Biased Metropolis-Heatbath Algorithm

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Introduction

In the Metropolis procedure transition probability from the configuration (k) to (l) is given as

$$W^{(l)(k)} = f(l,k)\, w^{(l)(k)} \;\text{ for }\; l \neq k$$

$$W^{(k)}(k) = f(k,k) + \sum_{l \neq k} f(l,k)(1 - w^{(l)(k)})$$

For the case of the non-symmetric proposal probabilities $f(l,k) \neq f(k,l)$ the acceptance probability can be modified as [Hastings (1970)]

$$w_b^{(l)(k)} = \min\left\{1, \frac{P_B^{(l)}}{P_B^{(k)}}\, \frac{f(k,l)}{f(l,k)}\right\}$$

Example: $U(1)$ Lattice Gauge Theory

Variables are complex numbers of unit length:

$$U = e^{i\phi}, \quad \phi \in [0, 2\pi)$$

The problem is reduced to sampling the probability density (PDF)

$$P_\alpha(\phi) = N_\alpha \, e^{\alpha \cos\phi}$$

where α is a parameter associated to the interaction of the link being updated with its environment. The corresponding cumulative distribution function (CDF) is

$$F_\alpha(\phi) = N_\alpha \int_0^\phi d\phi' \, e^{\alpha \cos\phi'}$$

where N_α ensures the normalization $F_\alpha(2\pi) = 1$.

Constructing the Algorithm

What are our options:

- HeatBath Algorithm (HBA)
- Metropolis (MA)
- Biased Metropolis-Heatbath Algorithm (BMHA)

$$\text{Acceptance rate (AR)} = \frac{\#\text{ of updated links}}{\text{total }\#\text{ of links}}$$

Constructing the Algorithm: HBA

The HBA generates ϕ by converting a uniformly distributed random number $0 \leqslant z < 1$ into

$$\phi = F_\alpha^{-1}(z) \ .$$

Implementation:

- Hattori and Nakajima
- Wensley

Repeat Until Accepted (RUA) step $\rightarrow$ acceptance rate $= 1$ ...
BUT may need several proposals!

Constructing the Algorithm: Metropolis

Generate ϕ_{new} uniformly in the range $0 \leqslant \phi_{new} < 2\pi$, accept with probability

$$p_{MA} = \min\left\{1, \frac{P_\alpha(\phi_{new})}{P_\alpha(\phi_{old})}\right\}$$

May have low acceptance rate.

Possible cures

- multihit Metropolis, but cannot be made RUA!
- shrinking of the proposal range

Constructing the Algorithm: BMHA

We need:

