Introduction to Monte Carlo Markov Chains (Part 2)

Class 20

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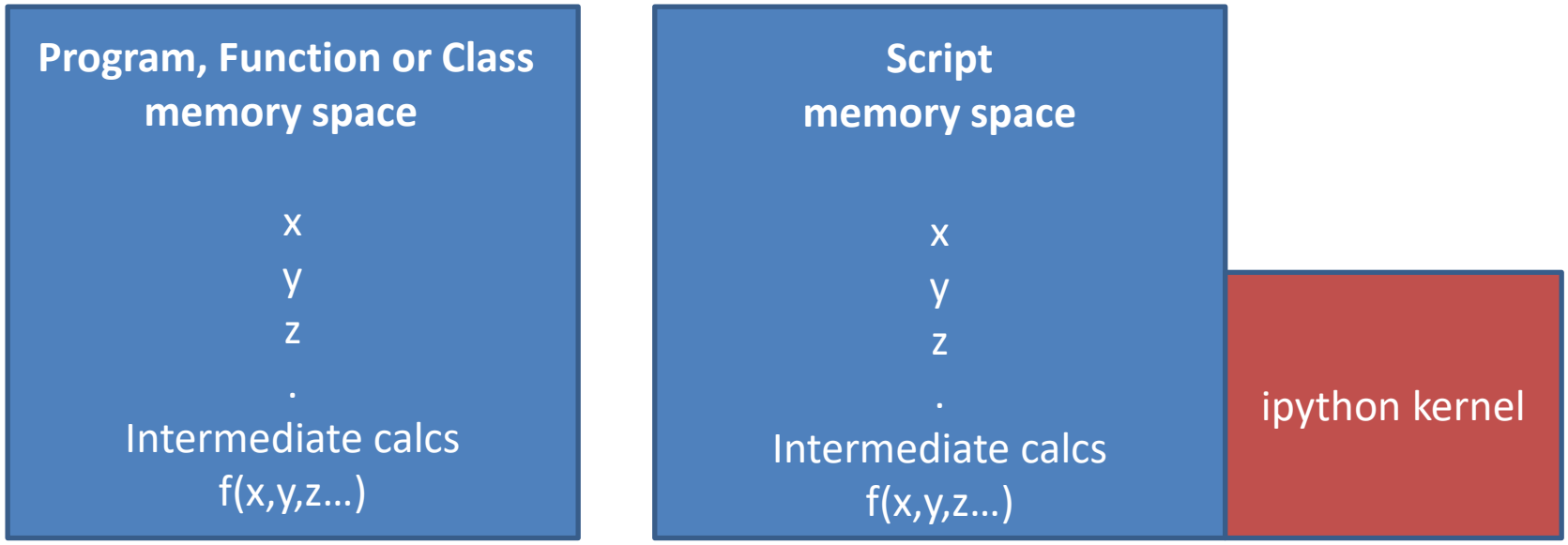
But first … scripts vs programs

```
def myfunc(x,y,z,…):
        do a bunch of stuff here
        return f(x,y,z,…)
```



My recommendations

Always write first drafts of code in script form.

Always do your code development in ipython.

- This makes debugging straightforward

Then … copy your useful (debugged) code into a function or class for long-term use.

- MCMC is a technique for taking a “biased random walk” through the space of $\pi(\vec{a})$

- It is “random” in the sense that we will draw from probability distributions to guess which way to go.

- It is “biased” in the sense that we will allow $\pi(\vec{a})$ to influence how often we choose the uphill direction.

