Approximate Markov Model for a Finite Population Genetic Algorithms

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Work in Progress

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Outline

1. **Introduction**
   - Motivation
   - Cumulant Approach

2. Approximate Markov Model
   - New Approach
   - Results
   - Future Work

Aims

- Modelling GA on a problem with a small number of states
- Want a ‘plug & play’ model
- The size of the search space, $\mathcal{S}$, might be $|\mathcal{S}| \approx 100$
- These states might correspond to many configurations
- E.g. **ones-max** where each state corresponds to a set of points in the search space grouped according to their Hamming distance from the all zeros string
- More interesting variants of ones-max, e.g. hurdle problem
- To model non-trivial problems we can amalgamate connected configurations with the same cost into a single state

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- To model non-trivial problems we can amalgamate connected configurations with the same cost into a single state—**coarse grained model of a problem**

Other Heuristics Search

- For some other heuristics search such as descent with a variable mutation rate or simulated annealing we can build an exact Markov Chain model
- This allows us to study the algorithm
- Can compute the expected performance
- Can compute the gradient in the expected performance as a function of the parameters
- Find optimal parameters

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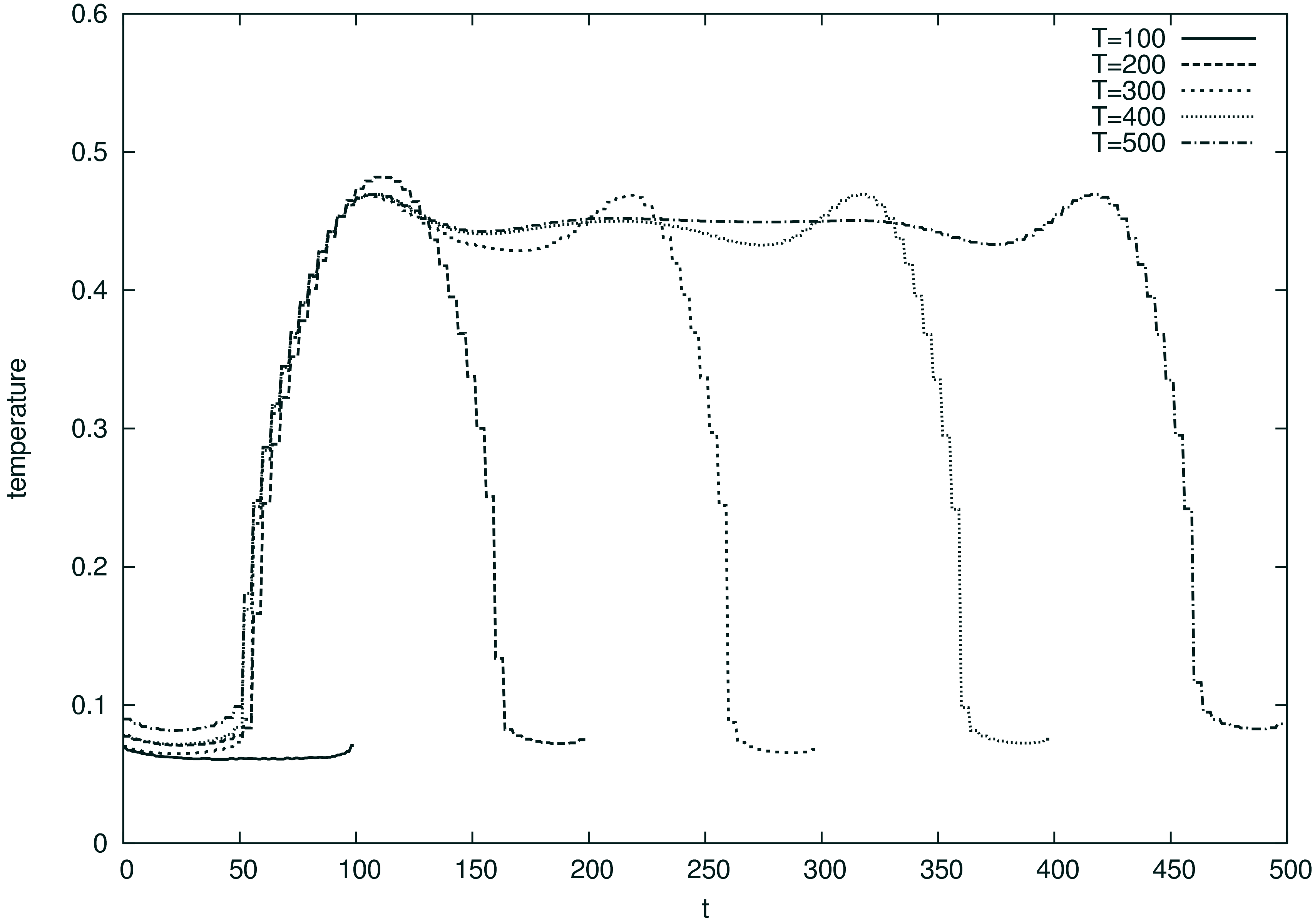
Max-Sat: Annealing Schedules with Best-So-Far



Exact Markov Model for a GA

- Describe the population by a vector

$$\boldsymbol{N} = (N_1, N_2, \cdots N_m) \qquad\qquad m = |\mathcal{S}|$$

  N_i is the number of individuals in state i.

- The probability of a population at time, t, is given by $\mathbb{P}\big(\boldsymbol{N}, t\big)$

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Problems with GAs

- Very useful to do this for a GA
  - ⋆ Provide a way to understand the interactions of many parameters
  - ⋆ Find optimal annealing schedule for mutation rate
- Crossover usually prevents coarse graining problems—care about correlation between members of the population
- There are $\binom{m+p-1}{p-1}$ different possible populations, $\boldsymbol{N}$

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  - ⋆ For $m = 100$, $p = 100$ the number of possible populations is 4.5×10^{58}

Infinite Population Approximation

- One way to avoid the problem caused by the large number of different possible populations is to consider an infinite population

- Because there are no fluctuations in the dynamics of an infinite population it suffices to consider the mean occupancy of each possible state $\mu_i = N_i/p$

- The infinite population approximation is very easy to work with but doesn't answer the questions of practical interest

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  Most practical issues arise because we are using a finite population

Statistical Mechanics Approach

- Approach developed in collaboration with Jonathan Shapiro, Magnus Rattray and Alex Rogers
- For simple problems the evolutionary dynamics can be modelled using statistical properties of distribution of fitness
- Principally these are the cumulants of the distribution of fitness
- Can also include fluctuation to describe an ensemble
- Possible to include more "macroscopic" variables to capture features of more complex problems
- Can also include crossover

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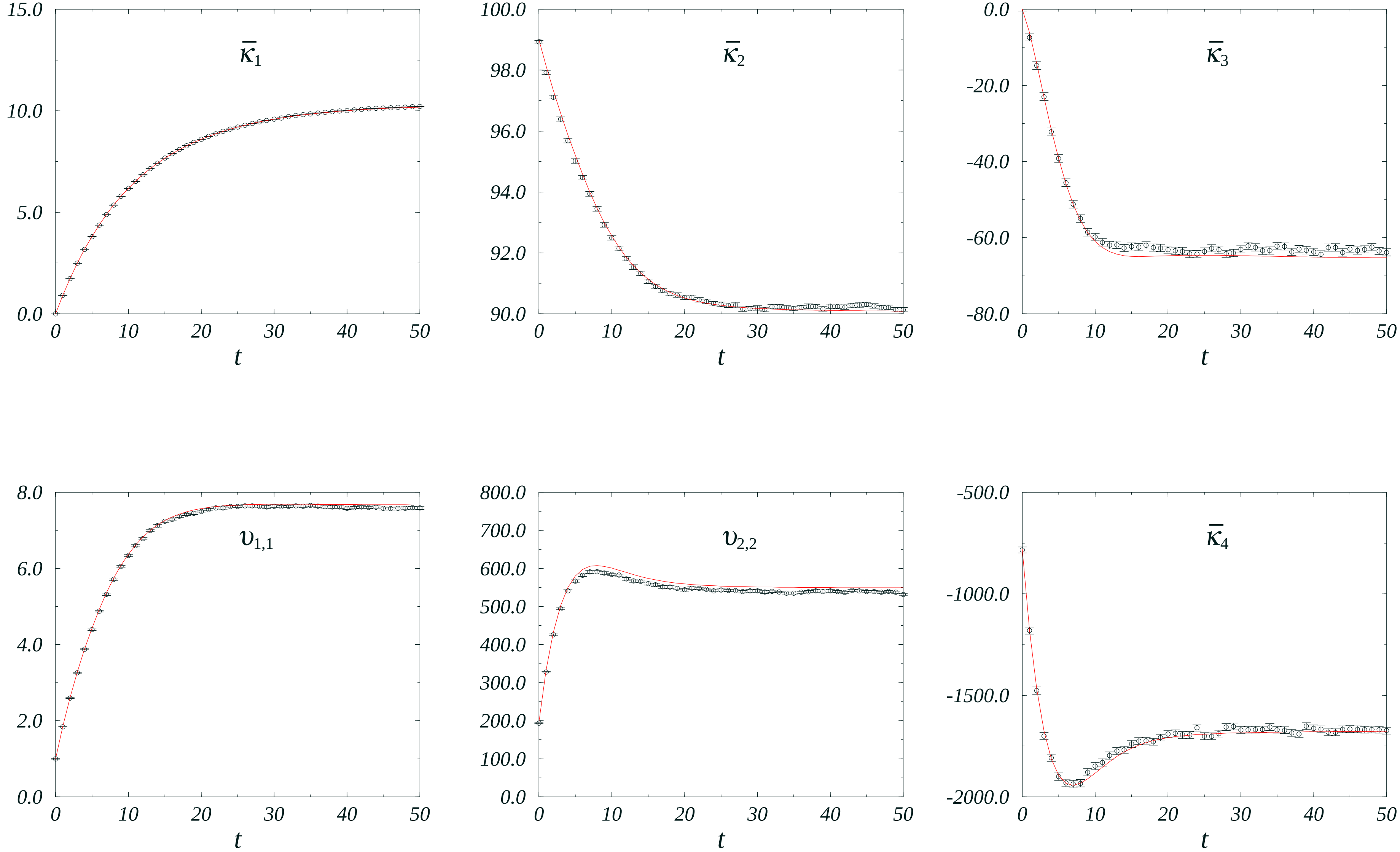
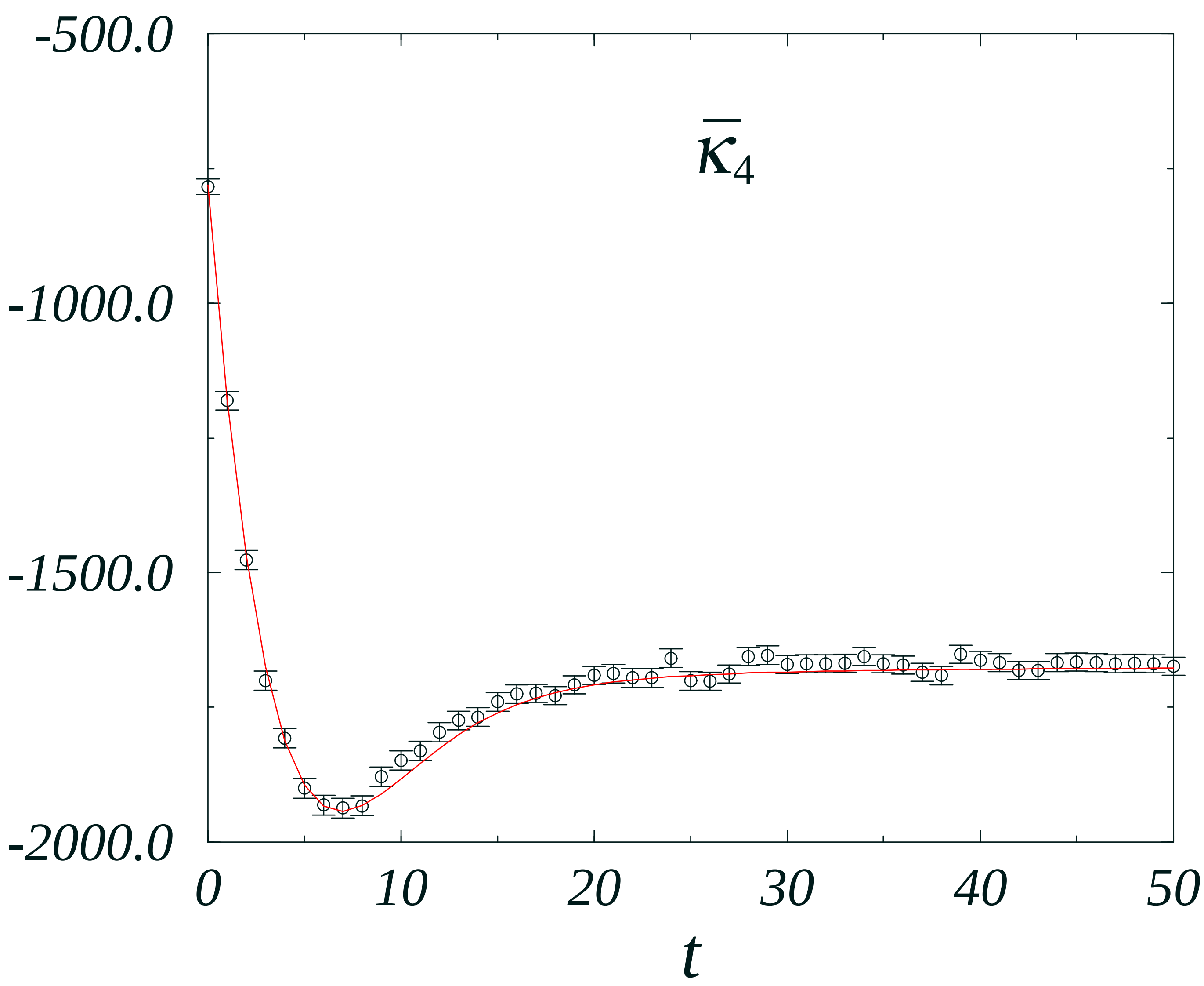
Example Dynamics: Ones-max



Asexual Evolution



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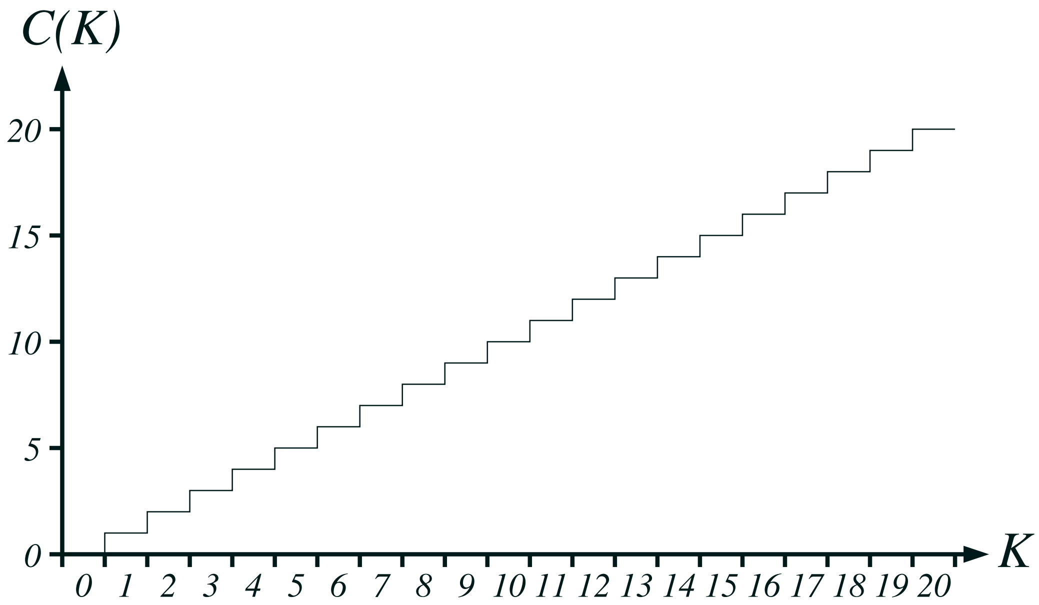

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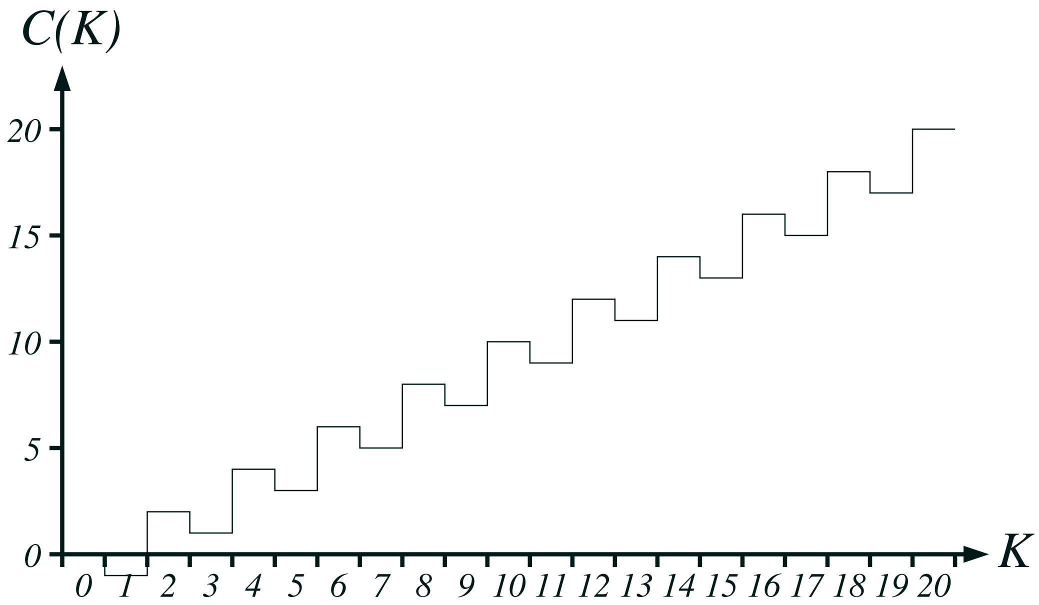

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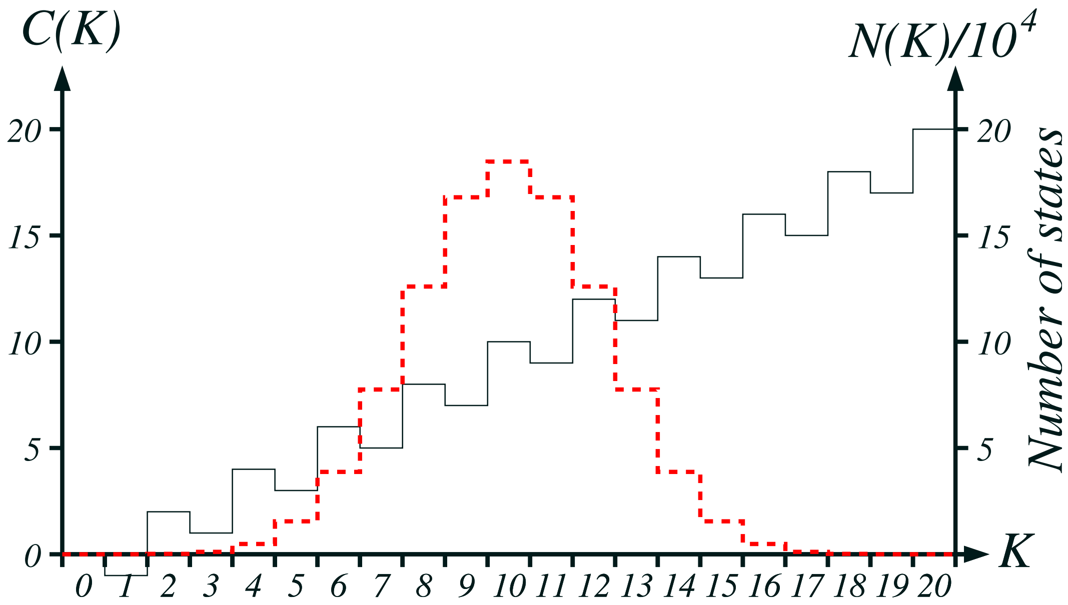

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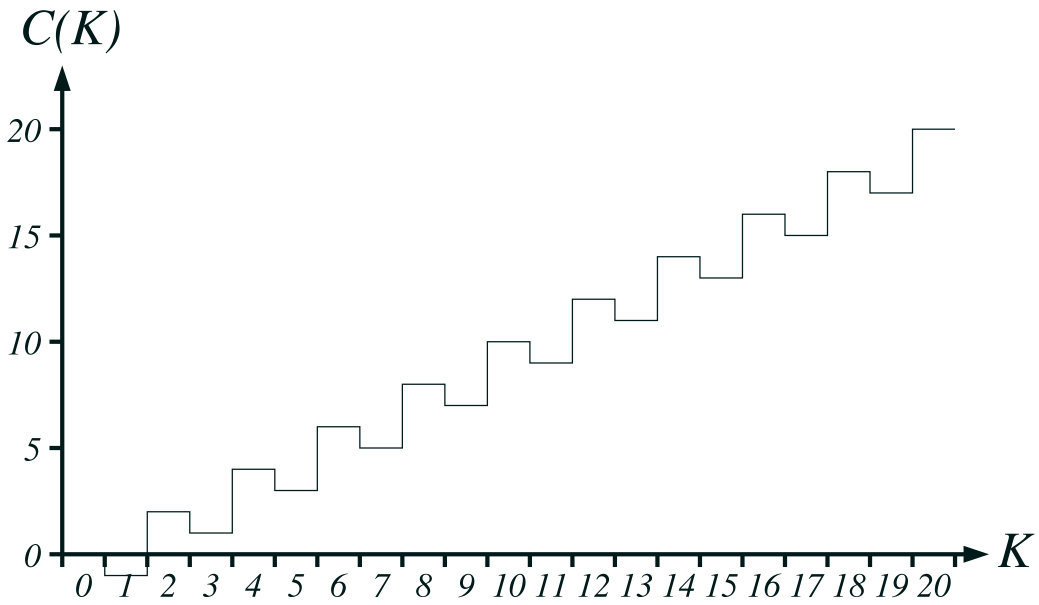

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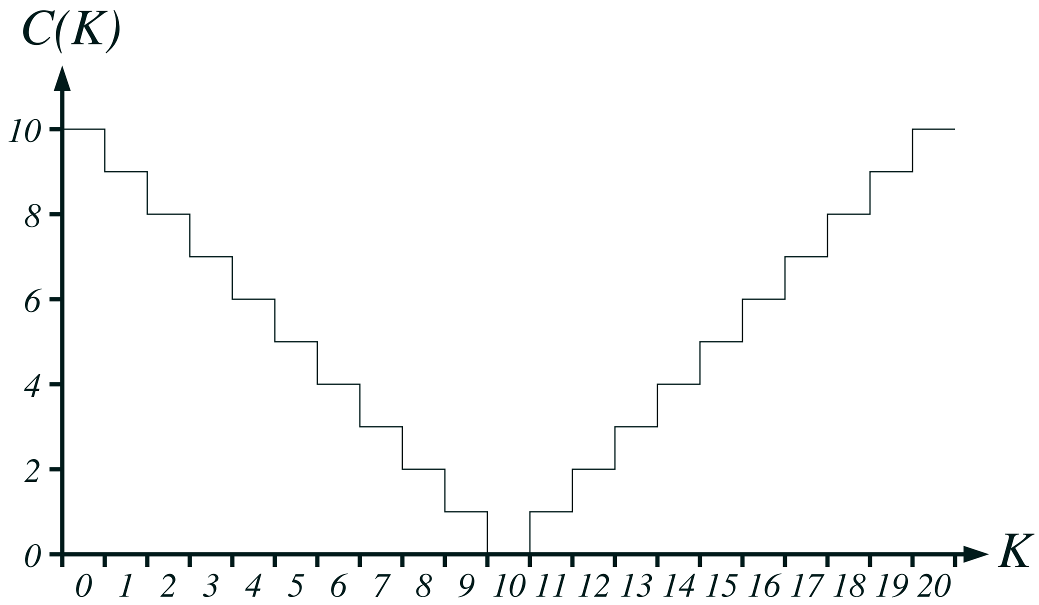

