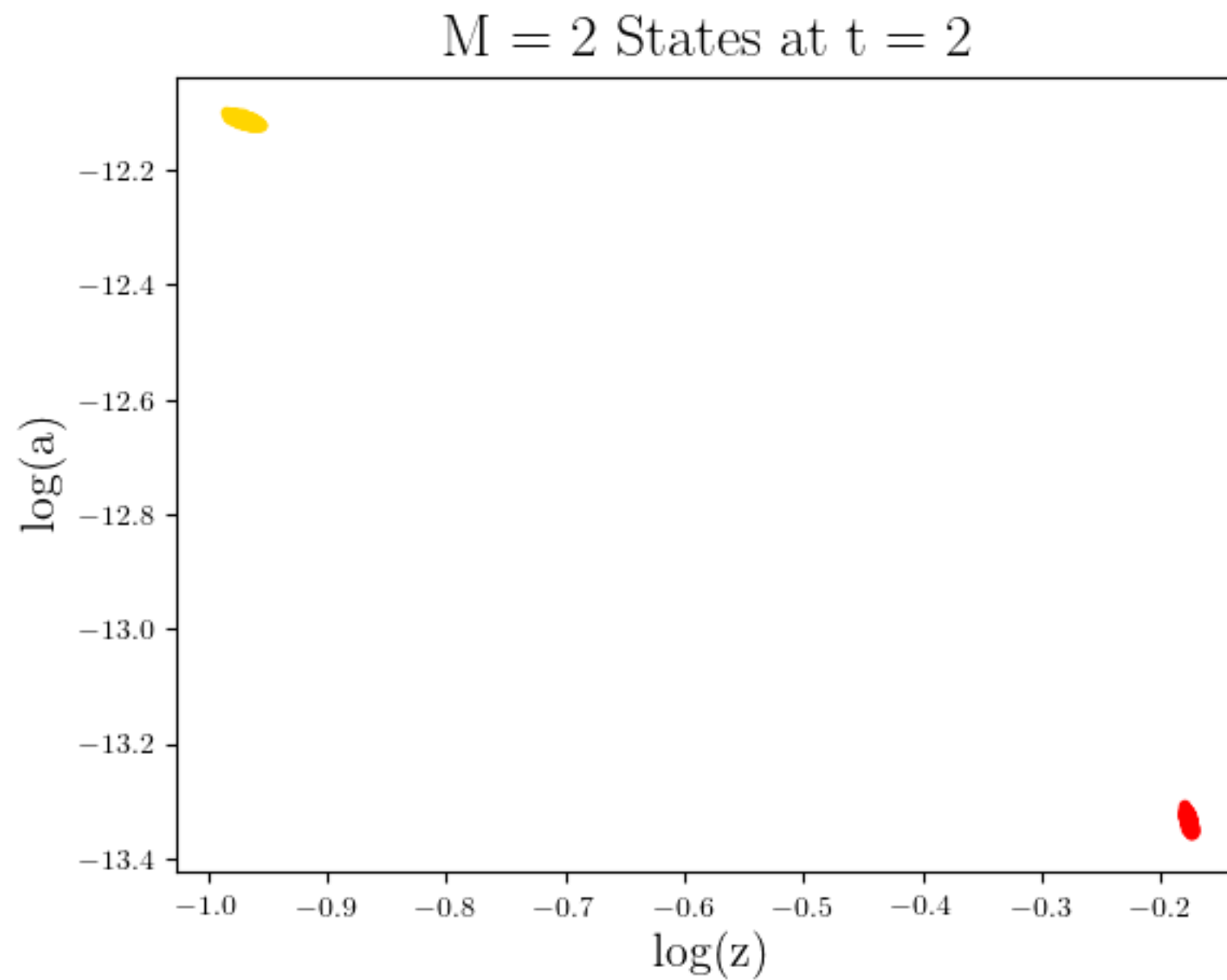
# From theory to practice: the bootstrap



