Distance between configurations in MCMC simulations and the emergence of AdS geometry in the simulated tempering algorithm

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"Matrix Models for Noncommutative Geometry and String Theory "

based on work with

N. Matsumoto (Kyoto Univ) **and N. Umeda** (PWC)

[arXiv:1705.0609, JHEP 1712 (2017) 001 (FMN1), arXiv:1806.10915 (FMN2)]

1. Introduction

Motivation (1/2)

There has long been an expectation
that quantum mechanics has its origin in randomness.

[Nelson, Parisi-Wu, ...]

⇩

Question:
Can quantum gravity be treated in such a framework?

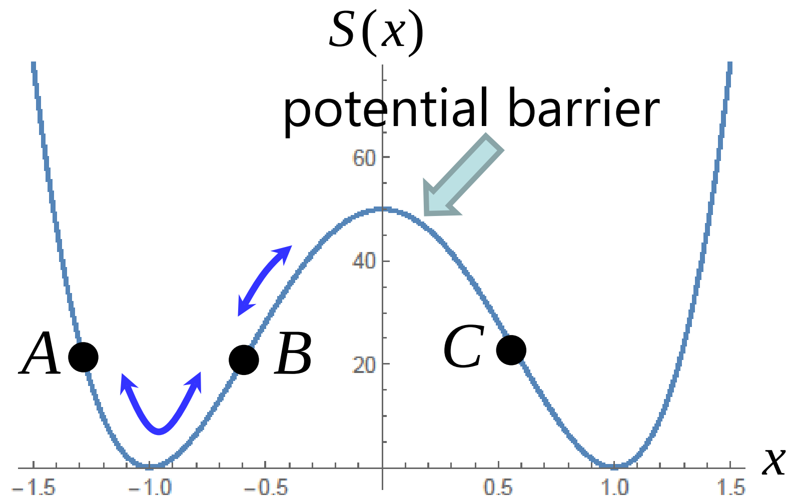
Main purpose of my talk is to show:

- One can introduce a geometry to any stochastic system which is based on Markov-chain Monte Carlo (MCMC), s.t. it reflects the difficulty of transitions between two configurations.
- Such geometry possesses a larger (or largest) symmetry if the algorithm is optimized s.t. distances are minimized.
- This distance gives another method to introduce a geometry to matrix models

Motivation (2/2)

To think more concretely,
let us consider the action

$$S(x) = \frac{\beta}{2}(x^2 - 1)^2 \quad (\beta \gg 1)$$



Separation of $A-B$ and that of $B-C$ are almost the same in x space.

However, in MCMC simulations,

A can be reached from B easily ⇦ "close" in MC

C cannot be reached from B easily ⇦ "far" in MC

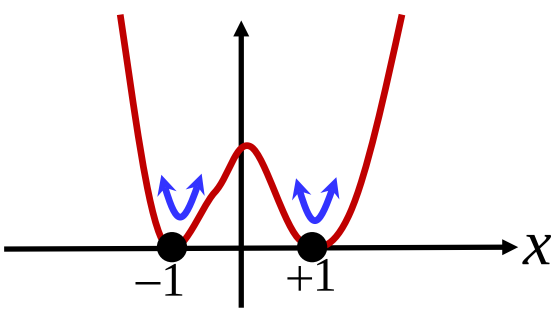
⇩

We introduce a measure that enumerates this "distance".

Main results

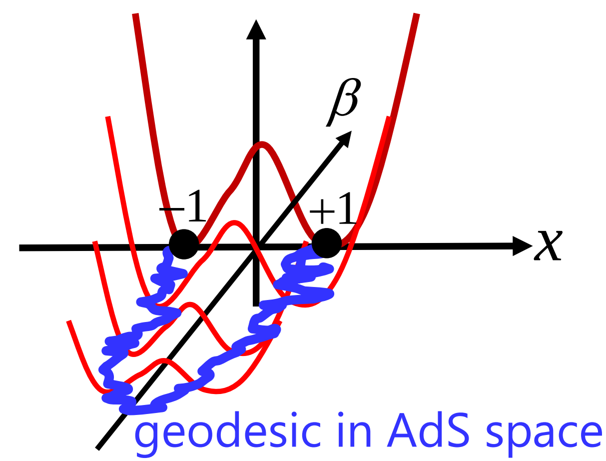
- This definition is universal for MCMC algorithms that generate local moves in configuration space
- The distance gives an AdS geometry when a simulated tempering is implemented for multimodal distributions with optimized parameters

original config space $\{x\}$



$$S(x) = \frac{\beta}{2}(x^2 - 1)^2 \quad (\beta \gg 1)$$

extended config space $\{(x, \beta)\}$



- This gives another method to introduce a distance in matrix models

Plan

1. Introduction (done)
2. Definition of distance
   - preparation
   - definition of distance
   - universality of distance
3. Examples
   - unimodal case
   - multimodal case
4. Distance for simulated tempering
   - simulated tempering
   - emergence of AdS geometry
   - AdS geometry from matrix models
5. Conclusion and outlook

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Preparation 1: MCMC simulation (1/3)

$\mathcal{M} = \{x\}$: configuration space

$S(x)$: action

We want to estimate VEVs of operators $\mathcal{O}(x)$:

$$\langle \mathcal{O}(x) \rangle \equiv \frac{1}{Z} \int dx\, e^{-S(x)}\, \mathcal{O}(x) \quad \left(Z = \int dx\, e^{-S(x)} \right)$$

In MCMC simulations:

- Regard $p_{\text{eq}}(x) \equiv \frac{1}{Z} e^{-S(x)}$ as a PDF
- Introduce a Markov chain

transition probability matrix

$$p_{n-1}(x) \to p_n(x) = \int dy\, P(x\,|\,y)\, p_{n-1}(y) = \int dy\, P^n(x\,|\,y)\, p_0(y)$$

s.t. $p_n(x)$ converges uniquely to $p_{\text{eq}}(x)$ in the limit $n \to \infty$

$\left[\text{i.e., } P^n(x\,|\,y) \simeq p_{\text{eq}}(x) \quad (n \geq n_0) \right]$

Preparation 1: MCMC simulation (2/3)

- Starting from an initial value x_0, generate $x_1, x_2, \ldots$ following the transition matrix $P(x_i \mid x_{i-1})$

$$x_0 \xrightarrow{P} x_1 \xrightarrow{P} \cdots \xrightarrow{P} x_{n_0} \xrightarrow{P} \underset{\equiv\, y_1}{x_{n_0+1}} \xrightarrow{P} \underset{\equiv\, y_2}{x_{n_0+2}} \xrightarrow{P} \cdots \xrightarrow{P} \underset{\equiv\, y_M}{x_{n_0+M}} \xrightarrow{P} \cdots$$

relaxation (for $x_0, \ldots, x_{n_0}$); generated with $\sim p_{\text{eq}}(x)$ (for $y_1, \ldots, y_M$)

- Take a sample $\{y_m\}_{m=1,\ldots,M}$ after the system is well relaxed

- Estimate VEVs of operators $\mathcal{O}(x)$ as a sample average:

$$\langle \mathcal{O}(x) \rangle \approx \frac{1}{M} \sum_{m=1}^{M} \mathcal{O}(y_m)$$

⇩

We first would like to establish a mathematical framework which enables the systematic understanding of relaxation

Preparation 1: MCMC simulation (3/3)