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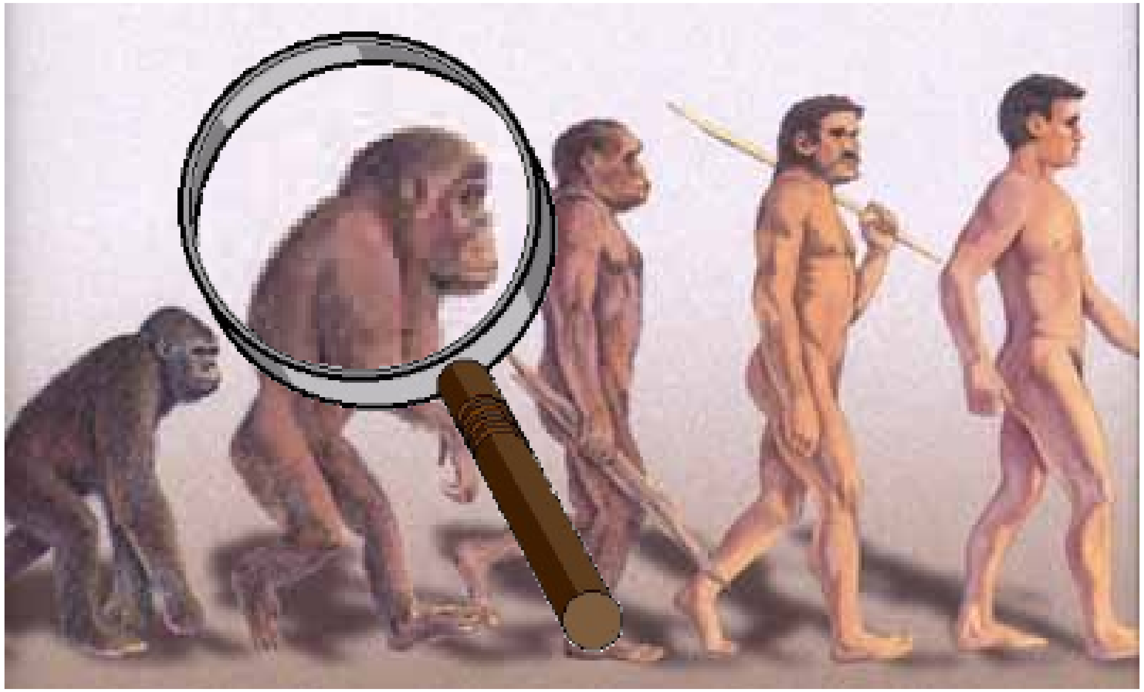

Approximate Markov Model

- Instead of describing the full probability distribution $\mathbb{P}(\boldsymbol{N}, t)$ we keep a 'small' set of statistics
  - ⋆ Average occupation $\boldsymbol{\mu} = \langle \boldsymbol{N} \rangle / p$
  - ⋆ Occupation covariance $\mathbf{C} = \left(\langle \boldsymbol{N}\, \boldsymbol{N}^T \rangle - \langle \boldsymbol{N} \rangle \langle \boldsymbol{N}^T \rangle \right) / p^2$
- These are *insufficient statistics* to compute the effect of selection, so we are forced to make approximations
- Can be considered an extension to the infinite population model which considers only $\boldsymbol{\mu} = \langle \boldsymbol{N} \rangle / p$

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Modelling a Simple GA

- We consider a population undergoing selection and mutation only
  - ⋆ We select a member of the population with a probability proportional to a selection strength s_i (which is some function of its cost/fitness)
  - ⋆ The probability of selecting from a state i is therefore

$$\frac{s_i N_i}{\sum_j s_j N_j}$$

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  - ⋆ Keep the population size, p, fixed

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Occupancy Distributions

- We can represent the probability of a population as

$$\mathbb{P}(\boldsymbol{N}, t) = \int f_{\boldsymbol{X}}(\boldsymbol{x}, t)\, \mathbb{P}(\boldsymbol{N}|\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$$

- where $\mathbb{P}(\boldsymbol{N}|\boldsymbol{x})$ is the multinomial

$$\mathbb{P}(\boldsymbol{N} = \boldsymbol{n}|\boldsymbol{x}) = p! \prod_{i \in \mathcal{S}} \frac{(x_i)^{n_i}}{n_i!} \left[\!\left[\sum_{i \in \mathcal{S}} n_i = p \right]\!\right]$$

- With the constraint $\sum_i X_i = 1$

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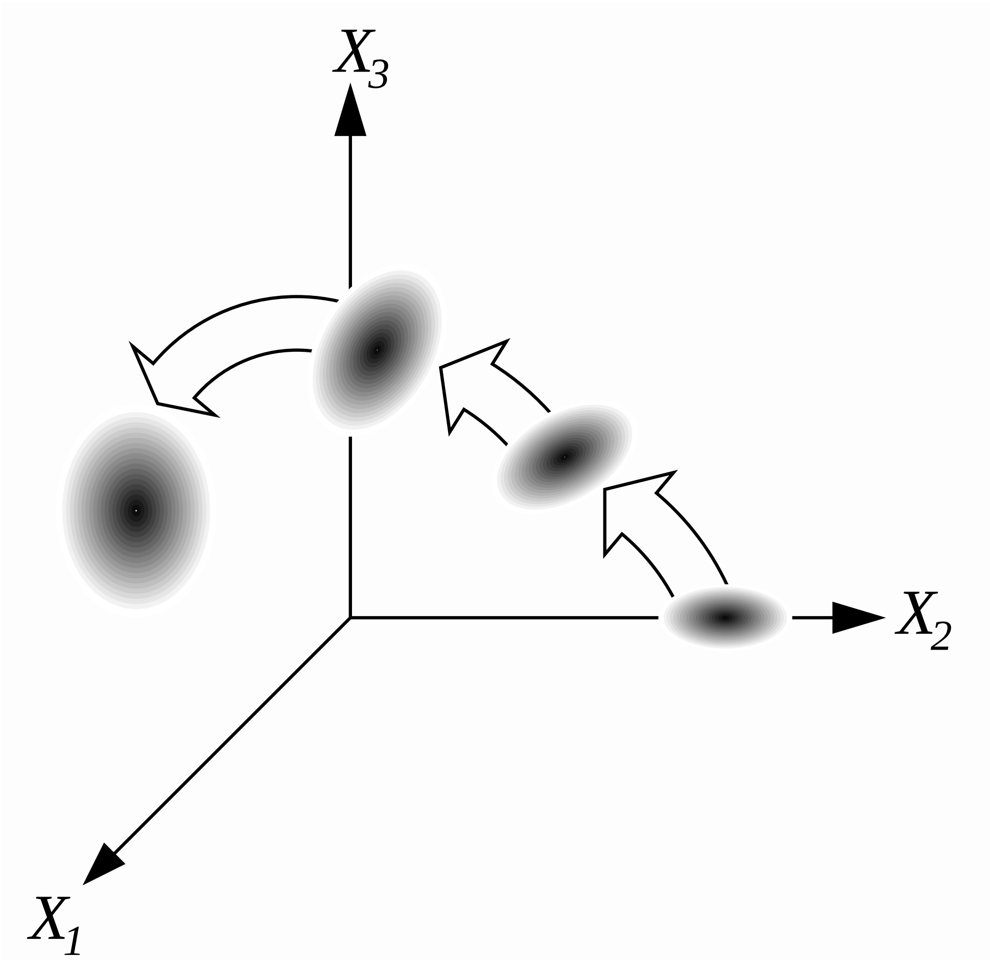
Distribution Ensemble

- $f_{\boldsymbol{X}}(\boldsymbol{x}, t)$ describes an ensemble of distributions $\boldsymbol{X}$



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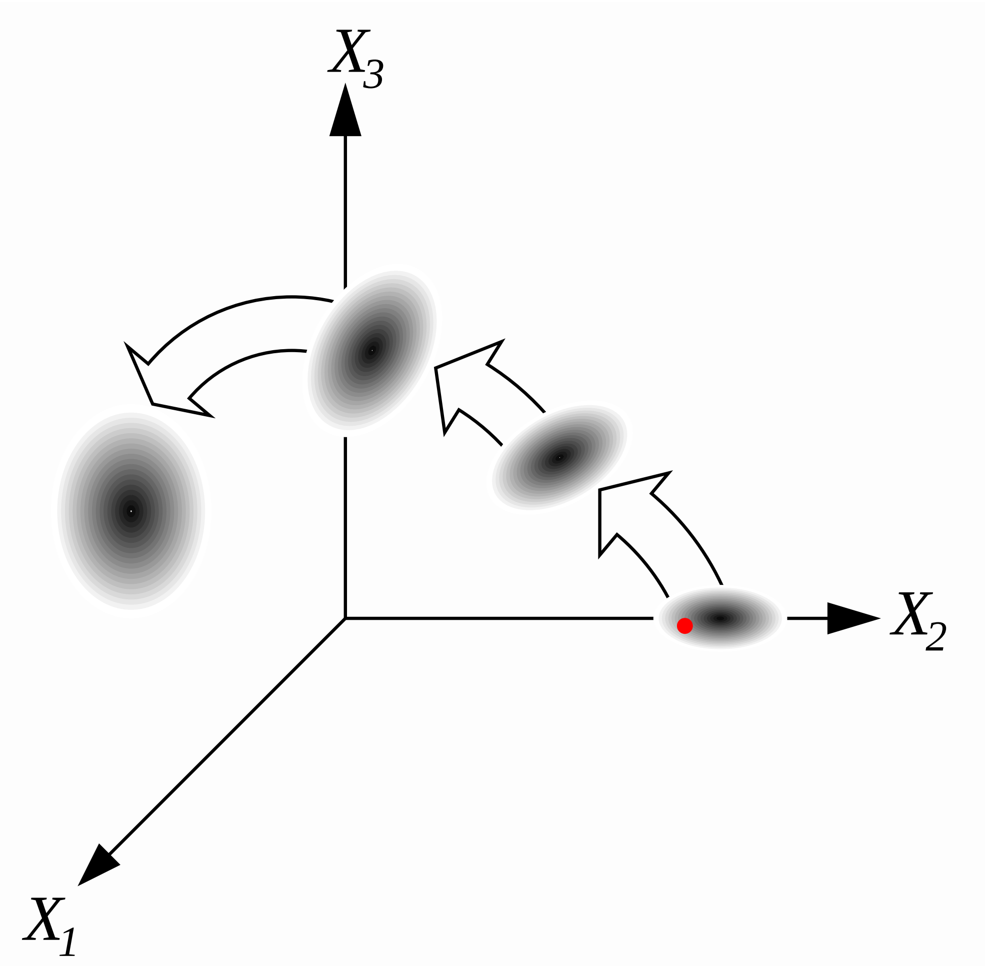

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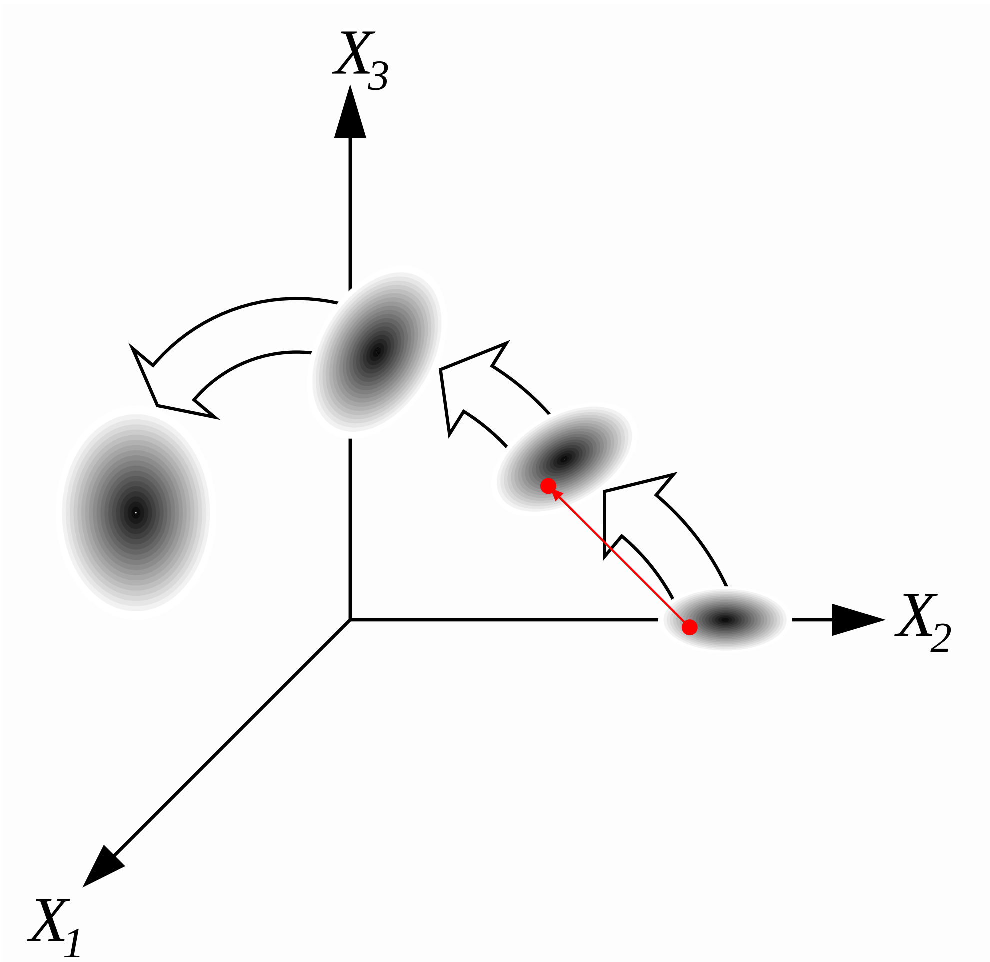

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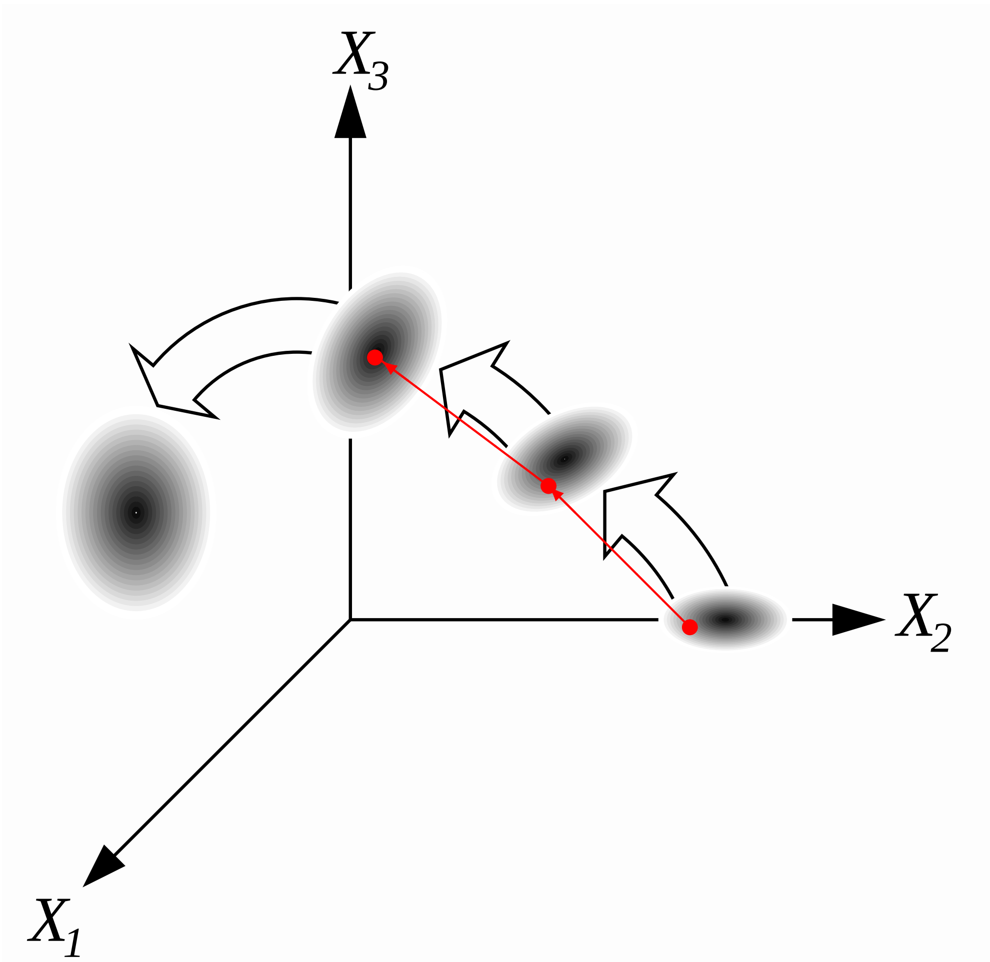

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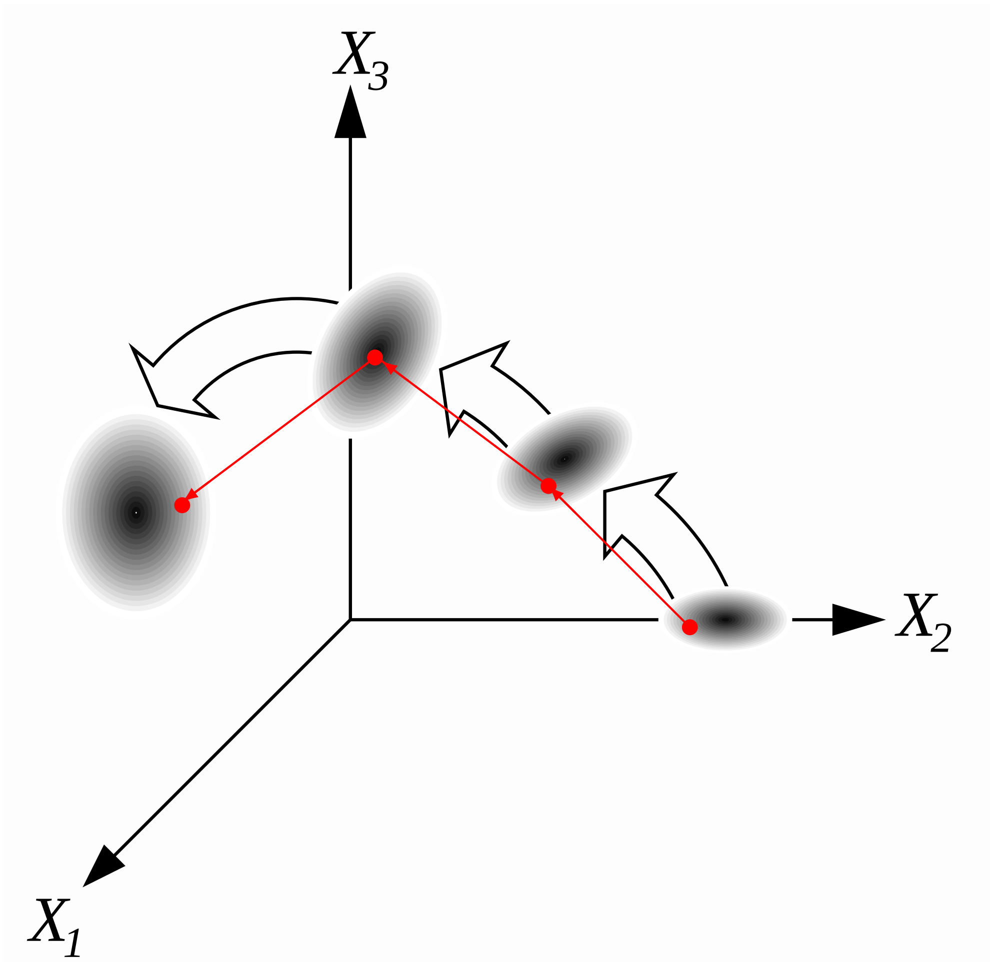

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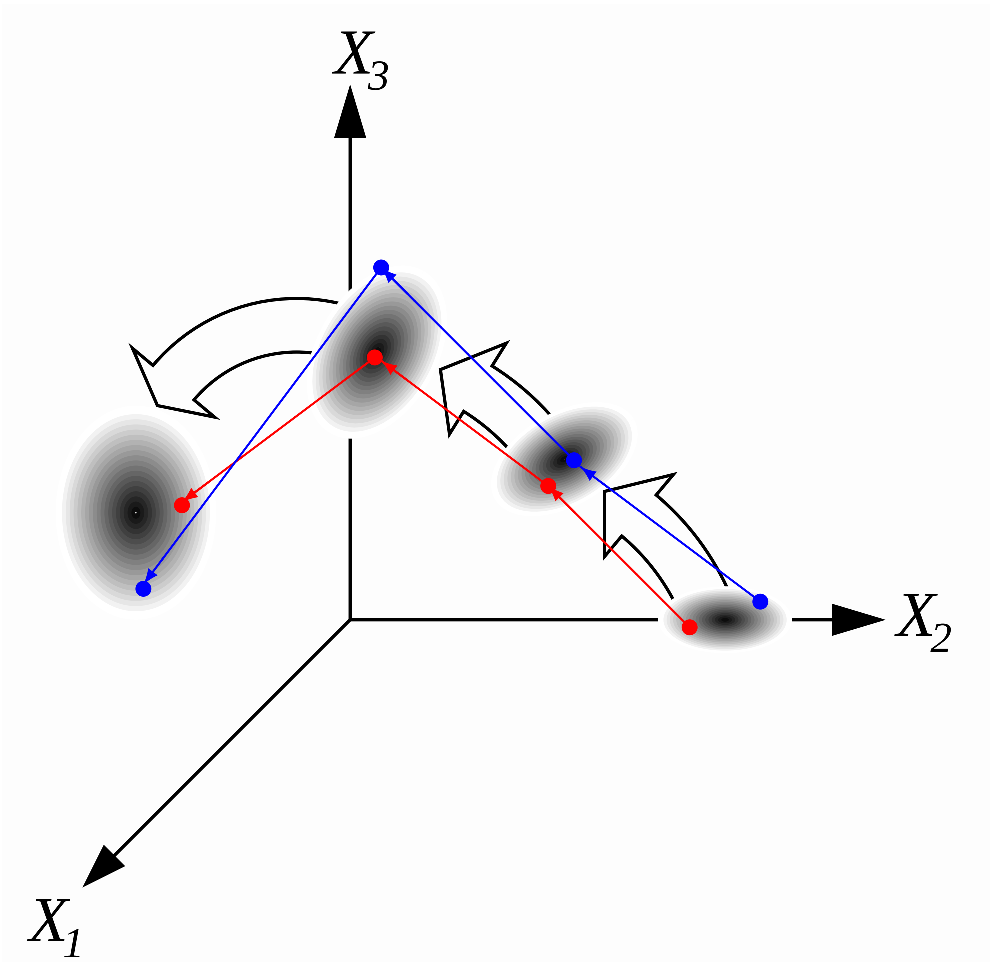

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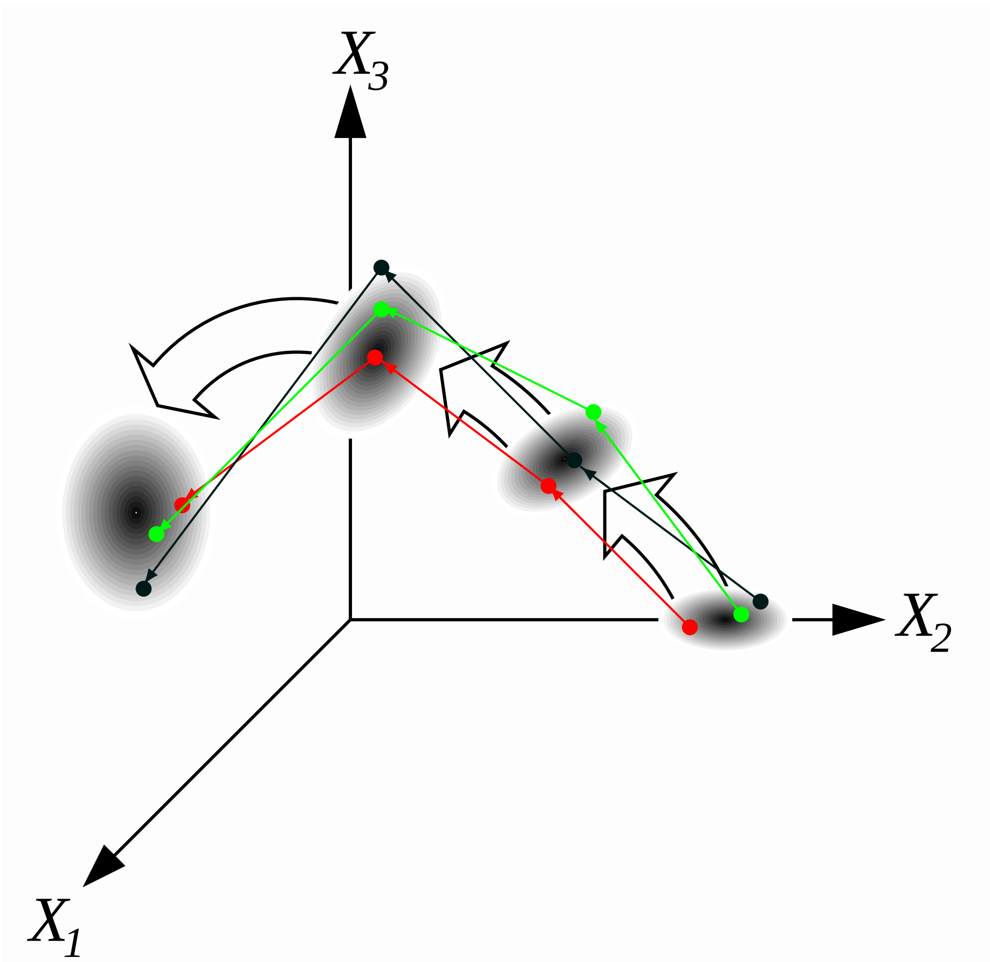