# From theory to practice: the bootstrap

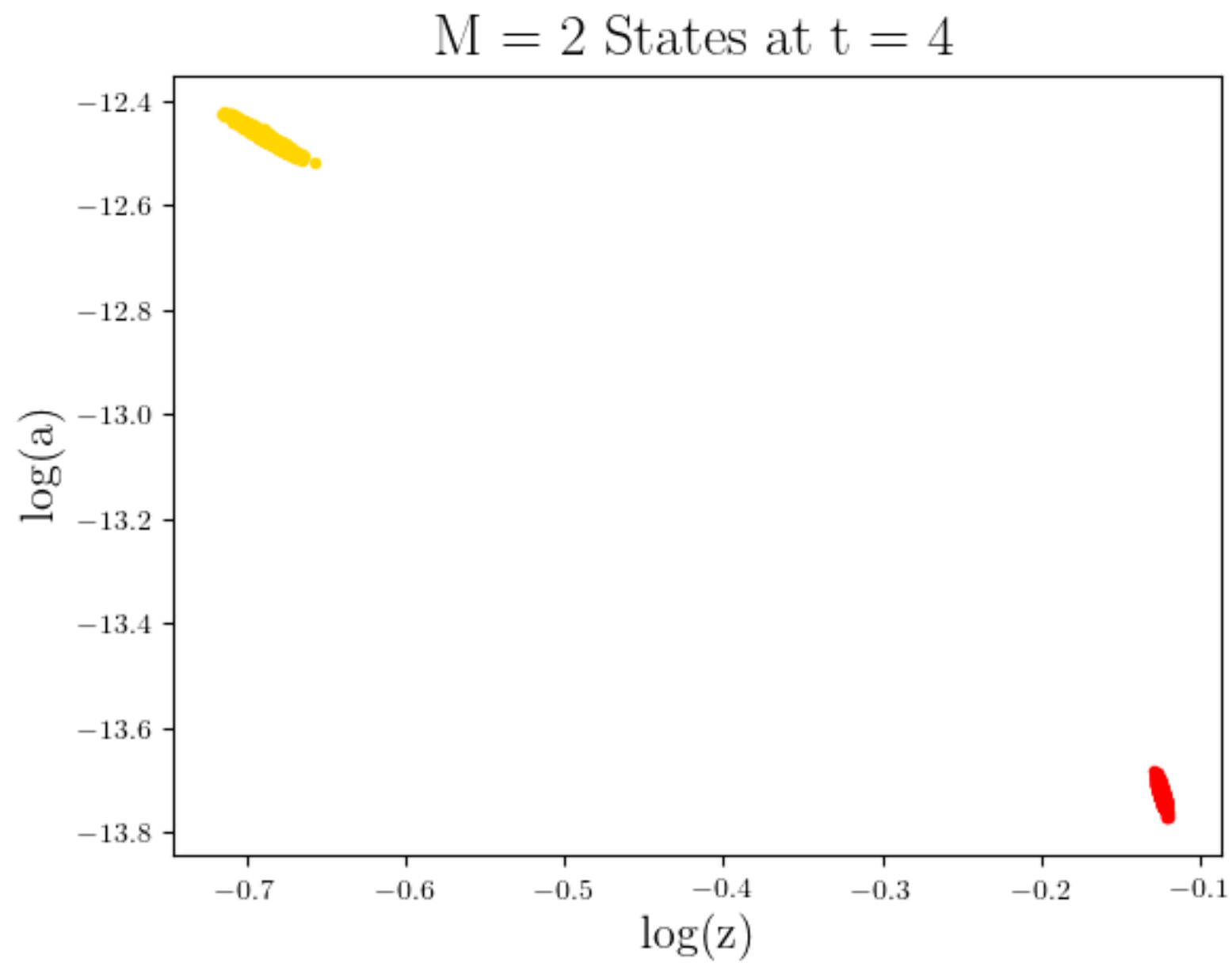


# M = 2 State Extraction

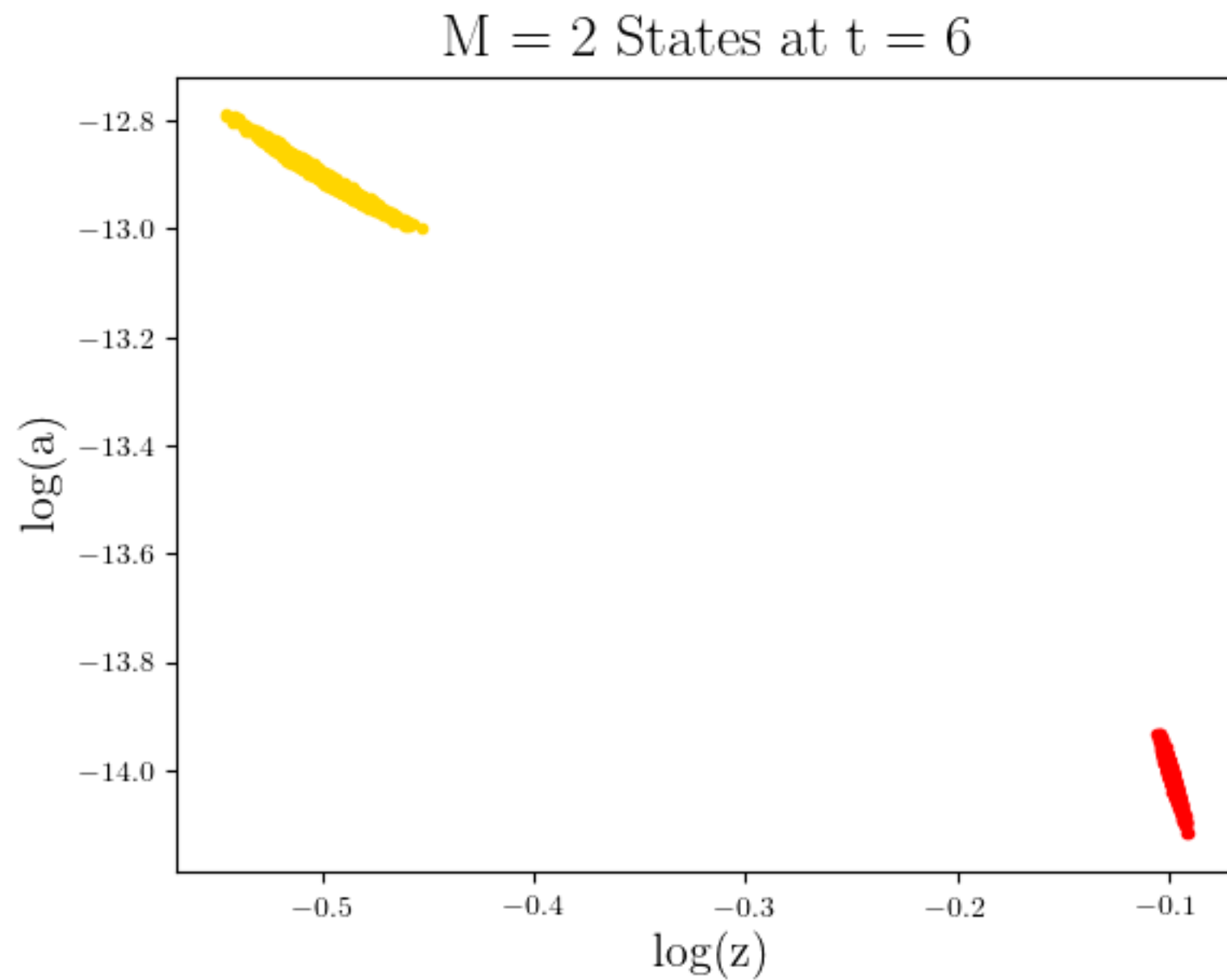




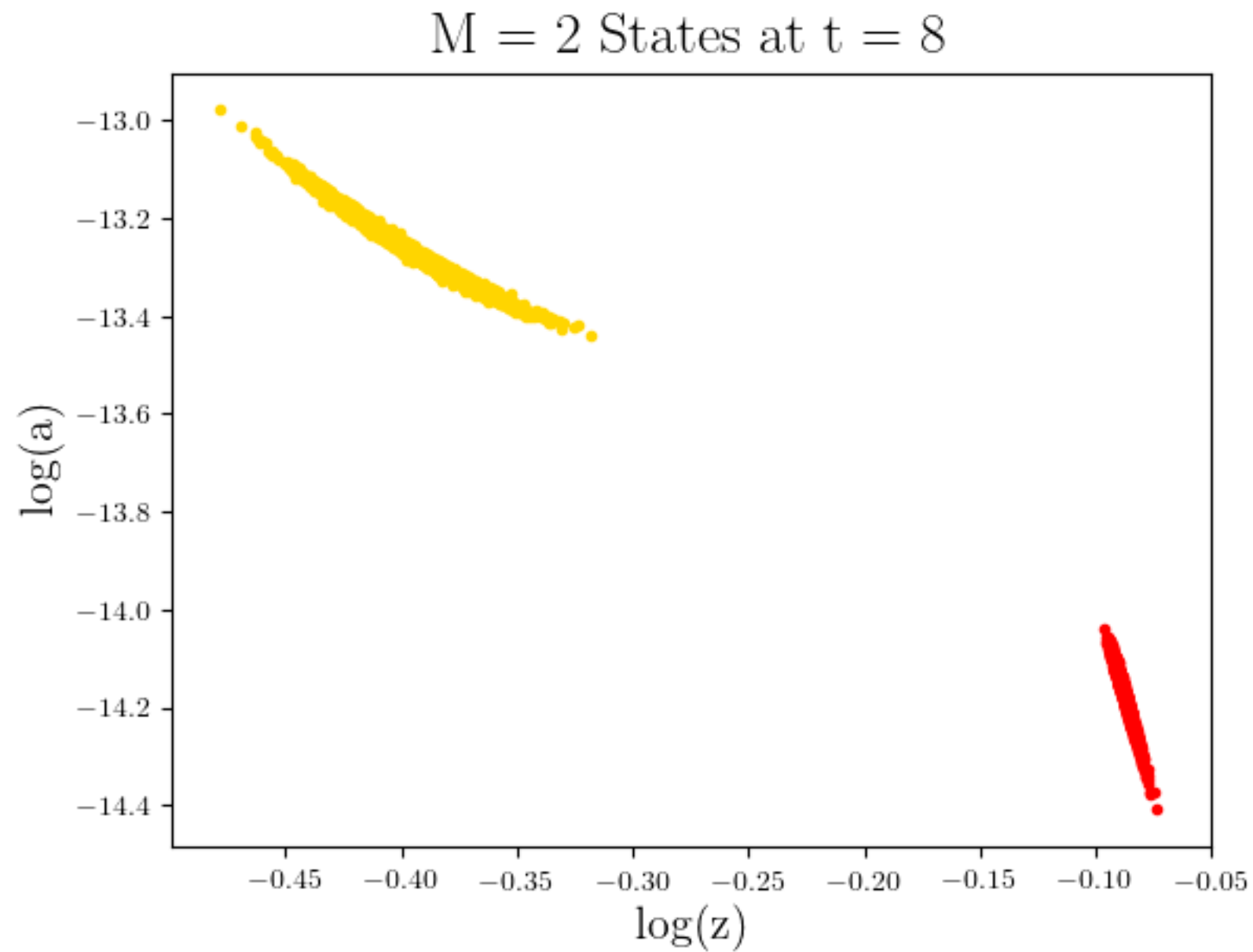
# M = 2 State Extraction



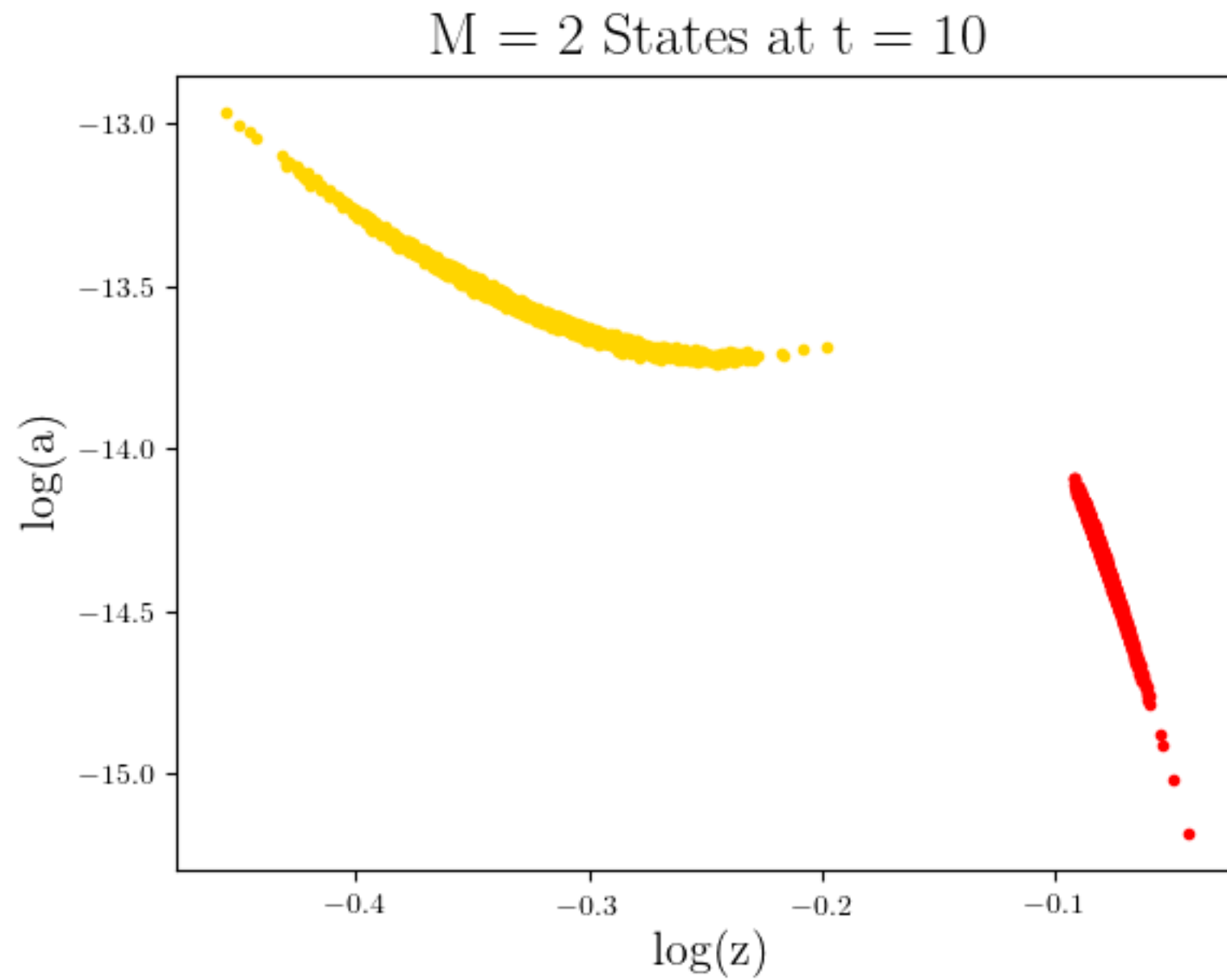
# M = 2 State Extraction



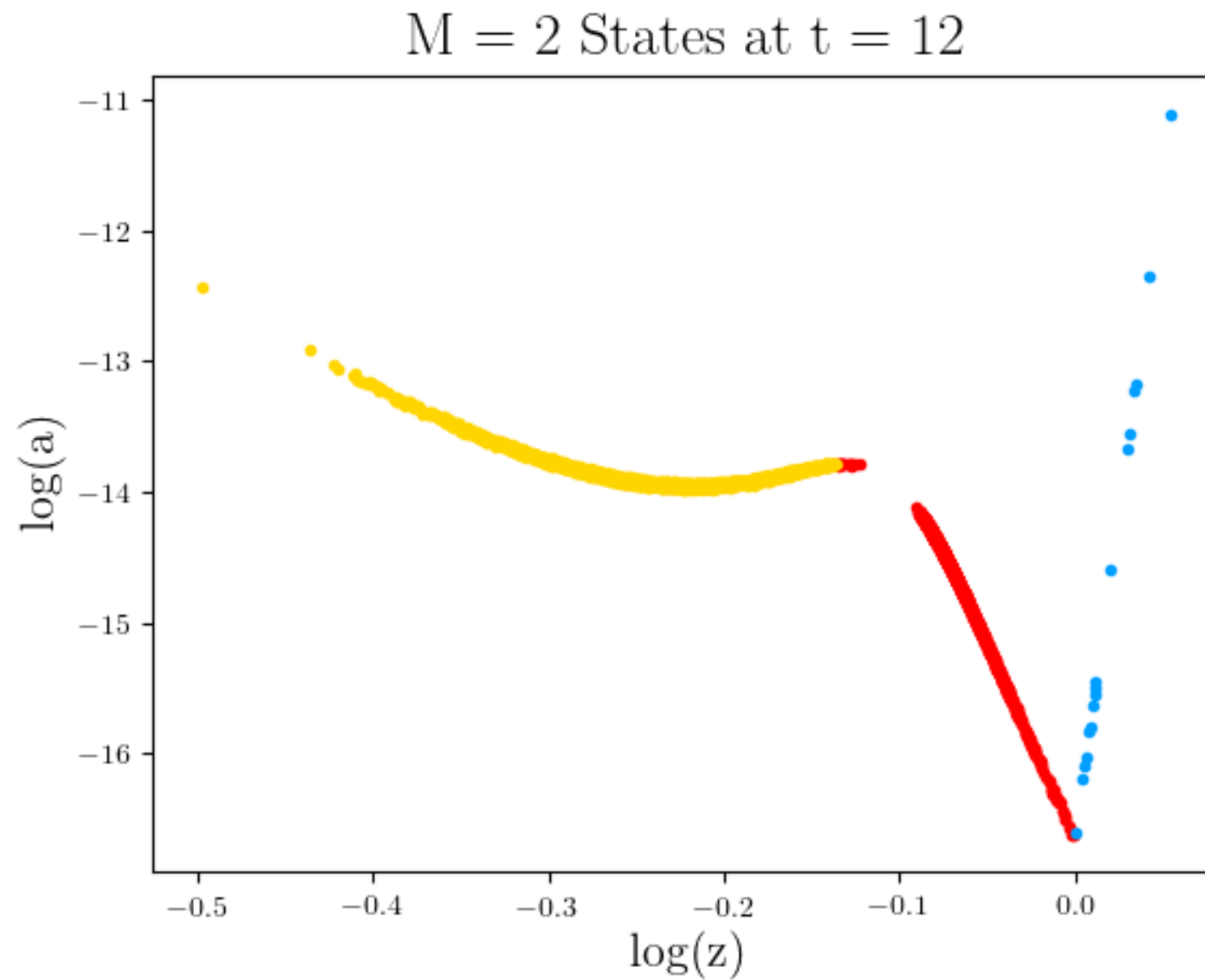
# M = 2 State Extraction



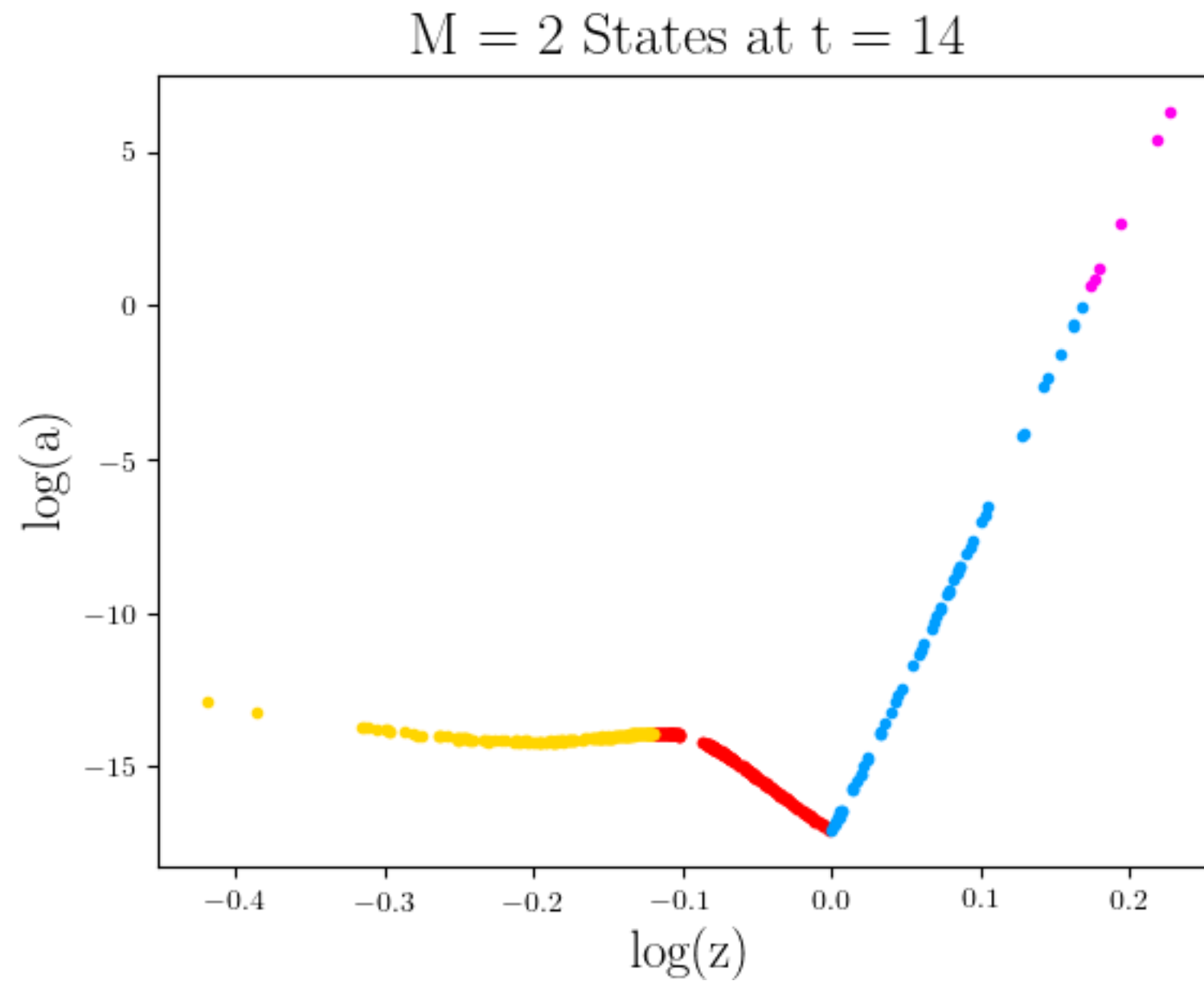
# M = 2 State Extraction



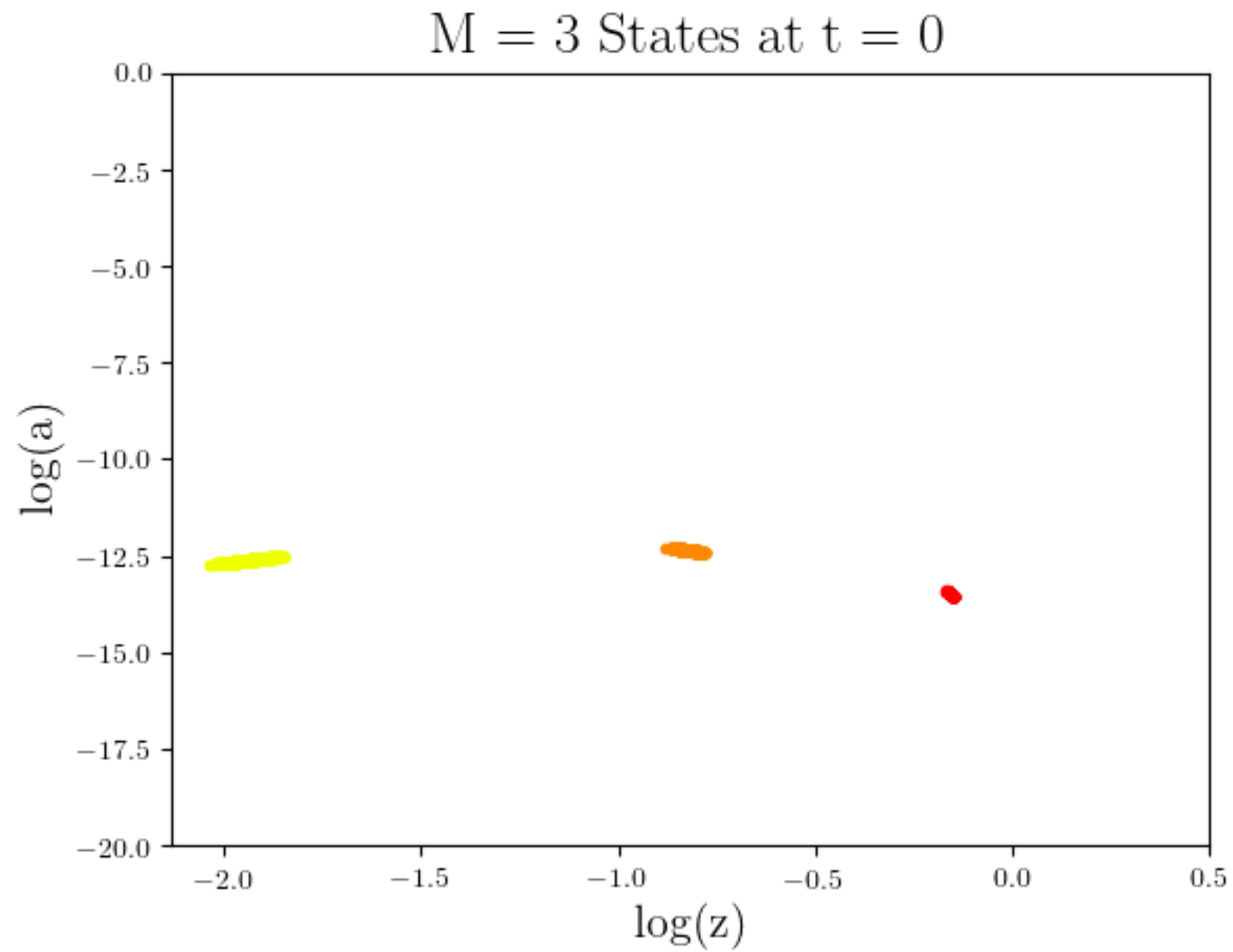
# M = 2 State Extraction



# M = 2 State Extraction

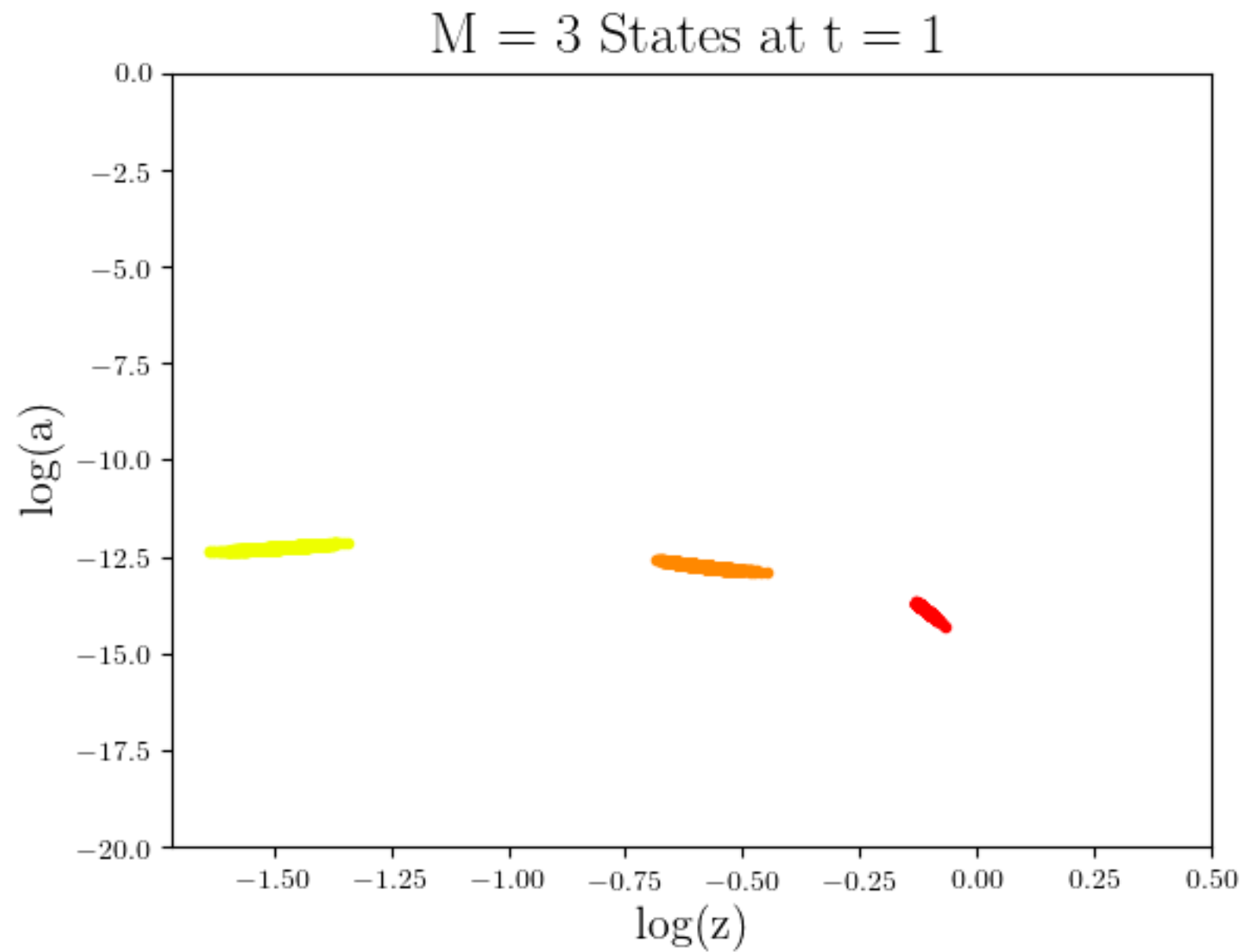


# M = 3 State Extraction

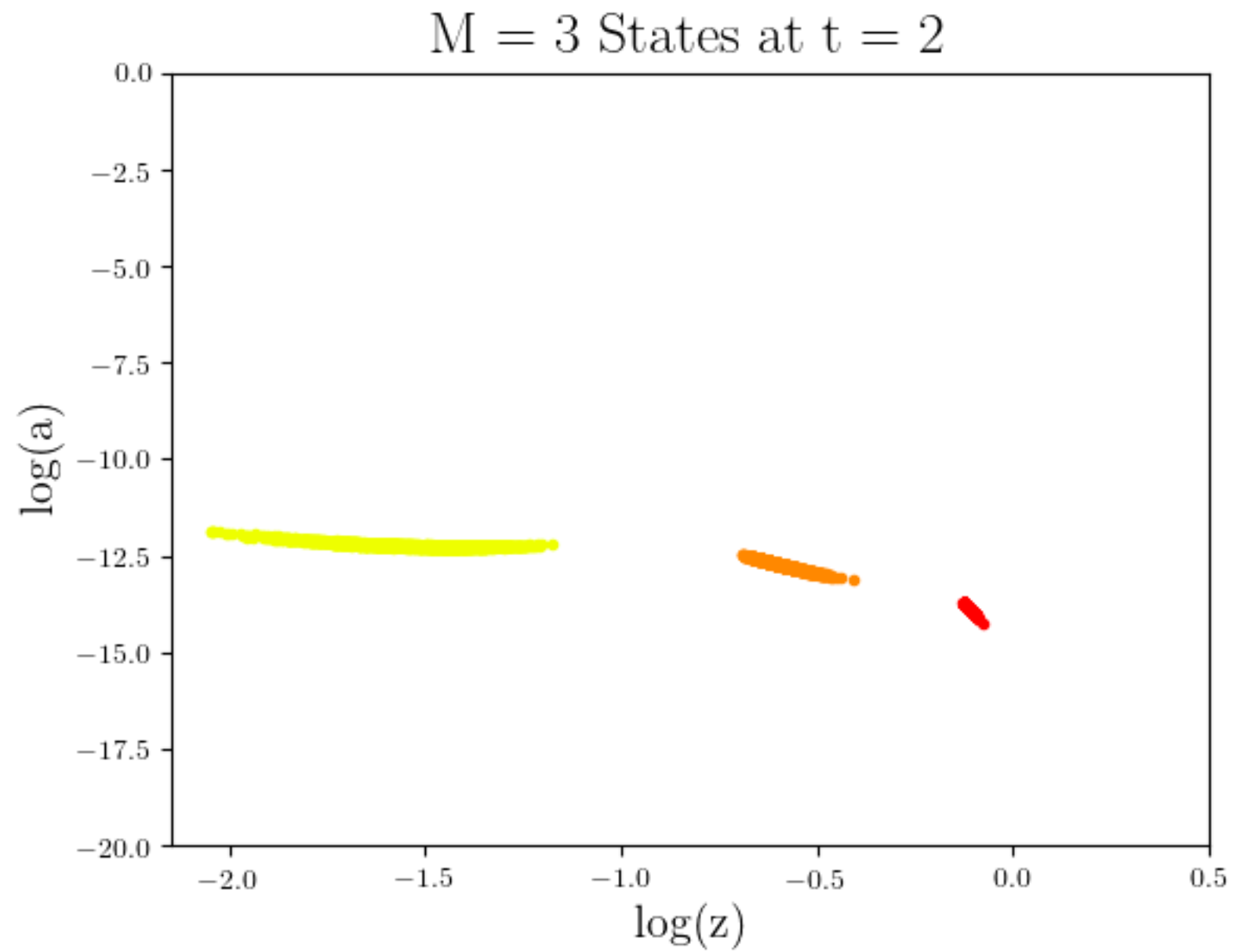




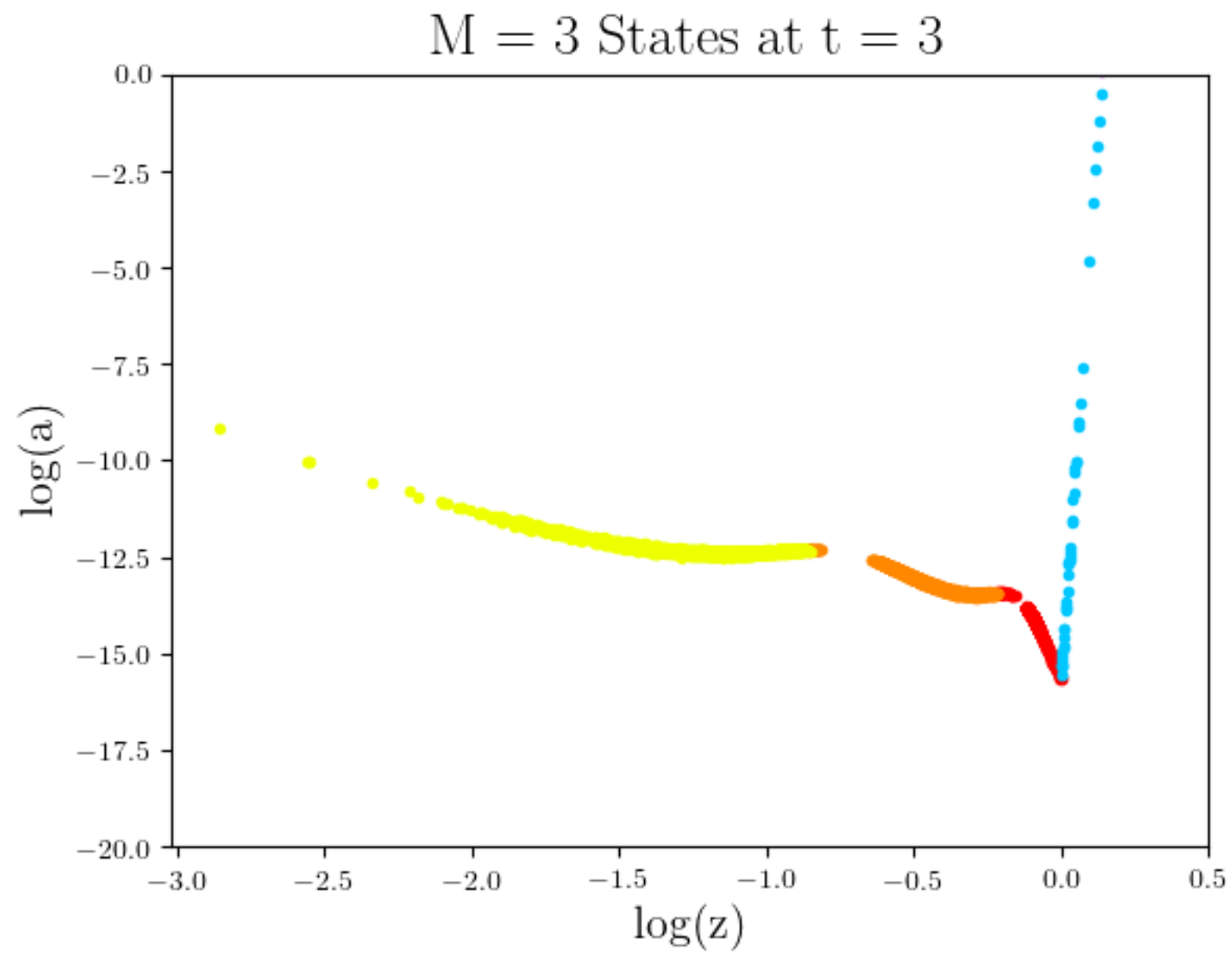
# M = 3 State Extraction



# M = 3 State Extraction



# M = 3 State Extraction



# Expectation Maximization Clustering

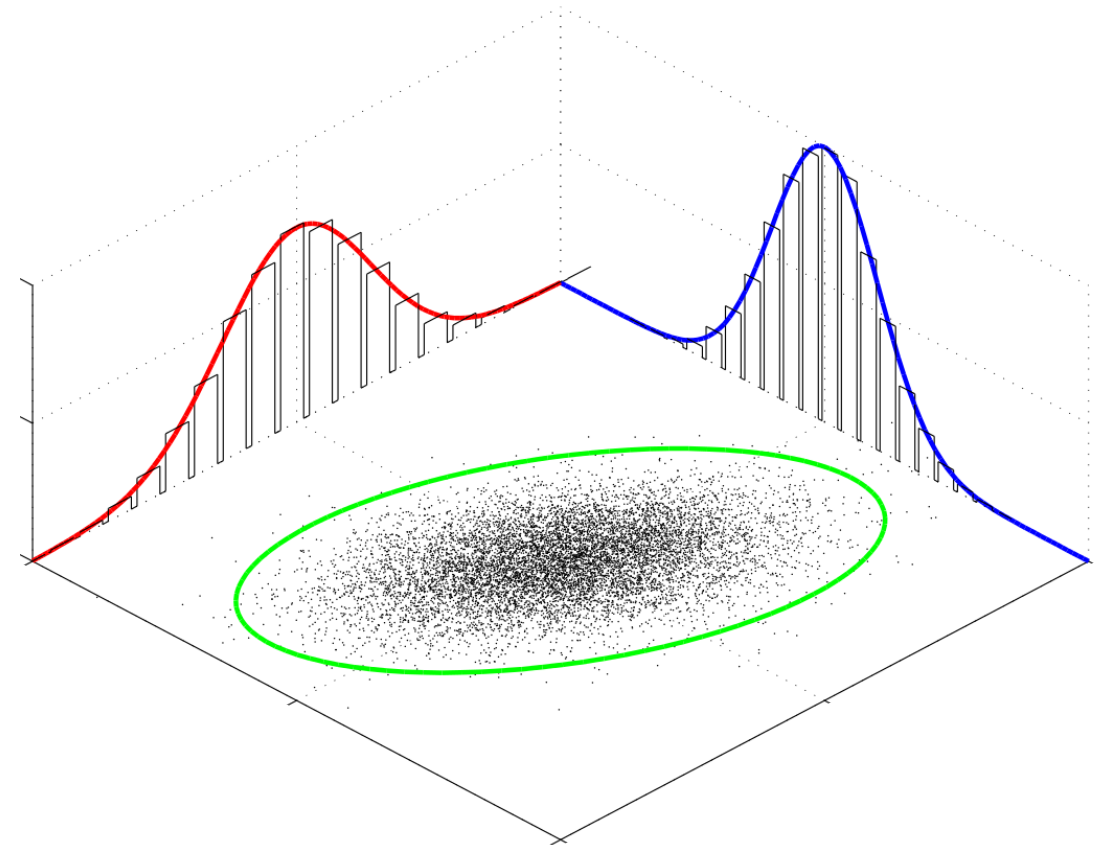
Dempster, A.P.; Laird, N.M.; Rubin, D.B. (1977). "Maximum Likelihood from Incomplete Data via the EM Algorithm". Journal of the Royal Statistical Society, Series B. 39 (1): 1–38.

$$\vec{\mu} = \left\langle \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle$$

$$\Sigma_{xx} = \sigma_x^2 = \langle (x - \mu_x)^2 \rangle$$

$$\Sigma_{yy} = \sigma_y^2 = \langle (y - \mu_y)^2 \rangle$$