We assume that

(1) $P(x\,|\,y)$ satisfies the detailed balance condition:

$$P(x\,|\,y)\,p_{\text{eq}}(y) = P(y\,|\,x)\,p_{\text{eq}}(x)\left(\Leftrightarrow P(x\,|\,y)e^{-S(y)} = P(y\,|\,x)e^{-S(x)}\right)$$

(2) all of the eigenvalues of P are positive

NB : (1) can be written as

$$\hat{P}e^{-S(\hat{x})} = e^{-S(\hat{x})}\,\hat{P}^T \qquad \left(\begin{aligned} &P(x\,|\,y) = \langle x\,|\,\hat{P}\,|\,y\rangle \\ &\hat{x} \equiv \int dx\, x\,|\,x\rangle\langle x\,| \end{aligned}\right)$$

NB : (2) is not too restrictive

In fact, if P has negative eigenvalues,
then we instead can use P^2 as the elementary transition matrix,
for which

- all the eigenvalues are positive
- the same detailed balance condition is satisfied as P :

$$P^2(x\,|\,y)e^{-S(y)} = P^2(y\,|\,x)e^{-S(x)}$$

Preparation 2: Transfer matrix (1/2)

[MF-Matsumoto-Umeda1]

We introduce the "transfer matrix" :

$$\boxed{\hat{T} \equiv e^{S(\hat{x})/2}\,\hat{P}\,e^{-S(\hat{x})/2}} \quad \left(\Leftrightarrow T(x\,|\,y) = e^{S(x)/2}\,P(x\,|\,y)\,e^{-S(y)/2} \right)$$

<u>properties</u>:

(1) $\hat{T} = \hat{T}^T \quad \left(\Leftrightarrow \hat{P} e^{-S(\hat{x})} = e^{-S(\hat{x})}\,\hat{P}^T \right)$

(2) same eigenvalue set as $\hat{P}$ (thus all positive)

We order the EVs as

$$\lambda_0 = 1 > \lambda_1 \geq \lambda_2 \geq \cdots > 0$$

<u>spectral decomposition</u>:

$$\hat{T} = \sum_{k\geq 0} \lambda_k\,|k\rangle\langle k| = |0\rangle\langle 0| + \sum_{k\geq 1} \lambda_k\,|k\rangle\langle k|$$

where

$$\langle x\,|\,0\rangle = \frac{1}{\sqrt{Z}}\,e^{-S(x)/2} = \sqrt{p_{\mathrm{eq}}(x)}$$

Preparation 2: Transfer matrix (2/2)

Note that $\hat{P}^n \Leftrightarrow \hat{T}^n = |0\rangle\langle 0| + \sum_{k\geq 1} \lambda_k^n |k\rangle\langle k| \quad (\lambda_0 = 1 > \lambda_1 \geq \lambda_2 \geq \cdots > 0)$

⇩

<u>relaxation to equilibrium</u>

$\Leftrightarrow$ relaxation of $\hat{T}^n$ to $|0\rangle\langle 0|$ in the limit $n \to \infty$

$\Leftrightarrow$ decoupling of modes $|k\rangle$ with $k \geq 1$

<u>NB</u>:

decoupling occurs earlier for higher modes (i.e. for larger k)

<u>NB</u>:

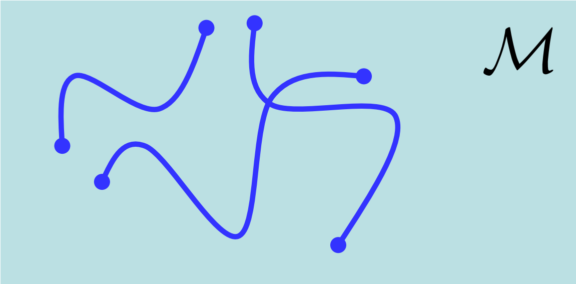
relaxation time τ can be estimated from $\lambda_1 \sim e^{-1/\tau}$

slow relaxation $\Leftrightarrow$ $\lambda_1 \sim 1$

Preparation 3: Connectivity between configs (1/3)

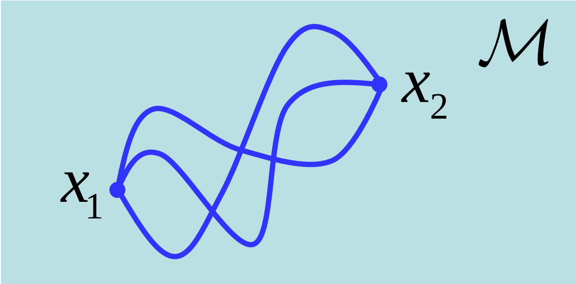
[MF-Matsumoto-Umeda1]

$\mathbf{X}_n \equiv$ (set of sequences of n processes in $\mathcal{M}$)



$\mathbf{X}_n(x_1, x_2)$

$\equiv \begin{pmatrix} \text{set of sequences of } n \text{ processes in } \mathcal{M} \\ \text{that start from } x_2 \text{ and end at } x_1 \end{pmatrix}$



We define the connectivity between two configs as

$$f_n(x_1, x_2) \equiv \frac{|\mathbf{X}_n(x_1, x_2)|}{|\mathbf{X}_n|}$$

$= (\text{prob to obtain } x_1 \text{ from } x_2) \times (\text{prob to have } x_2)$

det balance

$$= P^n(x_1 \,|\, x_2) \frac{1}{Z} e^{-S(x_2)} \left(= P^n(x_2 \,|\, x_1) \frac{1}{Z} e^{-S(x_1)} = f_n(x_2, x_1) \right)$$

Preparation 3: Connectivity between configs (2/3)

normalized connectivity ("half-time overlap"):

$$\left(\begin{aligned} & f_n(x_1, x_2) \\ & = P^n(x_1 \mid x_2) \frac{1}{Z} e^{-S(x_2)} \\ & = P^n(x_2 \mid x_1) \frac{1}{Z} e^{-S(x_1)} \end{aligned} \right)$$

$$F_n(x_1, x_2) \equiv \frac{f_n(x_1, x_2)}{\sqrt{f_n(x_1, x_1)\, f_n(x_2, x_2)}} = \sqrt{\frac{P^n(x_1 \mid x_2) P^n(x_2 \mid x_1)}{P^n(x_1 \mid x_1) P^n(x_2 \mid x_2)}} = \frac{K_n(x_1, x_2)}{\sqrt{K_n(x_1, x_1) K_n(x_2, x_2)}}$$

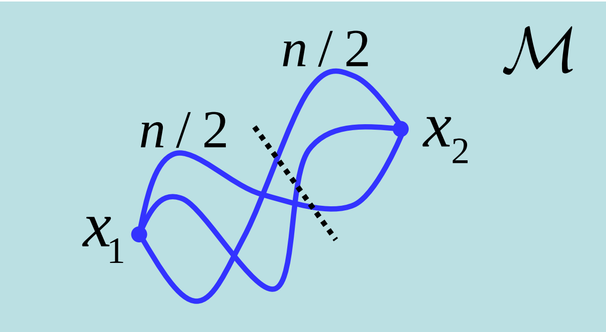
$$\left(K_n(x_1, x_2) \equiv \langle x_1 \mid \hat{T}^n \mid x_2 \rangle \right)$$