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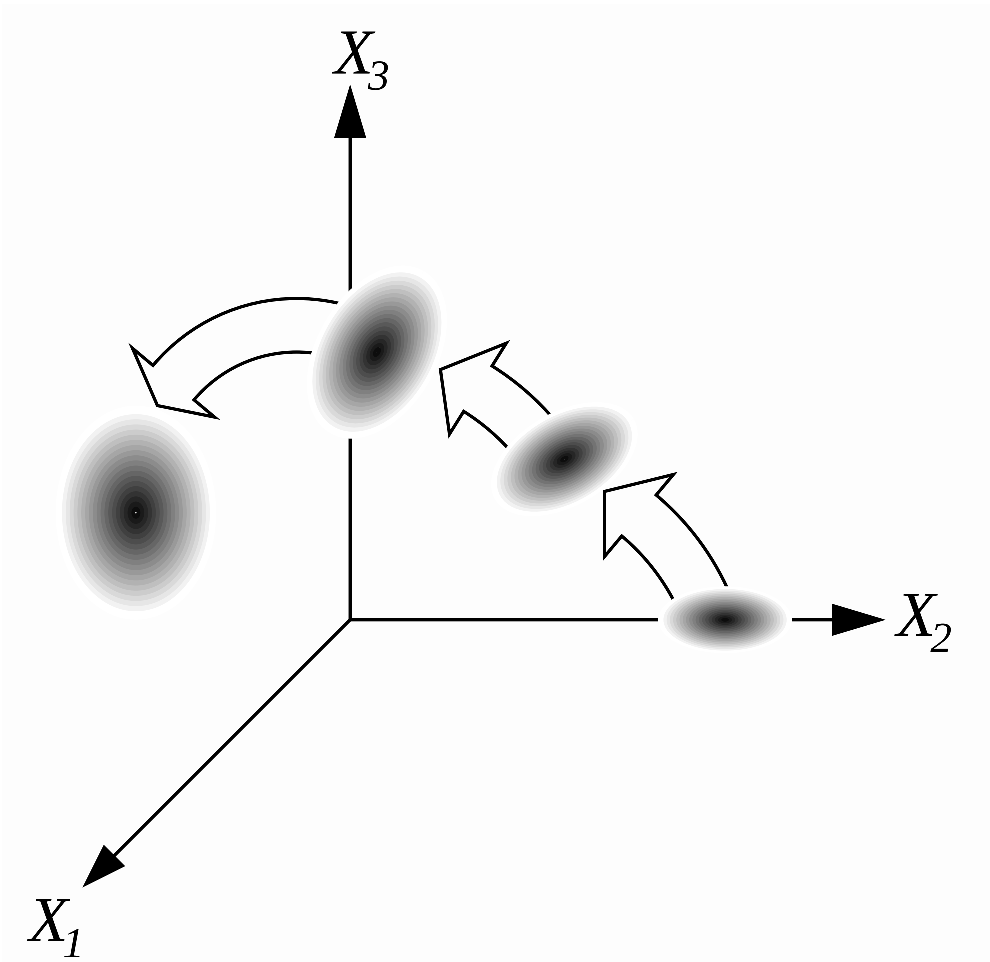

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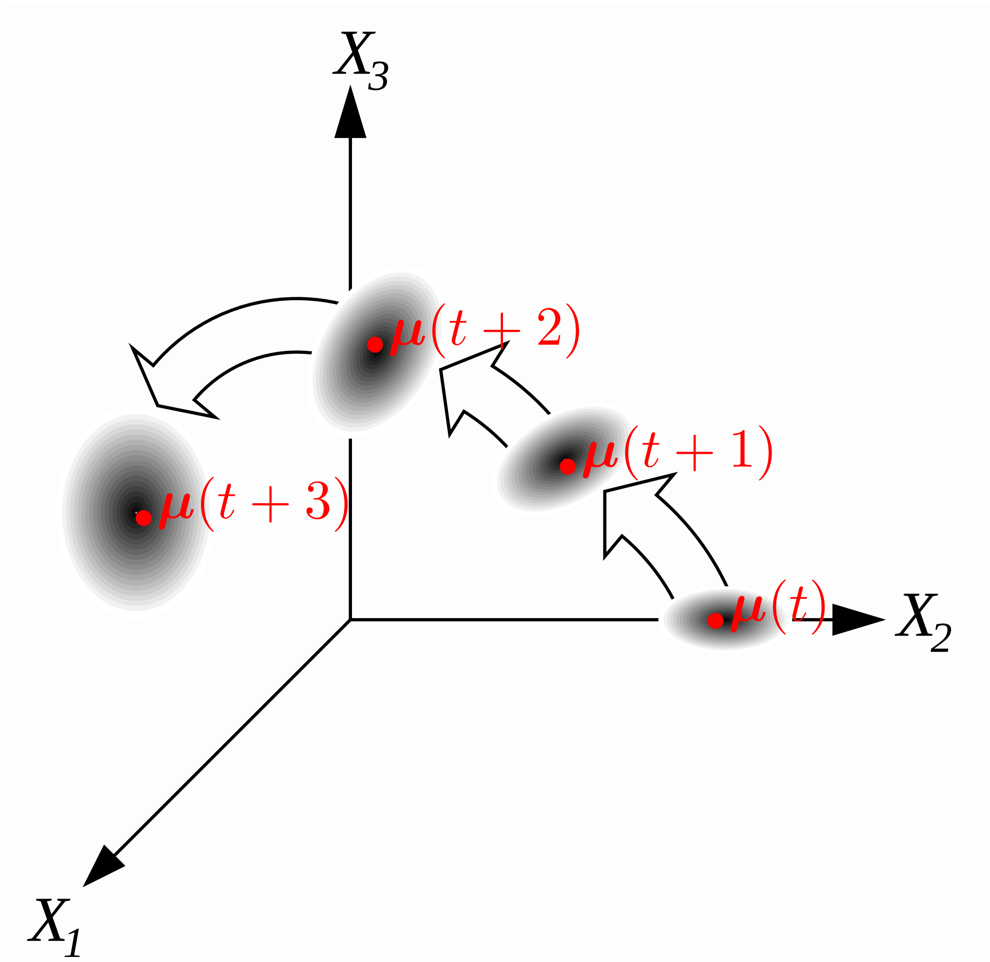

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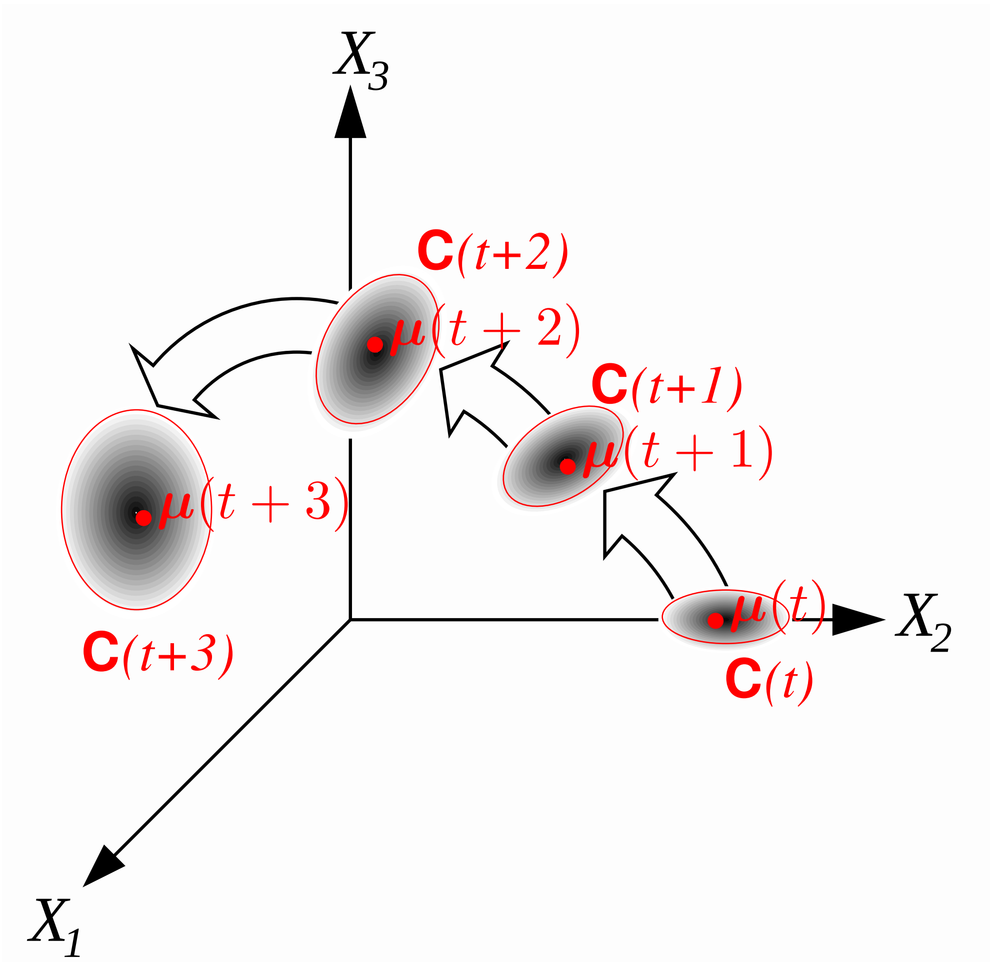

Four Phase Dynamics

- An ensemble of GAs can be modelled as follows

  1. Draw a distribution, $\boldsymbol{X}$, from $f_{\boldsymbol{X}}(\boldsymbol{x}, t)$
  2. Draw a sample, $\boldsymbol{N}$, of size p (the population size) from $\boldsymbol{X}$
  3. The occupation probability after selection is given by

  $$X_i^s = \frac{N_i s_i}{\sum_j N_j s_j}$$

  4. The occupation probability after mutation is given by

  $$\boldsymbol{X}^{sm} = \boldsymbol{W}\boldsymbol{X}^s$$

  where $\boldsymbol{W}$ is the mutation matrix with elements $W_{i,j}$

- To compute $f_{\boldsymbol{X}}(\boldsymbol{x}, t+1)$ we have to average over
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The Hard Part

- The only hard part is computing the distribution after selection
- We will only attempt to compute the mean and covariance of $f_{\boldsymbol{X}}(\boldsymbol{x}, t+1)$
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Stochastic Average

- A simple approach is to use the *stochastic expansion*

$$\left\langle f(\boldsymbol{N})\right\rangle = \left\langle f(\left\langle \boldsymbol{N}\right\rangle + \delta\boldsymbol{N})\right\rangle \qquad \delta\boldsymbol{N} = \boldsymbol{N} - \left\langle \boldsymbol{N}\right\rangle$$

$$\approx f(\left\langle \boldsymbol{N}\right\rangle) + \sum_i \left\langle \delta N_i\right\rangle \frac{\partial f(\left\langle \boldsymbol{N}\right\rangle)}{\partial \mu_i} + \frac{1}{2}\sum_{i,j}\left\langle \delta N_i \delta N_j\right\rangle \frac{\partial^2 f(\left\langle \boldsymbol{N}\right\rangle)}{\partial \mu_i \partial \mu_j}$$

$$= f(p\boldsymbol{\mu}) + \frac{1}{2}\sum_{i,j} p^2 C_{ij} \frac{\partial^2 f(p\boldsymbol{\mu})}{\partial \mu_i \partial \mu_j}$$

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Stochastic Expansion Approximation

- This lead to simple update equation for $\boldsymbol{\mu}$ and $\mathbf{C}$

$$\mu_i^s(t) \approx \frac{s_i}{m}\mu_i\left(1 + \sum_{k,l} s_k\, s_l\, c_{kl}(t)\right) - \frac{s_i}{m^2}\sum_k s_k\, c_{ik}(t)$$

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Can We Do Better?

- The quantities we are interested in can be obtained from

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- Using Euler's representation of the logarithm

$$\log(A) = \int_0^\infty \frac{\mathrm{e}^{-z} - \mathrm{e}^{-zA}}{z} \, \mathrm{d}z$$

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- In sampling we draw a population, $\boldsymbol{N}$, from a multinomial distribution

$$\mathbb{P}(\boldsymbol{N}=\boldsymbol{n}|\boldsymbol{x}) = \prod_{i=1}^{m} \frac{x_i^{n_i}}{n_i!} \left[\!\!\left[\sum_{i=1}^{m} n_i = p \right]\!\!\right]$$

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- For $p = 2$ we can compute this exactly

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Exact Update Equations for $p = 2$

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$$C_{ij}^s = \frac{2(\mu_i \mu_j + C_{ij}) s_i s_j}{(s_i + s_j)^2} + \sum_k \frac{2(\mu_i \mu_k + C_{ik}) s_i^2}{(s_i + s_k)^2} [\![i = j]\!] - \mu_i \mu_j$$

$$\boldsymbol{\mu}' = \mathbf{W} \boldsymbol{\mu}^s$$

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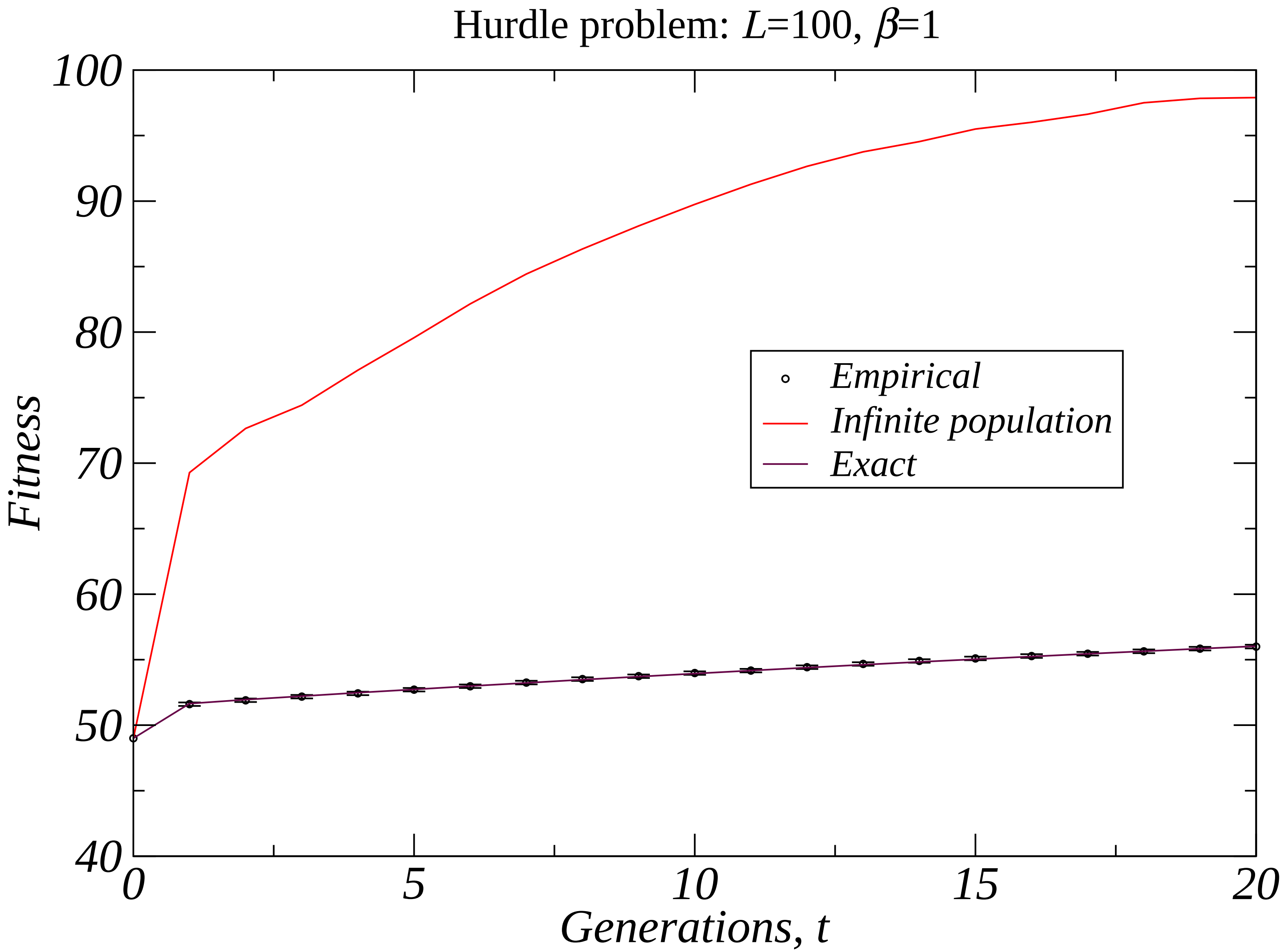
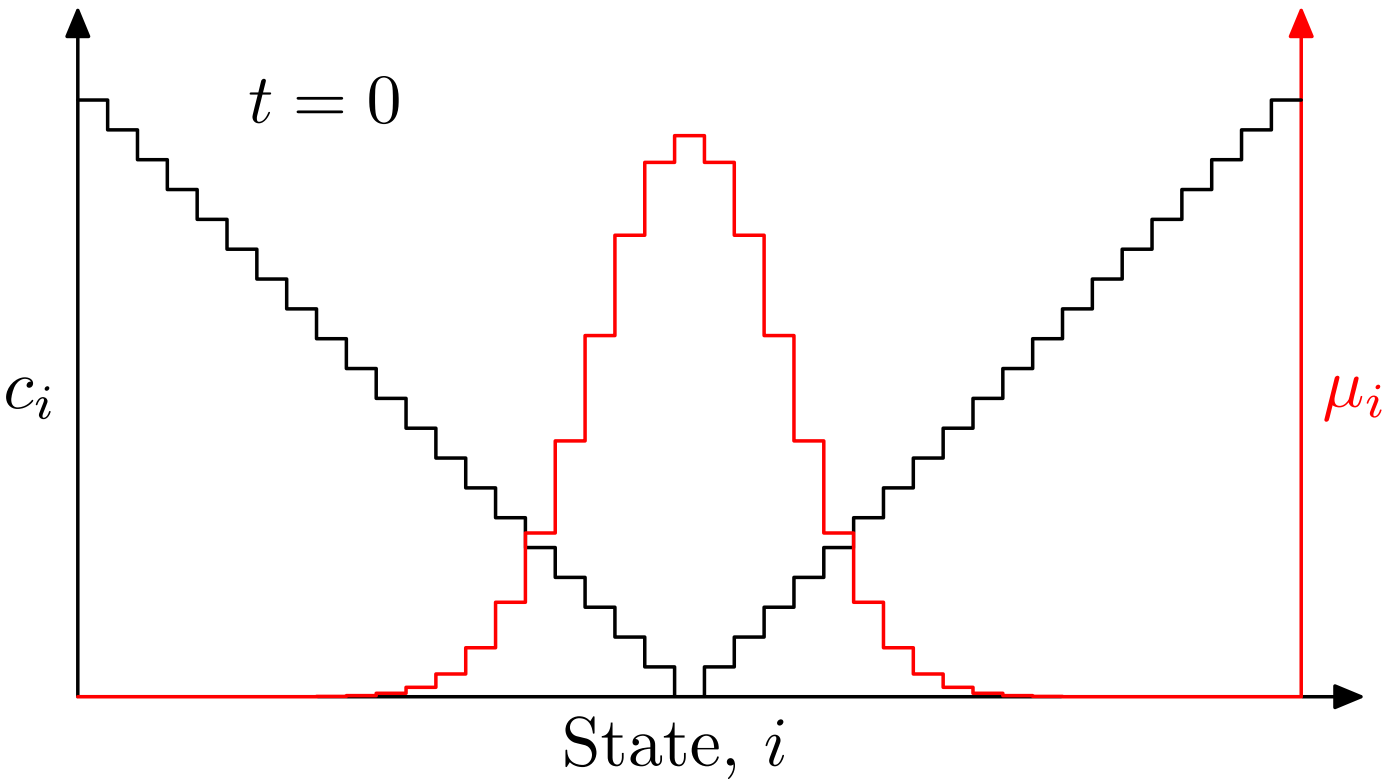


Symmetric Onemax $P = 2$



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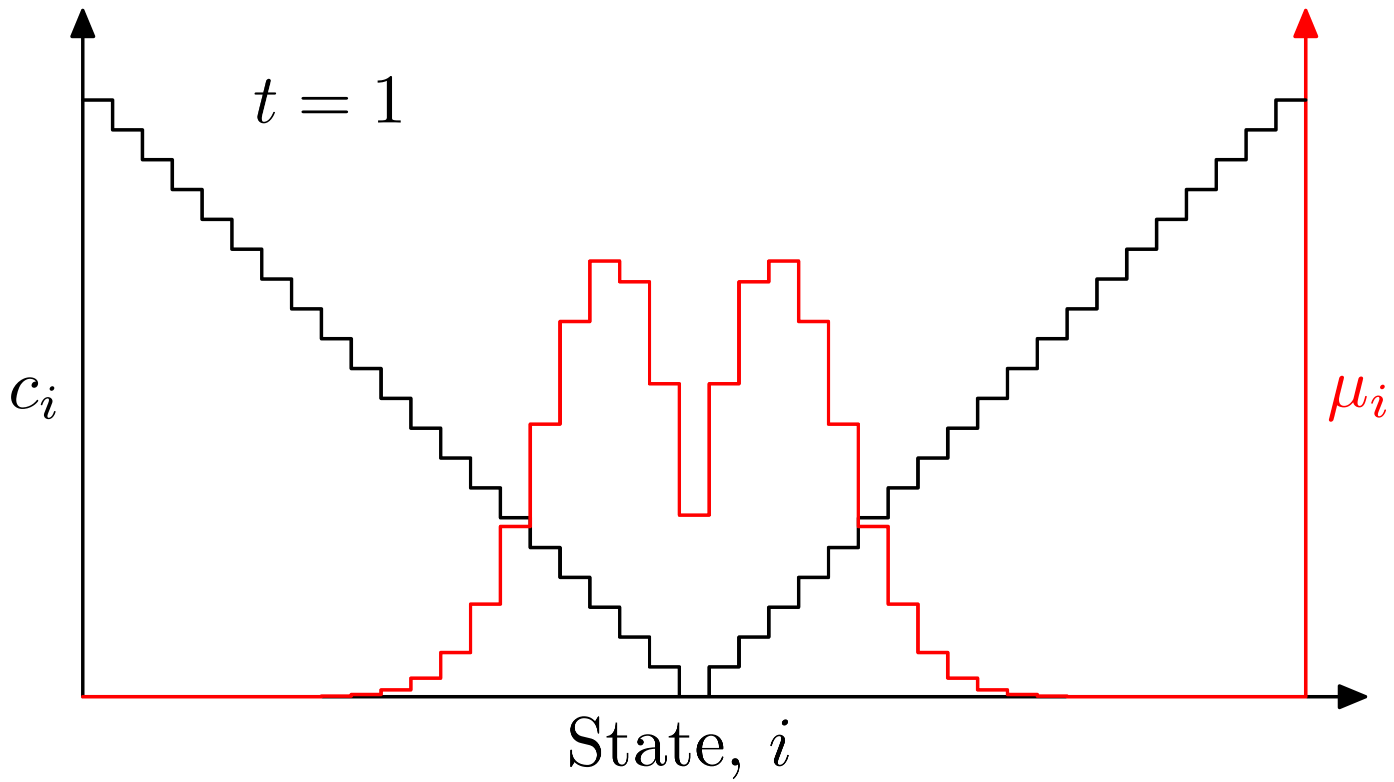