$$\Sigma_{xy} = \Sigma_{yx}^\dagger = \langle (x - \mu_x)(y - \mu_y) \rangle$$



$$p(\vec{x}) = \frac{1}{2\pi \sqrt{|\Sigma|}} e^{-\frac{1}{2} (\vec{x} - \vec{\mu})^T \Sigma^{-1} (\vec{x} - \vec{\mu})}$$

# K-Means Algorithm

Lloyd., S. P. (1982). "Least squares quantization in PCM"(PDF).  
IEEE Transactions on Information Theory. 28 (2): 129–137.

1. Assign points to initial clusters
2. Compute the mean and covariance matrix for each cluster
3. For each bootstrap sample, find most probably permutation of points among clusters
4. Repeat 2. and 3. until the process converges

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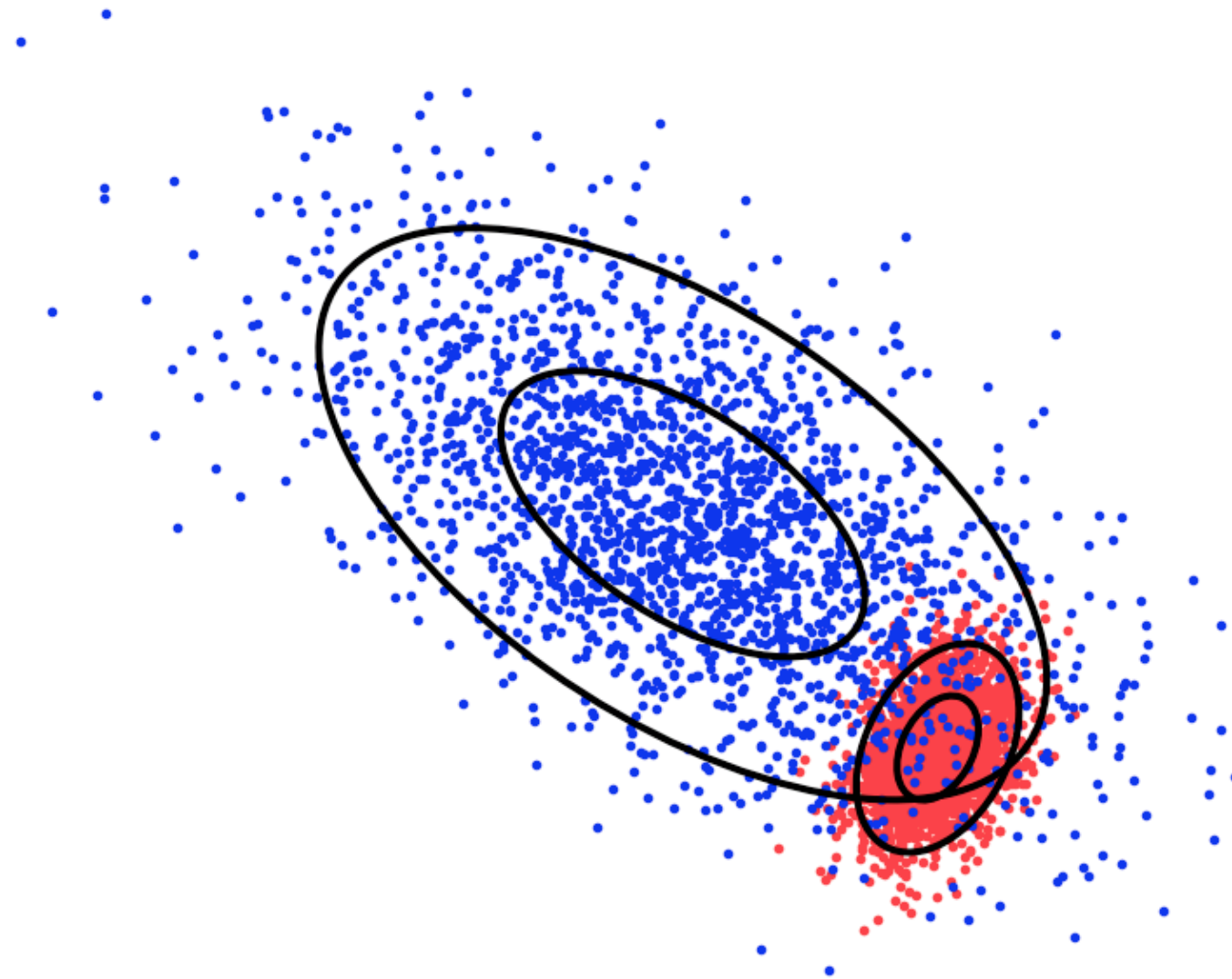
1. Assign points to initial clusters
2. Compute the mean and covariance matrix for each cluster
3. For each bootstrap sample, find most probably permutation of points among clusters
4. Repeat 2. and 3. until the process converges

$$p_1(\vec{x}) > p_2(\vec{x})$$

$$\Rightarrow \frac{1}{\sqrt{|\Sigma_1|}} e^{-\frac{1}{2}(\vec{x}-\vec{\mu}_1)^T \Sigma_1^{-1} (\vec{x}-\vec{\mu}_1)} > \frac{1}{\sqrt{|\Sigma_2|}} e^{-\frac{1}{2}(\vec{x}-\vec{\mu}_2)^T \Sigma_2^{-1} (\vec{x}-\vec{\mu}_2)},$$

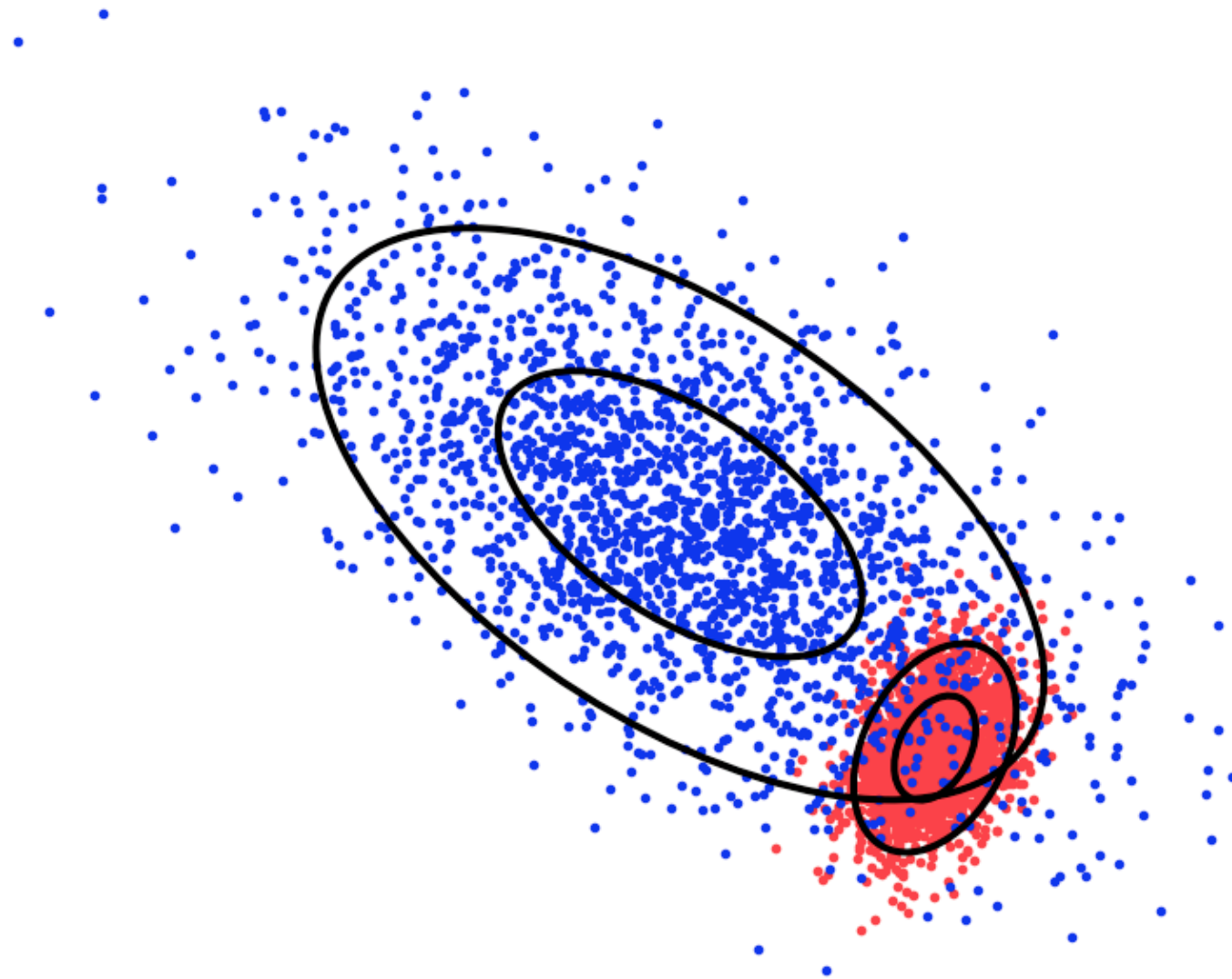
$$\Rightarrow d_1(\vec{x}) + \log|\Sigma_1| < d_2(\vec{x}) + \log|\Sigma_2|$$