$\Rightarrow$ $F_n(x_1, x_1) = 1$

$F_n(x_1, x_2)$ is actually the overlap between two normalized "half-time" elapsed states:

$$F_n(x_1, x_2) \equiv \langle x_1, n/2 \mid x_2, n/2 \rangle$$

$$\left(|x, n/2\rangle \equiv \hat{T}^{n/2} \mid x \rangle / \| \hat{T}^{n/2} \mid x \rangle \| \right)$$



Preparation 3: Connectivity between configs (3/3)

properties of $F_n(x_1, x_2)$

$$F_n(x_1,x_2) = \frac{K_n(x_1,x_2)}{\sqrt{K_n(x_1,x_1)K_n(x_2,x_2)}} = \langle x_1, n/2 \mid x_2, n/2 \rangle$$

(1) $F_n(x_1,x_2) = F_n(x_2,x_1)$

(2) $0 \le F_n(x_1,x_2) \le 1$

(3) $F_n(x_1,x_2) = 1 \Leftrightarrow x_1 = x_2$ (when n is finite)

(4) $\lim_{n\to\infty} F_n(x_1,x_2) = 1 \ (\forall x_1, x_2)$

+

(A) If x_1 can be easily reached from x_2 in n steps, then $F_n(x_1,x_2) \simeq 1$

(B) If x_1 and x_2 are separated by high potential barriers, then $F_n(x_1,x_2) \ll 1$

proof of (4):

In the limit $n \to \infty$, $\hat{T}^n \to |0\rangle\langle 0|$, and thus,

$$K_n(x_1,x_2) = \langle x_1 | \hat{T}^n | x_2 \rangle \to \langle x_1 | 0 \rangle \langle 0 | x_2 \rangle = \sqrt{K_n(x_1,x_1)K_n(x_2,x_2)}.$$

Definition of distance

[MF-Matsumoto-Umeda1]

$$\theta_n(x_1, x_2) \equiv \arccos(F_n(x_1, x_2))$$

properties of $\theta_n(x_1, x_2)$

$$\begin{cases} (1) & \theta_n(x_1, x_2) = \theta_n(x_2, x_1) \\ (2) & \theta_n(x_1, x_2) \geq 0 \\ (3) & \theta_n(x_1, x_2) = 0 \Leftrightarrow x_1 = x_2 \ \text{(when } n \text{ is finite)} \\ (4) & \lim_{n\to\infty} \theta_n(x_1, x_2) = 0 \ (\forall x_1, x_2) \\ (5) & \theta_n(x_1, x_2) + \theta_n(x_2, x_3) \geq \theta_n(x_1, x_3) \end{cases}$$

+

(A) If x_1 can be easily reached from x_2 in n steps, then $\theta_n(x_1, x_2)$: small

(B) If x_1 and x_2 are separated by high potential barriers, then $\theta_n(x_1, x_2)$: large

Alternative definition of distance

[MF-Matsumoto-Umeda1]

Instead of $\theta_n(x_1, x_2) = \arccos(F_n(x_1, x_2))$,
one can also use the following as distance:

$$d_n^2(x_1, x_2) \equiv -2\ln F_n(x_1, x_2)$$ ⇐ we will mainly use this

or $$D_n^2(x_1, x_2) \equiv 2[1 - \ln F_n(x_1, x_2)]$$

$$\left(\begin{array}{l} F_n(x_1, x_2) \\ = \cos\theta_n(x_1, x_2) = e^{-(1/2) d_n^2(x_1, x_2)} = 1 - \frac{1}{2} D_n^2(x_1, x_2) \\ \text{They agree when } \theta_n \approx 0 \end{array} \right)$$

<u>NB</u>: analogy in quantum information

$$\begin{cases} \theta_n(x_1, x_2) : \text{Bures length} \\ D_n(x_1, x_2) : \text{Bures distance} \end{cases}$$ for two pure states $\rho_{1,2} = | x_{1,2}, n/2 \rangle \langle x_{1,2}, n/2 |$

Universality of distance (1/4)

[MF-Matsumoto-Umeda1]

The above distance is expected to be universal
for MCMC algorithms that generate local moves in config space.

("universal" in the sense that differences of distance between two such local MCMC algorithms can always be absorbed into a rescaling of n)

In fact,

universality of $d_n^2(x_1, x_2) \Leftrightarrow$ univ. of $K_n(x_1, x_2) = \langle x_1 | \hat{T}^n | x_2 \rangle$

$\Leftrightarrow$ univ. of $\hat{T} \equiv e^{-\epsilon \hat{H}}$

and,

If algorithms are sufficiently local,
then $\hat{H}$ are expected to be local operators
acting on functions over $\mathcal{M}$ in almost the same way.

⇩

The wave functions $\langle x | k \rangle$ must be almost the same for small k

Universality of distance (2/4)

This expectation can be explicitly checked using a simple model.

algorithm 1: Langevin

$$x_{n+1} = x_n + \sqrt{\epsilon}\,\nu_n - \epsilon S'(x_n) \quad \text{with } \langle \nu_n \nu_m \rangle_\nu = 2\delta_{n,m}$$

$$\Rightarrow \langle x | \hat{T} | y \rangle = \langle x | e^{-\epsilon \hat{H}} | y \rangle \simeq \frac{1}{\sqrt{4\pi\epsilon}} e^{-\frac{1}{4\epsilon}(x-y)^2 - \epsilon V\left(\frac{x+y}{2}\right)}$$

$$\text{with } V(x) = (1/4)\big(S'(x)\big)^2 - (1/2)S''(x)$$

algorithm 2: Metropolis (with Gaussian proposal of variance σ^2)

$$\langle x | \hat{T} | y \rangle = \langle x | \hat{P} | y \rangle \times e^{S(x)/2 - S(y)/2}$$

$$= \min\left(1, e^{-S(x)+S(y)}\right) \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-y)^2} \times e^{S(x)/2 - S(y)/2}$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-y)^2 - \frac{1}{2}|S(x) - S(y)|}$$

Universality of distance (3/4)

With the identification $\sigma^2 \sim \epsilon$,

both Hamiltonians $\hat{H}\left(\equiv -\frac{1}{\epsilon}\ln \hat{T}\right)$ become local in the limit $\epsilon \to 0$,

and have the same tendency to enhance transitions

when $|x-y|$ and $|S(x)-S(y)|$ are small.

⇓

The low energy structure of $\hat{H}$ should be almost the same.

⇓

The global structure of distance should be almost the same.

(The argument for universality is more trustworthy as the DOF of the system become larger.)