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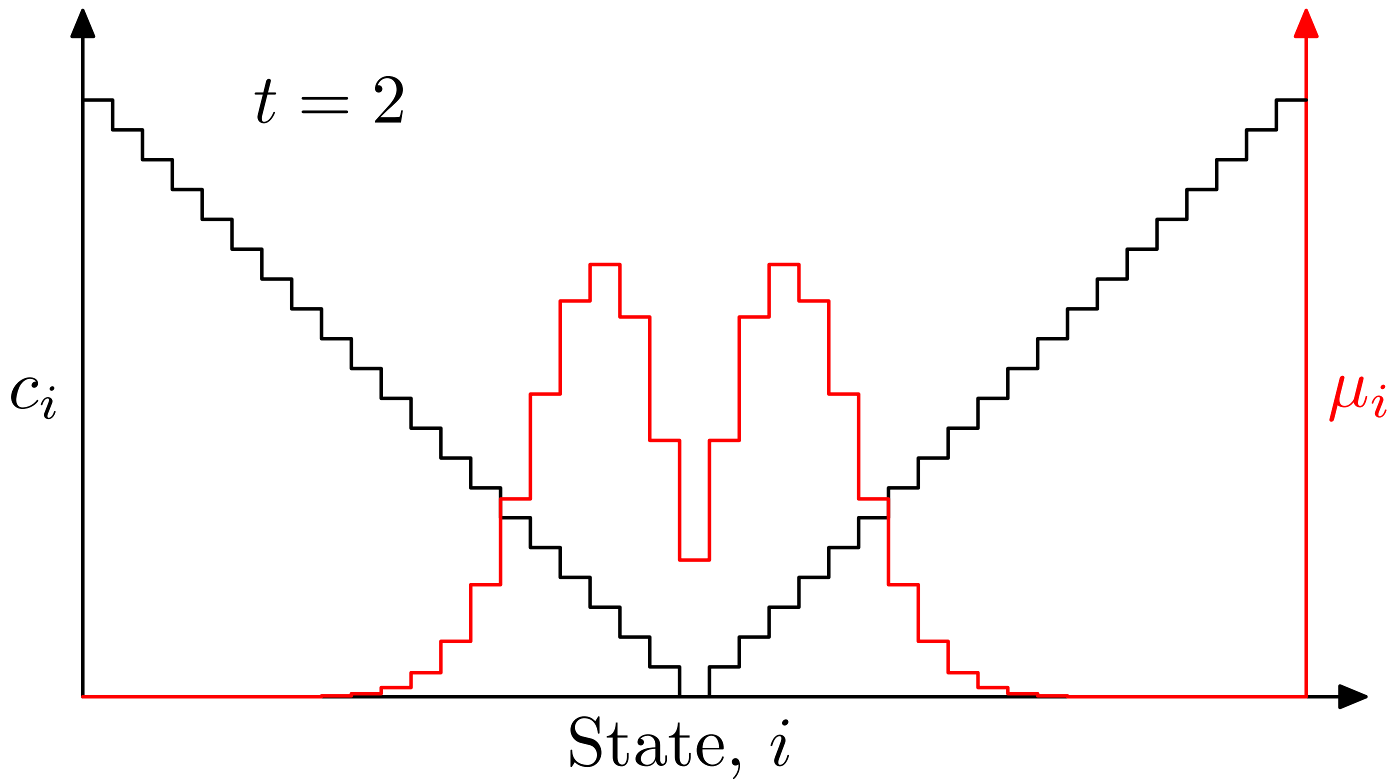

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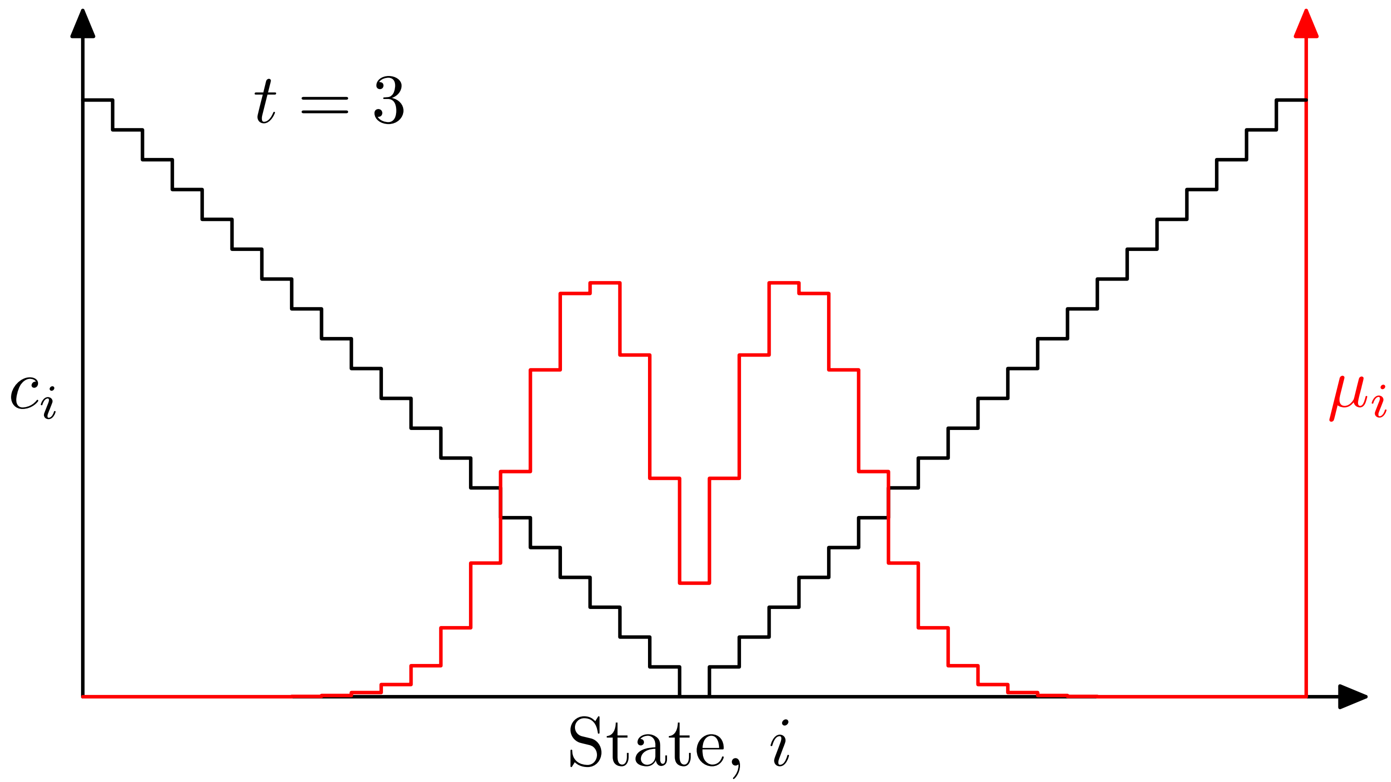

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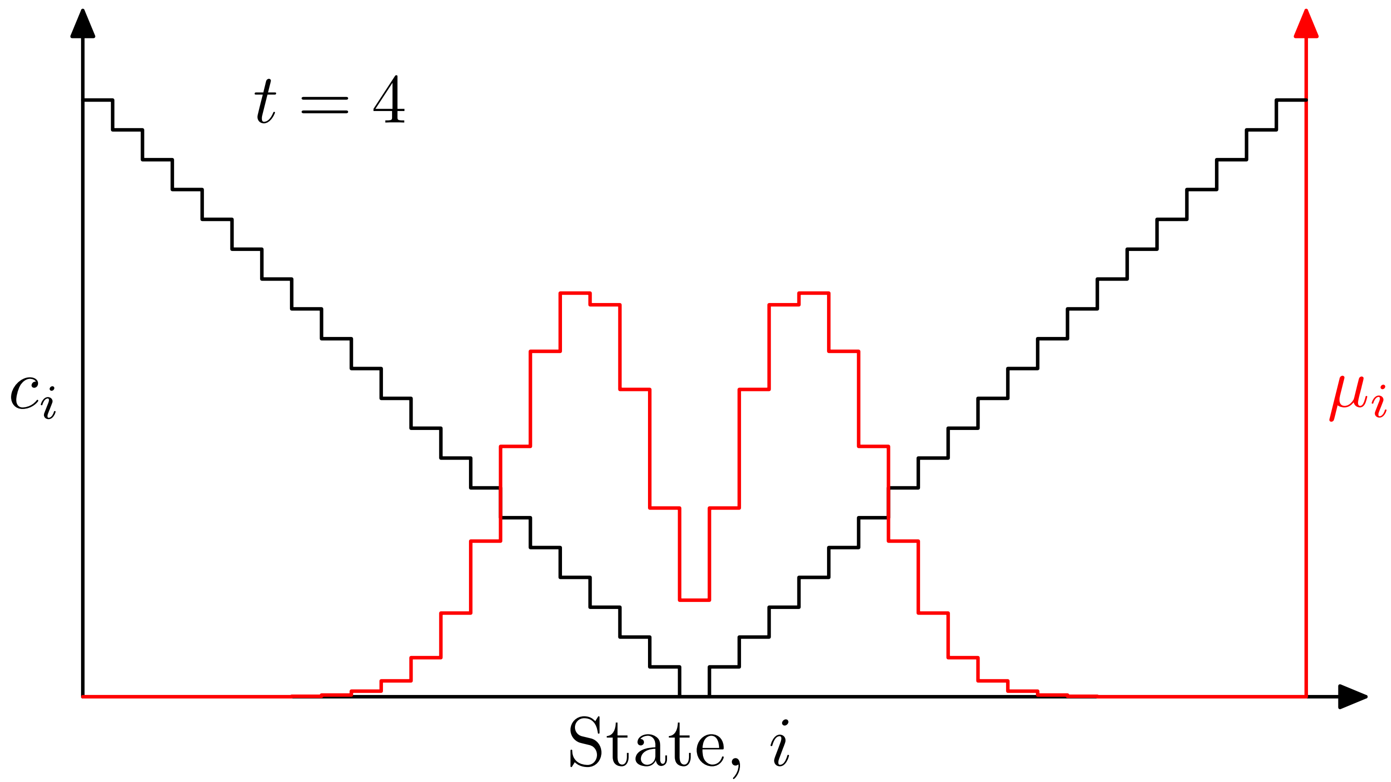

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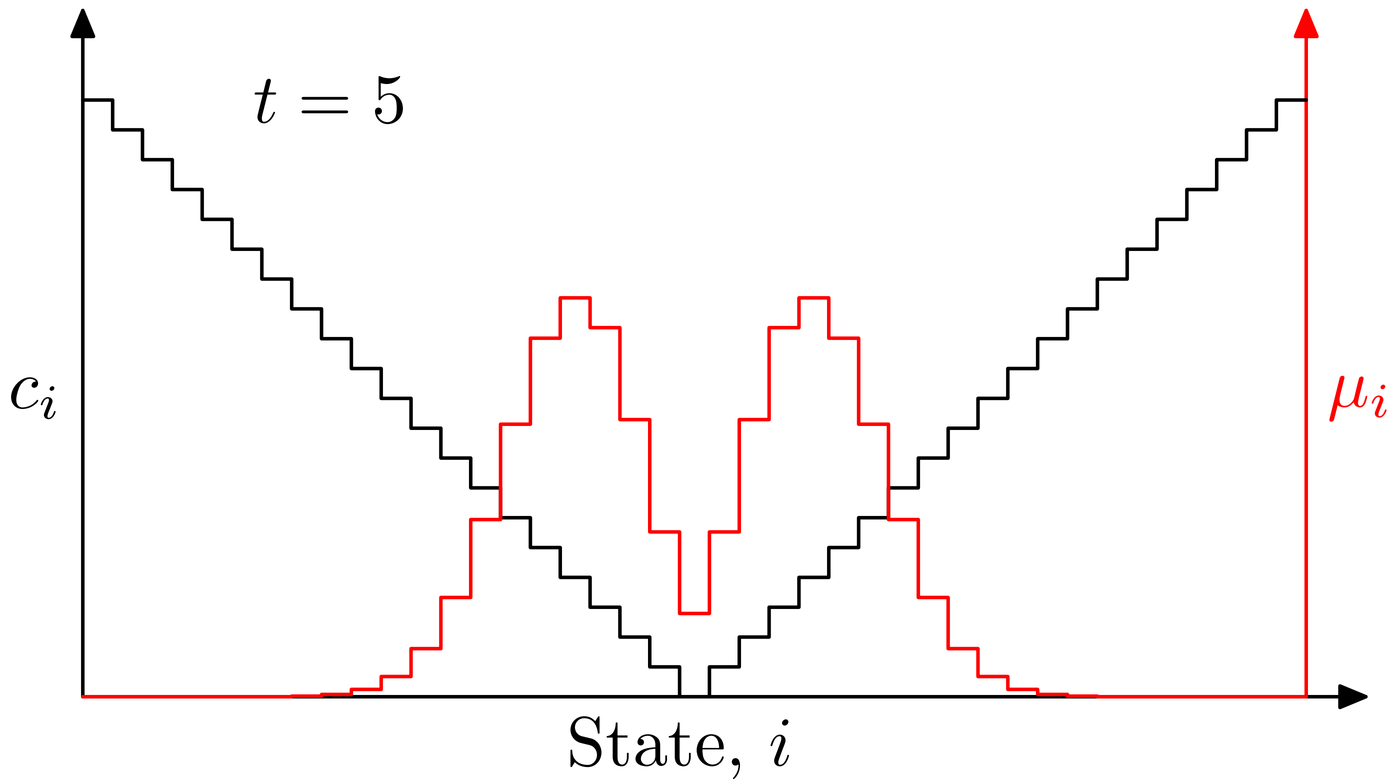

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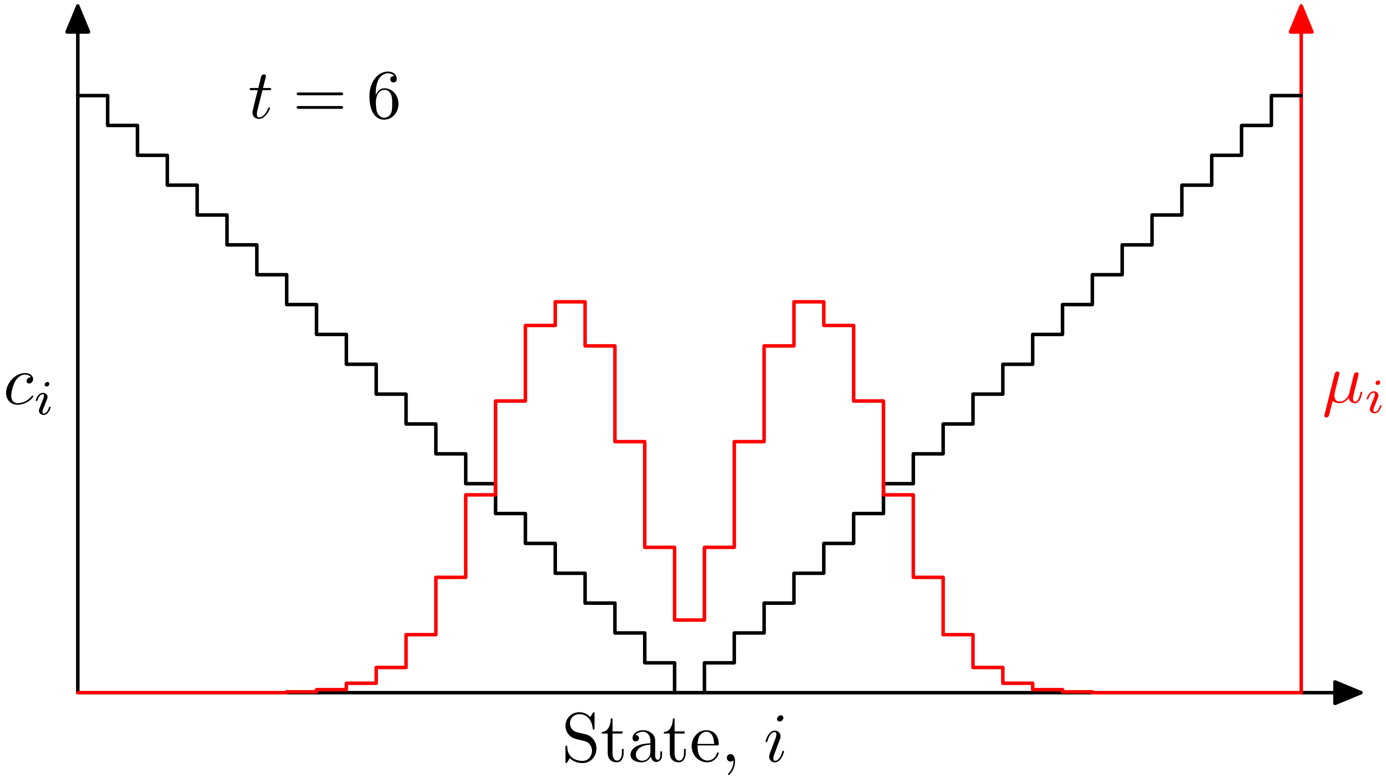

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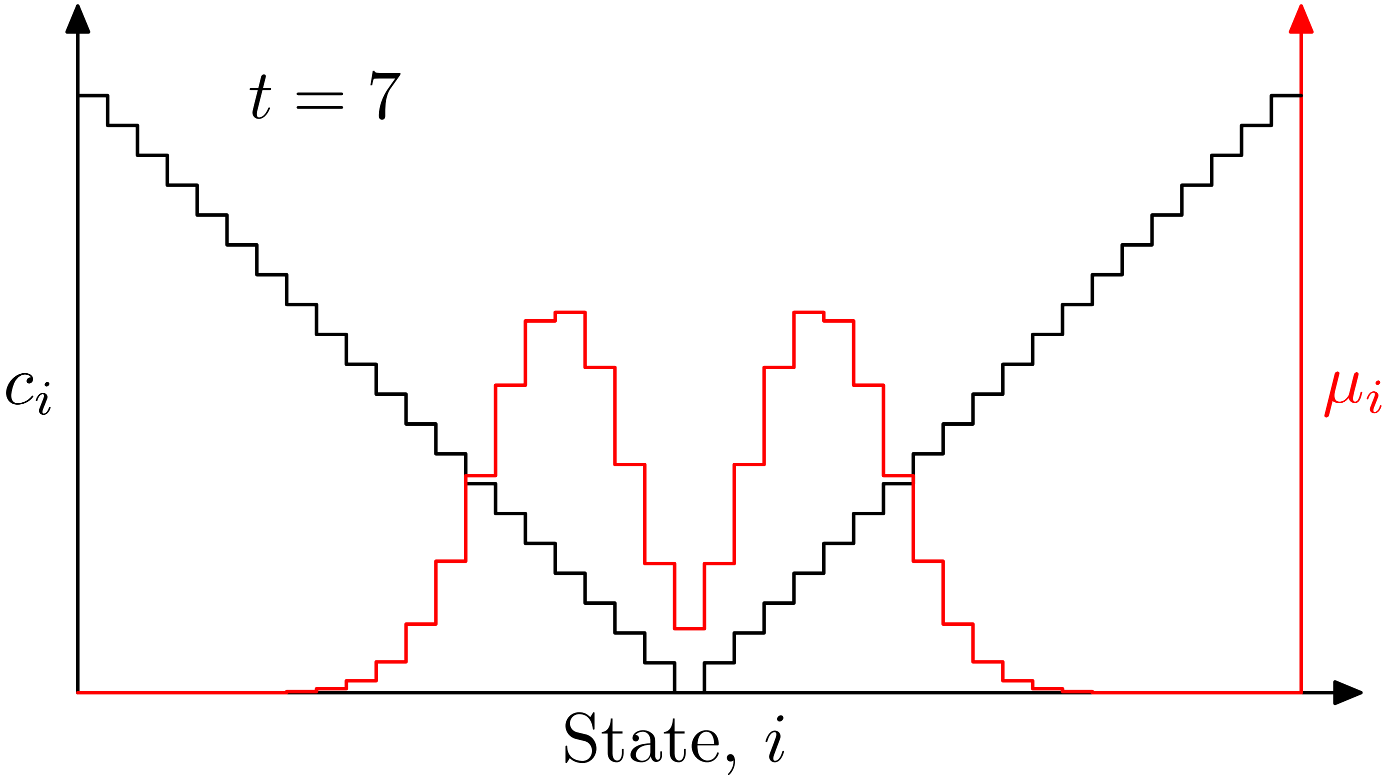

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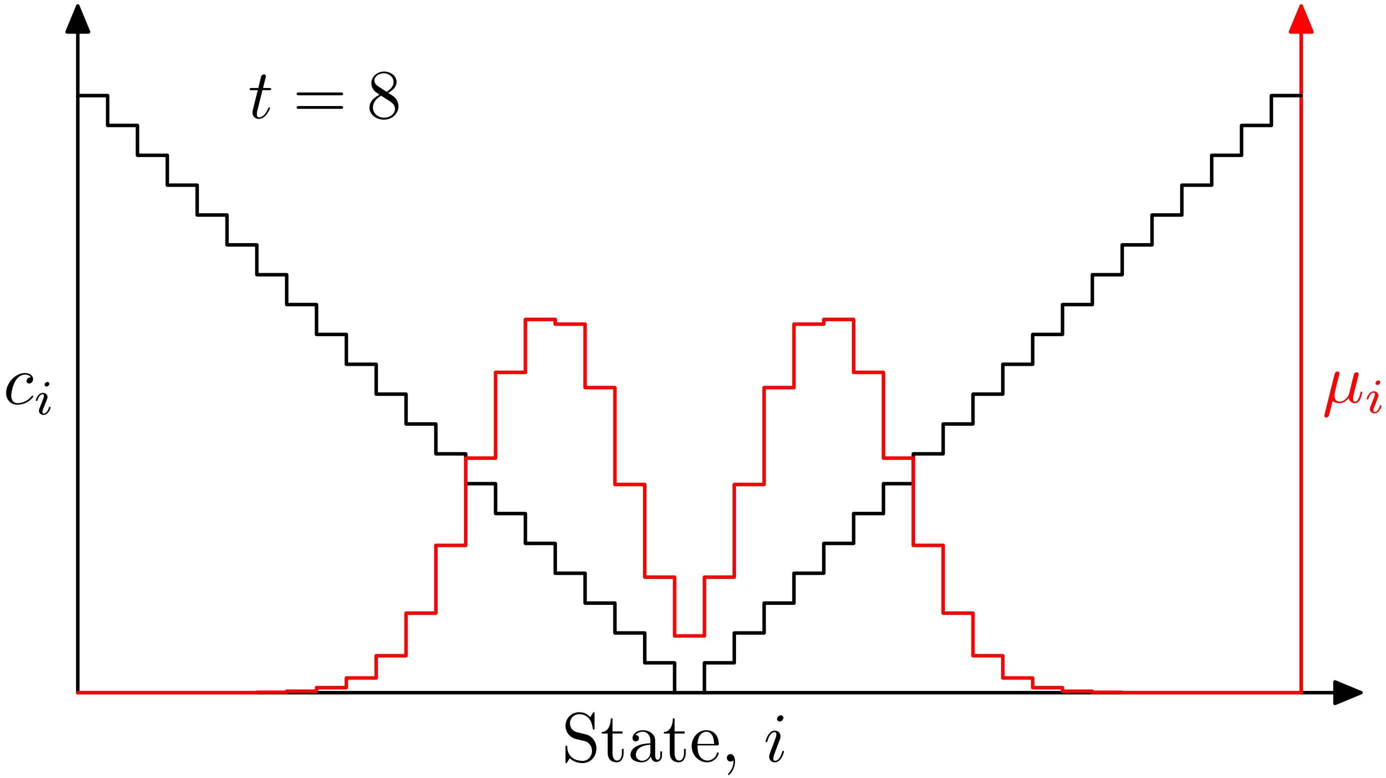

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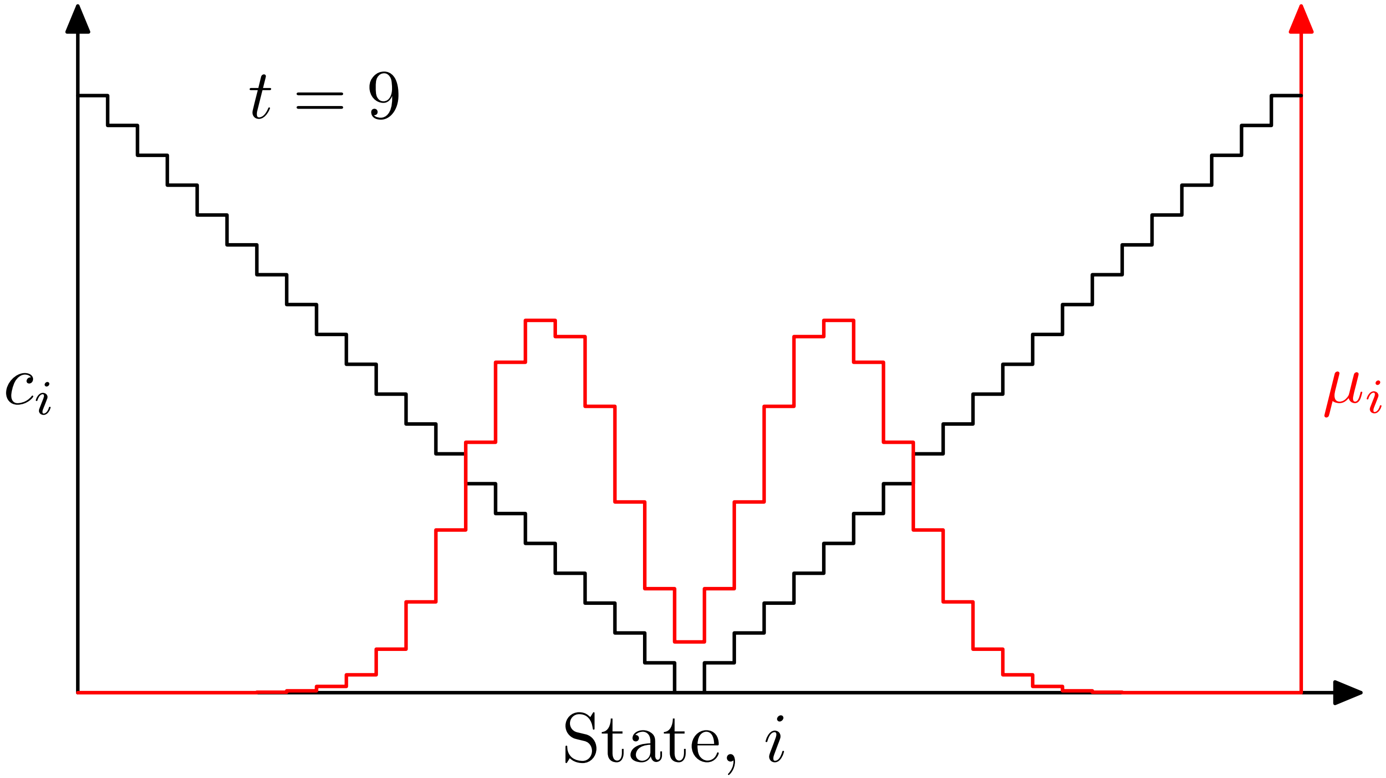