# K-Means Algorithm



$$\Rightarrow d_1(\vec{x}) + \log|\Sigma_1| < d_2(\vec{x}) + \log|\Sigma_2|$$

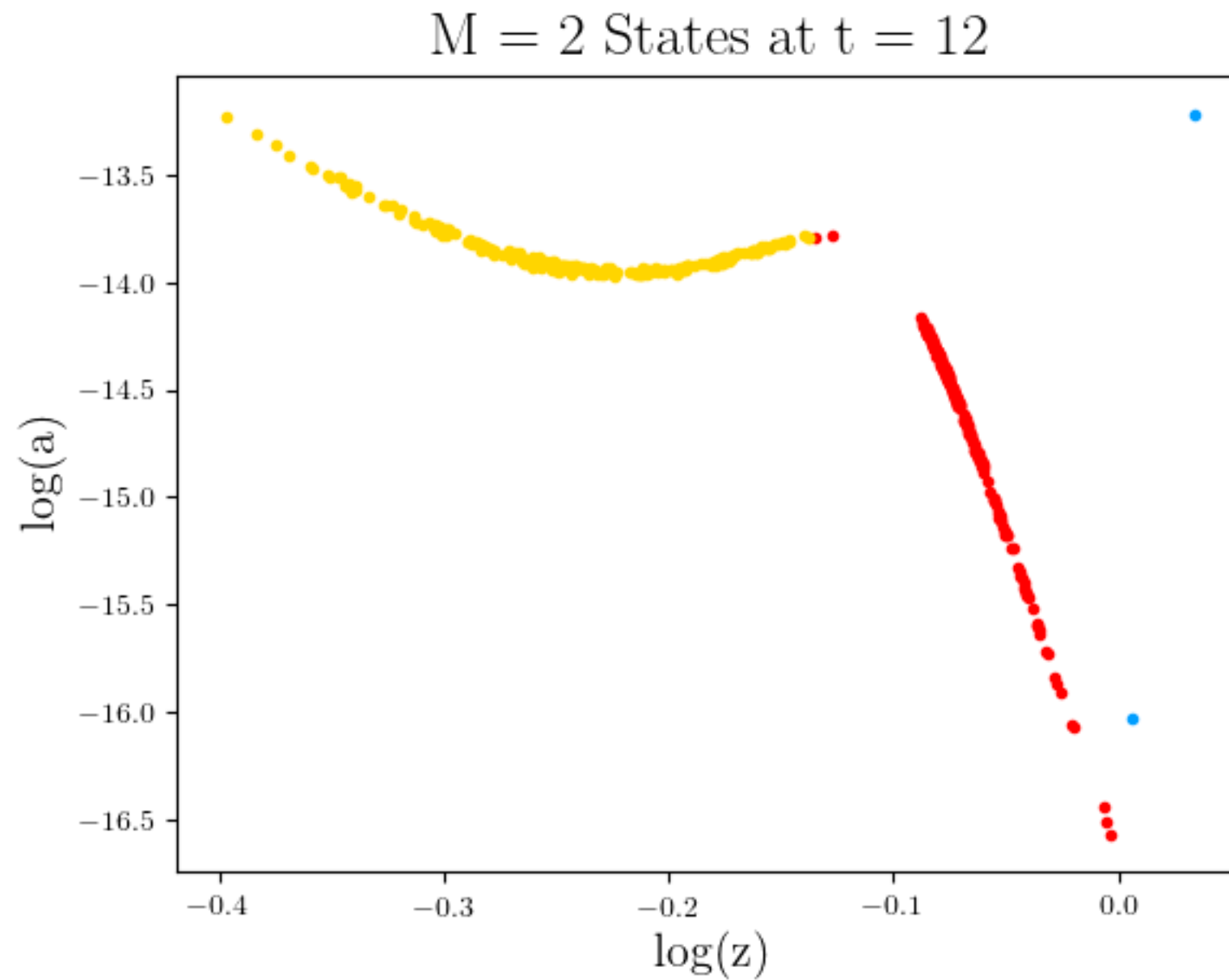
# K-Means Algorithm



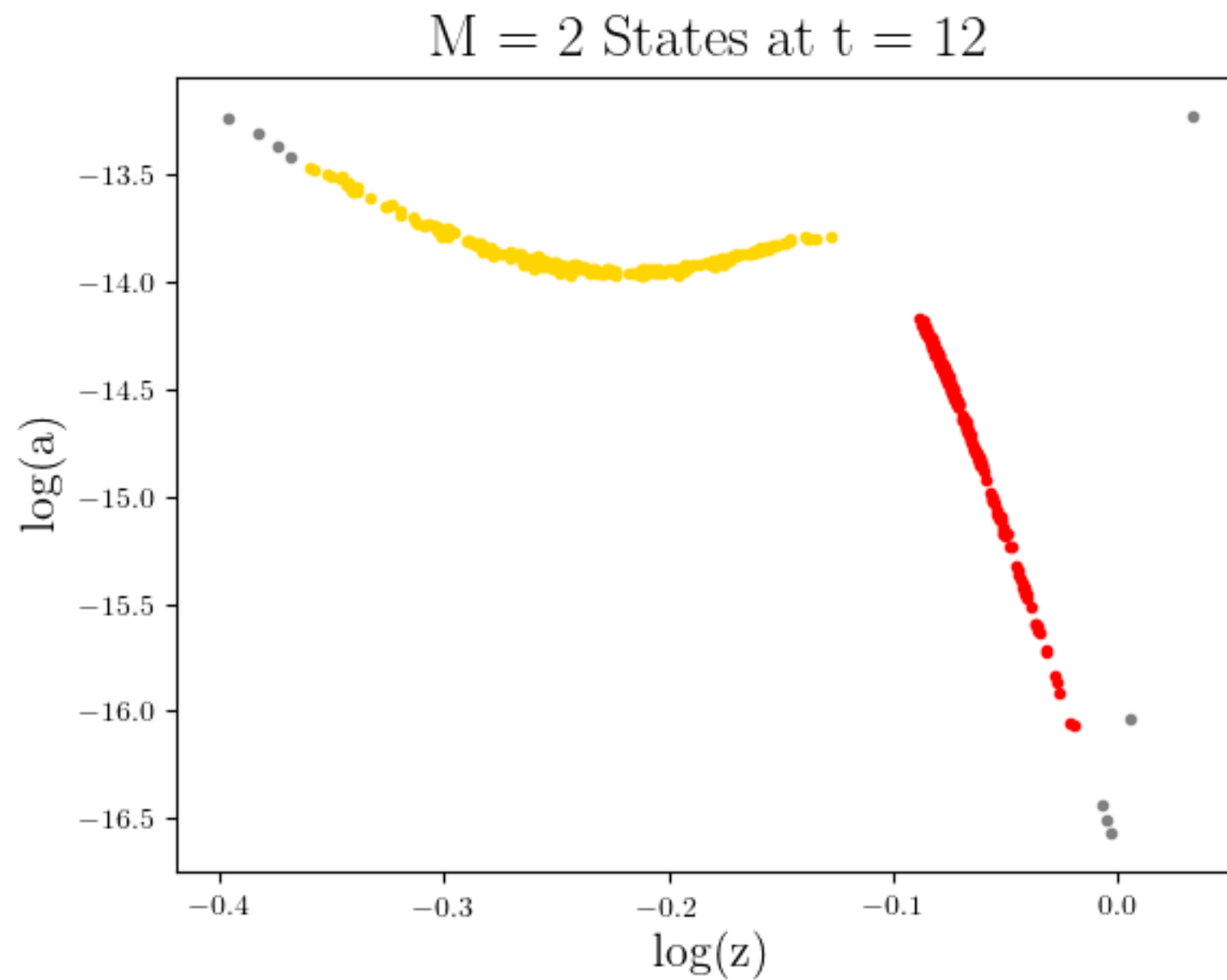
$$0 = p_0 + p_1 z + p_2 z^2$$

$$z_m = e^{-E_m}$$

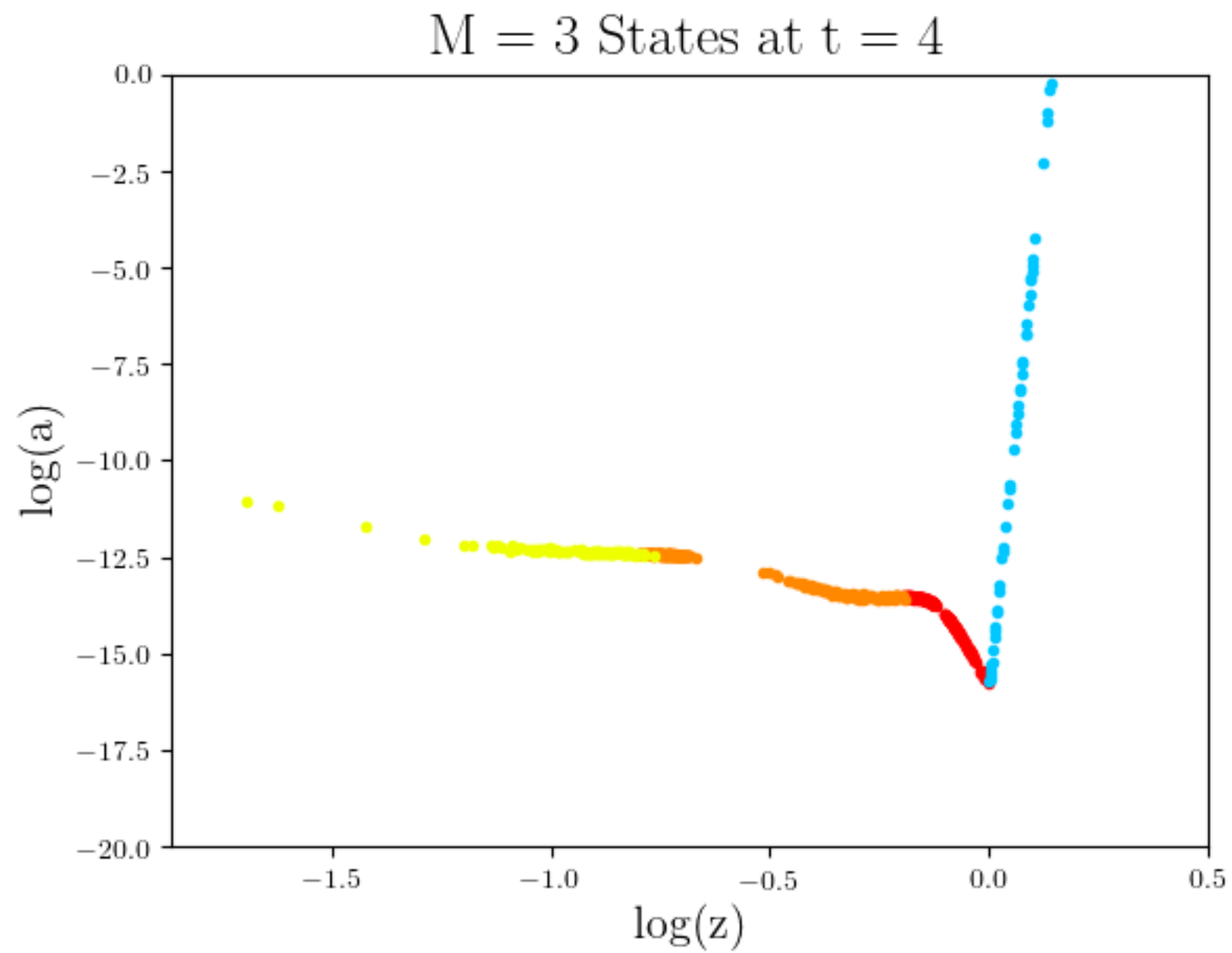
# Clustering M = 2, Initial



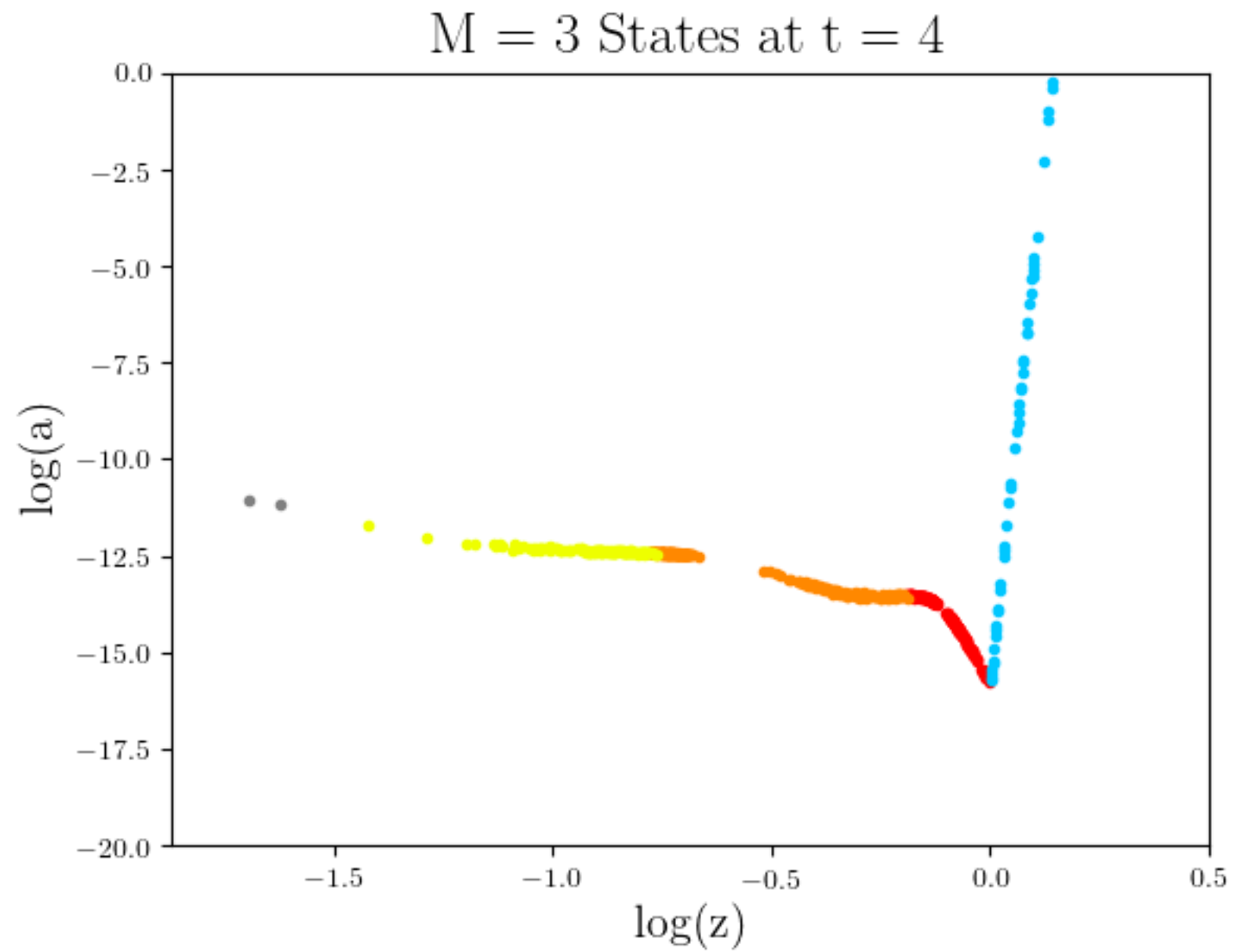
# Clustering $M = 2$ , 1 iteration



# Clustering $M = 3$ , Initial

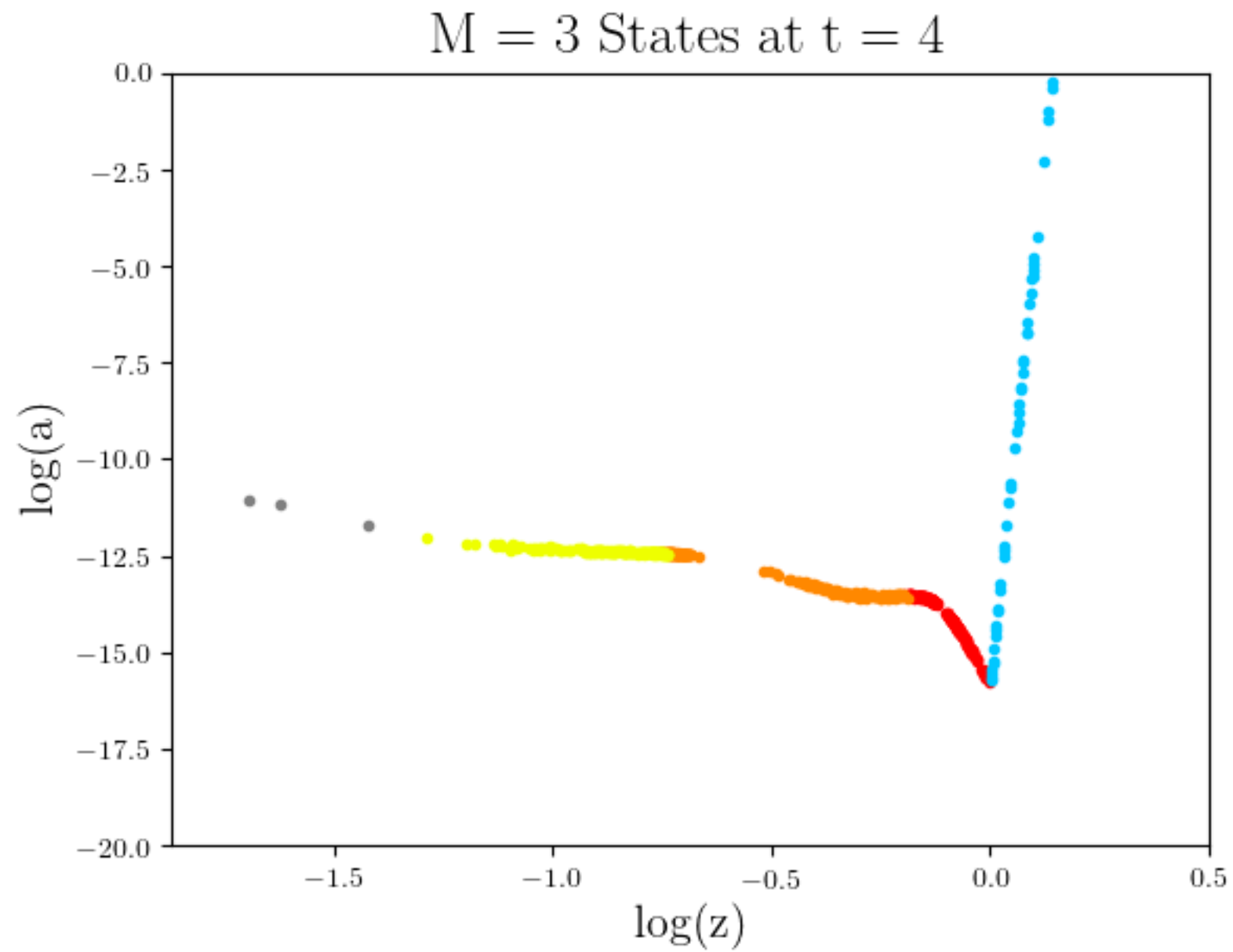


# Clustering $M = 3$ , 1 iteration

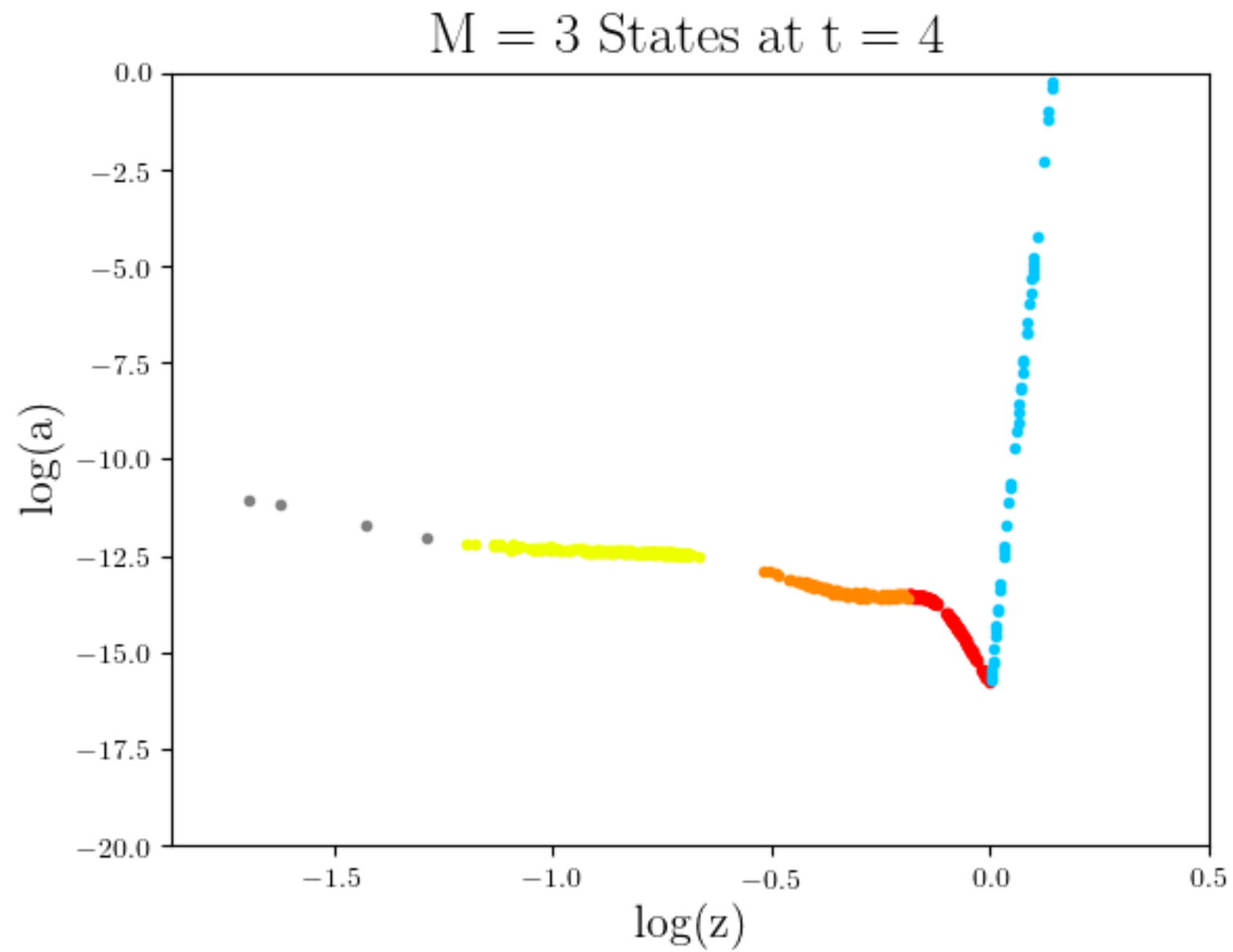




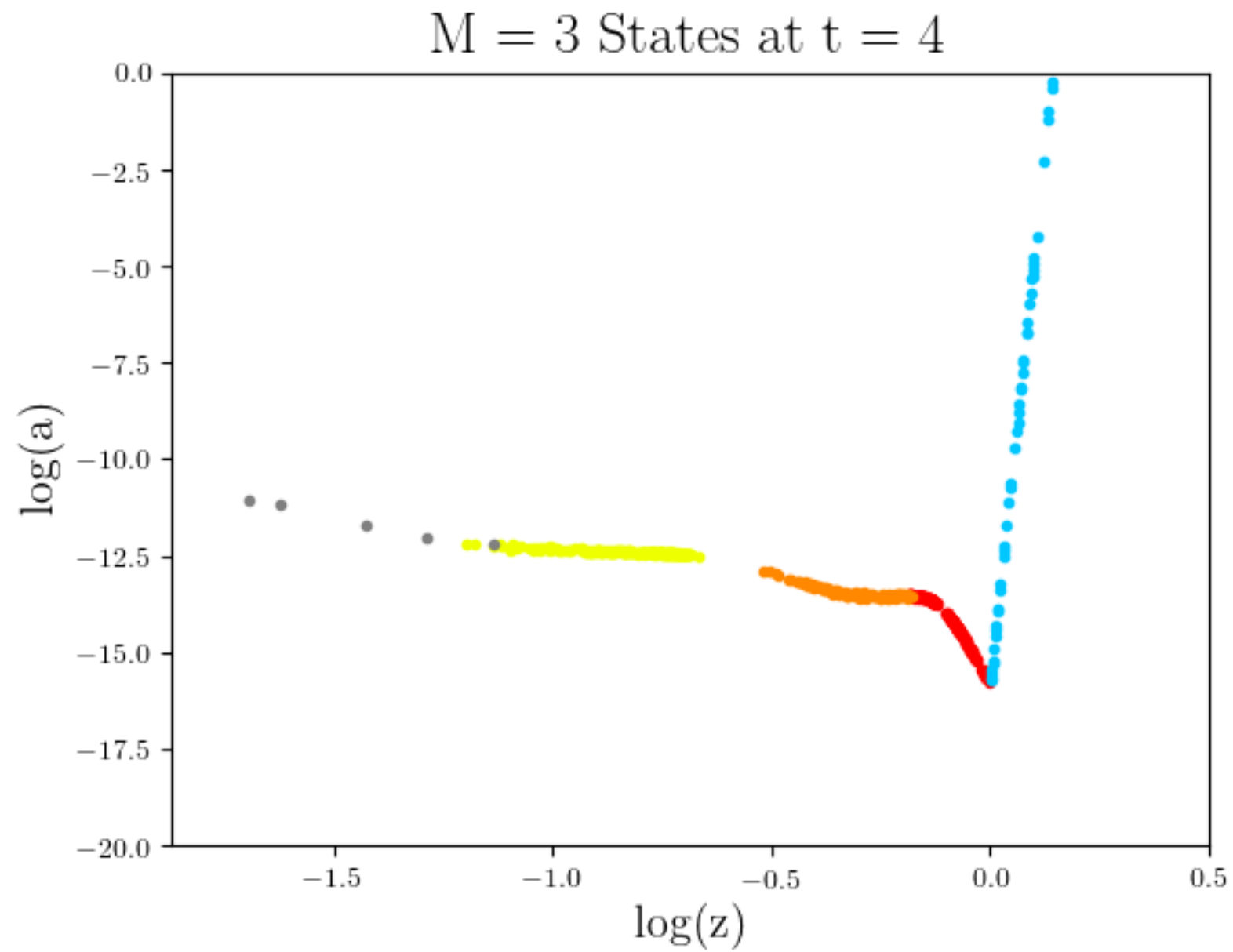