In fact,

the universality actually holds more than expected

even for a single DOF

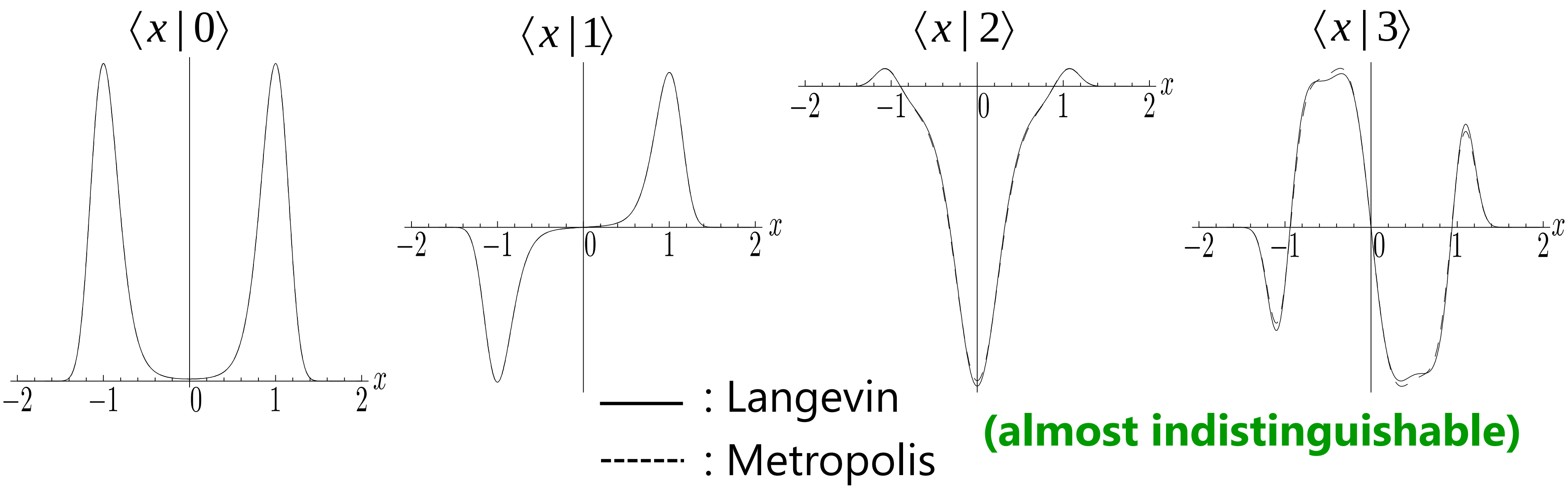
Universality of distance (4/4)

eigenvalues :

$$S(x)=\frac{\beta}{2}(x^2-1)^2 \quad (\beta=20)$$

	E_k (Lang)	E_k/E_1 (Lang)	E_k (Met)	E_k/E_1 (Met)
0	0	0	0	0
1	7.81 x 10^(-4)	1	7.62 x 10^(-4)	1
2	36.2	4.63 x 10^4	34.2	4.49 x 10^4
3	58.2	7.45 x 10^4	54.7	7.17 x 10^4

eigenfunctions :



(almost indistinguishable)

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Transfer matrix for Langevin

Langevin equation (continuum)

$$\dot{x}_t = \nu_t - S'(x_t) \text{ with} \begin{cases} x_{t=0} = x_0 \\ \langle \nu_t \nu_{t'} \rangle_\nu = 2\delta(t-t') \end{cases}$$

$$\Rightarrow \quad x_t = x_t(x_0, [\nu])$$

$$\Rightarrow \quad P_t(x \mid x_0) \equiv \left\langle \delta\left(x - x_t(x_0, [\nu])\right) \right\rangle_\nu = \langle x \mid e^{-t\hat{H}_{\mathrm{FP}}} \mid x_0 \rangle$$

$$\text{with } \hat{H}_{\mathrm{FP}} = -\partial_x [\partial_x + S'(x)]$$

$$\Rightarrow \quad K_t(x,y) = e^{S(x)/2} P_t(x \mid y) e^{-S(y)/2} = \langle x \mid e^{-\epsilon \hat{H}} \mid y \rangle$$

$$\text{with } \hat{H} = e^{S(\hat{x})/2} \hat{H}_{\mathrm{FP}} e^{-S(\hat{x})/2} = -\partial_x^2 + V(\hat{x})$$

$$\left[V(x) = (1/4)\left(S'(x)\right)^2 - (1/2) S''(x) \right]$$

$$\Rightarrow \quad F_t(x_1, x_2) = \frac{K_t(x_1, x_2)}{\sqrt{K_t(x_1, x_1) K_t(x_2, x_2)}} = e^{-\frac{1}{2} d_t^2 (x_1, x_2)}$$

Example 1: Unimodal distribution (Gaussian)

$$S(x) = \frac{\omega}{2} x^2$$

⇨ $\hat{H} = -\partial_x^2 + V(\hat{x})$ with $V(x) = (1/4)\big(S'(x)\big)^2 - (1/2)S''(x)$

$$= \frac{\omega^2}{4} x^2 - \frac{\omega}{2}$$

⇦ subtracts zero-point energy

⇨ $K_t(x,y) = \langle x | e^{-t\hat{H}} \,|\, y \rangle$

$$= \sqrt{\frac{\omega}{2\pi(1-e^{-2\omega t})}} \exp\left[-\frac{\omega}{4\sinh \omega t} [(x_1^2 + x_2^2)\cosh \omega t - 2x_1 x_2] \right]$$

⇨ $d_t^2(x_1, x_2) = \frac{\omega}{2\sinh \omega t} | x_1 - x_2 |^2 \sim e^{-\omega t} | x_1 - x_2 |^2$

We see that:

- geometry is flat and translationally invariant
- relaxation time τ is given by $\tau \sim 1/\omega \; \left[\omega^2 \sim V''(x) \right]$

Example 2: Unimodal dist. (non-Gaussian)

$$S(x) = \frac{\omega}{2} x^2 + \frac{\lambda}{4} x^4$$

⇨ perturbative expansion in λ :

$$d_t^2(x_1, x_2) = |x_1 - x_2|^2 \Big\{ \frac{\omega}{2s} - \frac{\lambda}{8\omega s^4} [12(s^3 - 3s^2 c + 3\omega t + 2\omega t s^3 - \omega t s^2 c) \\ + \omega(s^3 + 3s - 3\omega t c)(x_1 - x_2)^2 \\ + 3\omega(s^3 + 3s - 3\omega t c + 3\omega t - 3sc + 2\omega t s^2)(x_1 + x_2)^2] + O(\lambda^2) \Big\}$$

$$\left(c \equiv \cosh \omega t,\ s \equiv \sinh \omega t\right)$$

We see that:

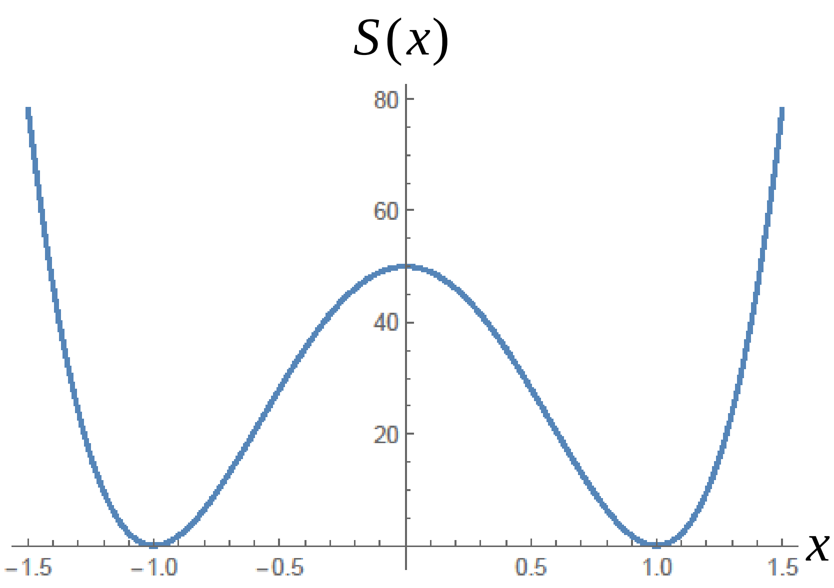
- geometry is no longer flat or translationally invariant
- relaxation time τ is again given by $\tau \sim 1/\omega$ $\left[\omega^2 \sim V''(x)\right]$