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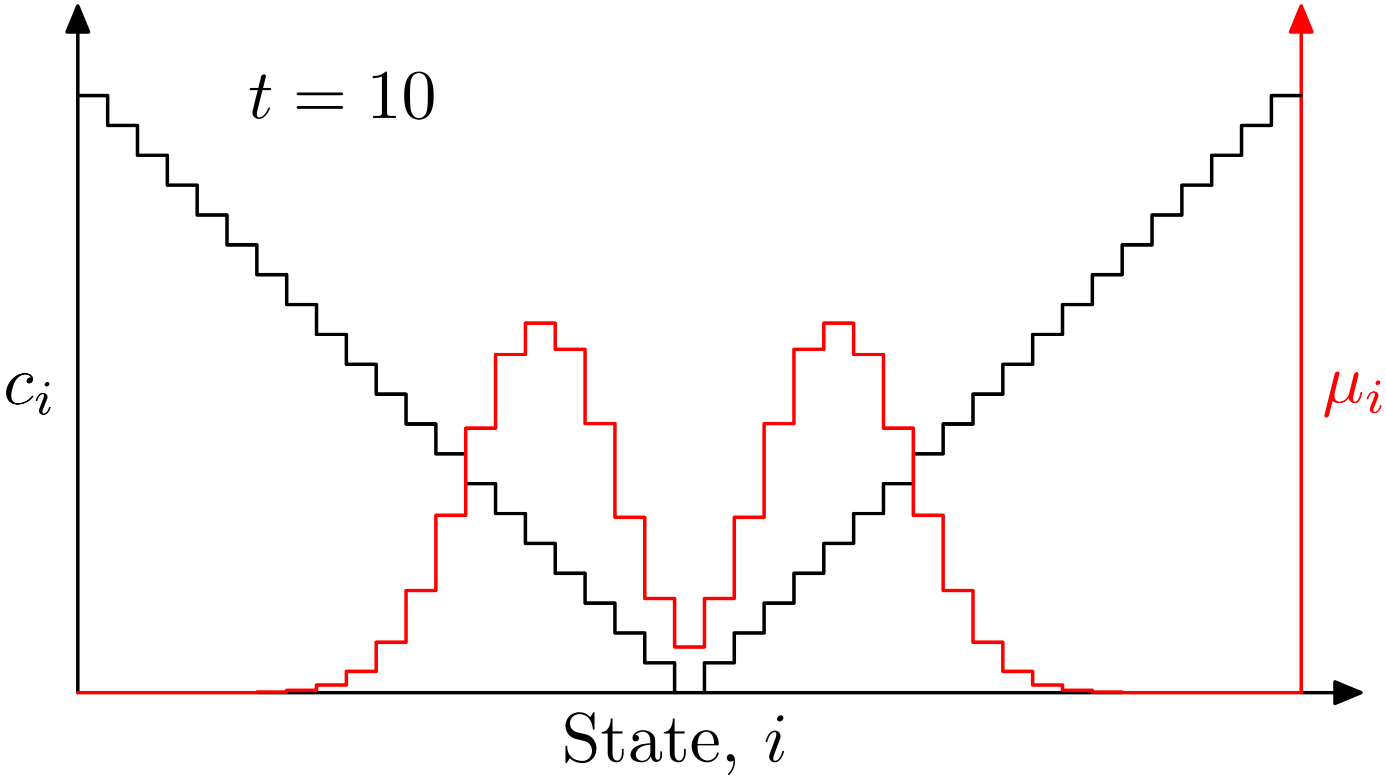

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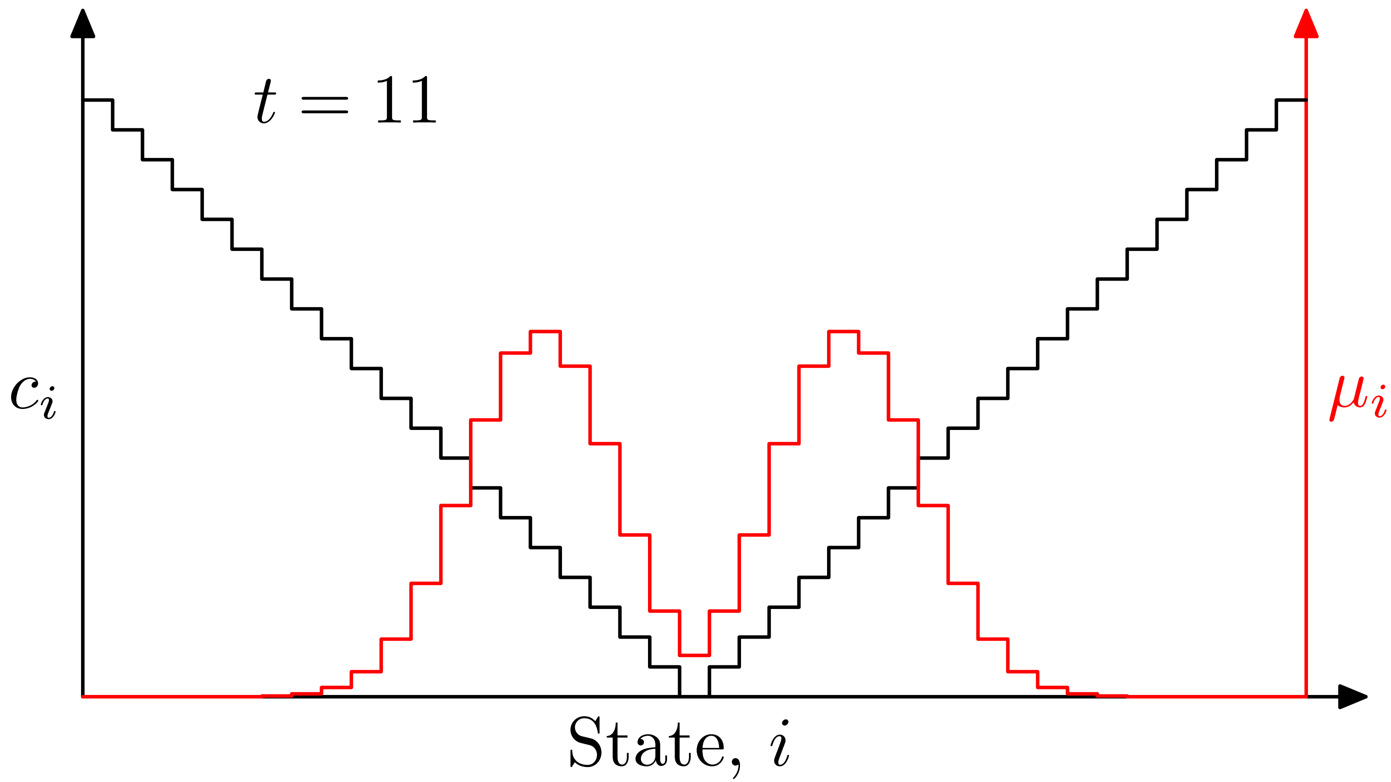

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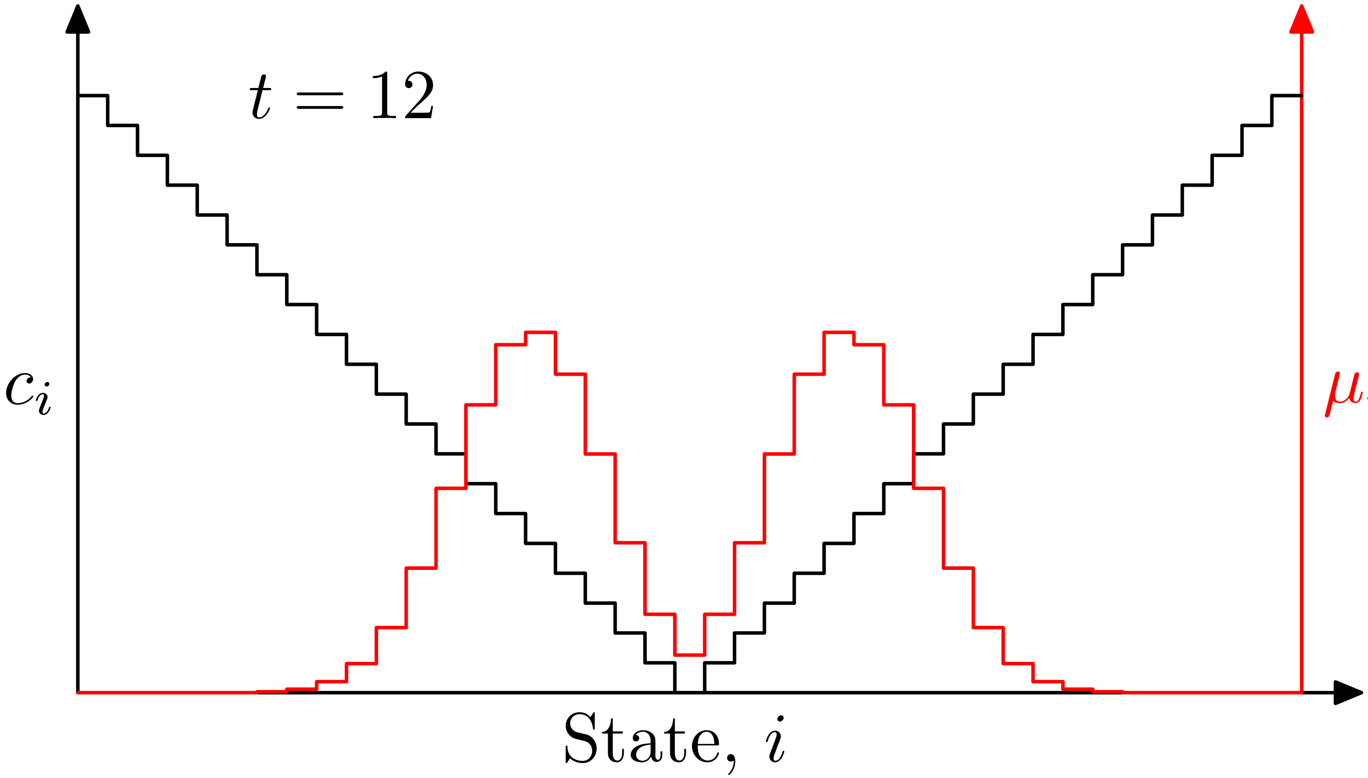

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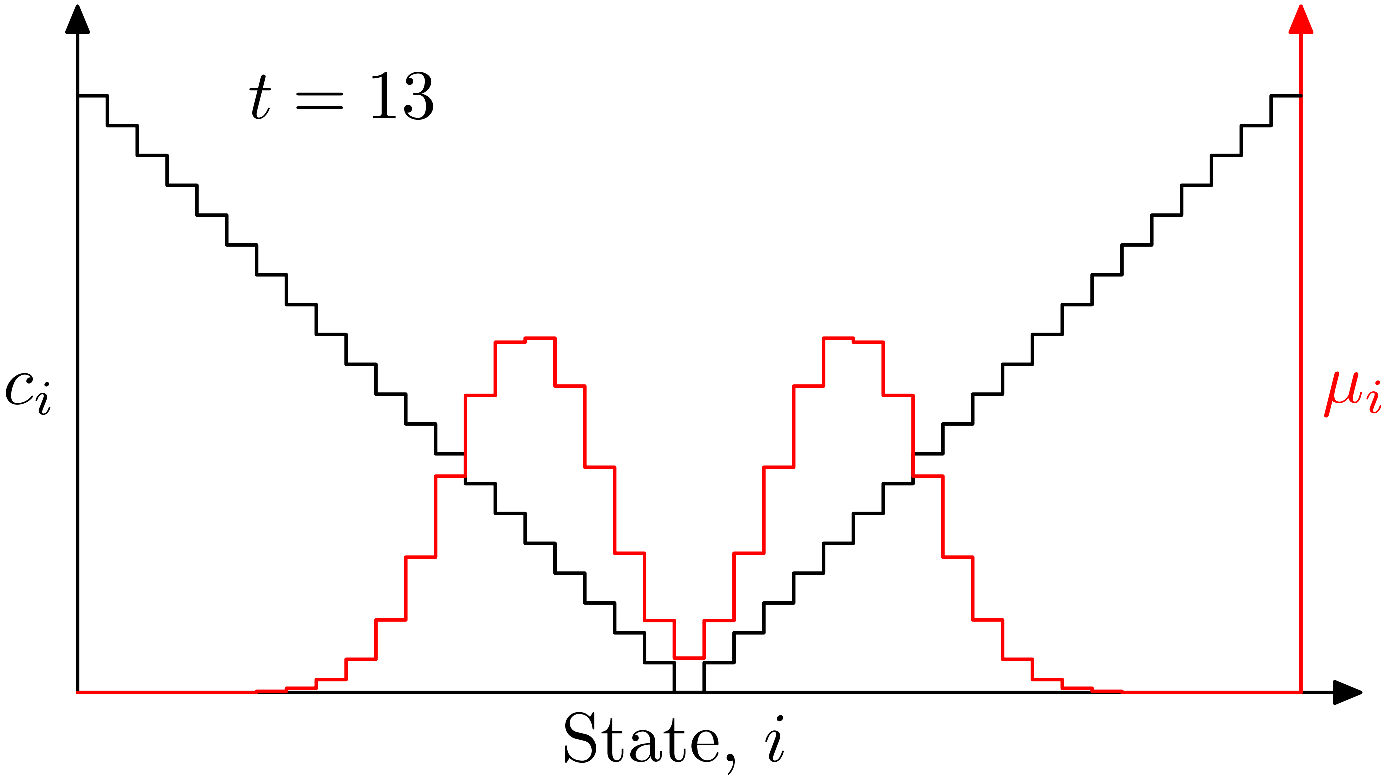

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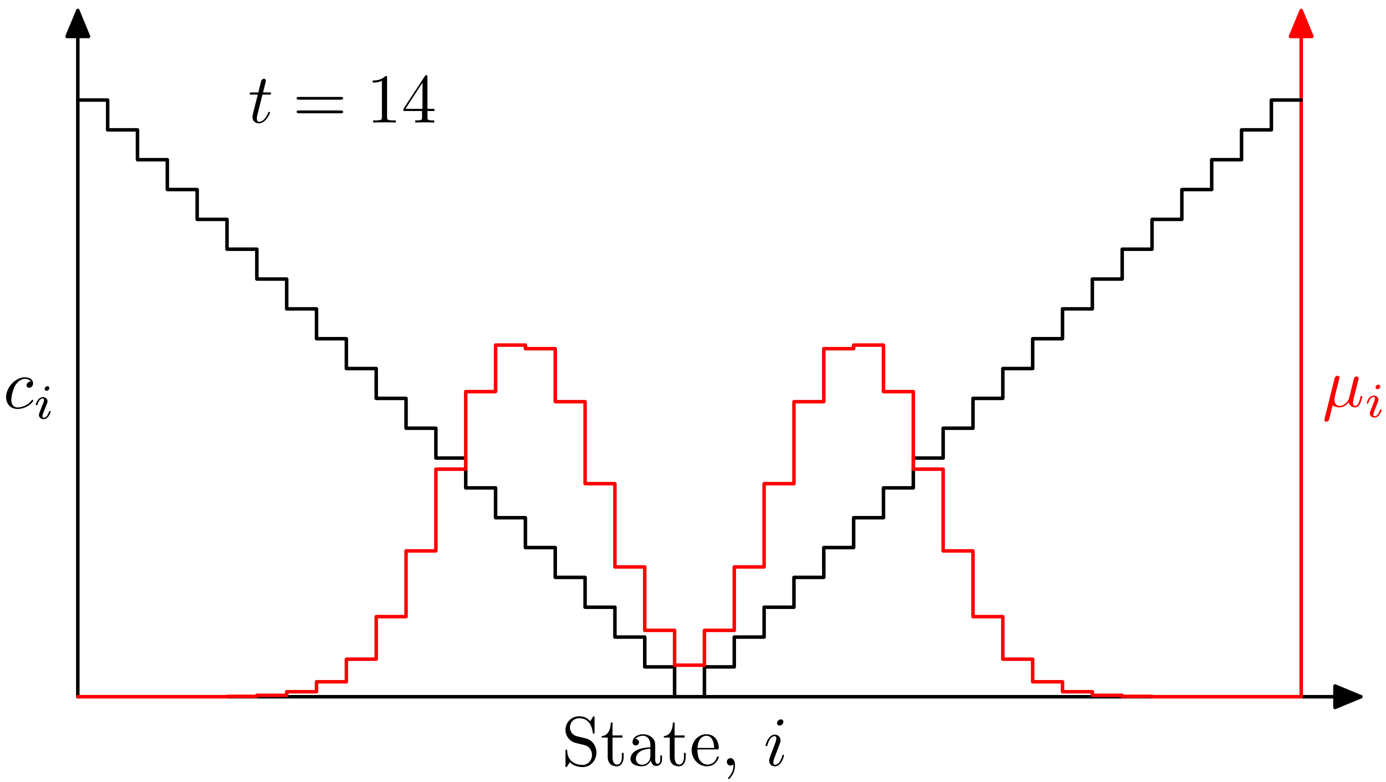

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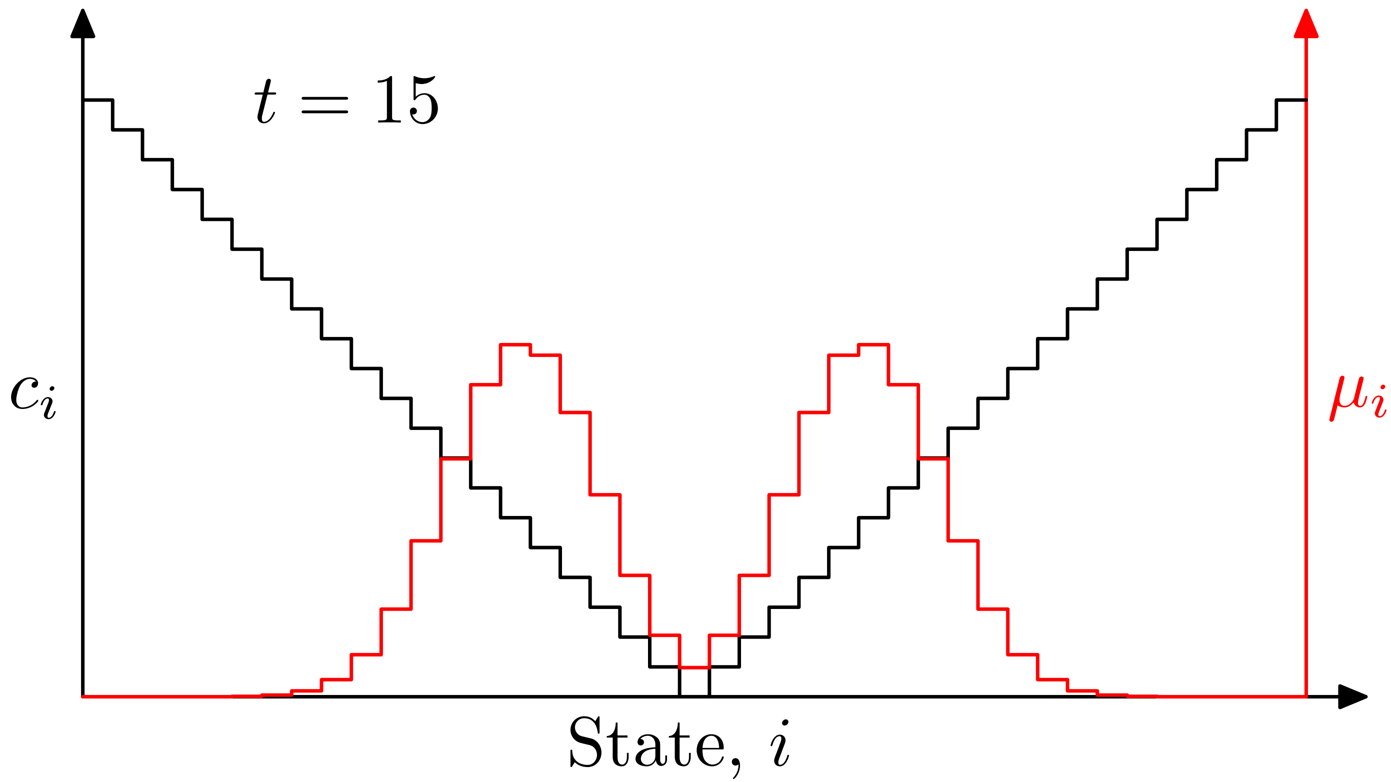

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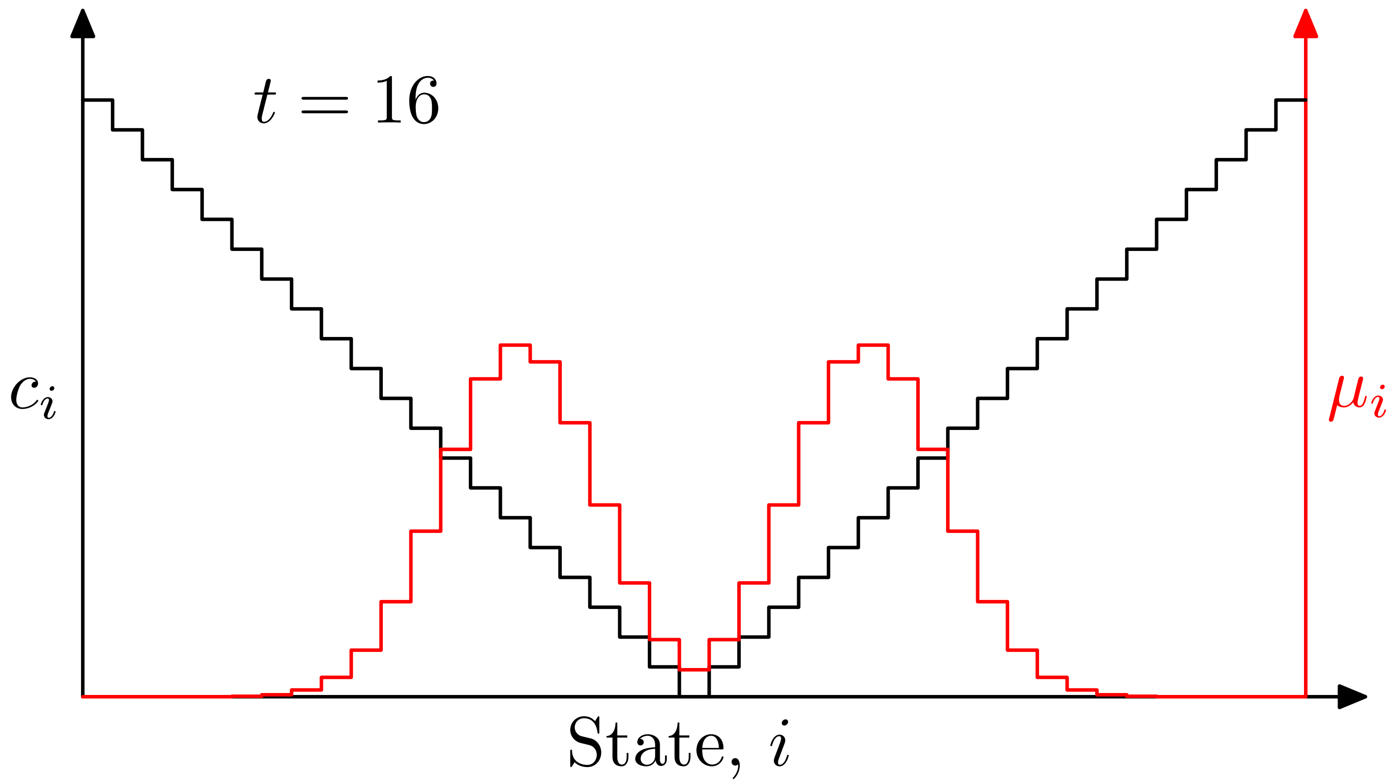