Metropolis - Hastings

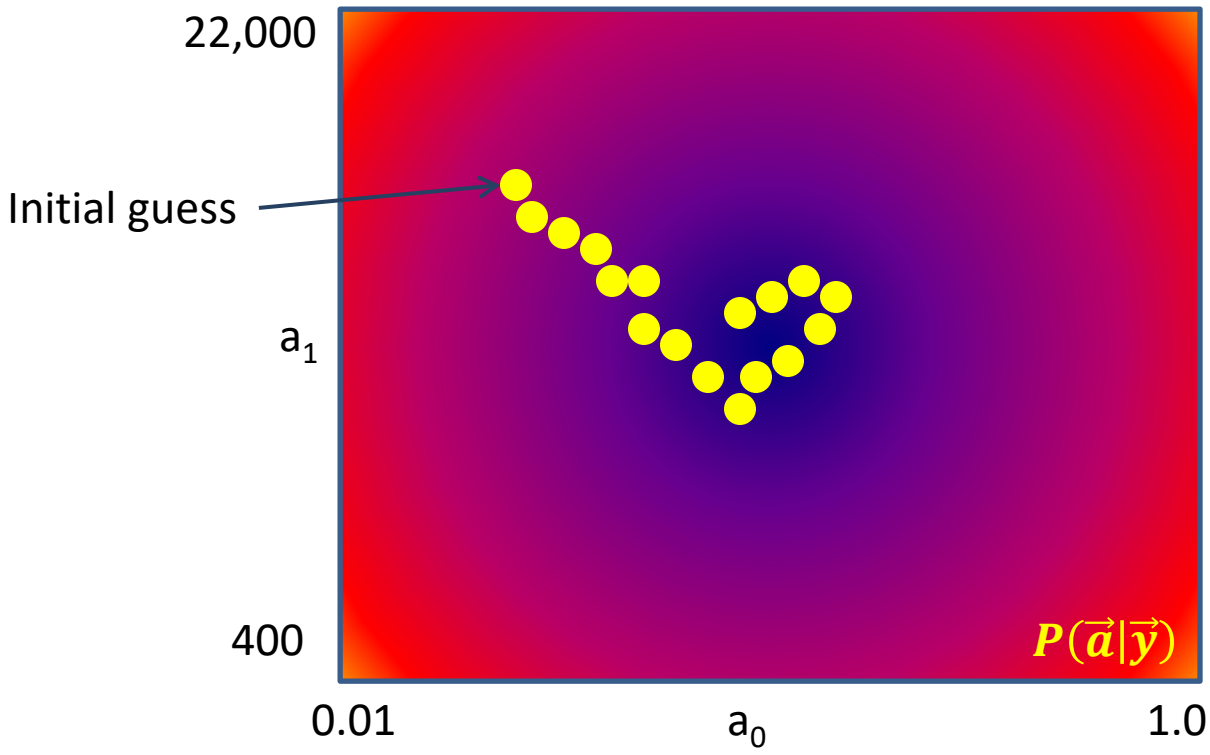
- Last time we implemented a simple Metropolis-Hastings algorithm for our sampler.

- Key points:
  - ergodic chains
  - transition probability satisfies detailed balance

- Challenges of M-H
  - for M free parameters there are a minimum of M parameters in the transition probability to be tuned by the user.

  - the autocorrelation time (# of samples required to achieve independent samples of the posterior distribution) is not optimally short.