# Clustering $M = 3$ , 2 iterations



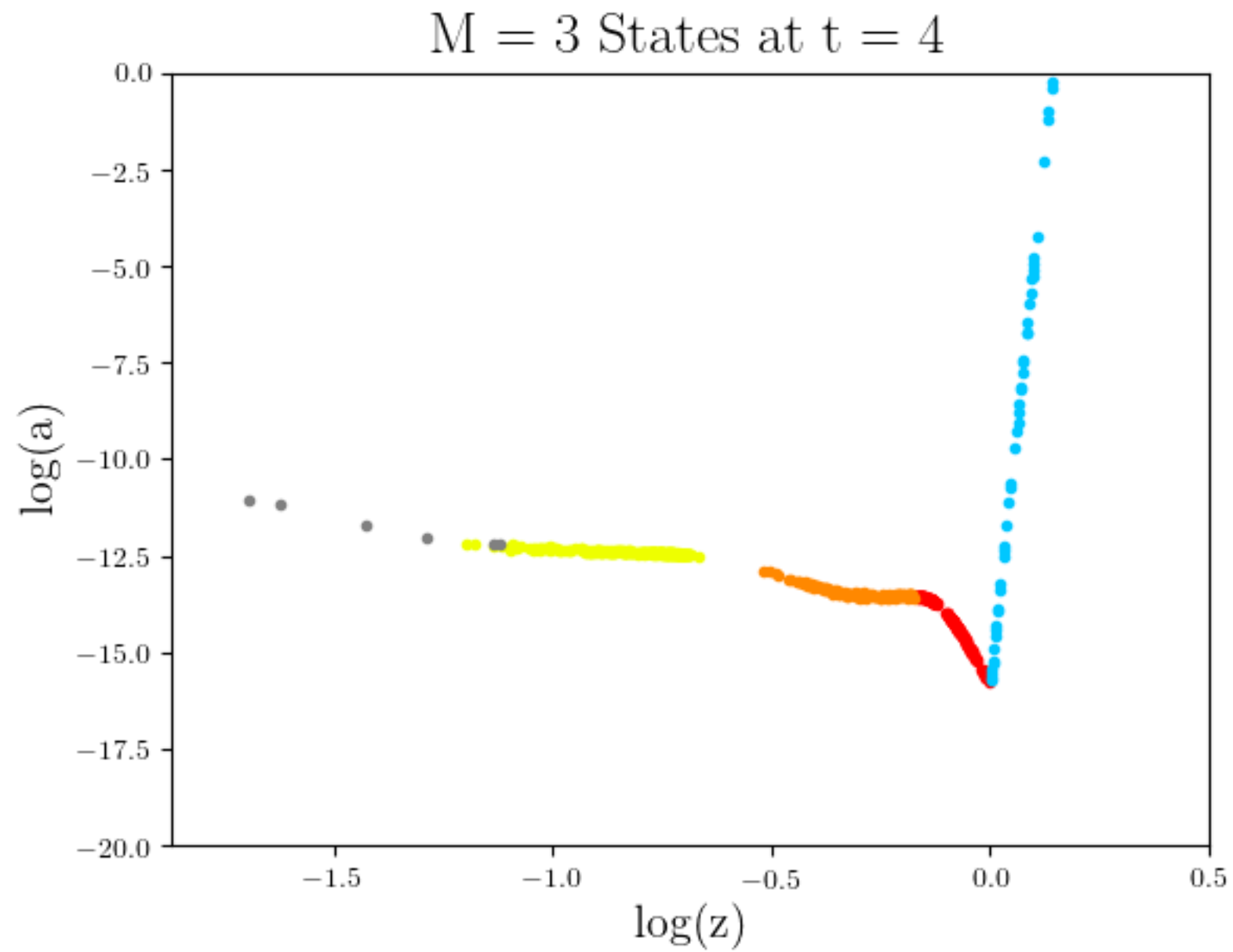
# Clustering $M = 3$ , 3 iterations



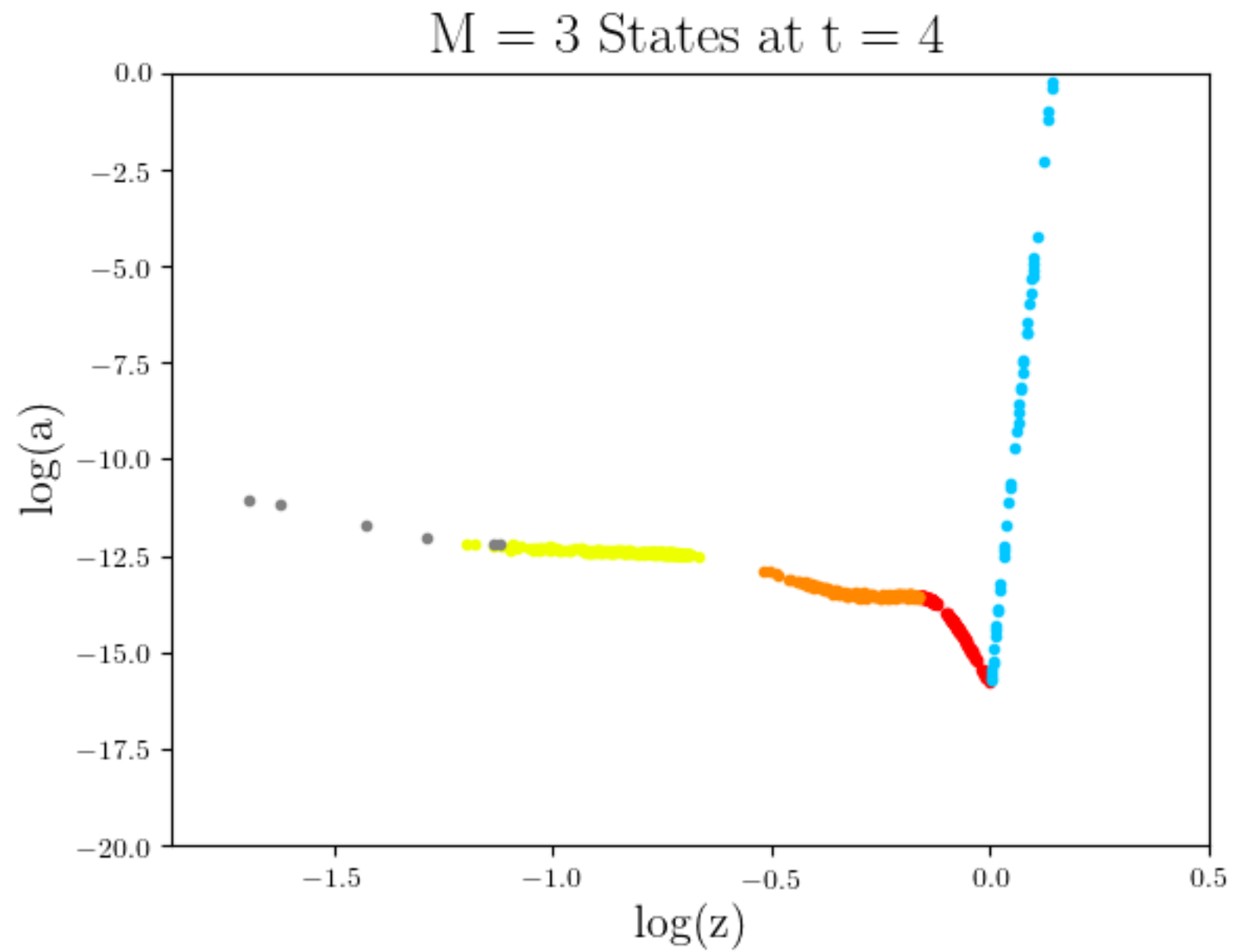
# Clustering M = 3, 4 iterations



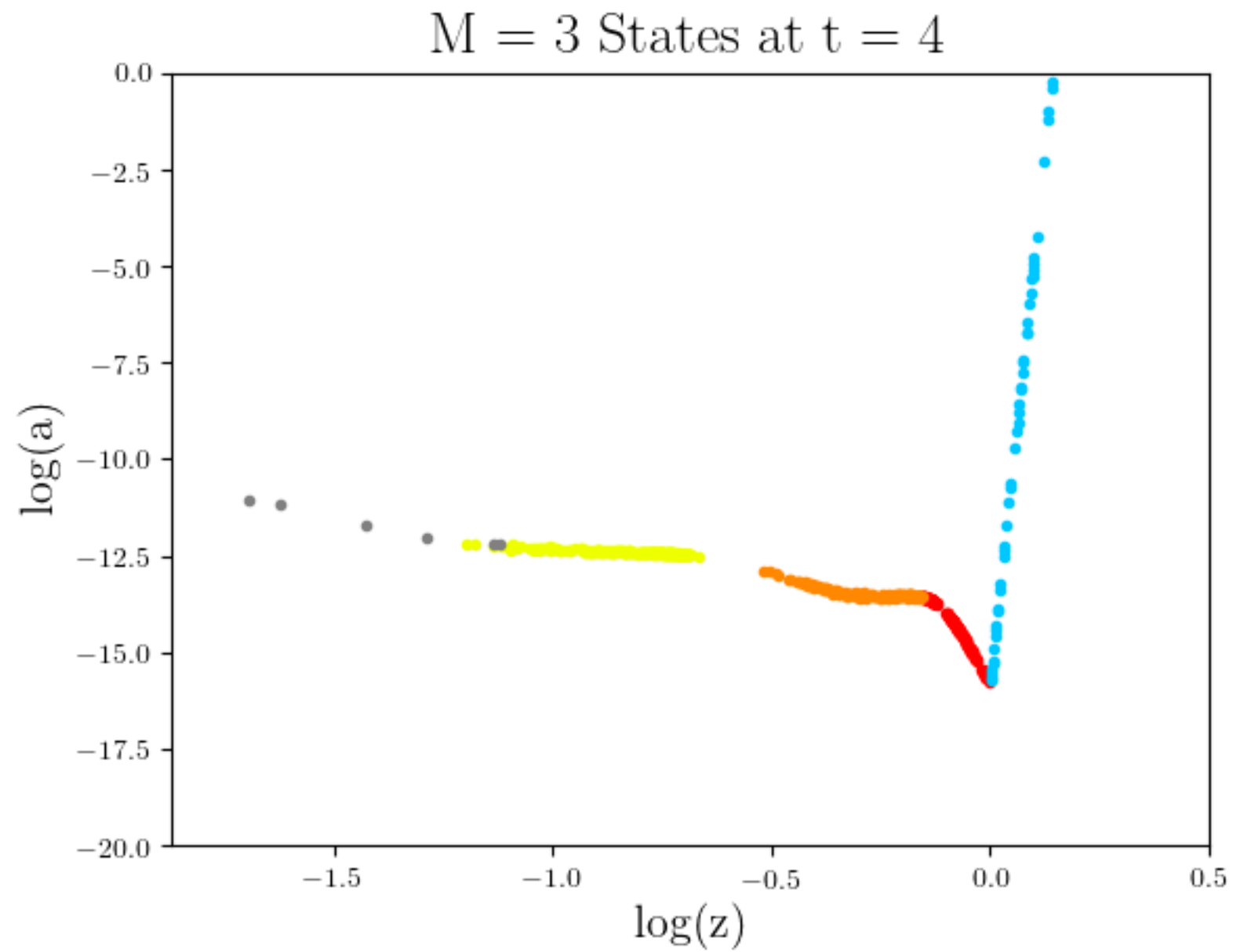
# Clustering M = 3, 5 iterations



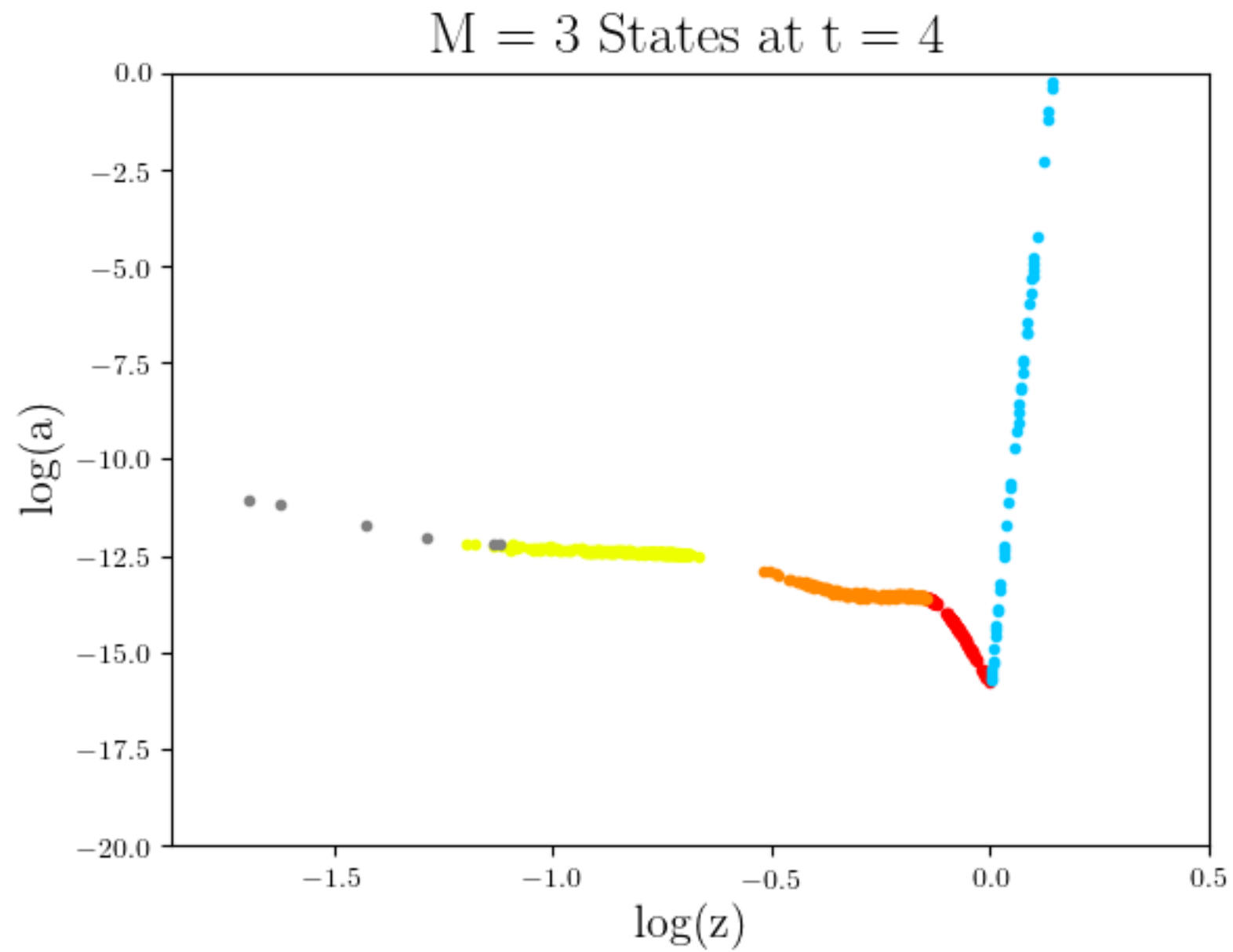
# Clustering M = 3, 6 iterations



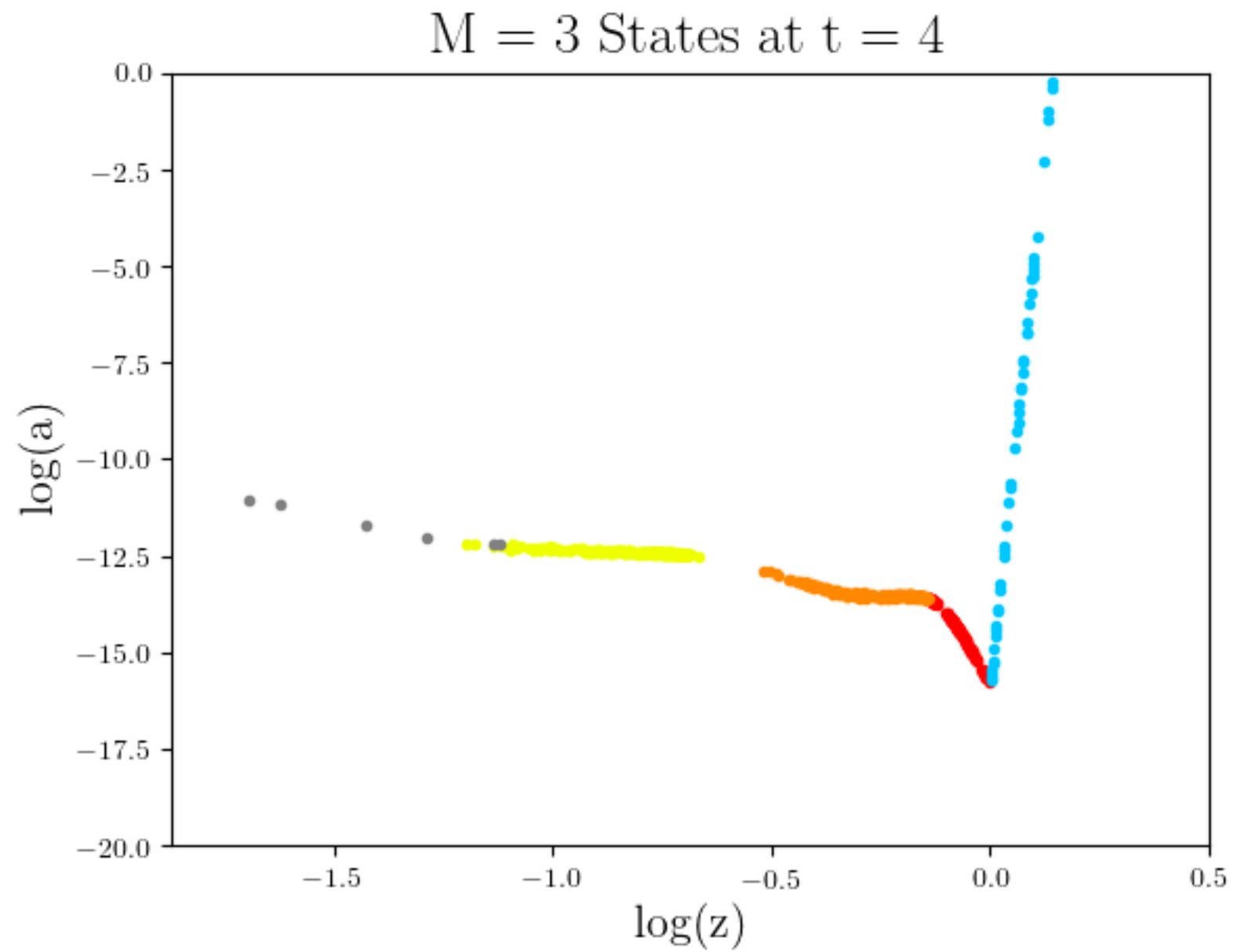
# Clustering $M = 3$ , 7 iterations



# Clustering $M = 3$ , 8 iterations

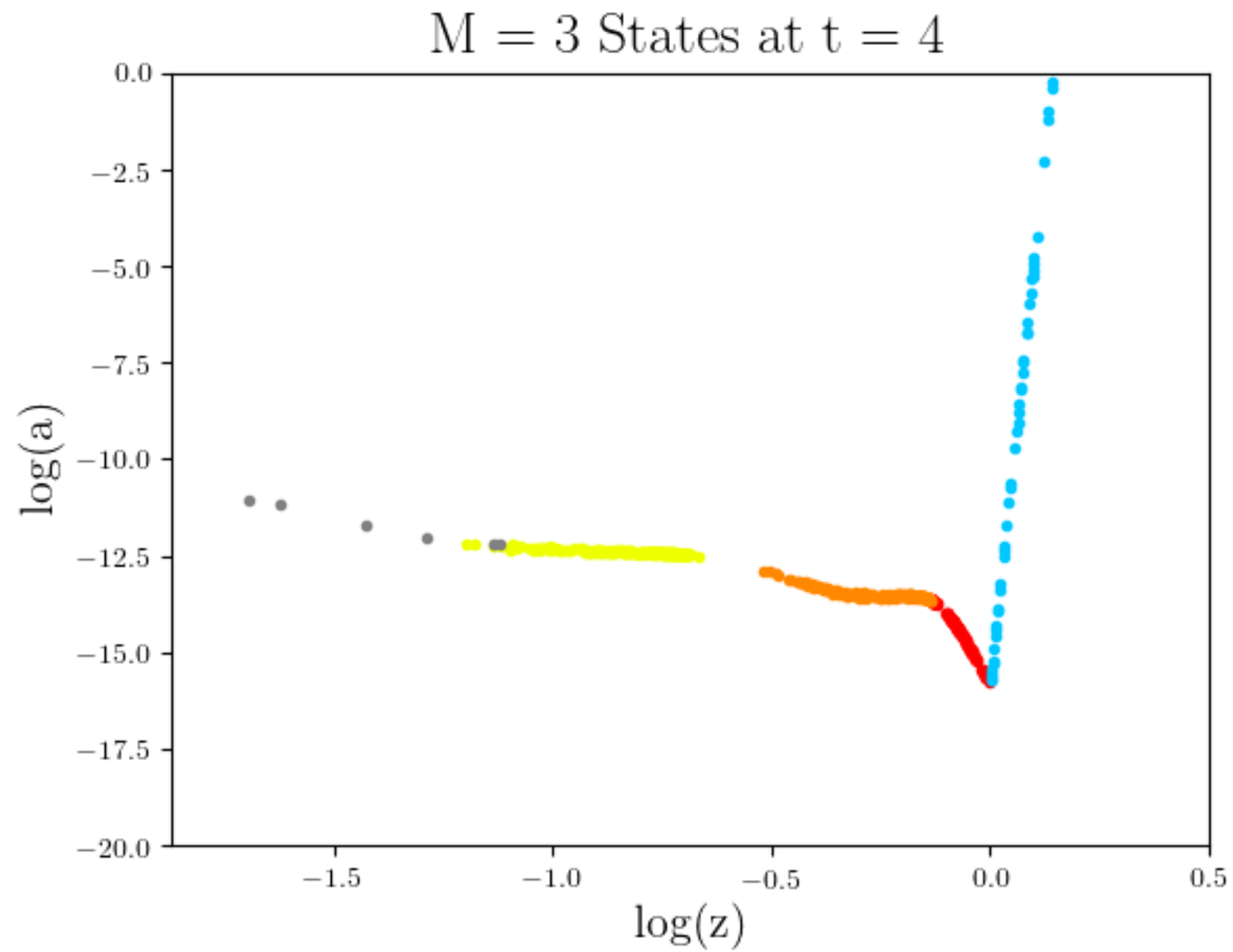


# Clustering $M = 3$ , 9 iterations

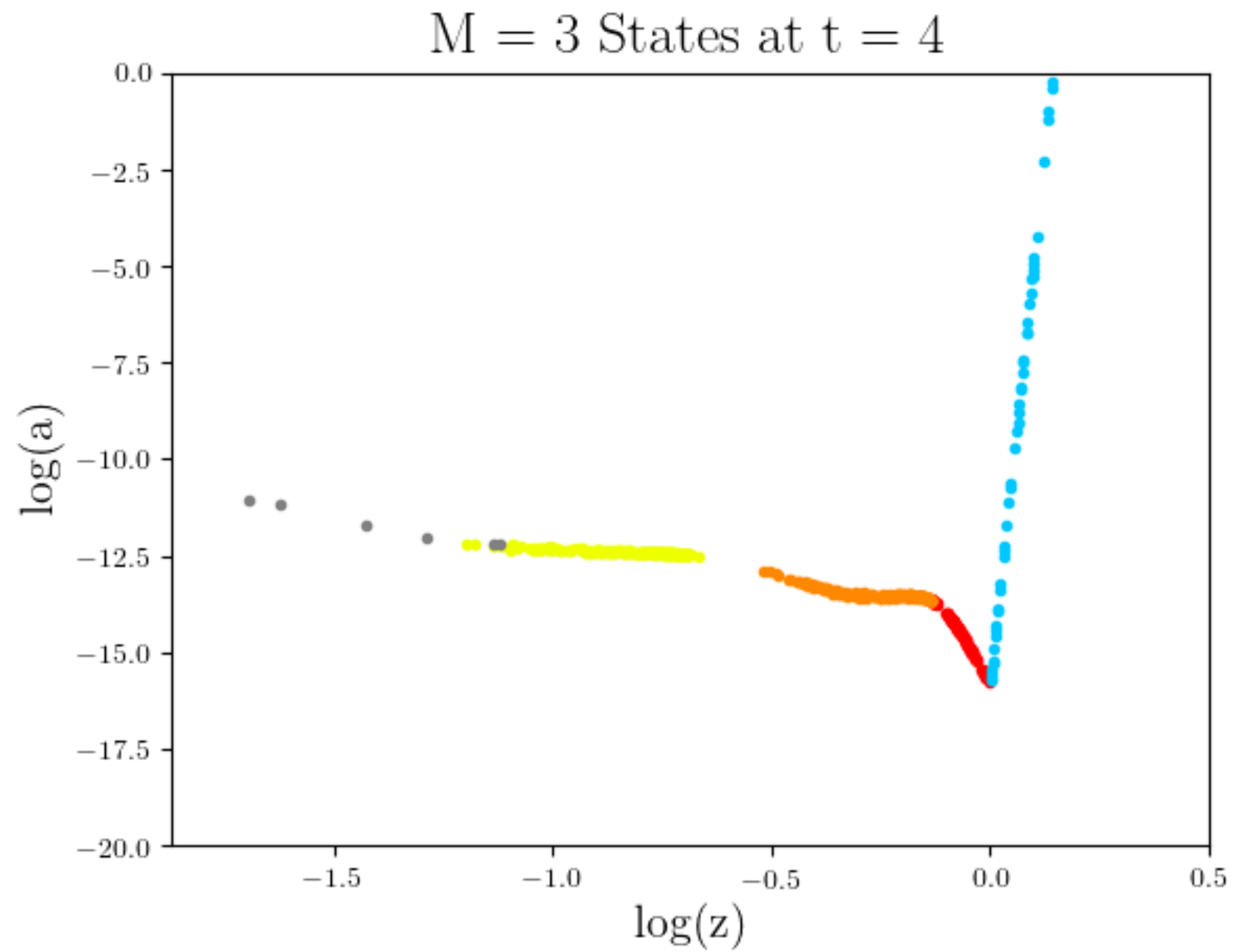




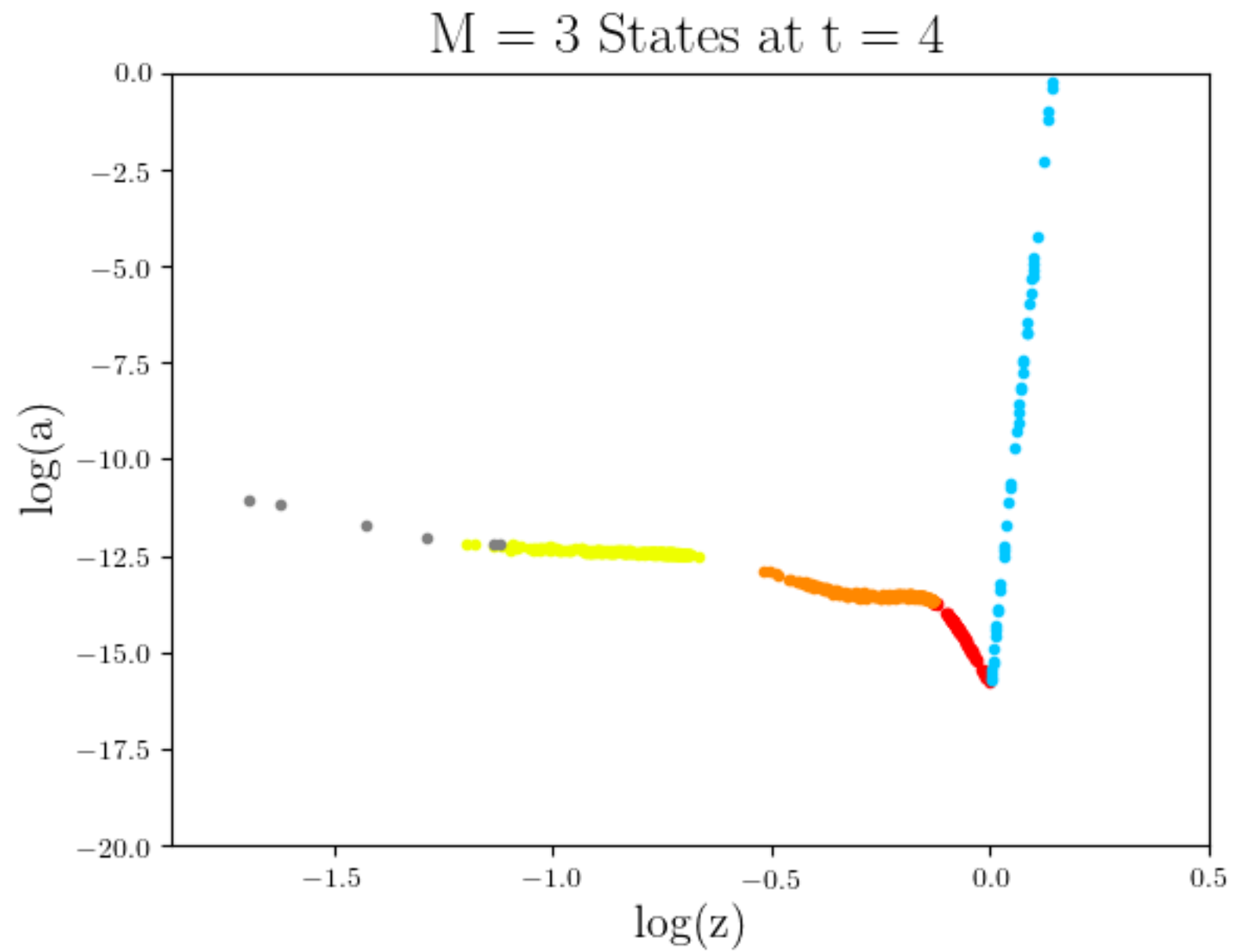