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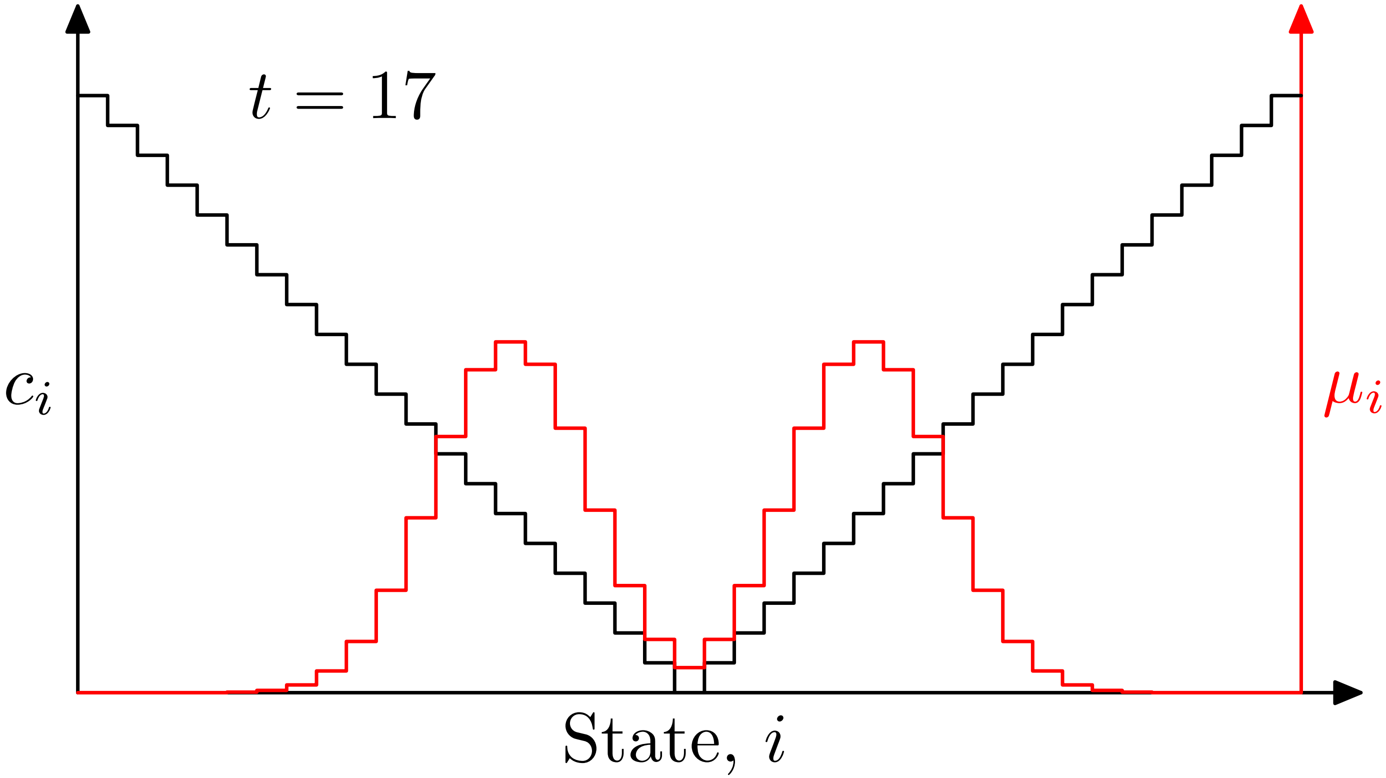

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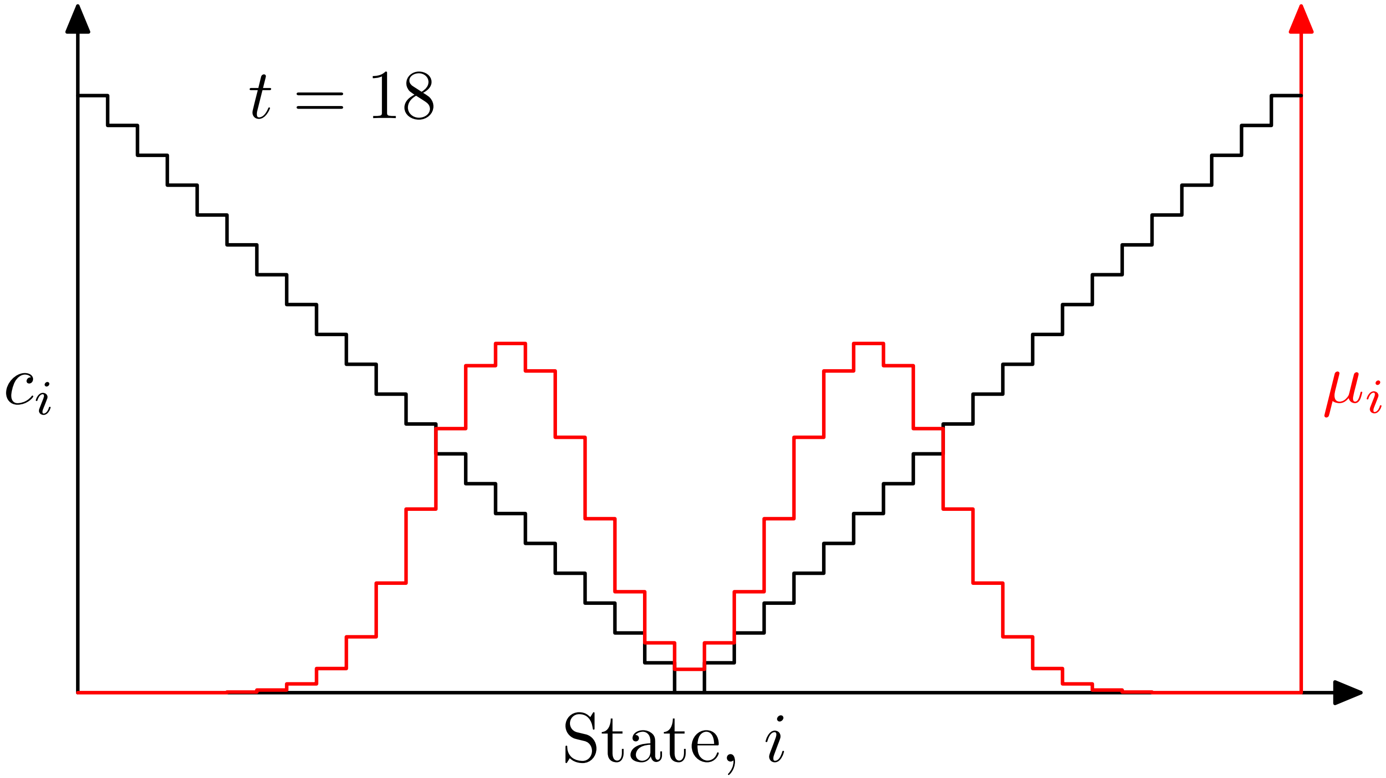

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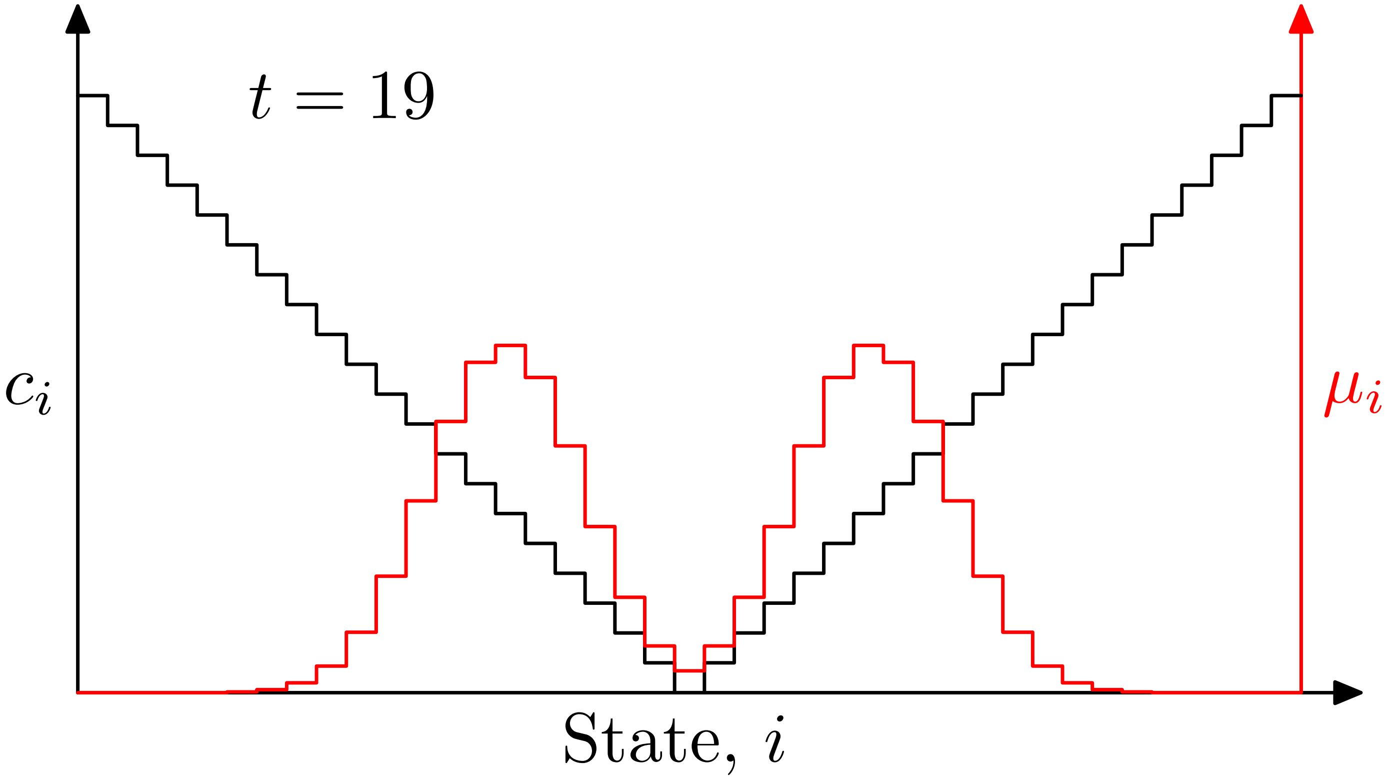

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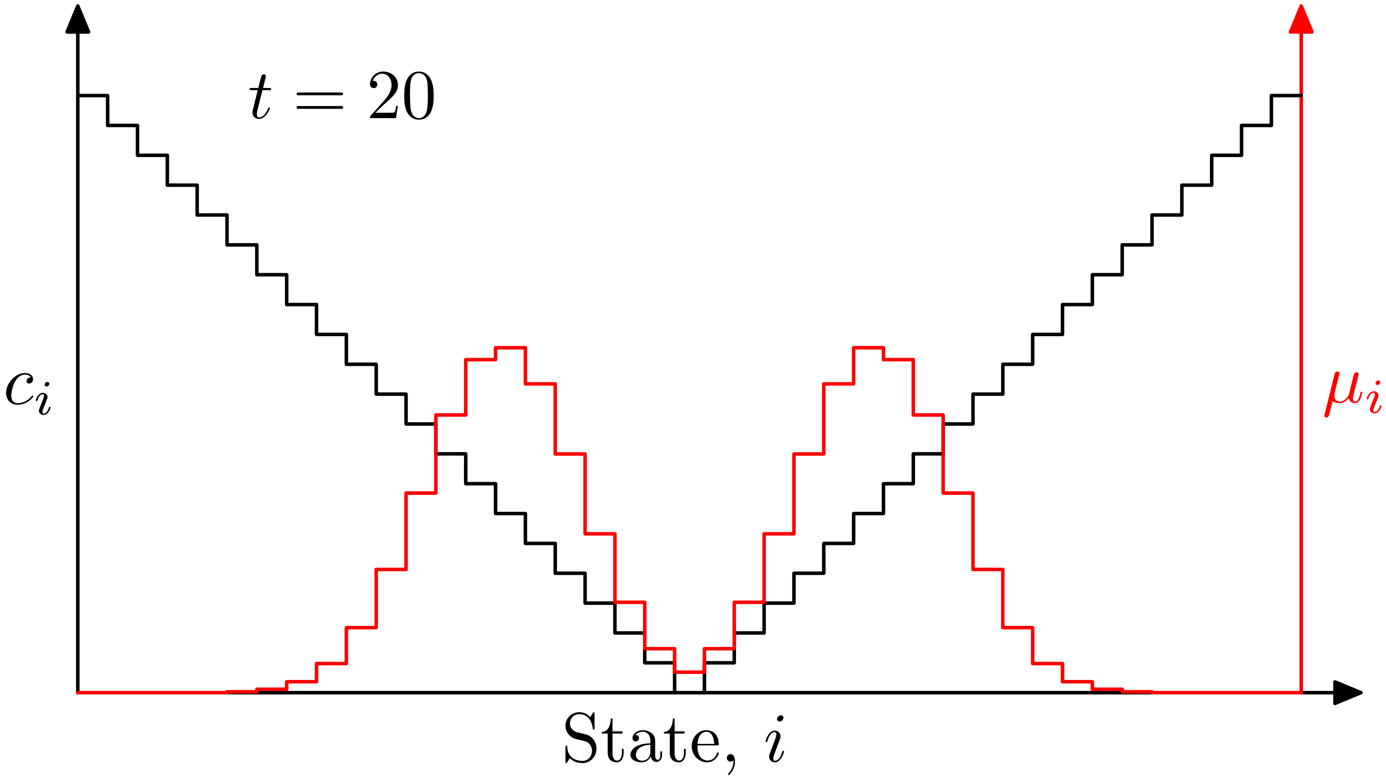

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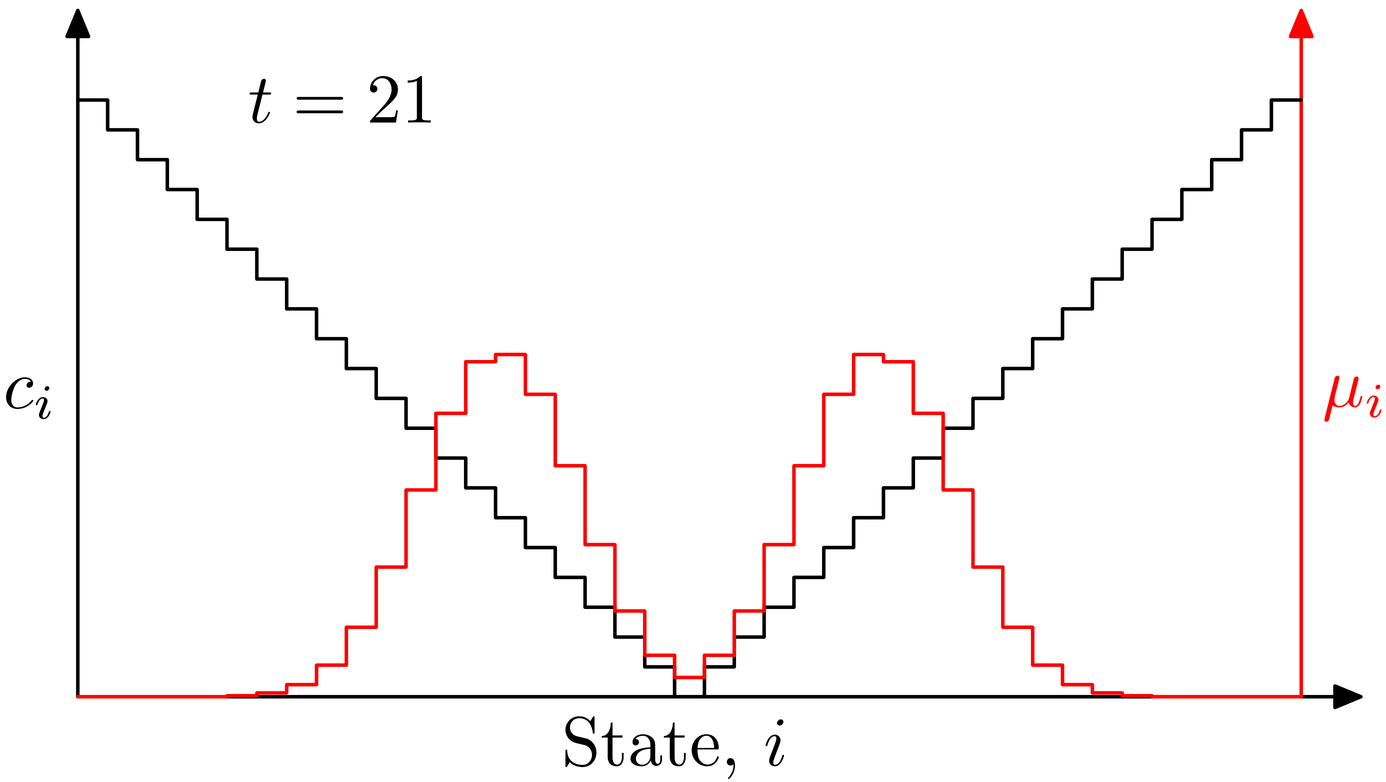

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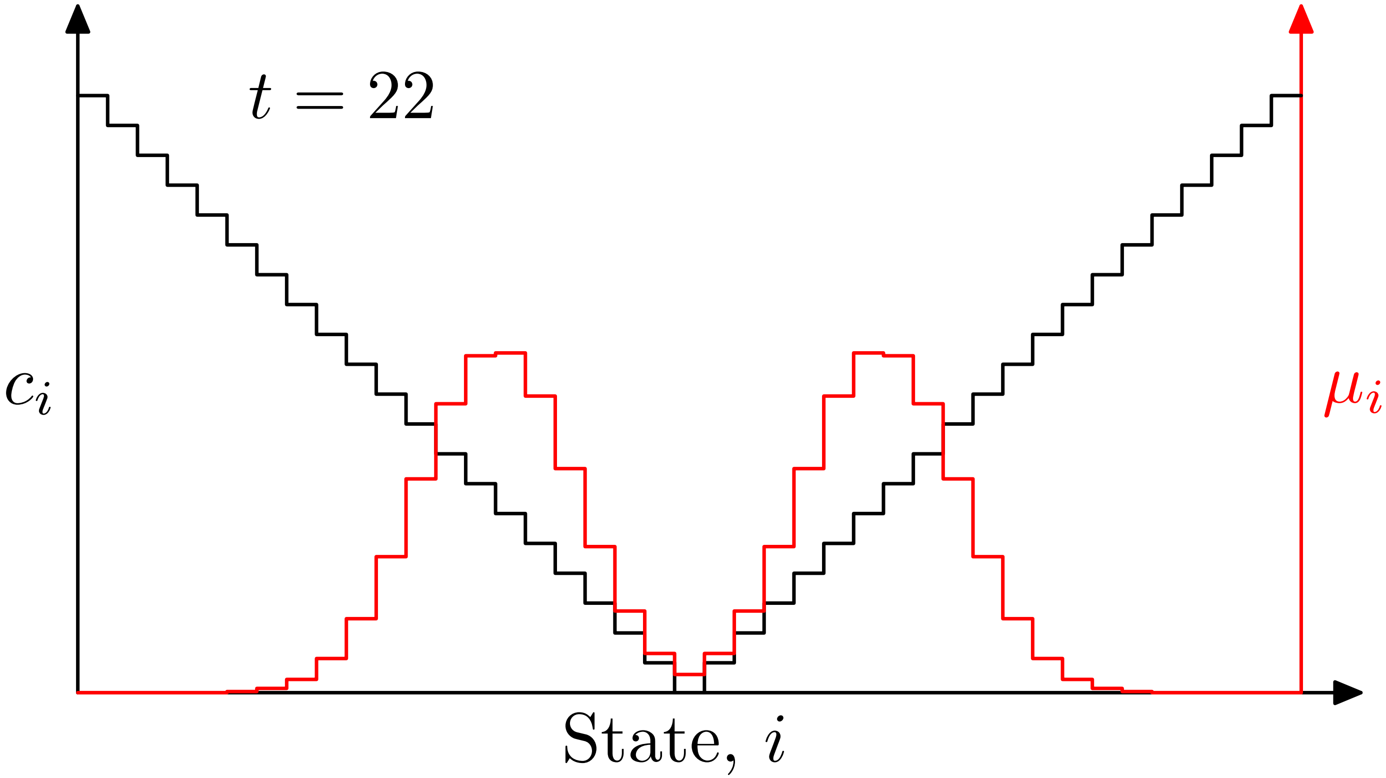

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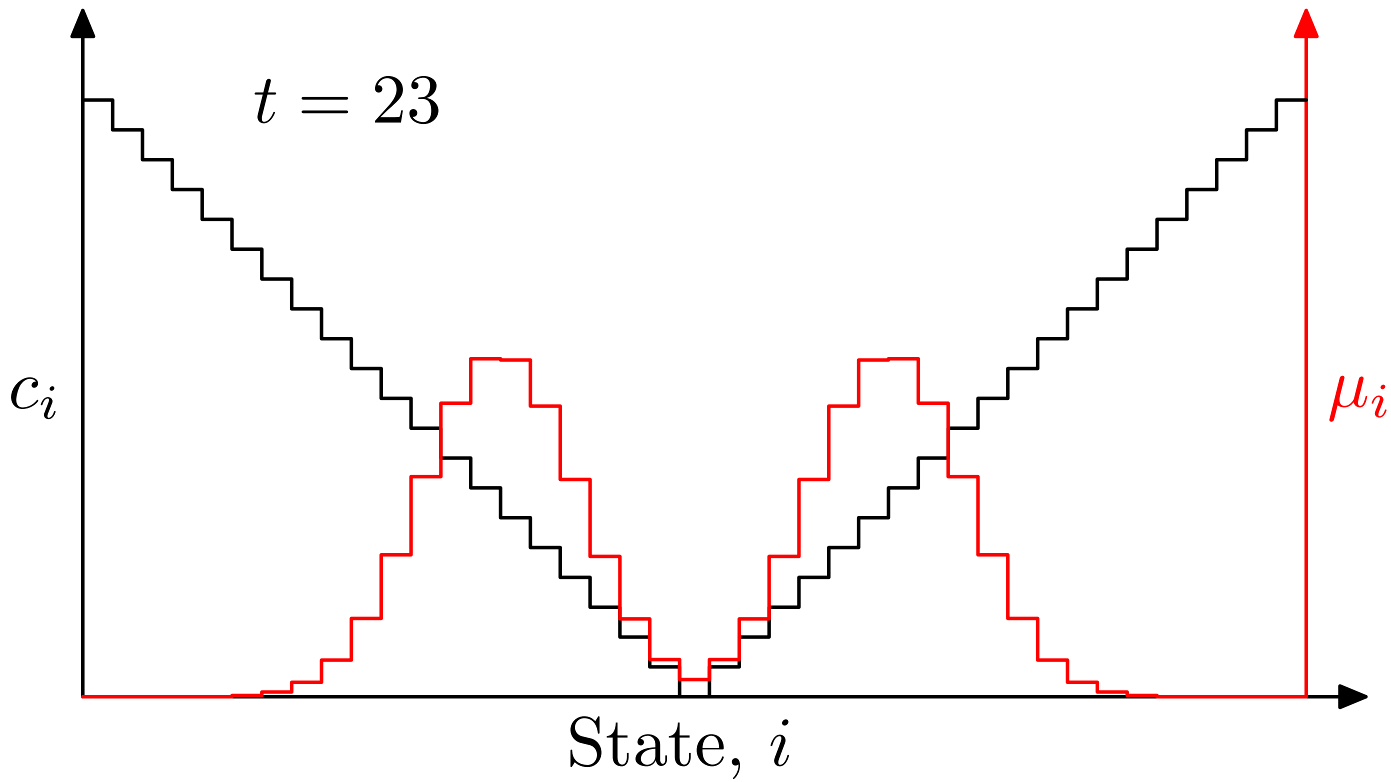