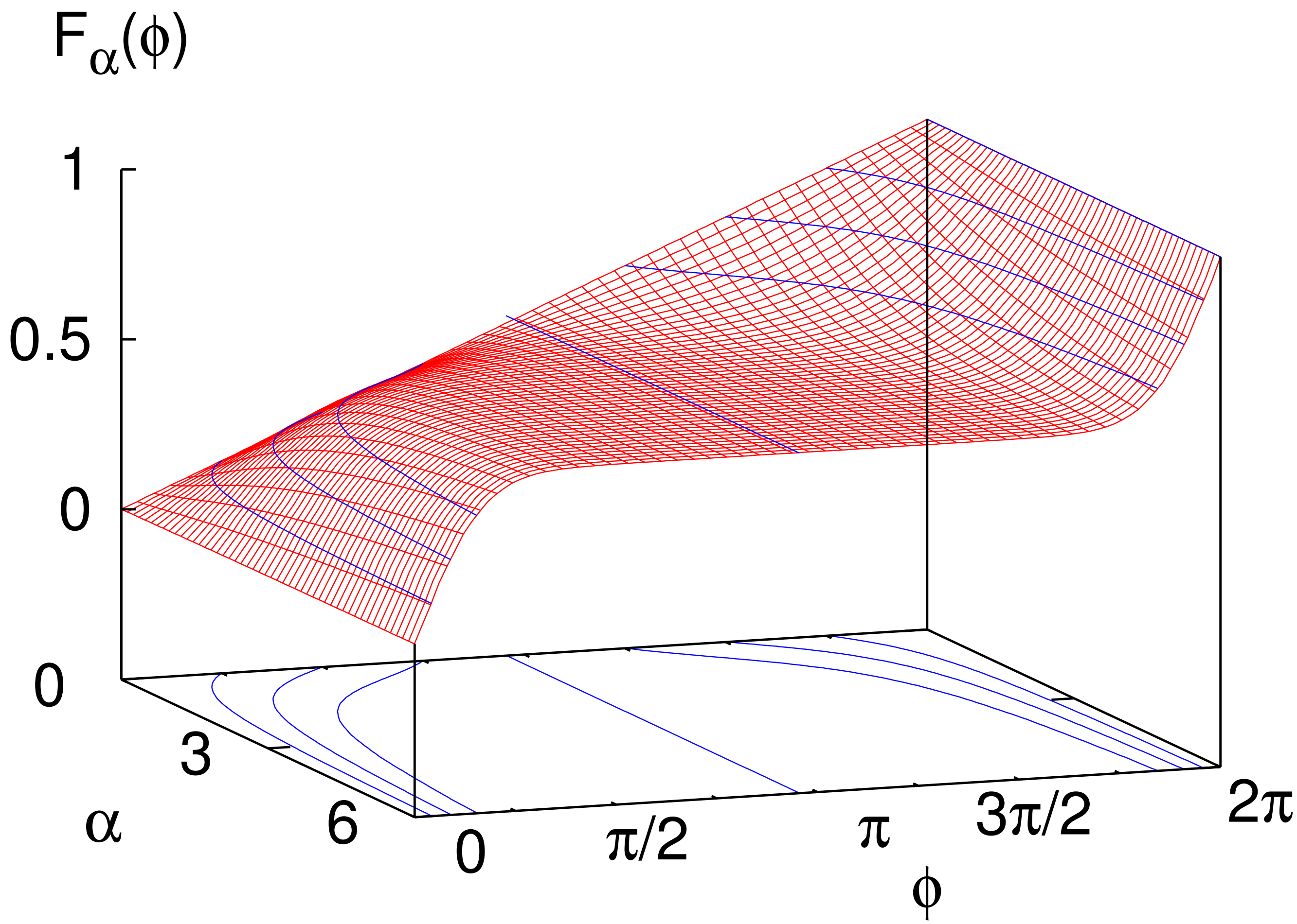
- discretization of the CDF
- table with the areas of equal probability
- modified proposal of ϕ_{new}
- modified accept/reject step