- M-H samplers require choice of step size for each parameter of interest

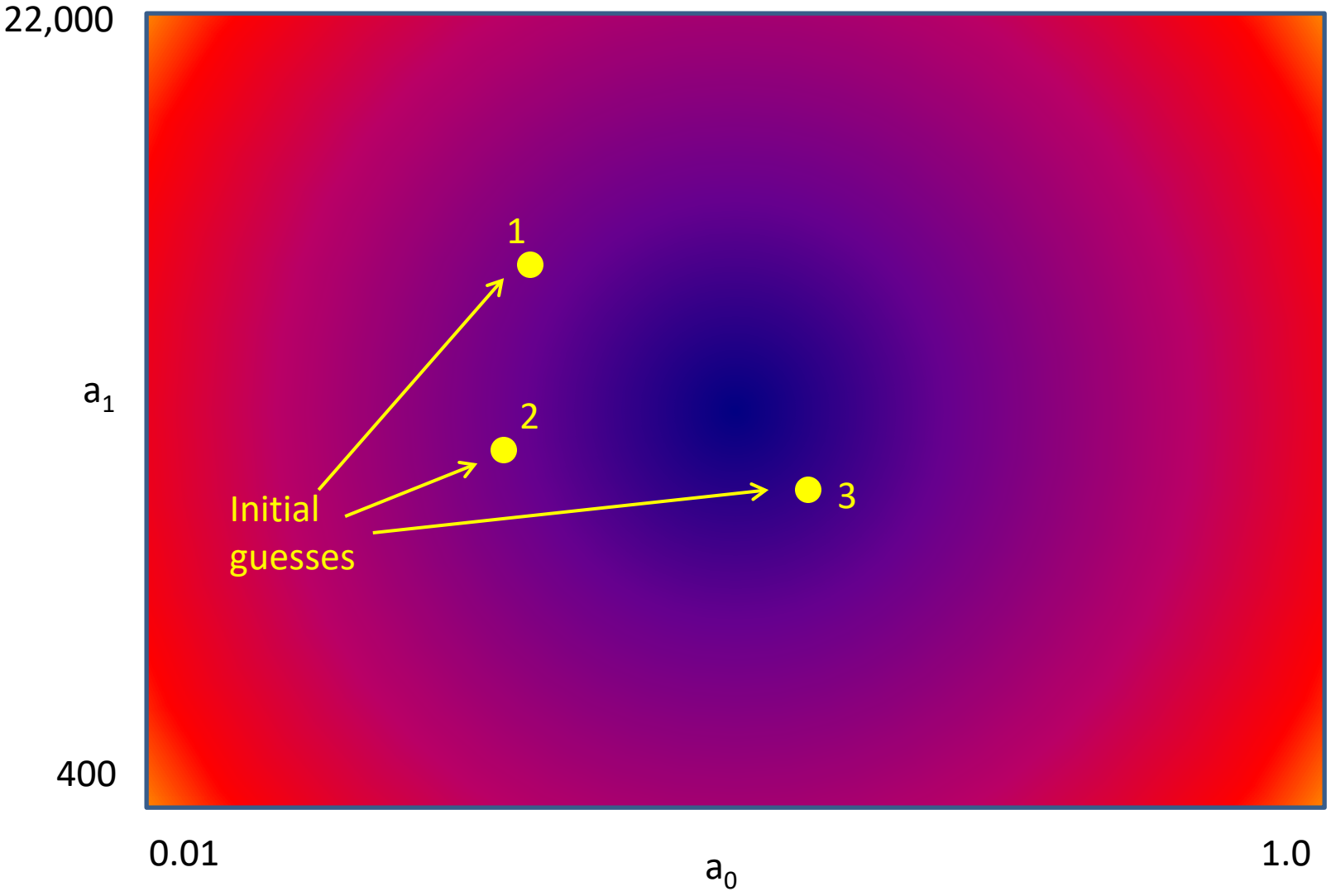


Over time, the chain will fill in the space with a density of visits proportional to the posterior probability distribution.

The Stretch Move Approach

- an affine-invariant ensemble sampling algorithm
- still generates ergodic chains
  - heads of chains are called “walkers”
- still satisfies detailed balance
- only one free parameter to set
  - set it to 2