# Clustering $M = 3$ , 10 iterations



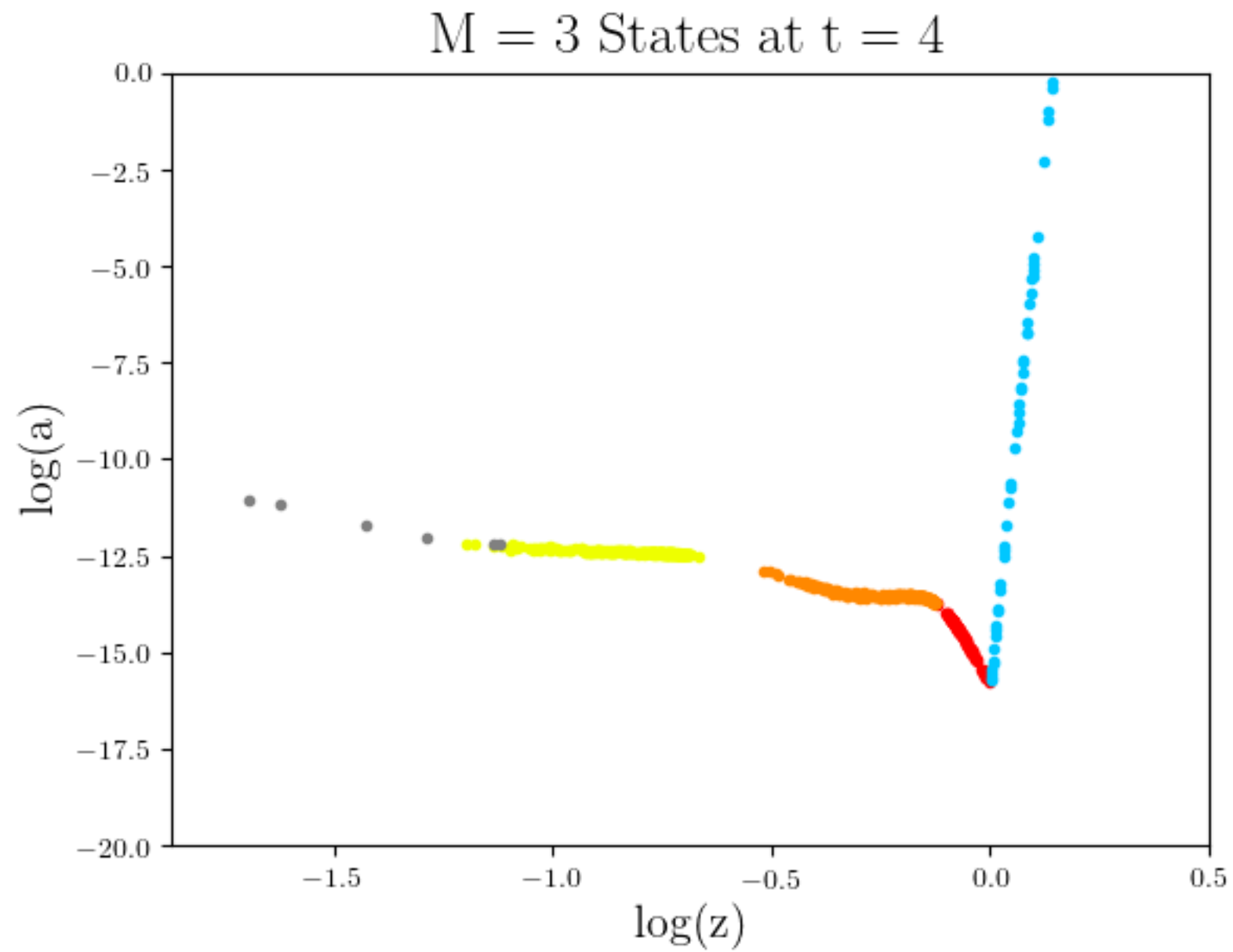
# Clustering $M = 3$ , 11 iterations



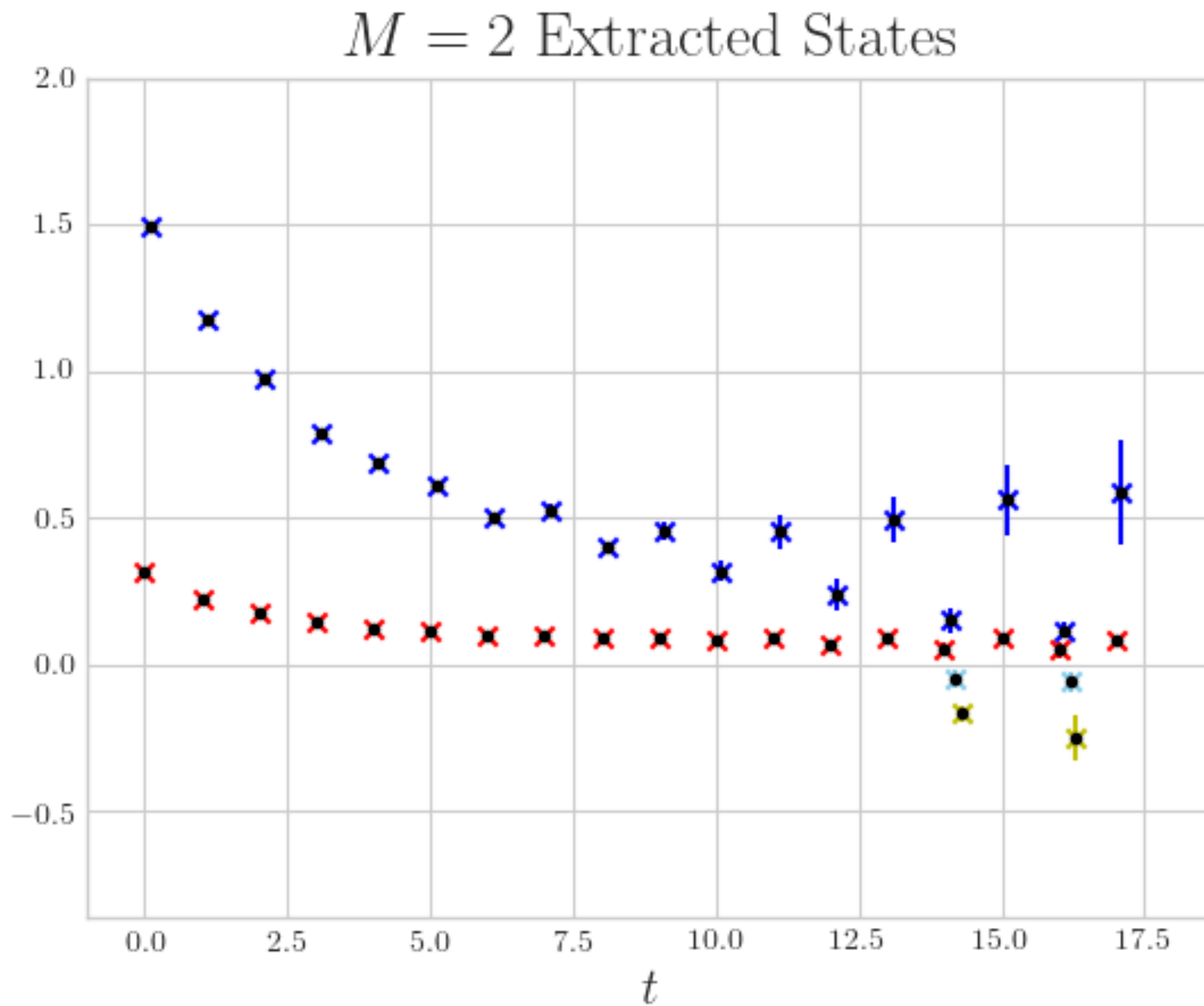
# Clustering $M = 3$ , 12 iterations



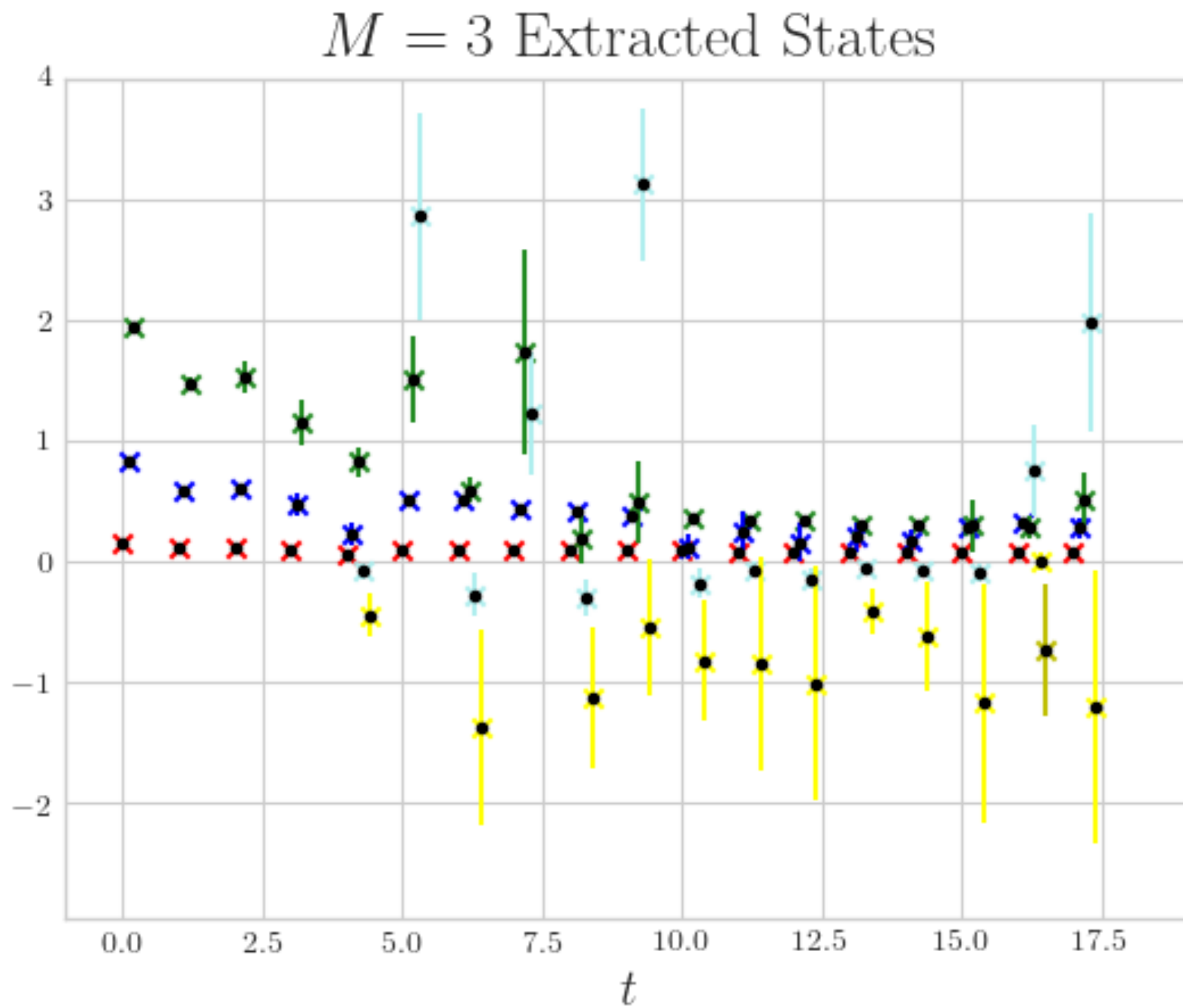
# Clustering $M = 3$ , 13 iterations



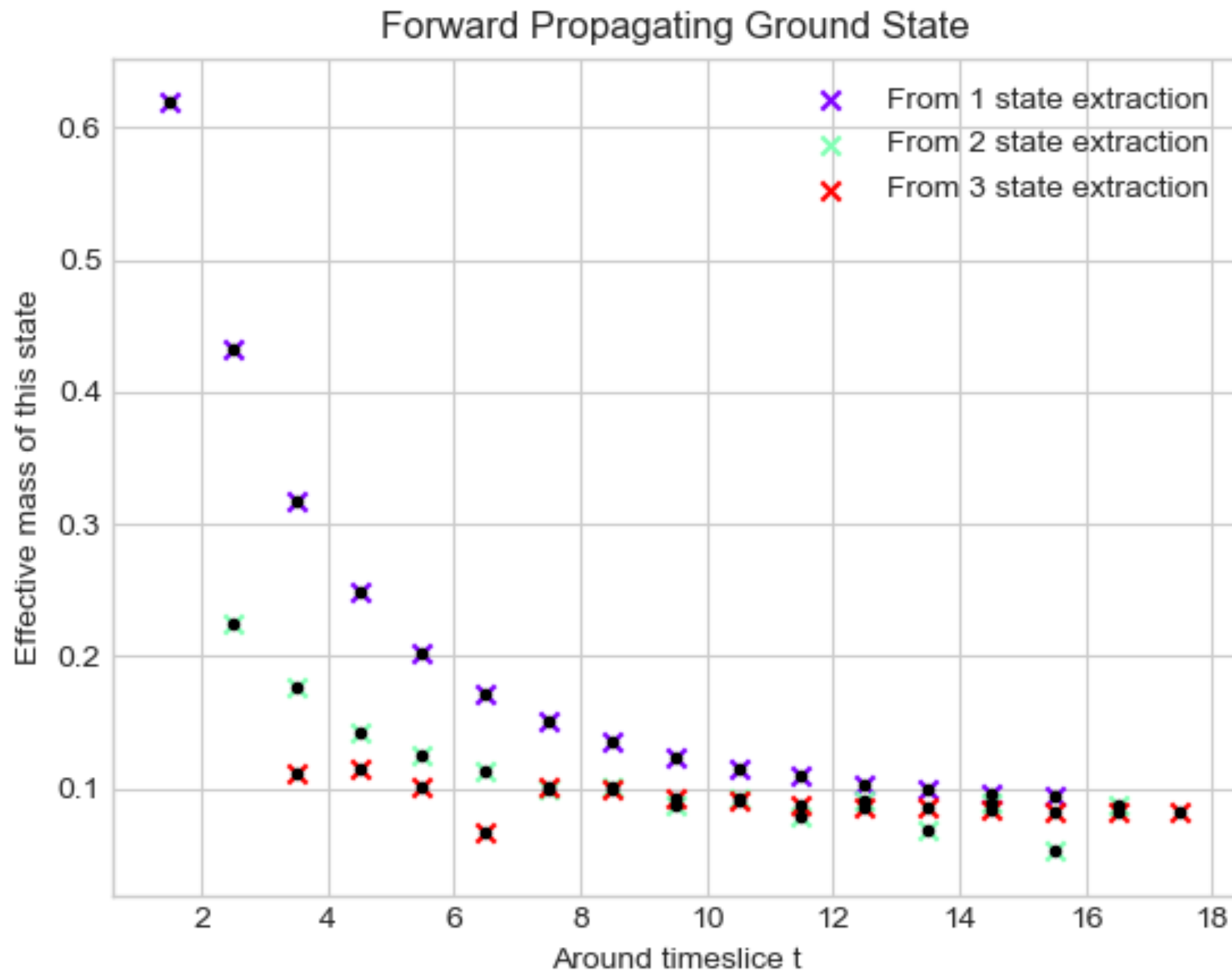
# Preliminary Results



# Preliminary Results

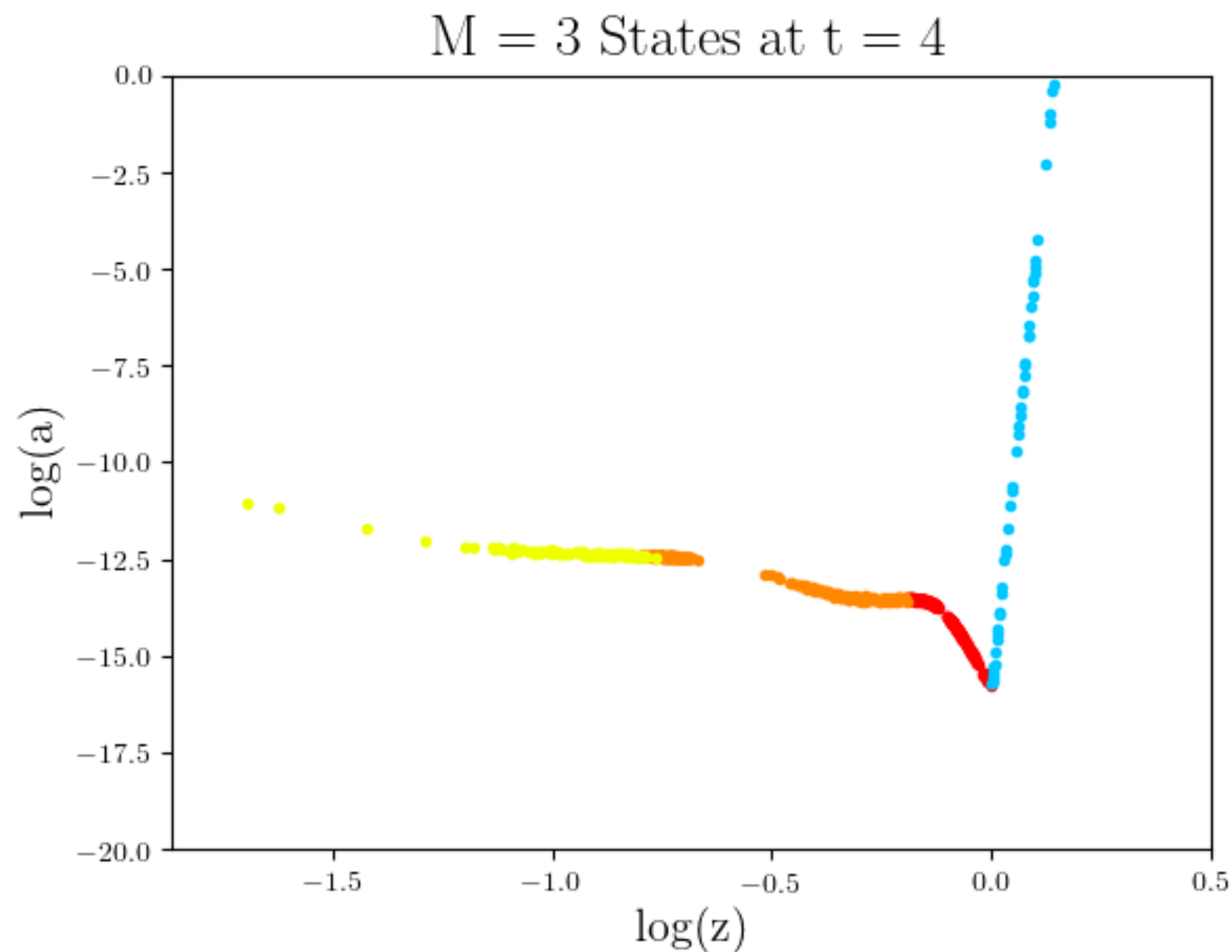


# Preliminary Results



# Future Work

- **Non-Gaussian clusters - try a new distance metric**  
-Don't worry about noisier time slices






# Future Work

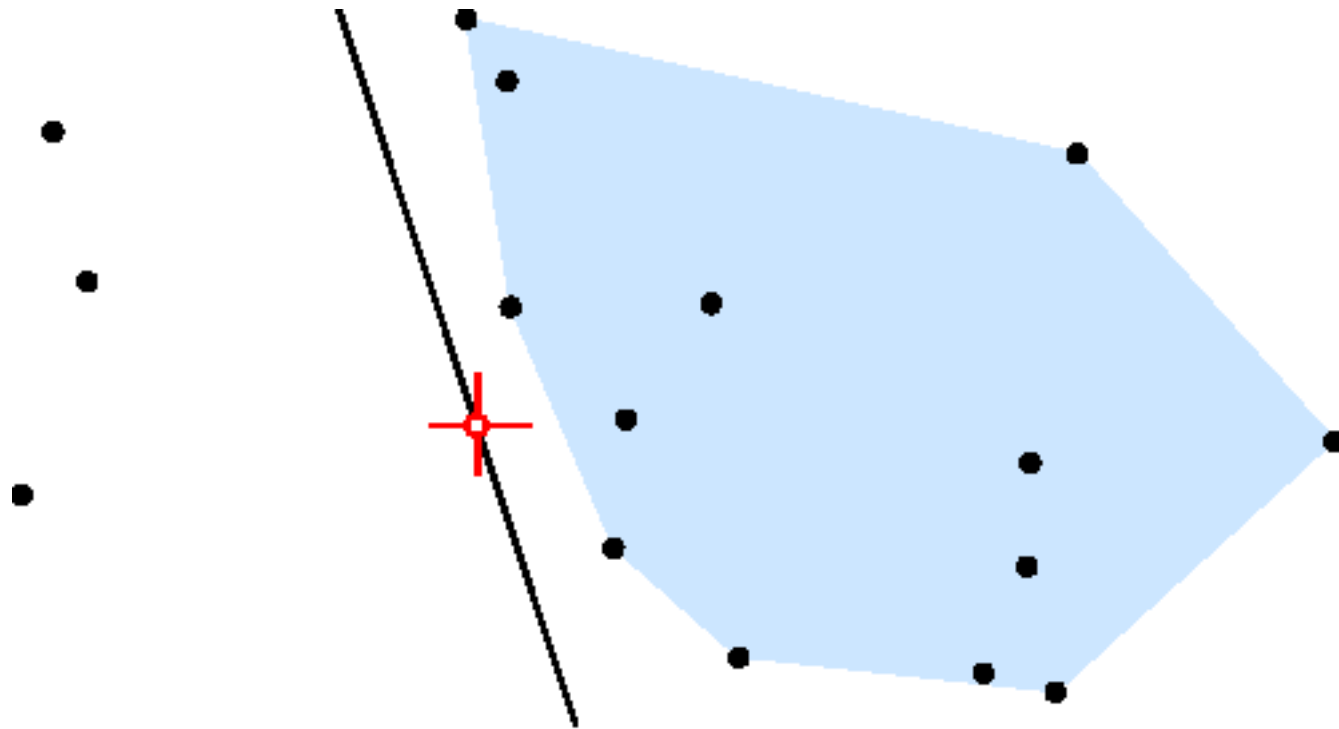