Example

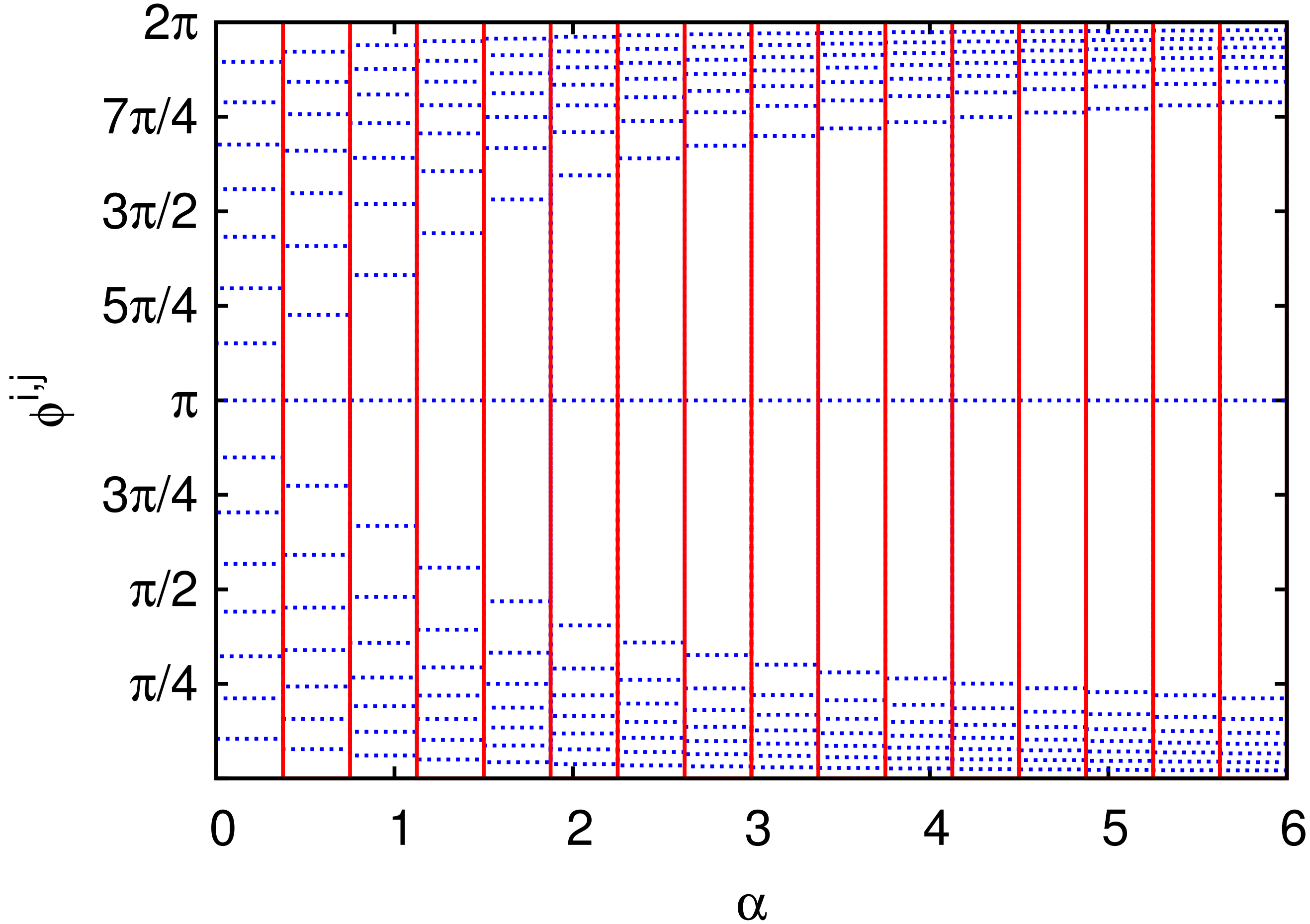
In 4D $0 \leqslant \alpha \leqslant 6\beta_g$. Let $\beta_g = 1.0 \quad \Rightarrow \quad 0 \leqslant \alpha \leqslant 6$

Discretize α in 16 bins, assume it is in 11th bin, use middle value.