- The stretch move with three walkers



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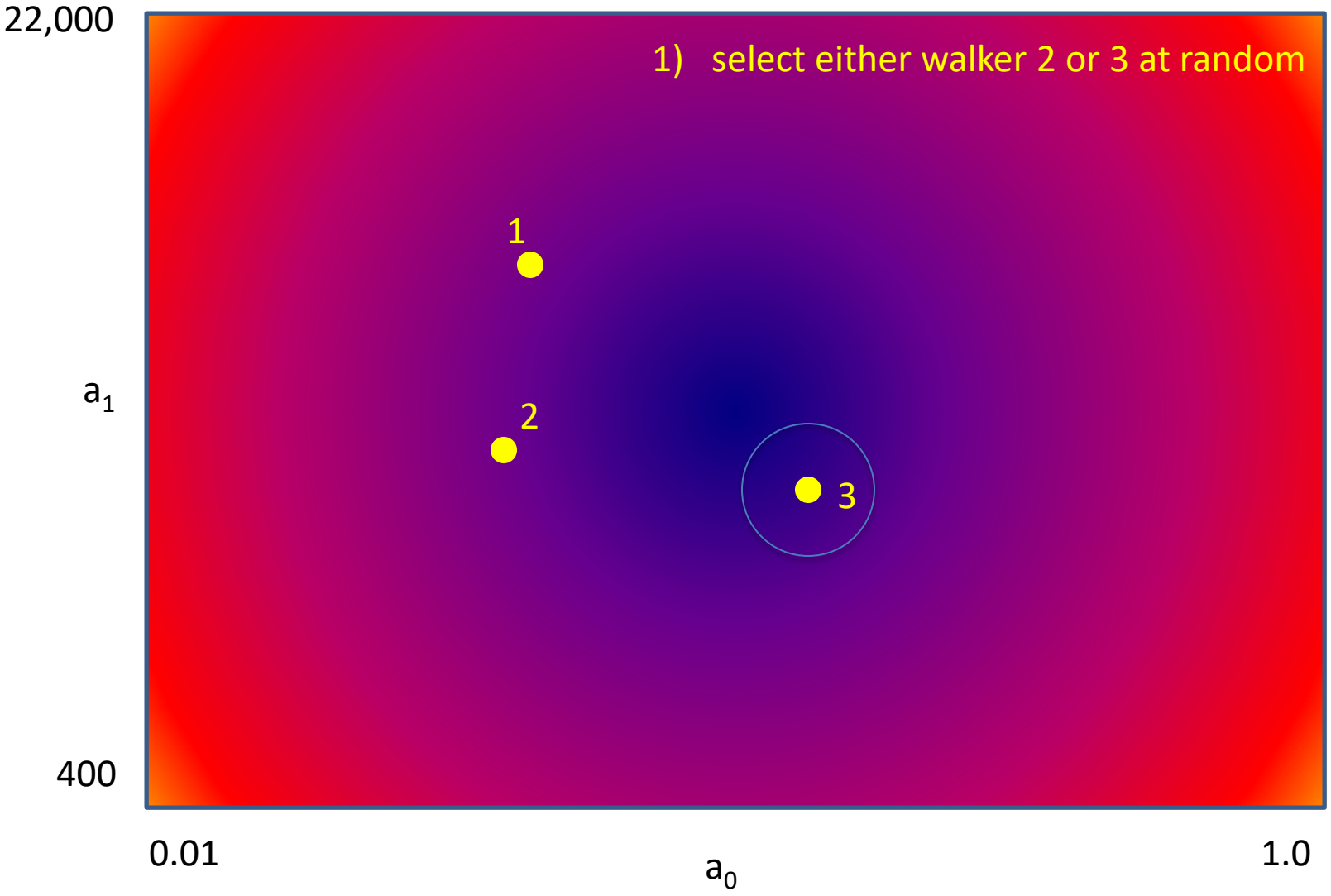

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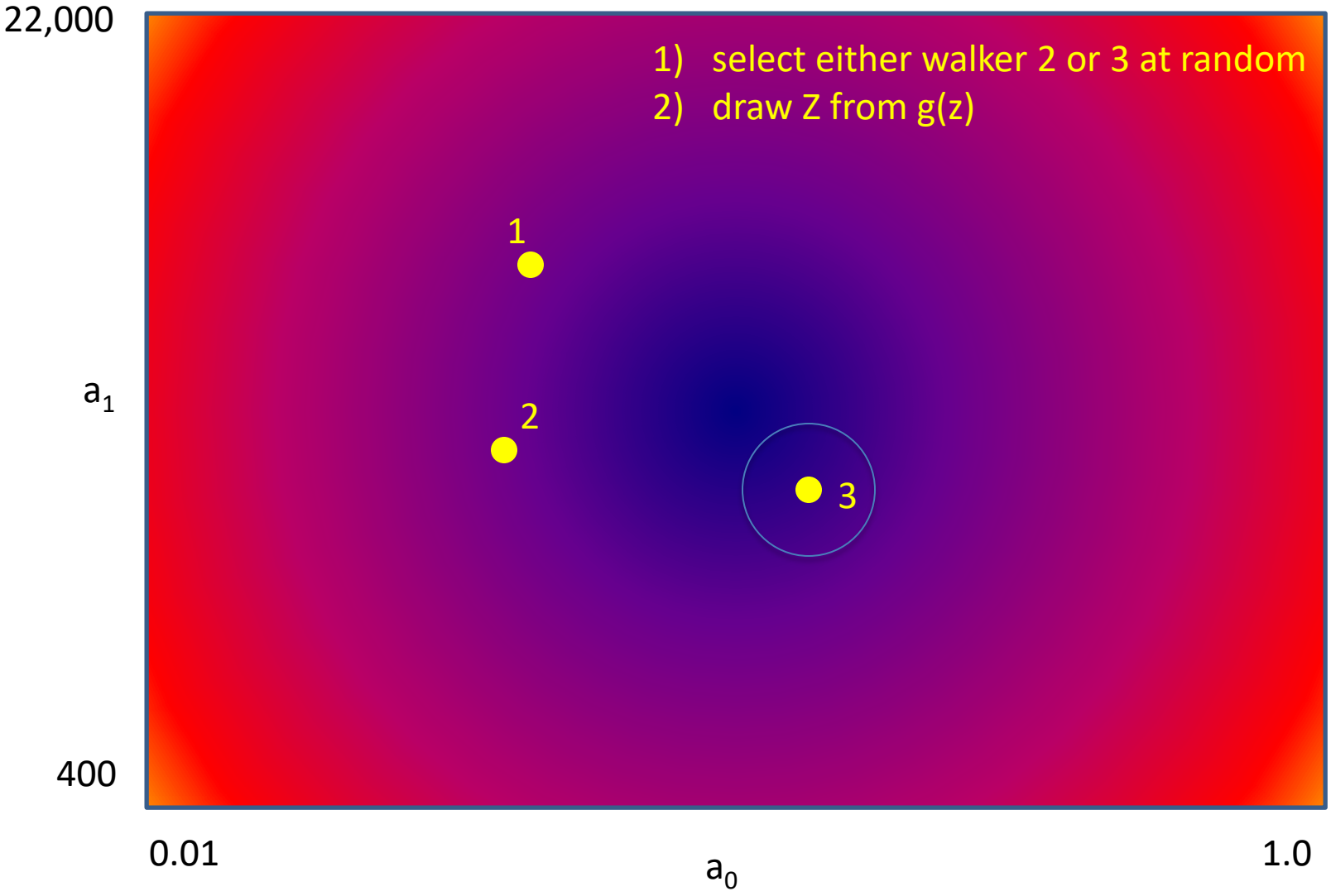