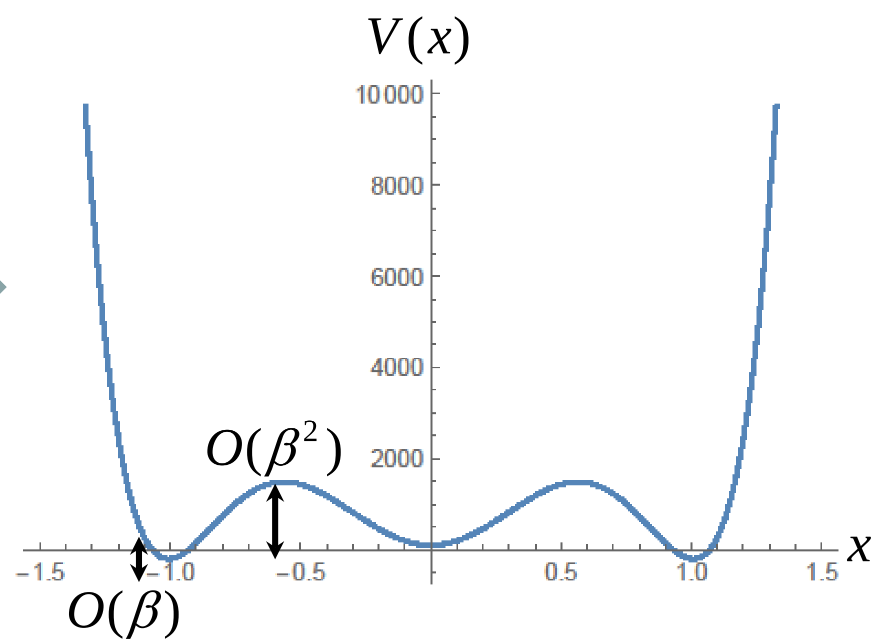
Example 3: Multimodal dist. (double well) (1/2)

$$S(x) = \frac{\beta}{2}(x^2 - 1)^2 \quad (\beta \gg 1)$$

$$\Rightarrow \quad \hat{H} = -\partial_x^2 + V(\hat{x})$$

with $V(x) = \beta^2 x^6 - 2\beta^2 x^4 + (\beta^2 - 3\beta)x^2 + \beta$
$= \beta^2 x^2 (x^2 - 1)^2 + O(\beta)$





Example 3: Multimodal dist. (double well) (2/2)

For $\beta = 20$:

$E_0 = 0$

$E_1 = 7.81\times10^{-4}$

instanton $e^{-O(\beta)}$

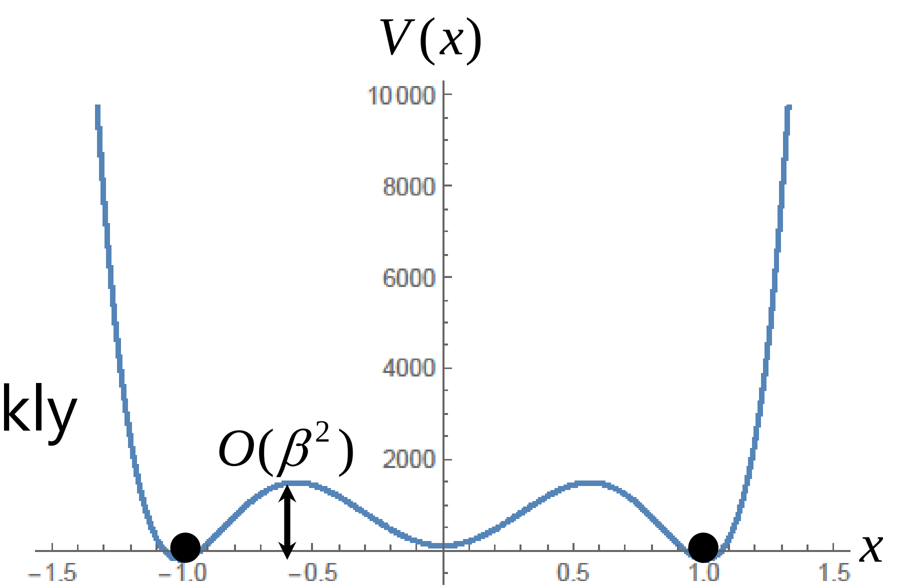
$E_2 = 36.2$

$E_3 = 58.2$

$\langle x|k\rangle \ (k=2,3,\ldots)$: decouple quickly

$\langle x|1\rangle$: decouples very slowly

$\hat{H} = -\partial_x^2 + V(\hat{x})$



In fact,

n	$d_n^2(-1,+1)$
10	39.1
50	19.2
100	16.9
500	13.2
1,000	11.7
5,000	8.46

decreases only very slowly

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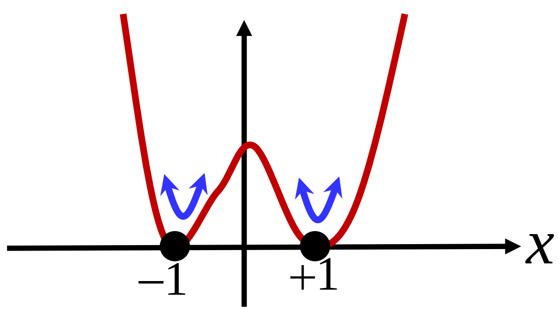
Simulated tempering (1/3)

Basic idea of tempering : **[Marinari-Parisi]**

Even when the original action $S(x;\beta_0)$ is multimodal, it often happens that $S(x;\beta)$ becomes less multimodal if we take smaller β.

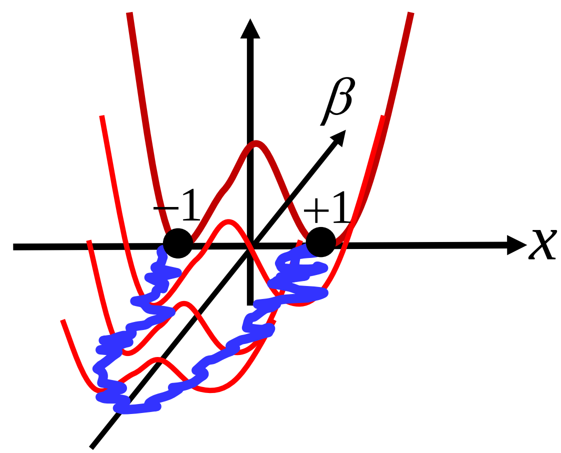
We extend the configuration space s.t. configurations in different modes can be reached from each other by passing through small β's.

original config space $\{x\}$



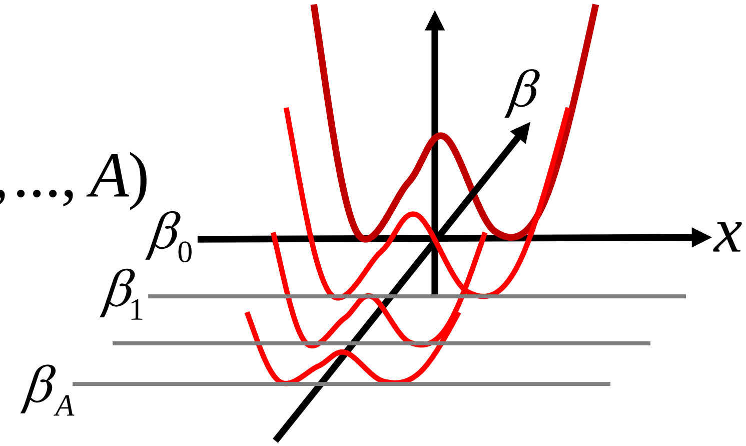
$$S(x;\beta_0)=\frac{\beta_0}{2}(x^2-1)^2 \quad (\beta_0 \gg 1)$$

extended config space $\{(x,\beta)\}$



Simulated tempering (2/3)