- **Non-Gaussian clusters - try a new distance metric**  
-Don't worry about noisier time slices
- **All data in “stencil” - extract  $M = T/2$  states**  
-Remove all operator bias

$$0 = \begin{vmatrix} y_0 & y_1 & \cdots & y_{M-2} & y_{M-1} & 1 \\ y_1 & y_2 & \cdots & y_{M-1} & y_M & z \\ y_2 & y_3 & \cdots & y_M & y_{M+1} & z^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ y_M & y_{M+1} & \cdots & y_{2M-2} & y_{2M-1} & z^M \end{vmatrix}$$


  
Hankel matrix

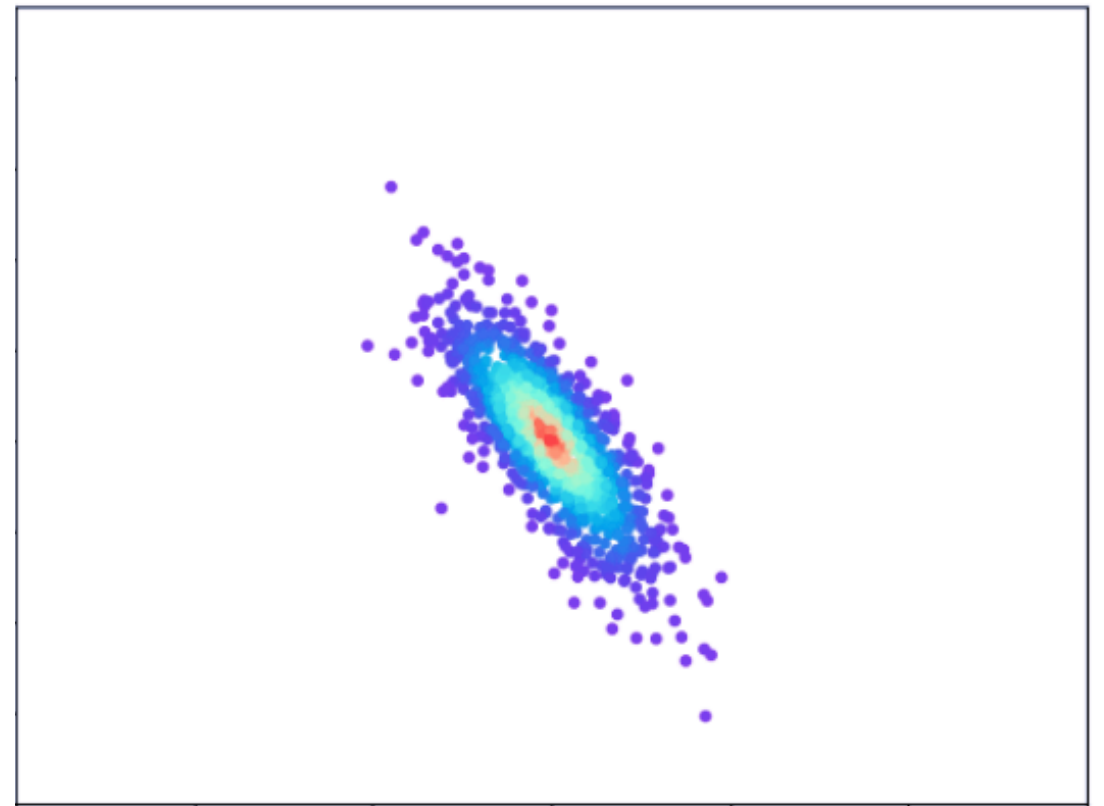
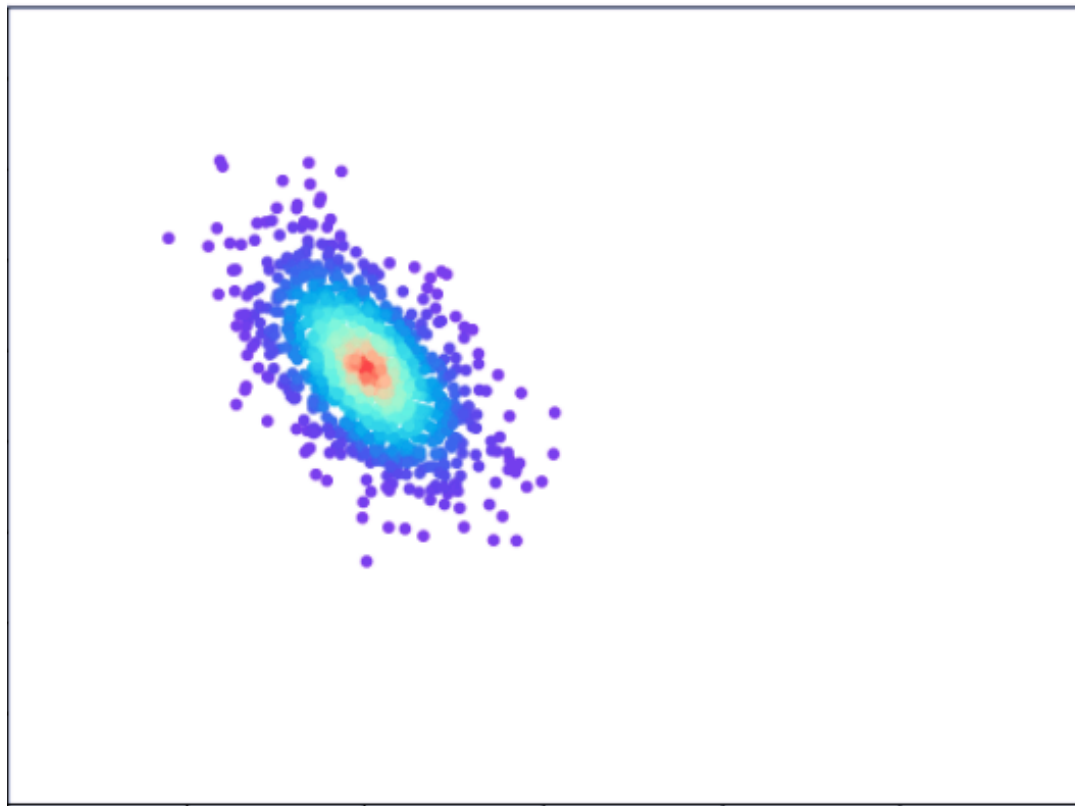
# Possible solution: Tukey Depth