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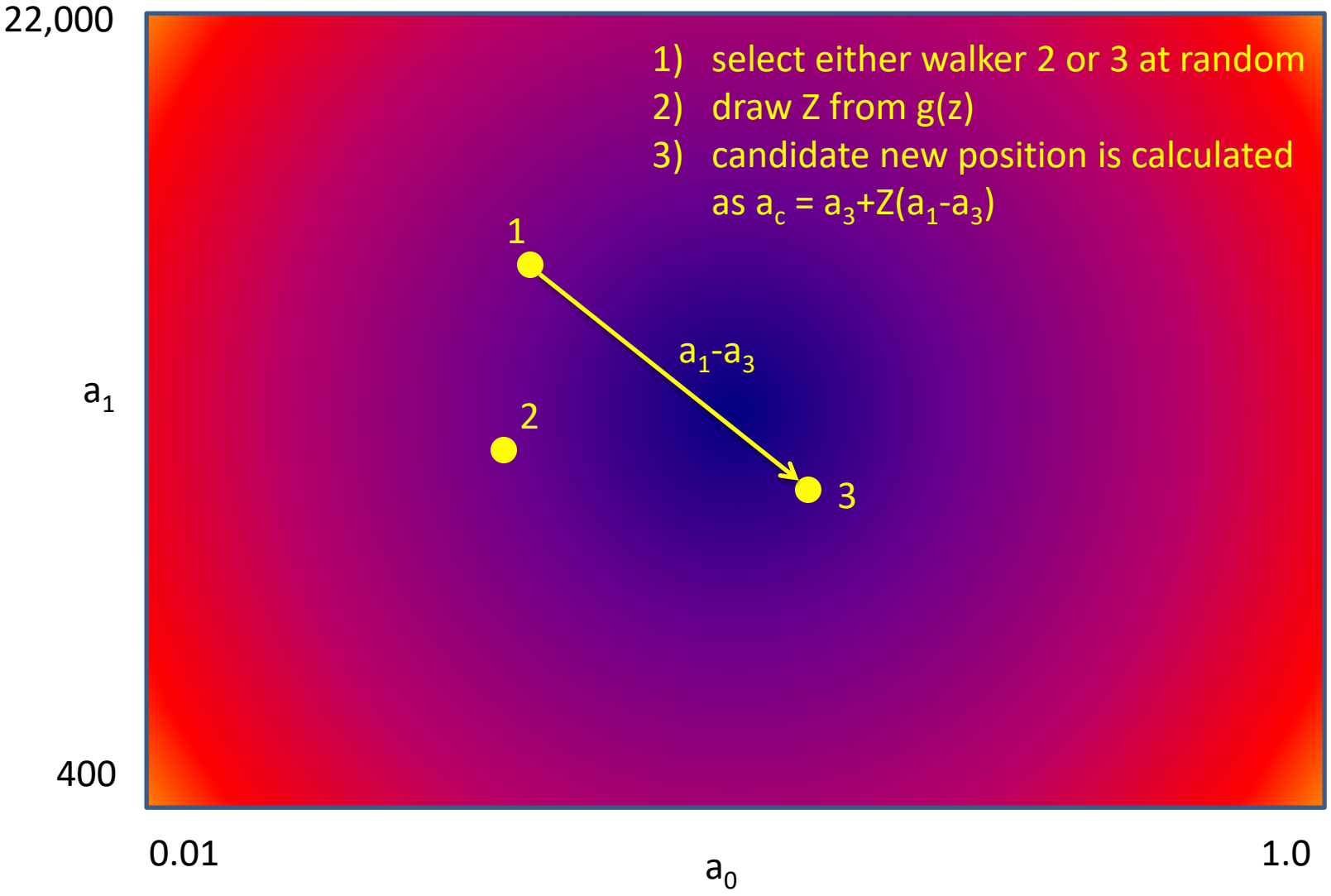