<u>Realization</u>



- Extend the config space $\mathcal{M}=\{x\}$
  to $\mathcal{M}\times\mathcal{A}=\{X=(x,\beta_a)\}(x\in\mathcal{M};\ a=0,1,\ldots,A)$

- Introduce a stochastic process

$$P_n(X)\rightarrow P_{n+1}(X)$$

s.t. $P_n(X)\xrightarrow{n\to\infty}P_{\mathrm{eq}}(X)=P_{\mathrm{eq}}(x,\beta_a)=w_a e^{-S(x;\beta_a)}$

- Estimate the VEV by only using the subsample with $\beta_{a=0}$

<u>NB</u> : (appearance probability of a-th subsample)

$$=\int dx\, P_{\mathrm{eq}}(x,\beta_a)=w_a Z_a \quad \left(Z_a=\int dx\, e^{-S(x;\beta_a)}\right)$$

⇩

w_a is often set as $w_a\propto 1/Z_a$,
which ensures that the desired 0-th configs appear
with nonvanishing probability $(=1/(A+1))$

consideration not necessary for parallel tempering

Simulated tempering (3/3)

<u>Algorithm</u>

(1) Generate a transition in the x direction,

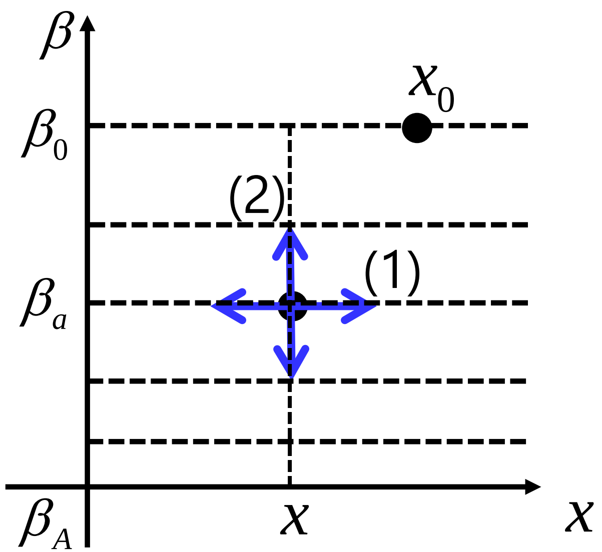
$$X=(x,\beta_a)\to X'=(x',\beta_a)$$

with some proper algorithm
(such as Langevin or Metropolis)

(2) Generate a transition in the β direction,

$$X=(x,\beta_a)\to X'=(x,\beta_{a'=a\pm 1})$$

with the probability $\min\left(1,\dfrac{w_{a'}\,e^{-S(x,\beta_{a'})}}{w_a e^{-S(x,\beta_a)}}\right)$



(3) Extract a subsample with $\beta_{a=0}$; $\{(x_m,\beta_0)\}\ (m=1,\ldots,M)$

(4) Evaluate VEVs as $\langle \mathcal{O}(x)\rangle_{\beta_0}\simeq \dfrac{1}{M}\sum_{m=1}^{M}\mathcal{O}(x_m)$

<u>NB</u> : a-dependence of β_a should be chosen
s.t. the transition in the β-direction is easy.
This adjustment is usually done manually or adaptively.
We will show that this can be done geometrically.

Distance for simulated tempering

[MF-Matsumoto-Umeda1]

The introduction of tempering should be seen as the reduction of distance.

In fact,

w/o tempering

n	$d_n^2(-1,+1)$
10	39.1
50	19.2
100	16.9
500	13.2
1,000	11.7
5,000	8.46

w/ tempering

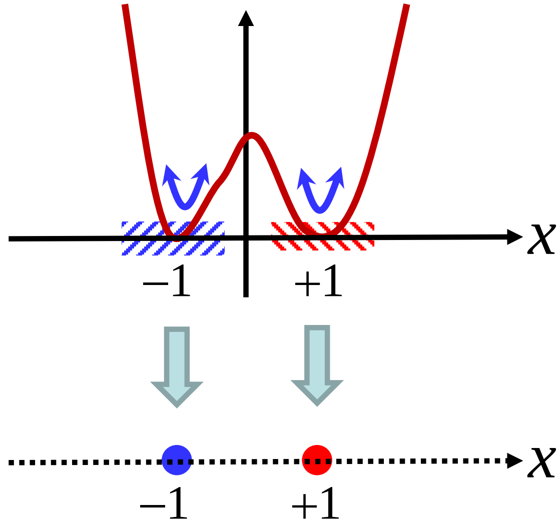
$d_n^2(-1,+1)$
26.5
7.16
4.35
0.708
0.106
2.78 x 10^(-8)

rapid decreasing

Coarse-grained configuration space (1/4)

[MF-Matsumoto-Umeda1,2]

In MCMC simulations,
the most expensive part is the transitions between configs in different modes,
and thus, configs in the same mode can be effectively treated as a point.



⇩

This leads us to the idea of "coarse-grained config space" $\overline{\mathcal{M}}$

⇩

We would like to show that

> when the original config space is multimodal with high degeneracy,
> the extended coarse-grainined config space $\overline{\mathcal{M}} \times \mathcal{A}$
> naturally has an AdS geometry

Coarse-grained configuration space (2/4)

[MF-Matsumoto-Umeda2]

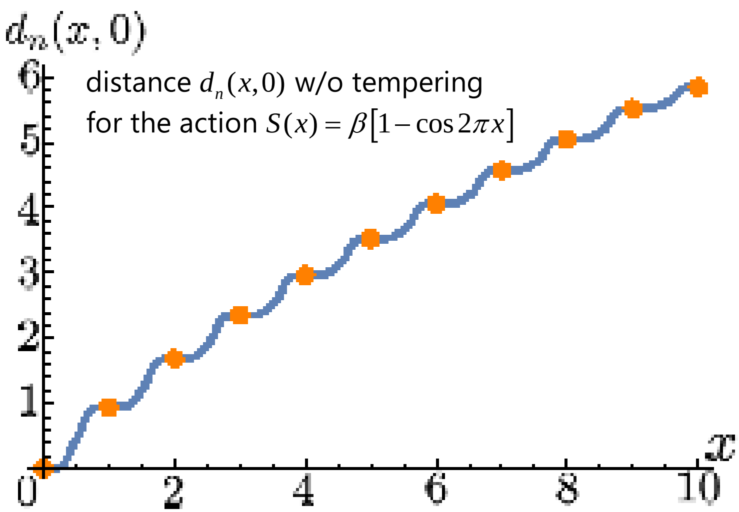
NB

We have two different distances, $\theta_n(x_1, x_2)$ and $d_n(x_1, x_2)$ that are related with the half-time overlap $F_n(x_1, x_2)$ as

$$F_n(x_1, x_2) = \cos\theta_n(x_1, x_2) = e^{-d_n^2(x_1, x_2)/2}$$

$\theta_n(x_1, x_2)$ always satisfies triangle inequality but takes a complicated form even for Gaussian distribution.