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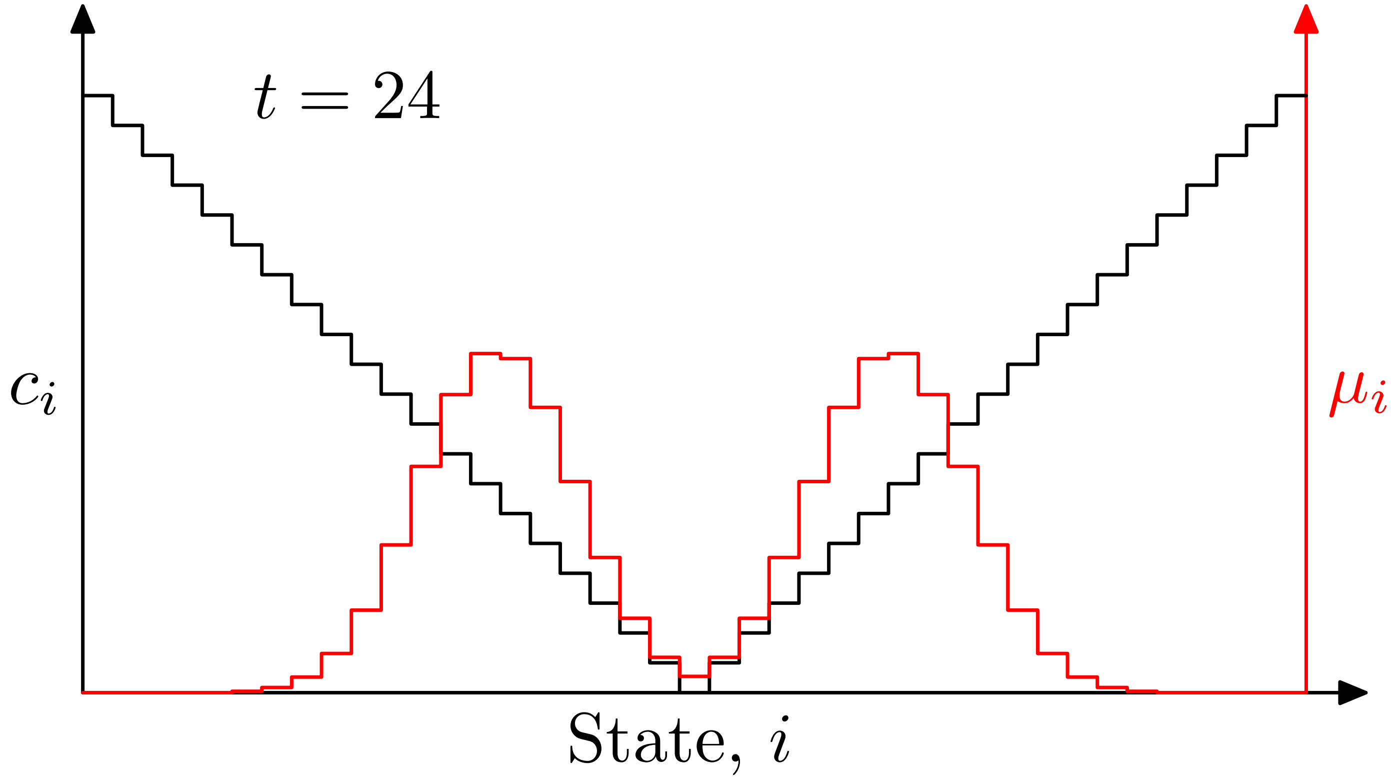

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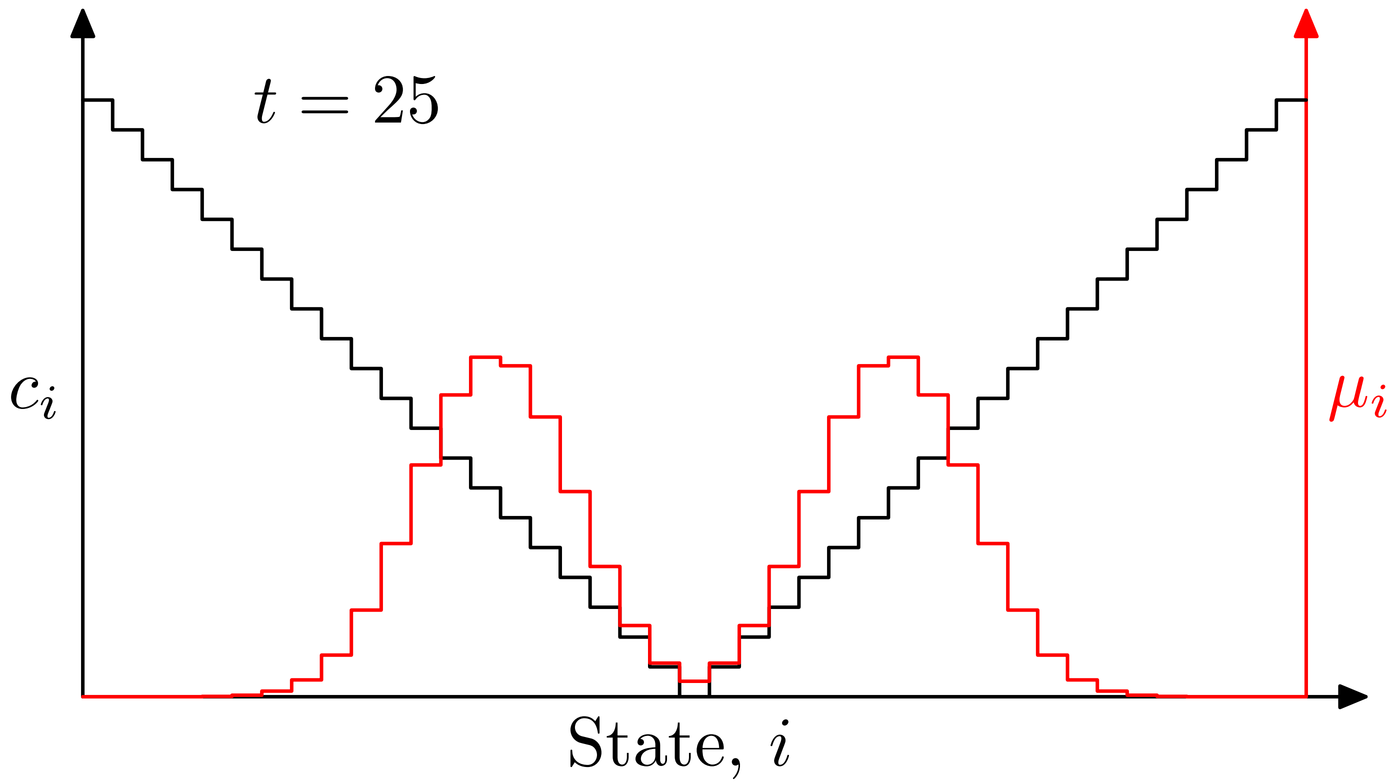

Approximating $g(\boldsymbol{S}, z)$

- For $p > 2$ we don't have enough information to compute $g(\boldsymbol{S}, z)$ exactly
- Many different approaches to approximating $g(\boldsymbol{S}, z)$
- E.g. can use stochastic expansion
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$$f_{\boldsymbol{X}}(\boldsymbol{x}, t) = \frac{1}{\sqrt{|2\pi \mathbf{C}|}} \mathrm{e}^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \mathbf{C}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}$$

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Results

- The approximation usually **breaks down!**
- We discuss why latter
- Using the exact sampling approach gives slightly more accurate model than stochastic expansion
- Finding a robust approximation is still unsolved—although I will talk about a possible approach to cure this
- In problems below I use a selection pressure

$$s_i = \mathrm{e}^{\beta c_i}$$

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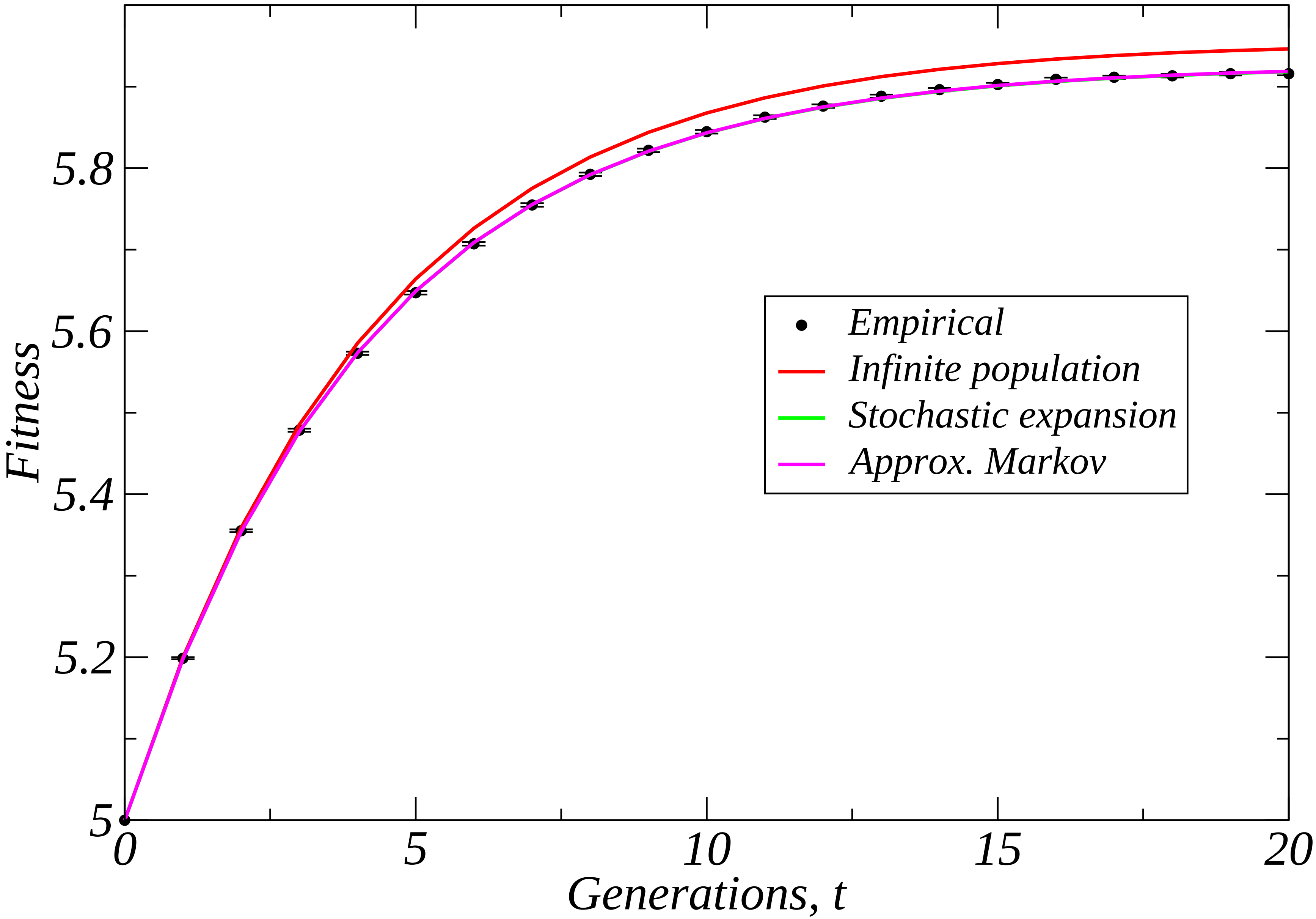
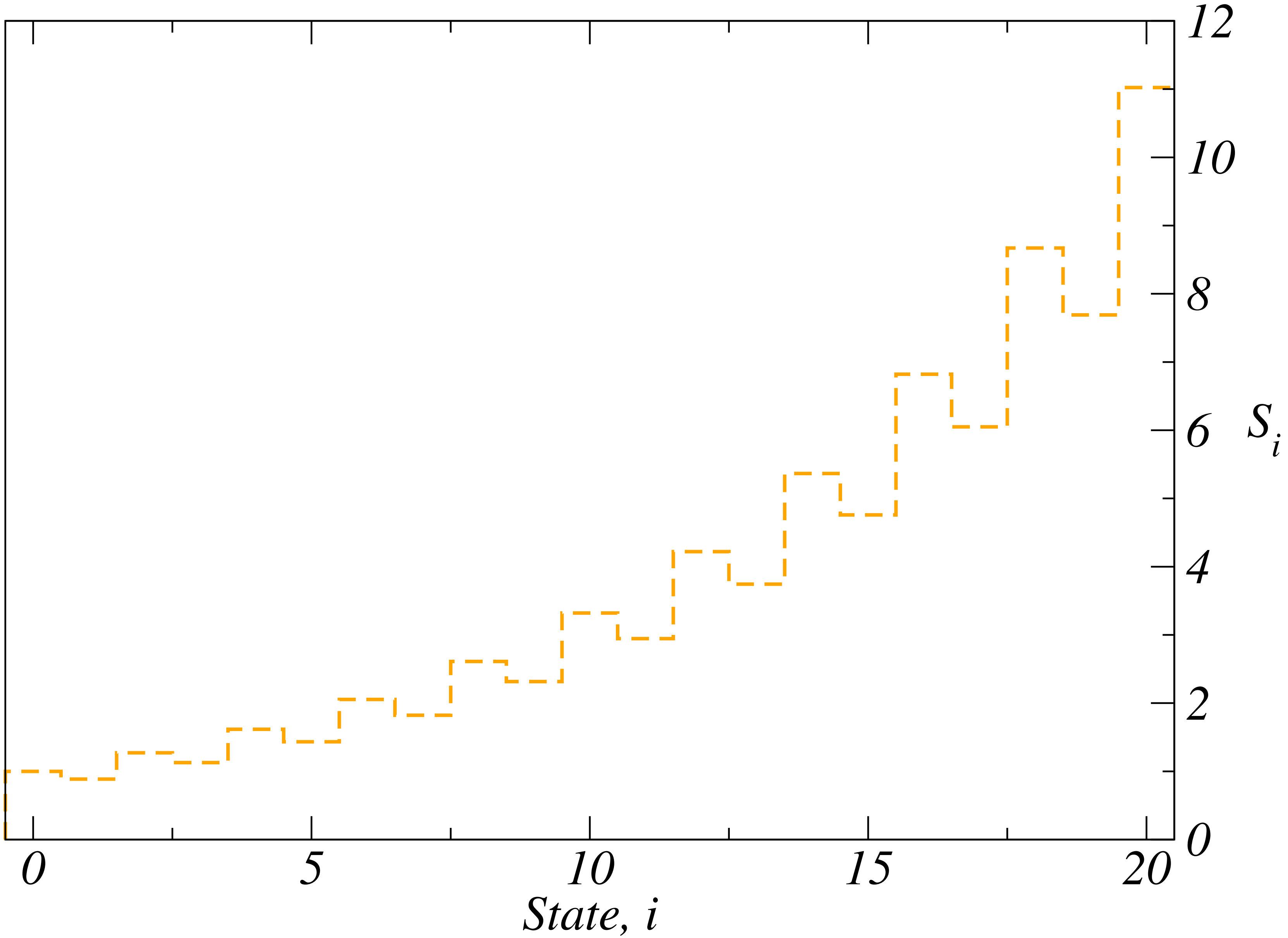


Hurdle Problem After 5 Generations



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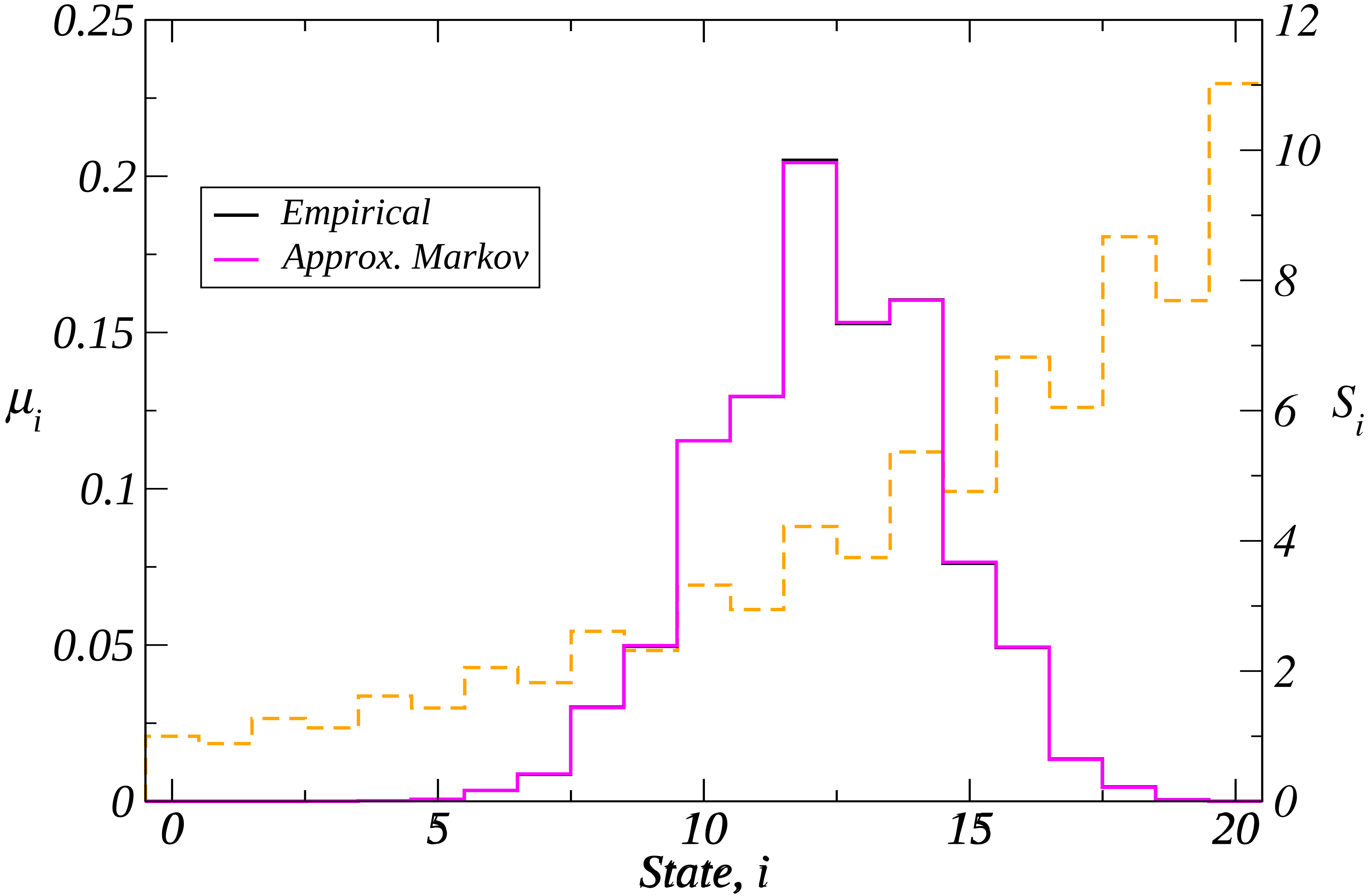
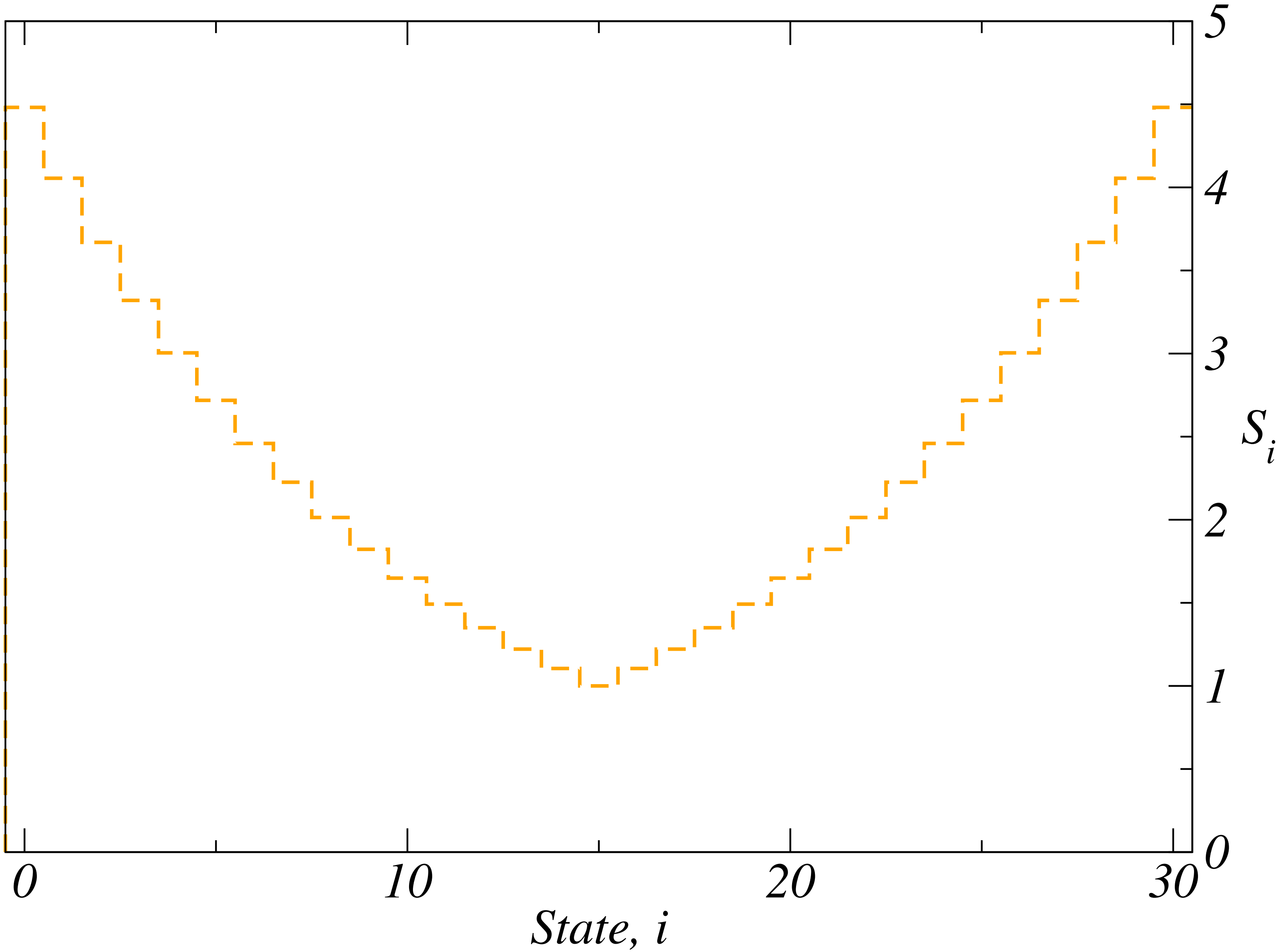