Multidimensional generalization of *percentiles*



# Possible solution: Tukey Depth

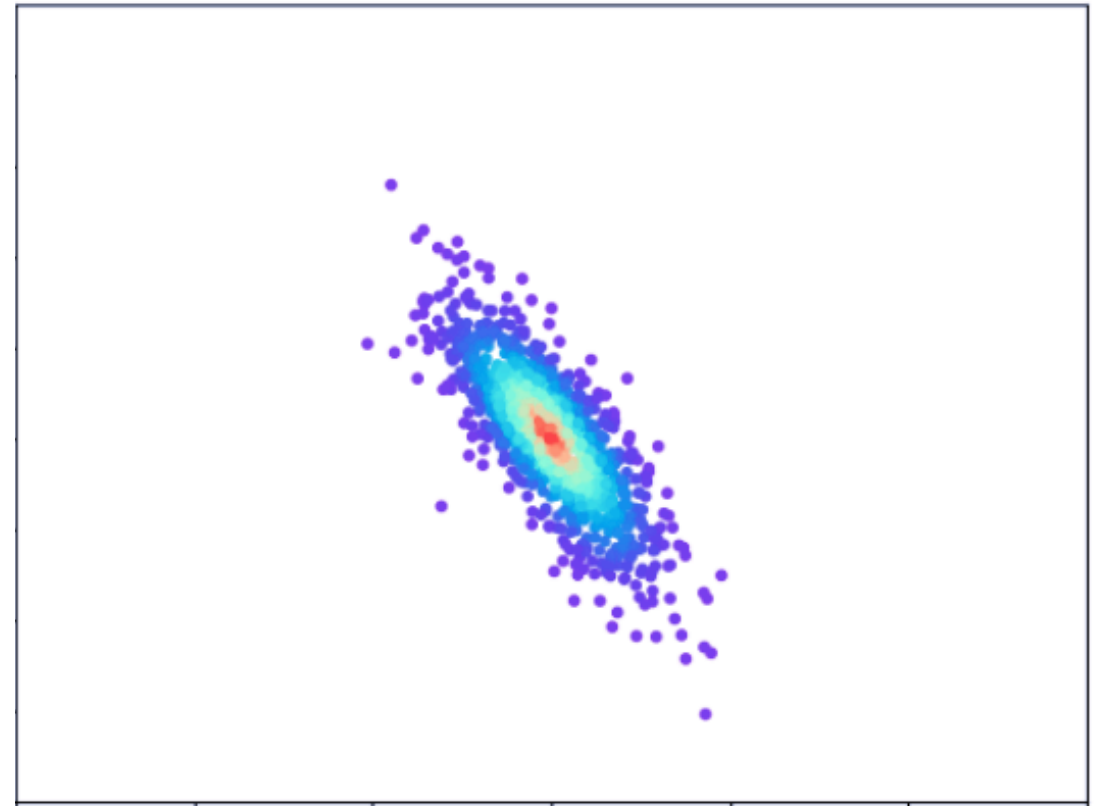
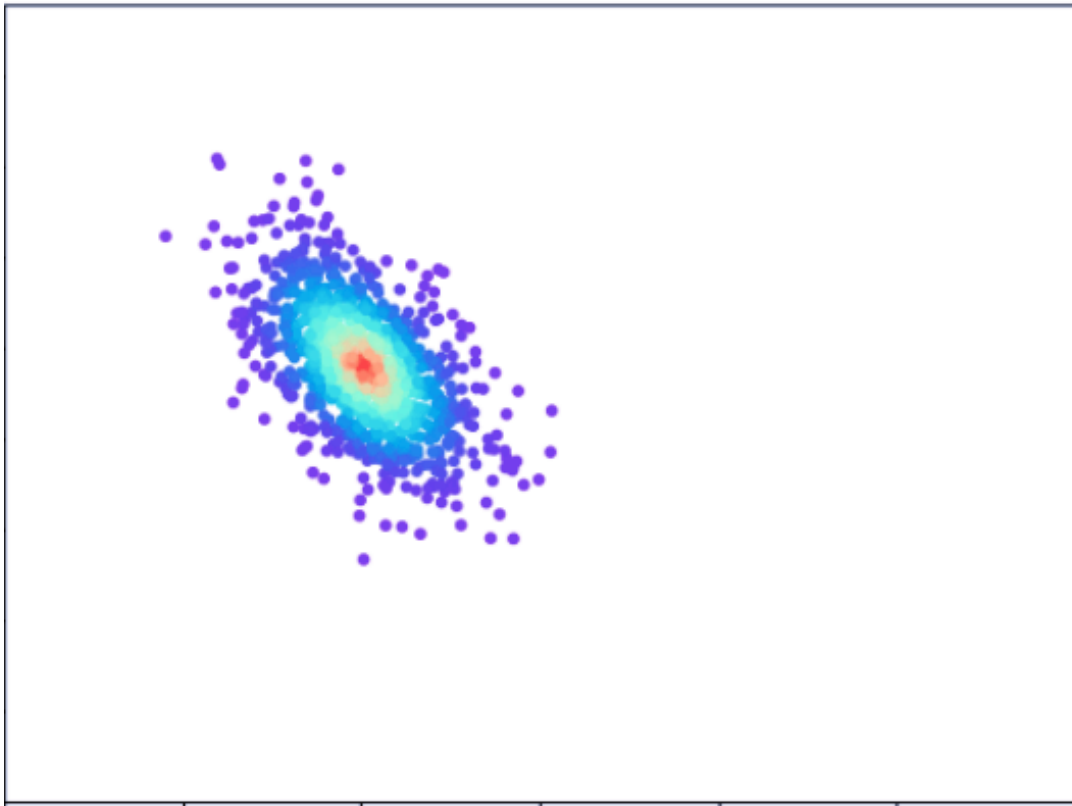
Multidimensional generalization of *percentiles*



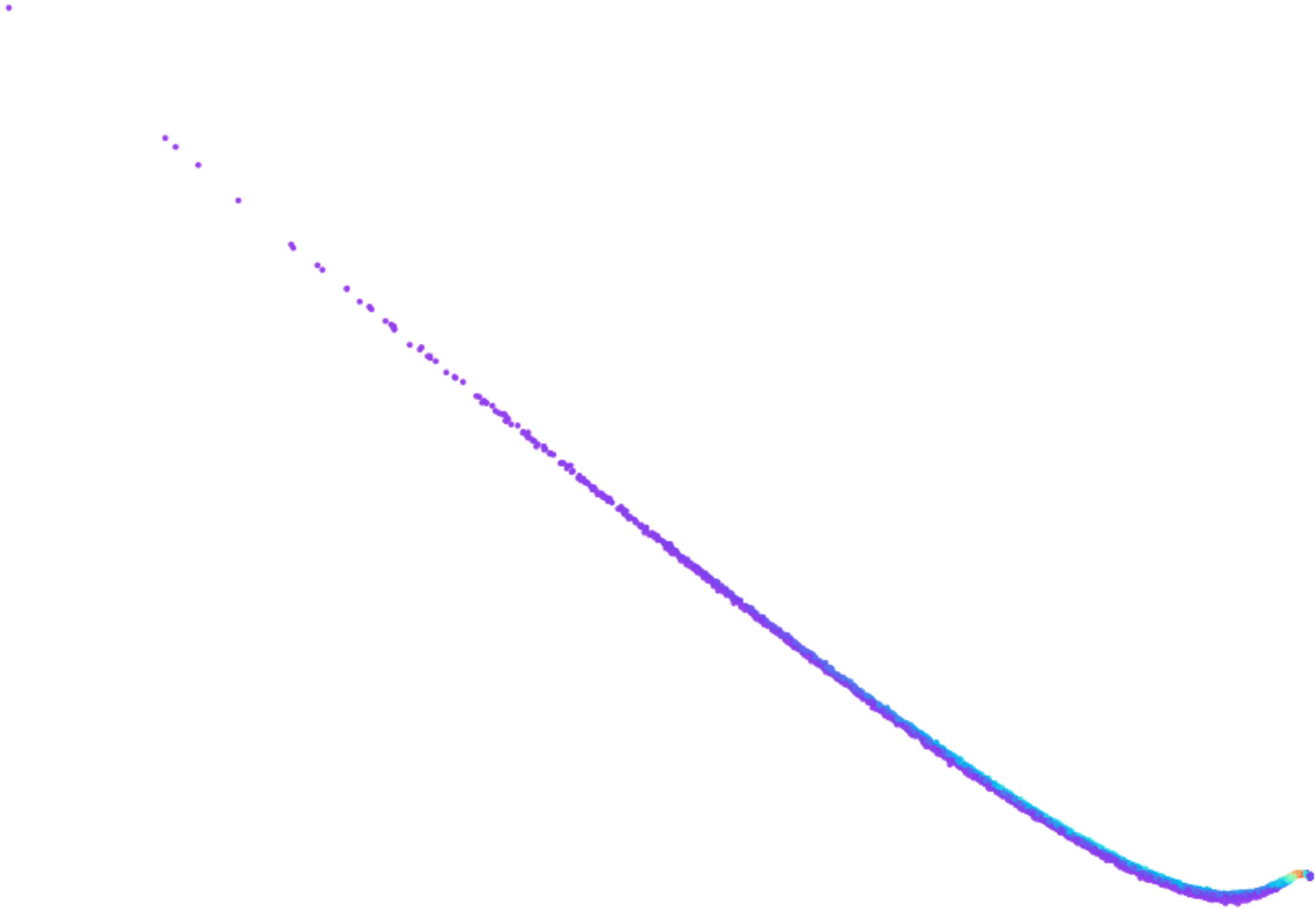
# Possible solution: Tukey Depth

Multidimensional generalization of *percentiles*

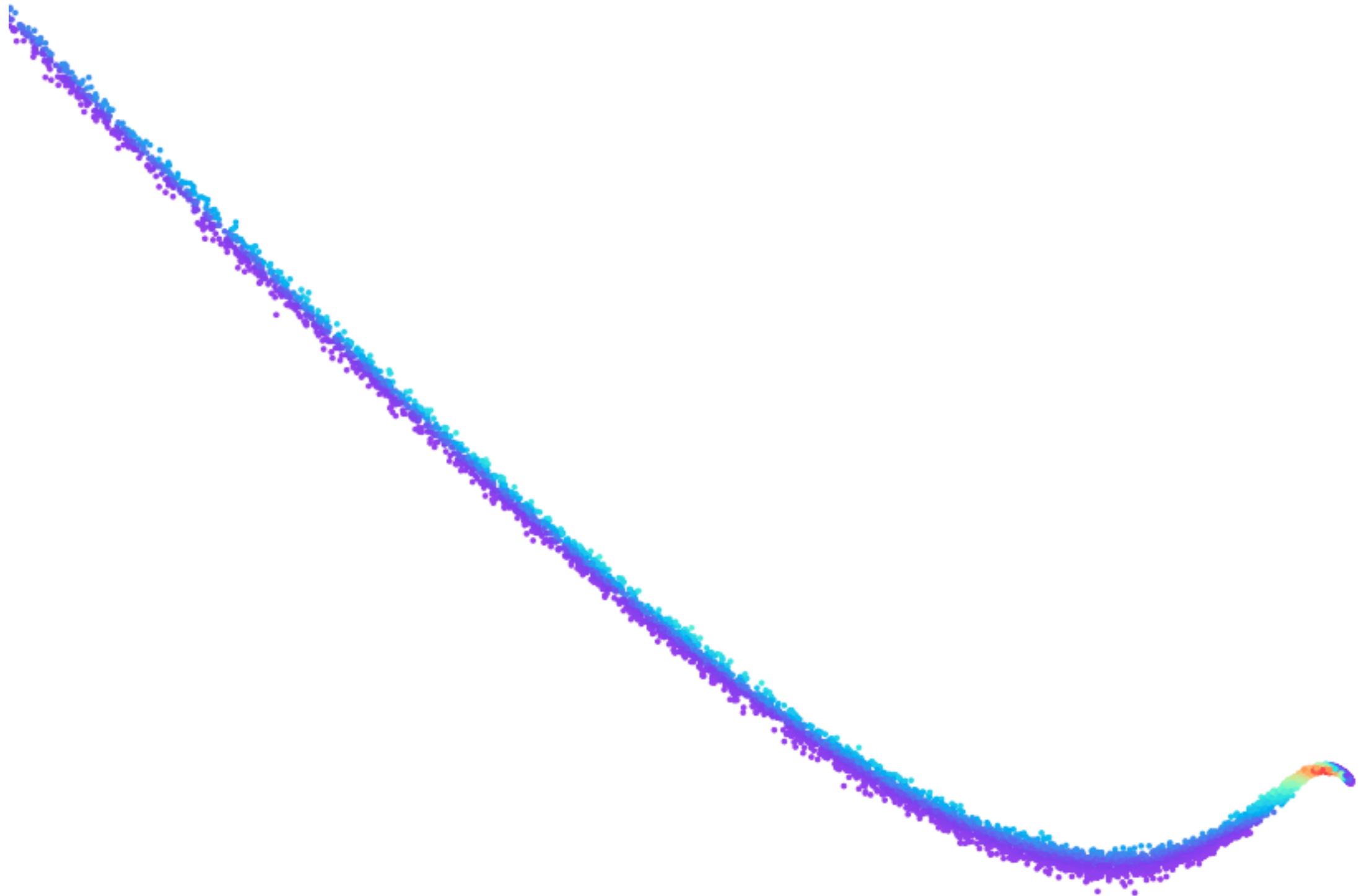
Non-parametric statistic!



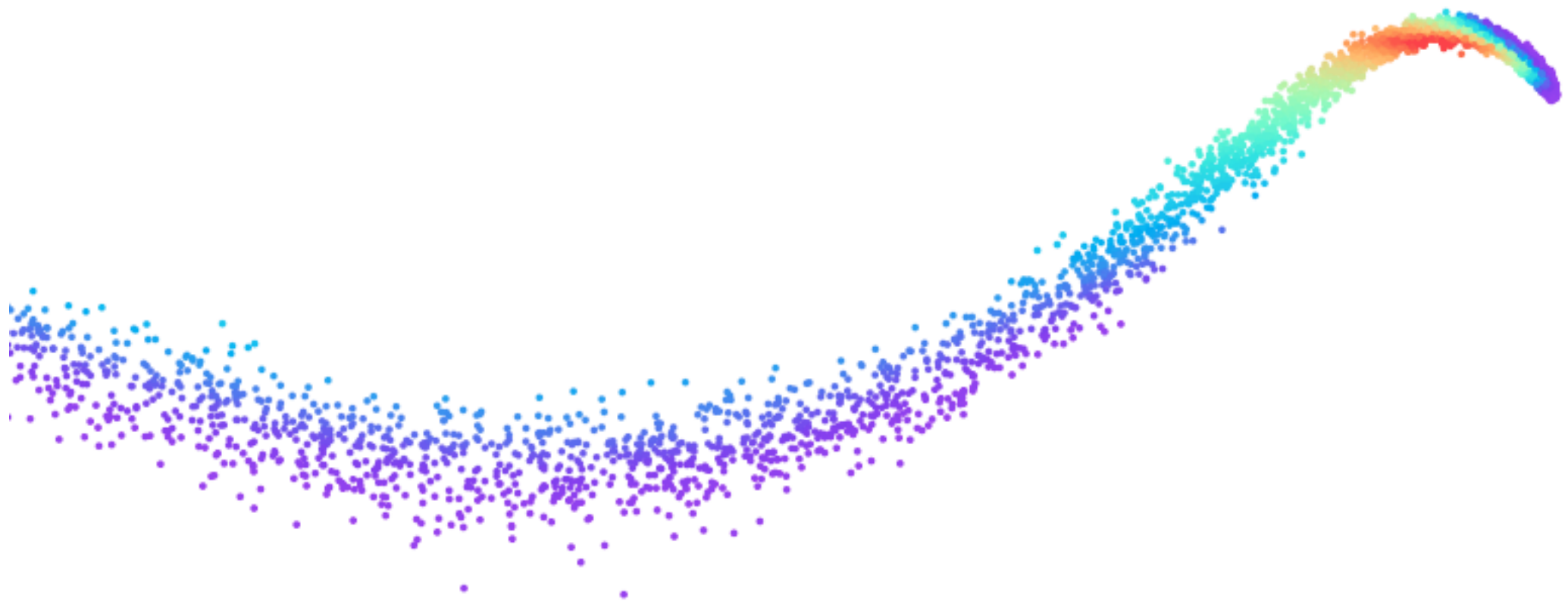
# Tukey Depth Example with non-Gaussian Data



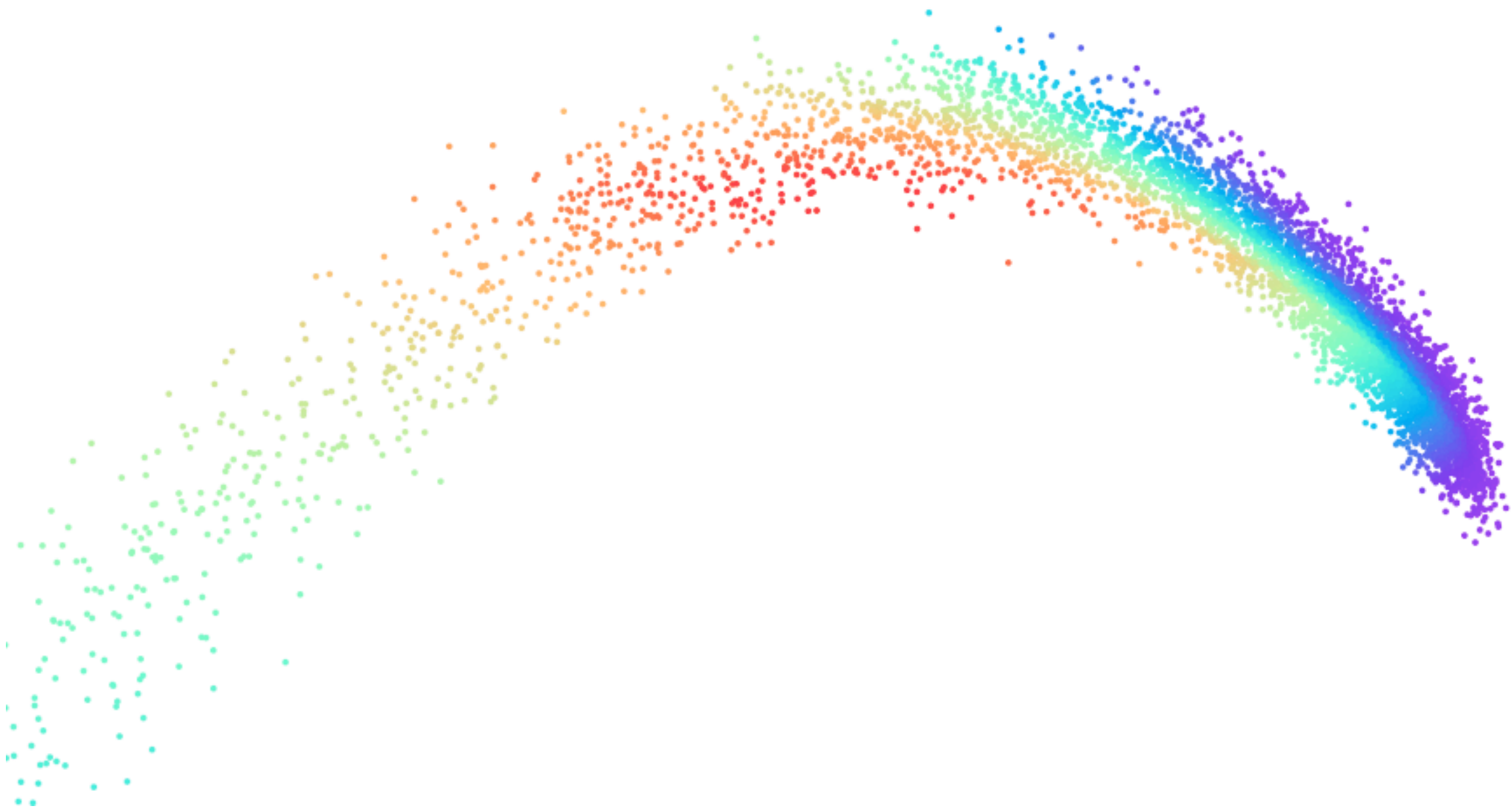
# Tukey Depth Example with non-Gaussian Data



# Tukey Depth Example with non-Gaussian Data



# Tukey Depth Example with non-Gaussian Data





# Conclusion

- **Extracting excited states is important for lattice QCD and BSM lattice**
- **Standard method involves fitting to exponentials and has many known problems**
- **Prony's method may be a better approach if we can identify clusters**
- **We will need a better clustering algorithm to account for weirdly shaped clusters**

**Thanks!**