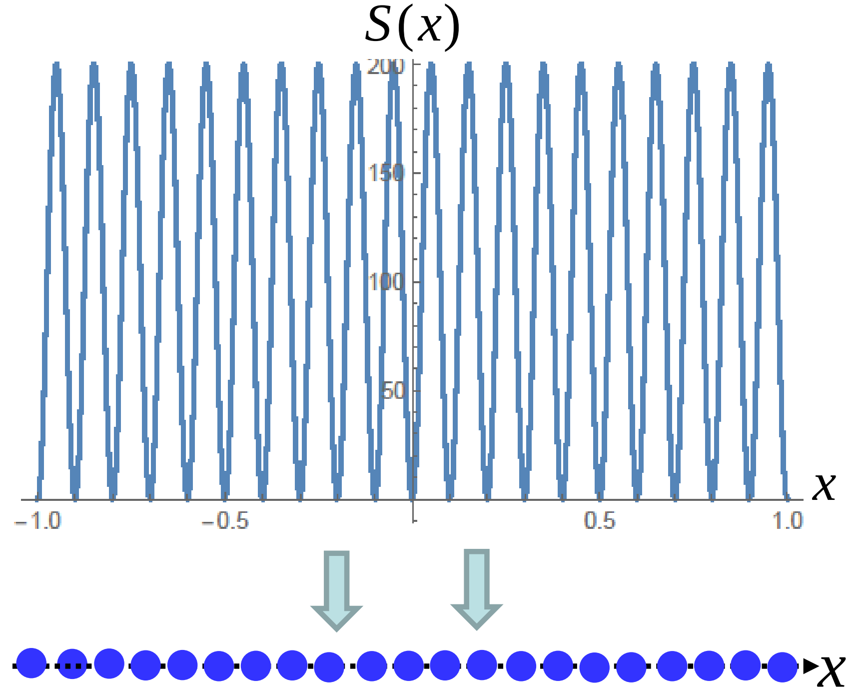
$d_n(x_1, x_2)$ does not satisfy triangle ineq generically, but gives a flat geometry for Gaussian distribution. This does satisfy triangle ineq in the coarse-grained config space.



We will regard $d_n(x_1, x_2)$ as more fundamental when discussing coarse-grained config space

Coarse-grained configuration space (3/4)

action: $S(x;\beta_0)=\beta_0\left[1-\cos\left(\frac{2\pi x}{\epsilon}\right)\right]$



original config space: $\mathcal{M}=\mathbb{R}$

coarse-grained config space:

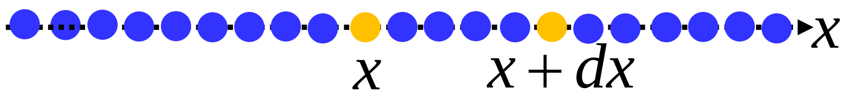
$\overline{\mathcal{M}}=$ (1D lattice with spacing ϵ)

$\oplus$ sim temp

extended coarse-grained config space:

$\overline{\mathcal{M}}\times\mathcal{A}=\{X=(x,\beta_a)\}$ $[x\in$ (1D lattice with spacing ϵ)$]$

Coarse-grained configuration space (4/4)

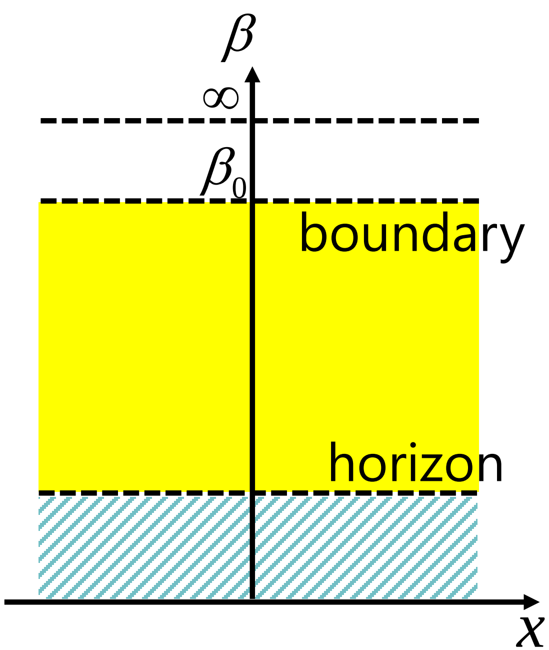


We assume that

$$d_n^2\big((x,\beta),(x+dx,\beta)\big) = \text{const.}\,\beta^q\,dx^2 \quad \begin{pmatrix} q=1 \text{ when not tempered} \\ q<1 \text{ when tempered} \end{pmatrix}$$

and set

$$d_n^2\big((x,\beta),(x,\beta+d\beta)\big) = f(\beta)\,d\beta^2 \qquad \text{---- (\#)}$$



Then we have

$$ds^2 \equiv d_n^2\big((x,\beta),(x+dx,\beta+d\beta)\big)$$
$$= \text{const.}\,\beta^q\,dx^2 + f(\beta)\,d\beta^2$$

If (#) is scale invariant (i.e., $f(\beta)\propto 1/\beta^2$),
this gives an AdS metric:

$$ds^2 = \text{const.}\,\beta^q\,dx^2 + \text{const.}\frac{d\beta^2}{\beta^2} = \frac{\text{const}}{z^2}\left(dx^2+dz^2\right) \quad \left(z\propto\beta^{-q/2}\right)$$

(This is actually an asymptotic AdS with a horizon)

AdS geometry as a result of optimization (1/4)

[MF-Matsumoto-Umeda2]

If $\beta_a \ (a = 0, 1, \ldots, A)$ is chosen as

$$\beta_a = \beta_0 \left(\frac{\beta_A}{\beta_0} \right)^{a/A}, \qquad \text{-------------------- (\#\#)}$$

obeying (##) !

one can show that geometry in β direction becomes scale invariant, so that we will obtain an AdS geometry, as we saw before.

One can actually confirm that (##) is the best choice for minimizing the distance in simulated tempering:

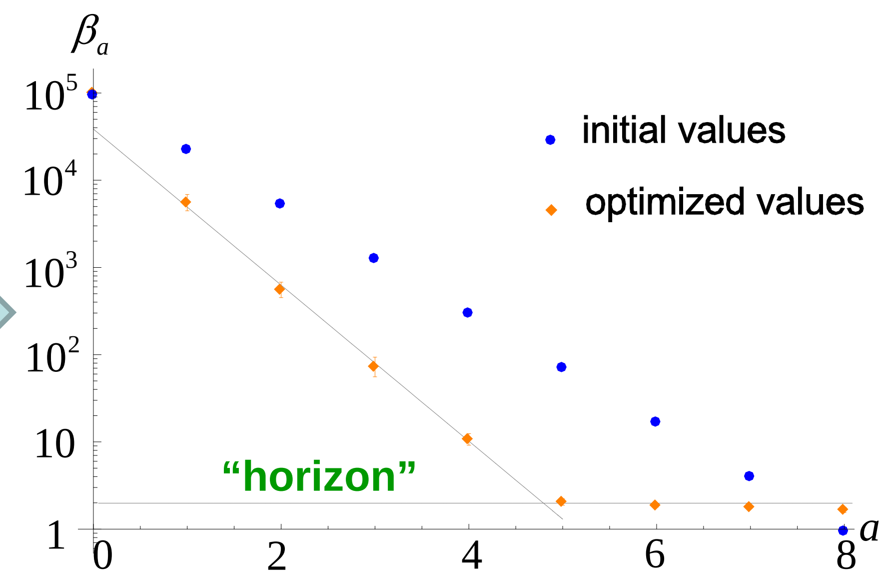
Consider the action :

$$S(\mathbf{x}; \beta_0) = \beta_0 \sum_{i=1}^{2} [1 - \cos(2\pi x_i)]$$

$$\left(\beta_0 = 10^5 \right)$$

Search for $\{\beta_1, \beta_2, \ldots, \beta_8\}$

that minimize $d_n^2 \left((0, \beta_0), (+1, \beta_0) \right)$



AdS geometry as a result of optimization (2/4)