Symmetry Breaking After 5 Generations



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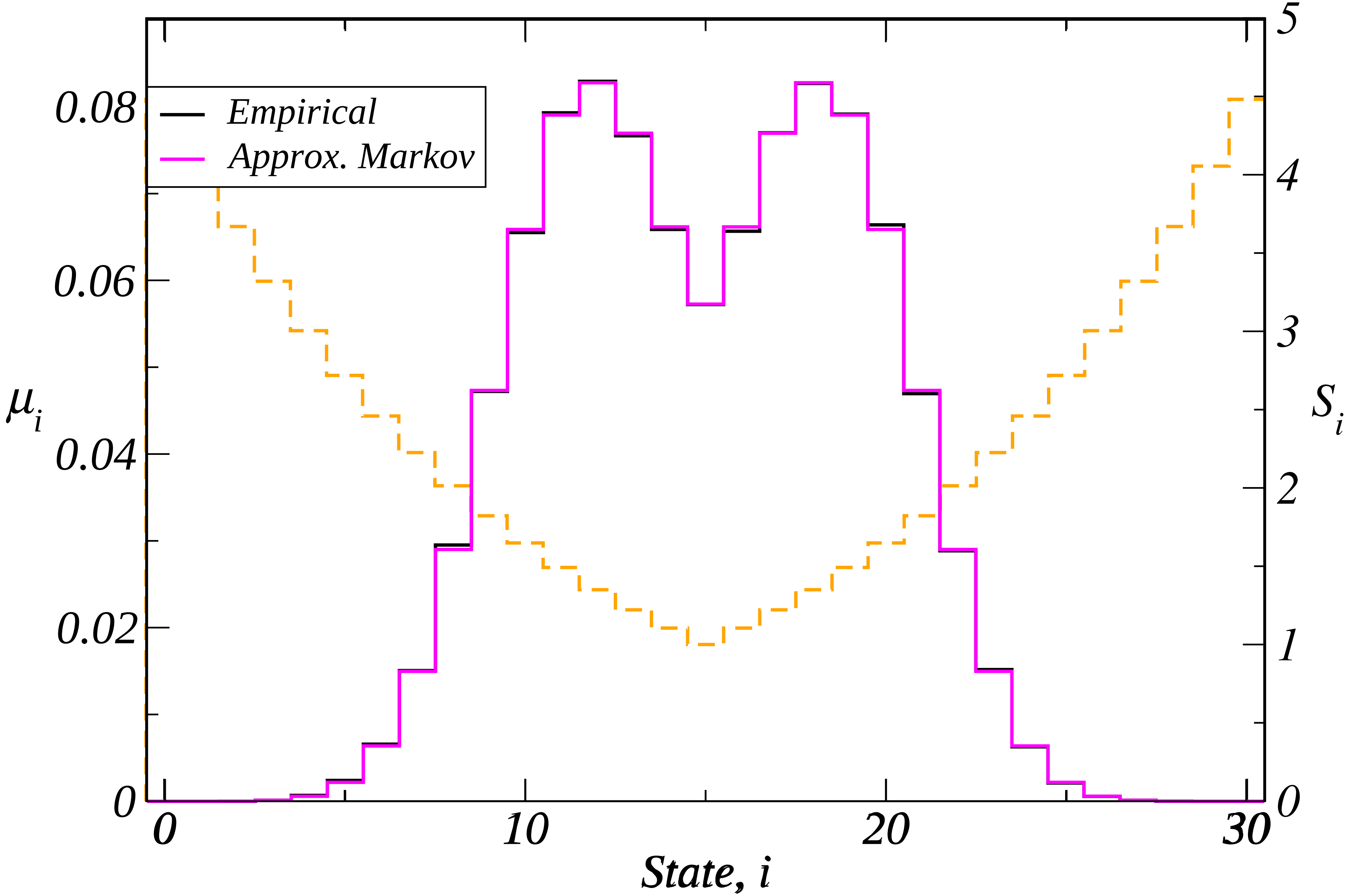
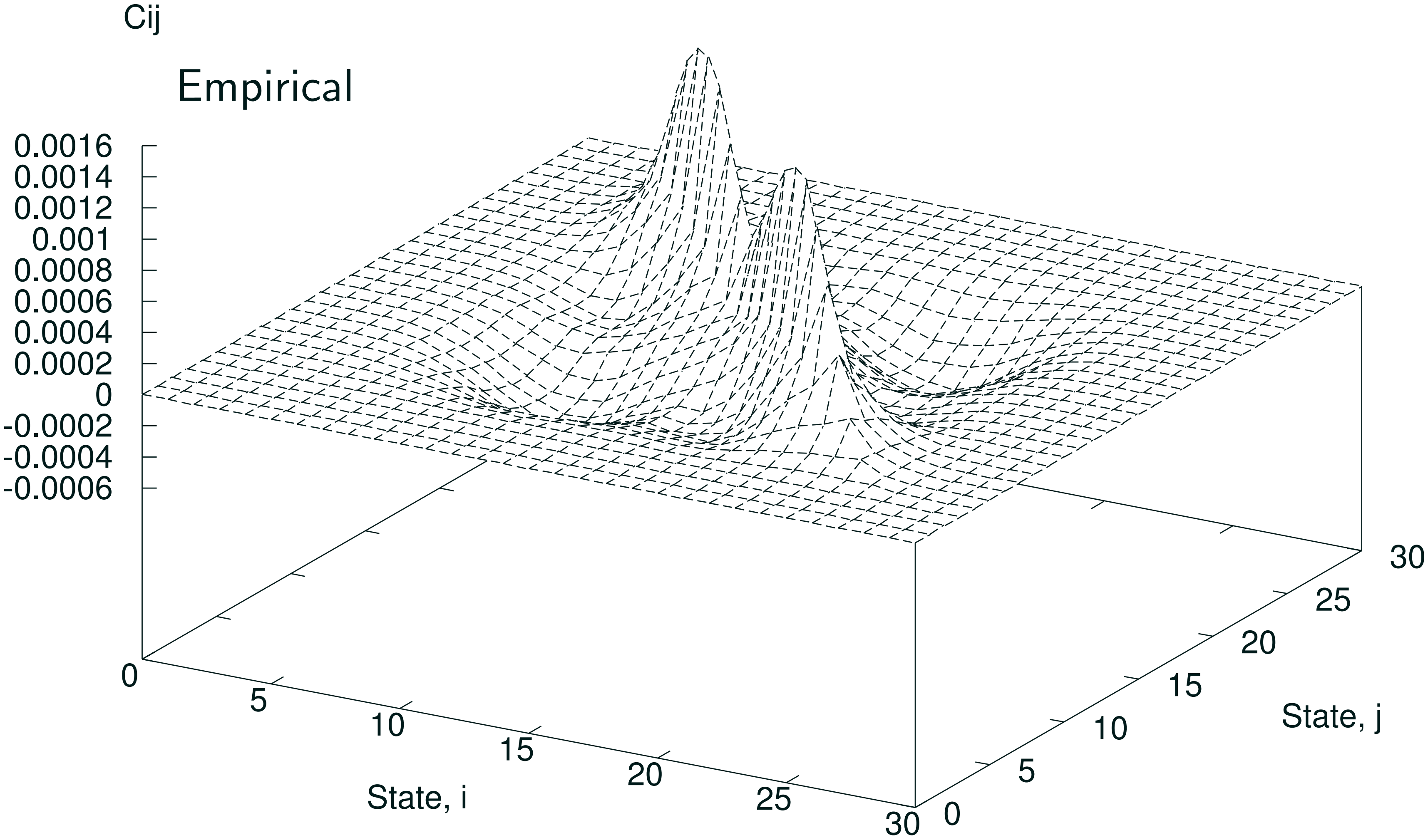
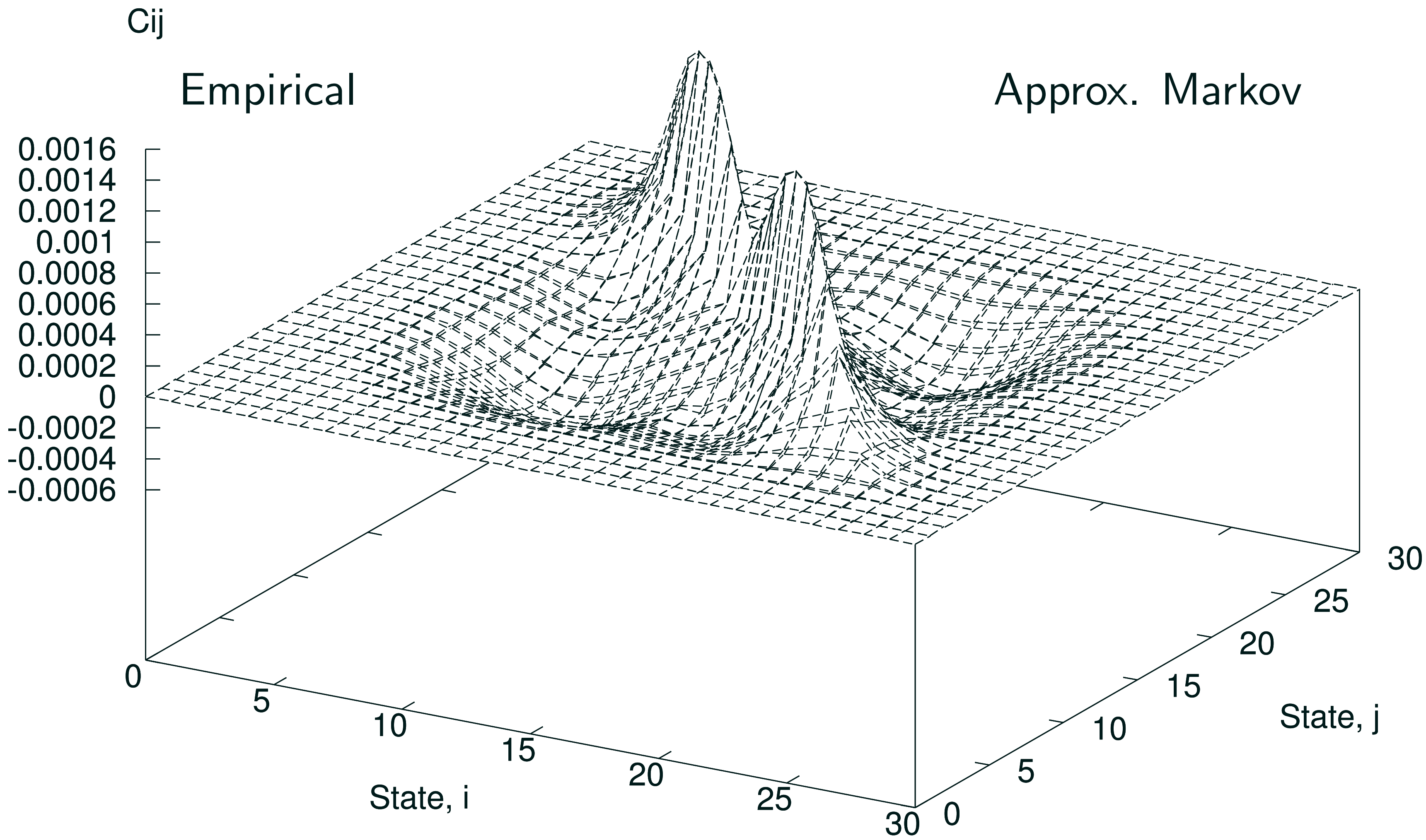


Covariance


Cij
Empirical
0.0016
0.0014
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
-0.0002
-0.0004
-0.0006
0
5
10
15
20
25
30
State, i
0
5
10
15
20
25
30
State, j

Covariance


Cij
Empirical
Approx. Markov
0.0016
0.0014
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
-0.0002
-0.0004
-0.0006
0
5
10
15
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0
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Break down

- Both the stochastic expansion and exact sampling approach break down for large selection rates or large problems
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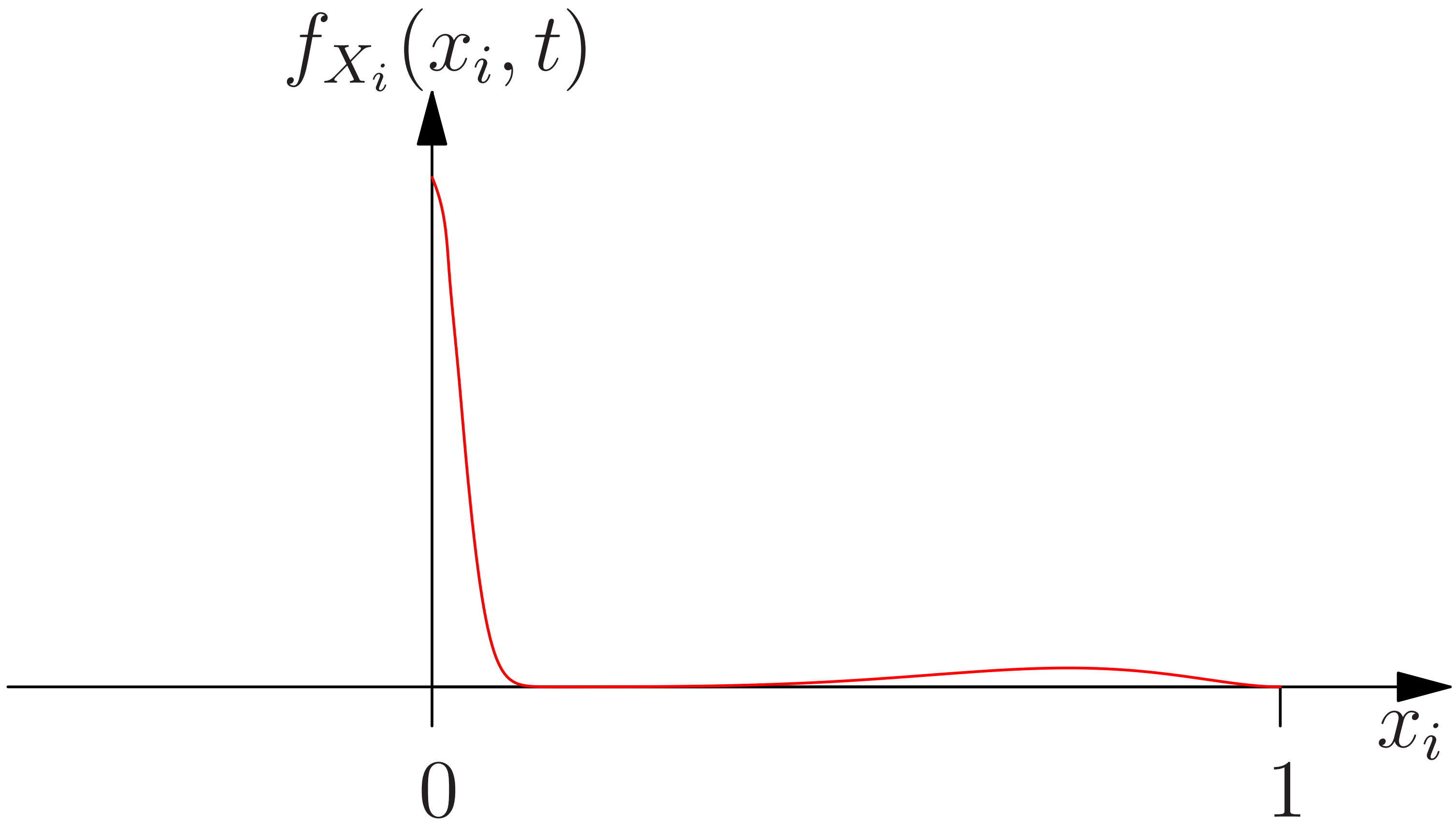

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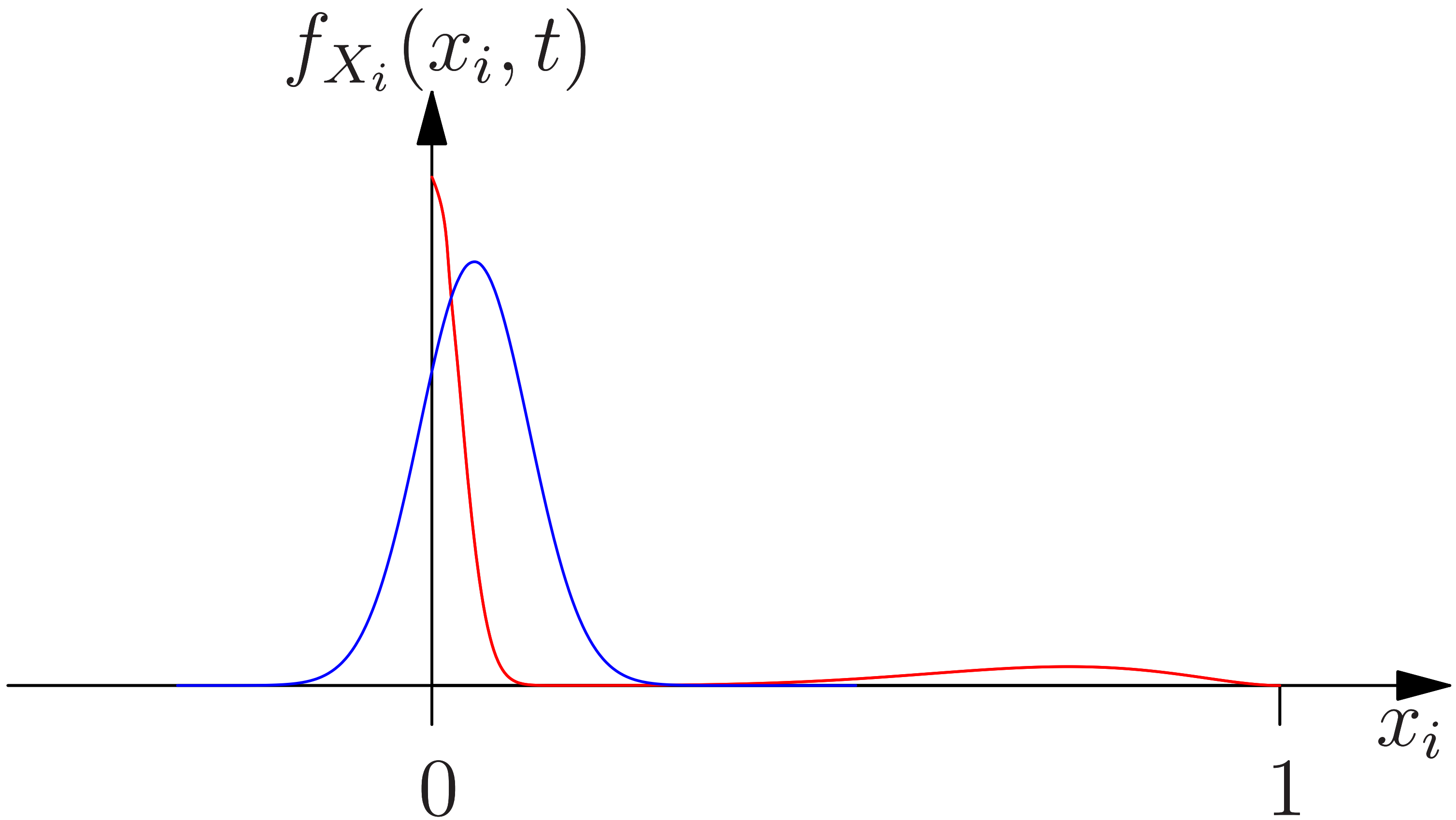
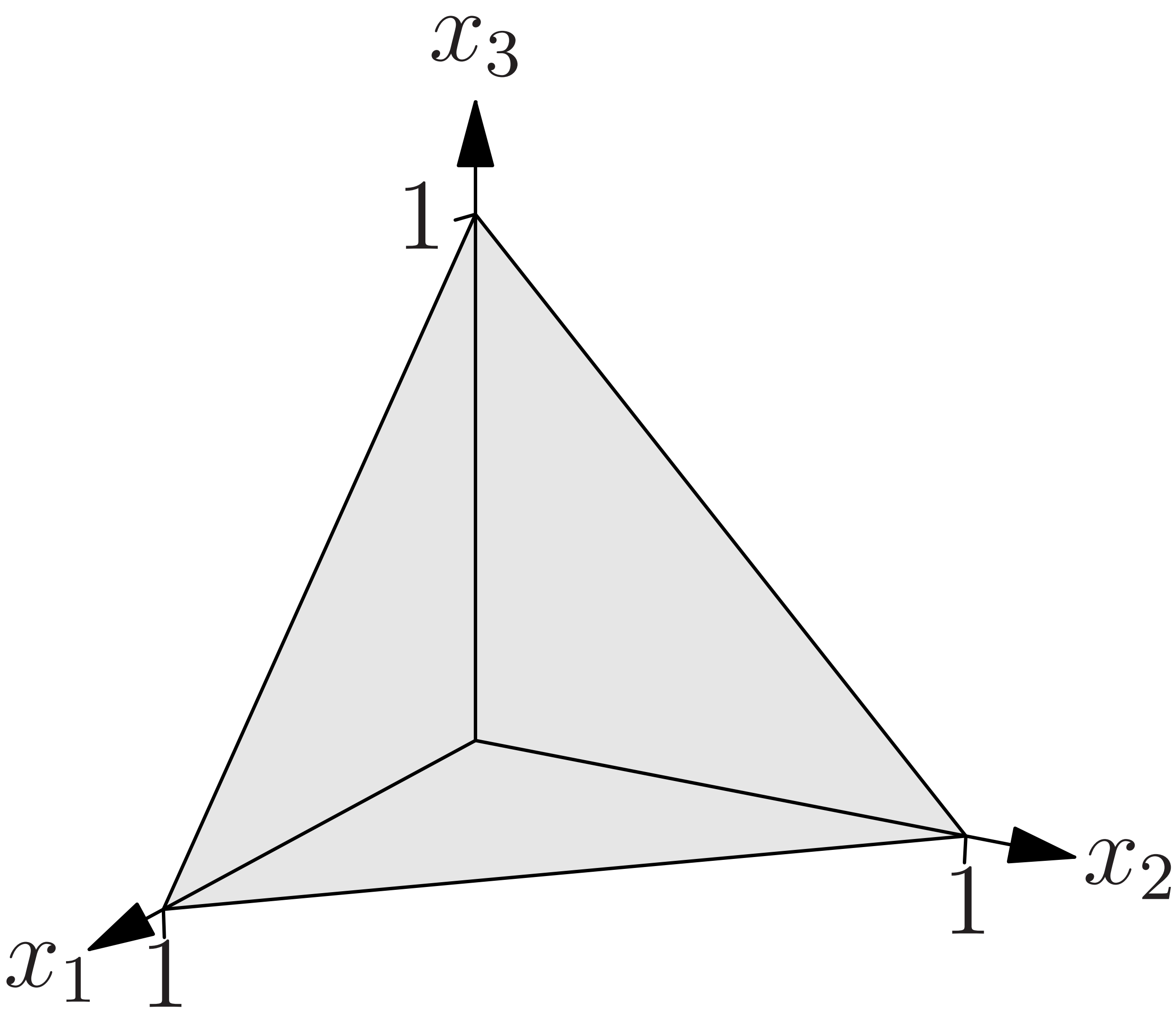
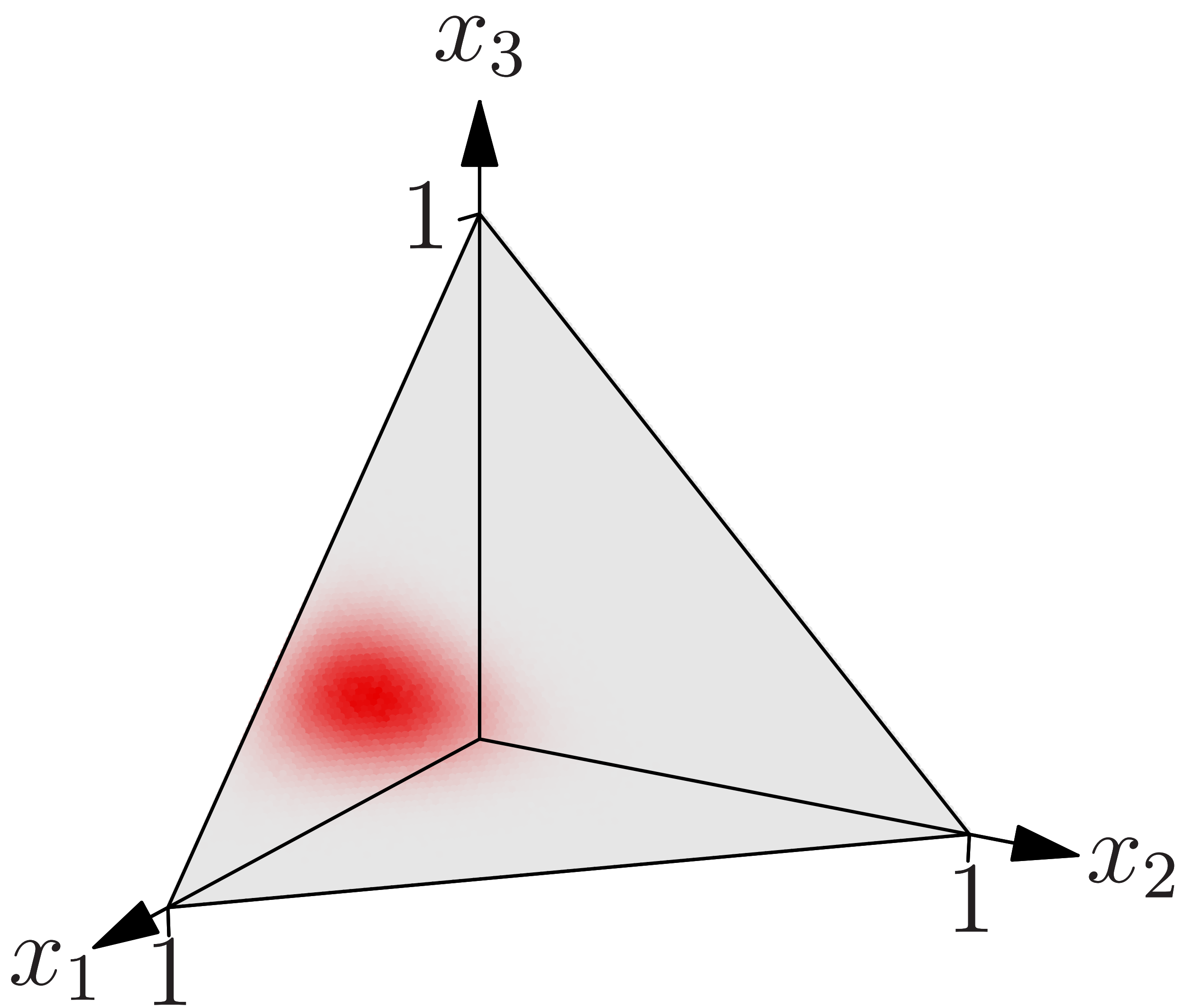


c.f. Foga 2002

Distribution on the Simplex



Distribution on the Simplex



Multivariate Distribution on Simplex

- Require a multivariate distribution defined on the unit simplex
- No standard distribution
- Easy to define

$$f_{\boldsymbol{X}}(\boldsymbol{x}|\boldsymbol{\mu}, \mathbf{L}) = \int_{-\infty}^{\infty} N_{\boldsymbol{Y}}(\boldsymbol{y}|\boldsymbol{\mu}, \mathbf{L}) \prod_{i=1}^{n} \delta\left(x_i - \frac{y_i^2}{\sum_j y_j^2}\right) \mathrm{d}\boldsymbol{y}$$

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Averages Over Simplex Distribution

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- However, to be practical it must be possible to compute average quantities

$$\langle g(\boldsymbol{X}) \rangle = \int g(\boldsymbol{X}) f_{\boldsymbol{X}}(\boldsymbol{x}|\boldsymbol{\mu}, \mathbf{L}) \mathrm{d}\boldsymbol{x}$$

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Conclusions

- An approximate Markov model would be desirable for studying GAs
- Need to go beyond infinite population model
- Plausible that using the means and covariances an approximate Markov model can be made
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