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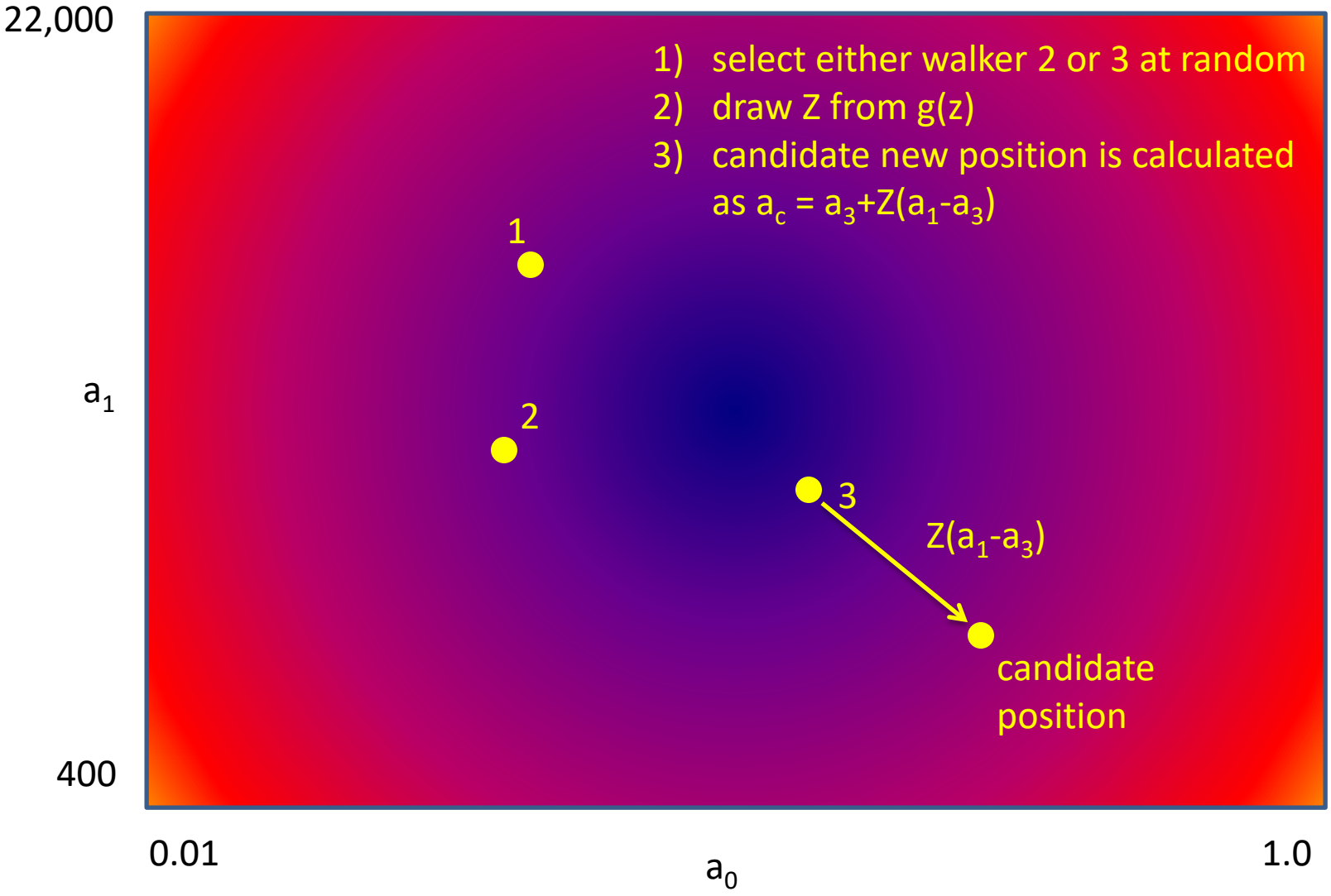