That is,

optimize β_a s.t. the distance is minimized

⇓

$$\beta_a = \beta_0 \left(\frac{\beta_A}{\beta_0} \right)^{a/A} \quad (a = 0, 1, 2, \ldots,) \text{ for large } \beta_a$$

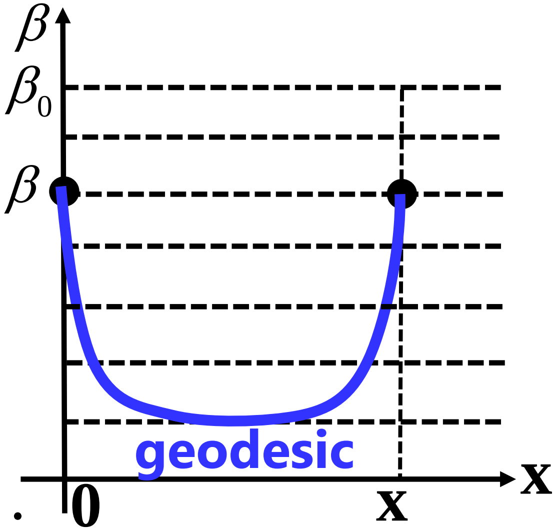
⇓

<u>AdS metric</u> :

$$ds^2 = \text{const.}\, \beta^q dx_i^2 + \text{const.} \frac{d\beta^2}{\beta^2} = \frac{\text{const}}{z^2}\left(dx_i^2 + dz^2\right) \quad \left(z \propto \beta^{-q/2}\right)$$

This is the first example of the "emergence of AdS geometry" in nonequilibrium systems.

AdS geometry as a result of optimization (3/4)



Algorithm to determine the metric

(1) Set an ansatz: $ds^2 = \ell^2 \left(\frac{d\beta^2}{\beta^2} + \alpha \beta^q \sum_{i=1}^{N} dx_i^2 \right)$

⇩

geodesic distance between $(\mathbf{0}, \beta)$ and $(\mathbf{x}, \beta)$:

$$I(\mathbf{x}, \beta; \ell, \alpha, q) = \frac{4\ell}{q} \ln \frac{\sqrt{\left(q\sqrt{\alpha}\,|\mathbf{x}|\right)^2 + 16\beta^{-q}} + q\sqrt{\alpha}\,|\mathbf{x}|}{4\beta^{-q/2}}$$

(2) Calculate distances $d_n\left((\mathbf{0}, \beta_a), (\mathbf{x}, \beta_a)\right)$ for various $\mathbf{x}$ and β_a

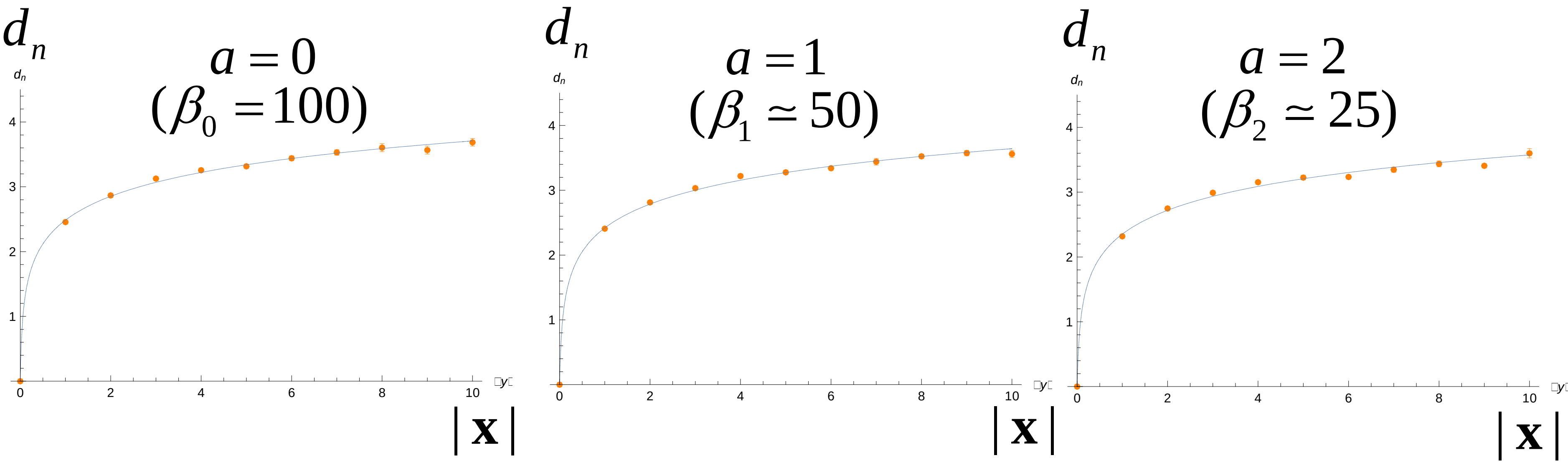
(3) Find the values of (ℓ, α, q) that minimize the cost function

$$C(\ell, \alpha, q) \equiv \sum_{\mathbf{x}} \sum_{a} \left[d_n\left((\mathbf{0}, \beta_a), (\mathbf{x}, \beta_a)\right) - I(\mathbf{x}, \beta_a; \ell, \alpha, q) \right]^2$$

AdS geometry as a result of optimization (4/4)

Result $(N=2)$

$$ds^2 = \ell^2\left(\frac{d\beta^2}{\beta^2} + \alpha\,\beta^q \sum_{i=1}^{2} dx_i^2\right) \qquad \begin{cases} \ell = (5.3 \pm 0.3)\times 10^{-3} \\ \alpha = (4.1 \pm 1.0)\times 10^{4} \\ q = 0.39 \pm 0.02 \end{cases}$$



Plan

1. Introduction
2. Definition of distance
   - preparation
   - definition of distance
   - universality of distance
3. Examples
   - unimodal case
   - multimodal case
4. Distance for simulated tempering
   - simulated tempering
   - emergence of AdS geometry
   - AdS geometry from matrix models
5. Conclusion and outlook

Conclusion and outlook

What we have done:

- We introduced the concept of "distance between configs" in MCMC simulations
- The distance satisfies desired properties as distance
- This can be used for the optimization of parameters, and AdS geometry appears as a result of optimization

Future work:

- Establish a systematic method for optimization

  e.g., $\beta_a = \beta(a)$ would be found by simply solving
  the E-L eq of some functional $I[\beta(a)]$

- Investigate the relationship between the obtained result and the Einstein equation
- Investigate the geometry of matrix models further

Thank you.