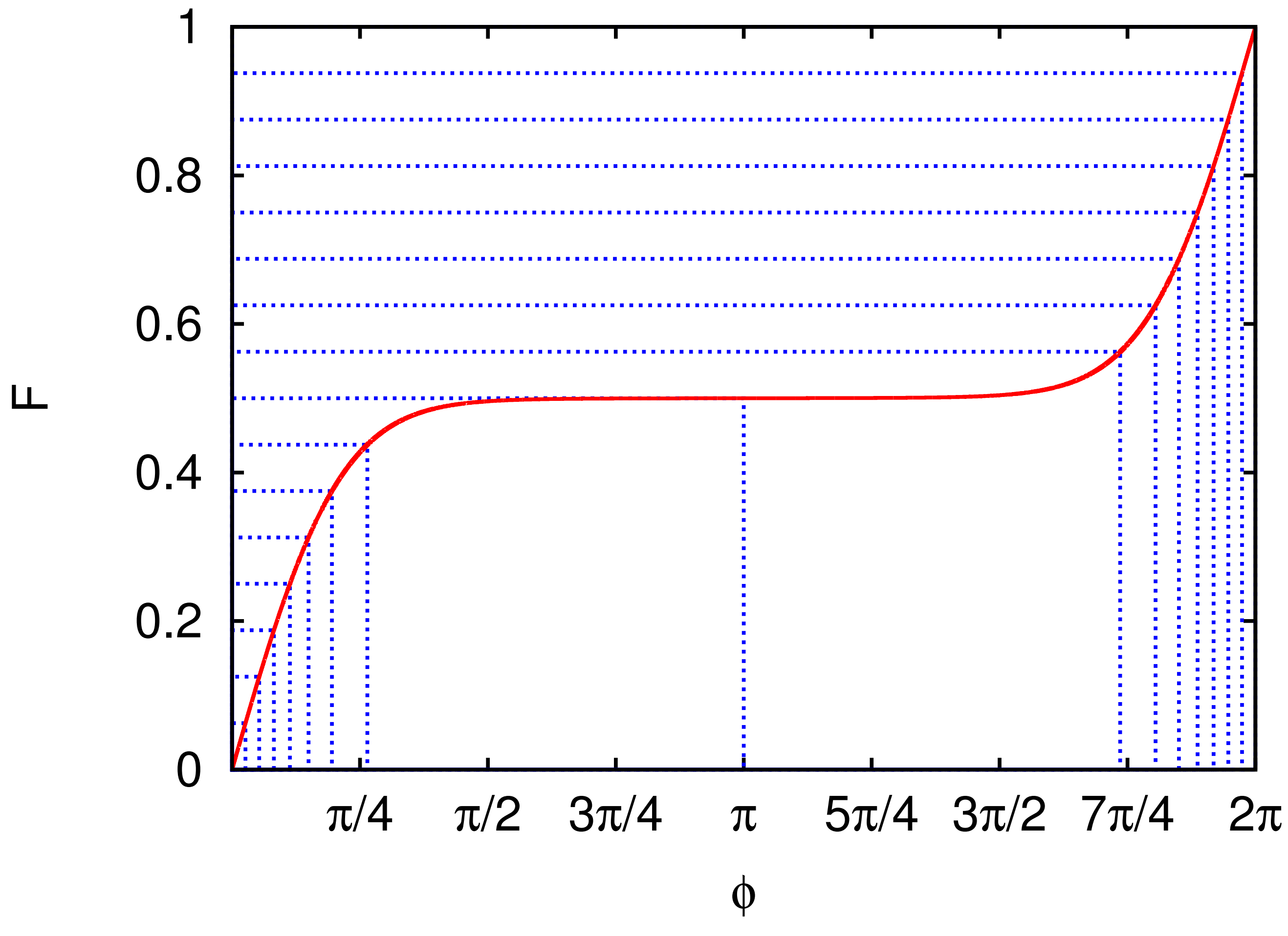
Cumulative distribution function $F_\alpha(\phi)$ with the level map in the $\alpha - \phi$ plane



Partition of the $\triangle\phi^{i,j}$ values



Discretization of the cumulative distribution function for $U(1)$



BMHA update procedure

1. Find the α^i value nearest to the actual α ($i = 11$ in ex.)

2. Place the old ϕ_{old} value on the discretization grid, i.e., find integer j such that $\phi^{i,j-1} \leqslant \phi_{old} < \phi^{i,j}$ (for $n = 2^{n_2}$ the label j can be determined in n_2 steps with recursion).

3. Pick an integer j' from 1 to n ($n = 16$ in example)

4. Propose $\phi_{new} = \phi^{i,j'-1} + x^r \triangle\phi^{i,j'}$, $0 \leqslant x^r < 1$.

5. Accept ϕ_{new} with the probability

$$p_{BMHA} = \min\left\{1, \frac{P_\alpha(\phi_{new})}{P_\alpha(\phi_{old})} \frac{\boldsymbol{\Delta}\phi^{\mathbf{i},\mathbf{j}'}}{\boldsymbol{\Delta}\phi^{\mathbf{i},\mathbf{j}}}\right\}$$

U(1) BMHA performance

Lattice: 4×16^3

Coupling: $\beta_g = 1.0$

Sweeps: $16384 + 32 \times 20480$

CDF discretization: 32×128

	HBA	Metropolis	BMHA
CPU time [s]	131,111	84,951	107,985
AR	1 (1.093 proposals)	0.286	0.972
$\langle \cos \phi_\Box \rangle$	0.59113 (8)	0.59103 (16)	0.59106 (12)
τ_{int}	127 (7)	341 (26)	142 (10)

Summary: Biased Metropolis-Heatbath Algorithm (BMHA)

- Sampling with BMHA is essentially equivalent to HBA but can be numerically faster
- BMA can be used when CDF is not a priori known (making HBA impossible)
- BMA can be extended to a multi-variable case