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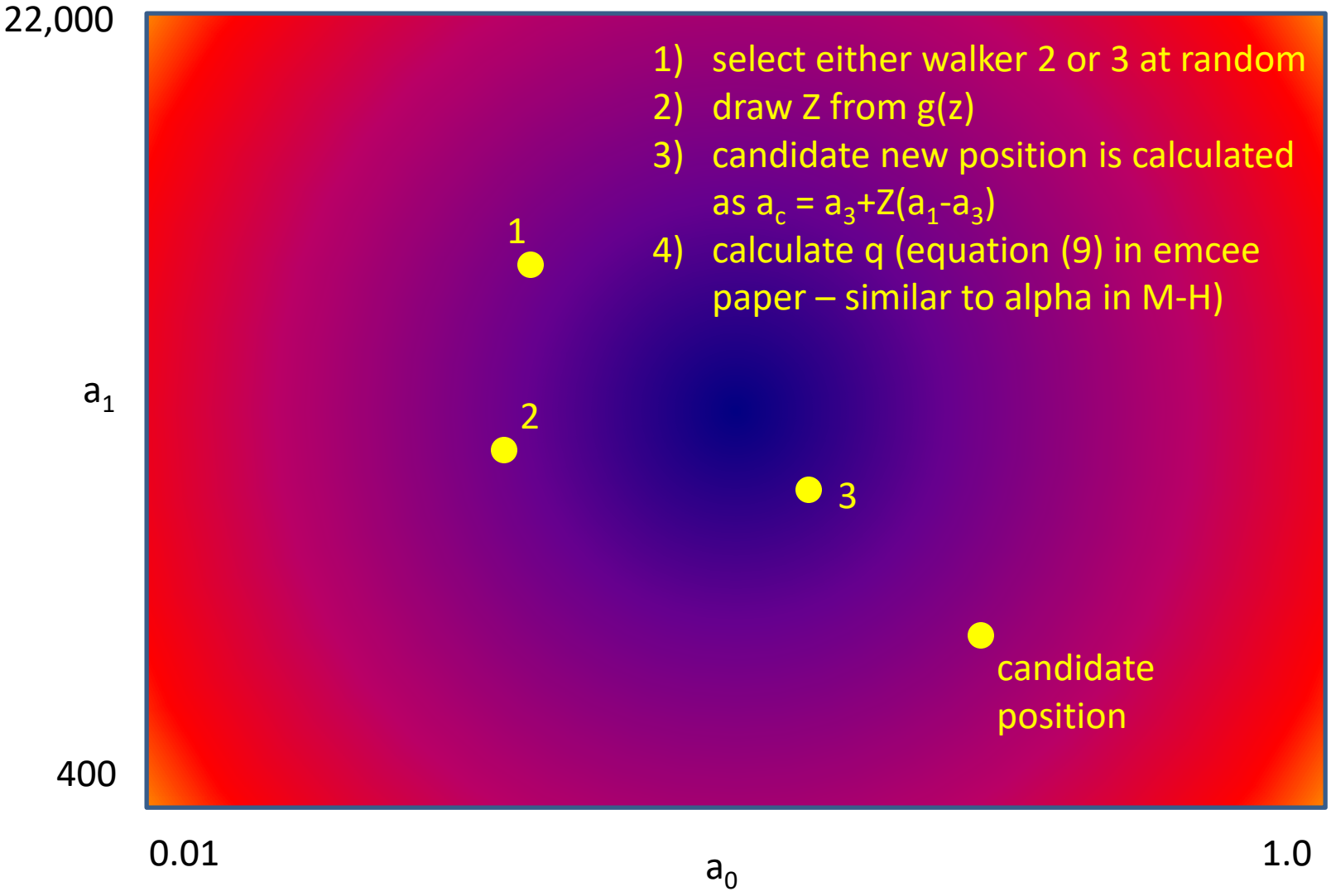

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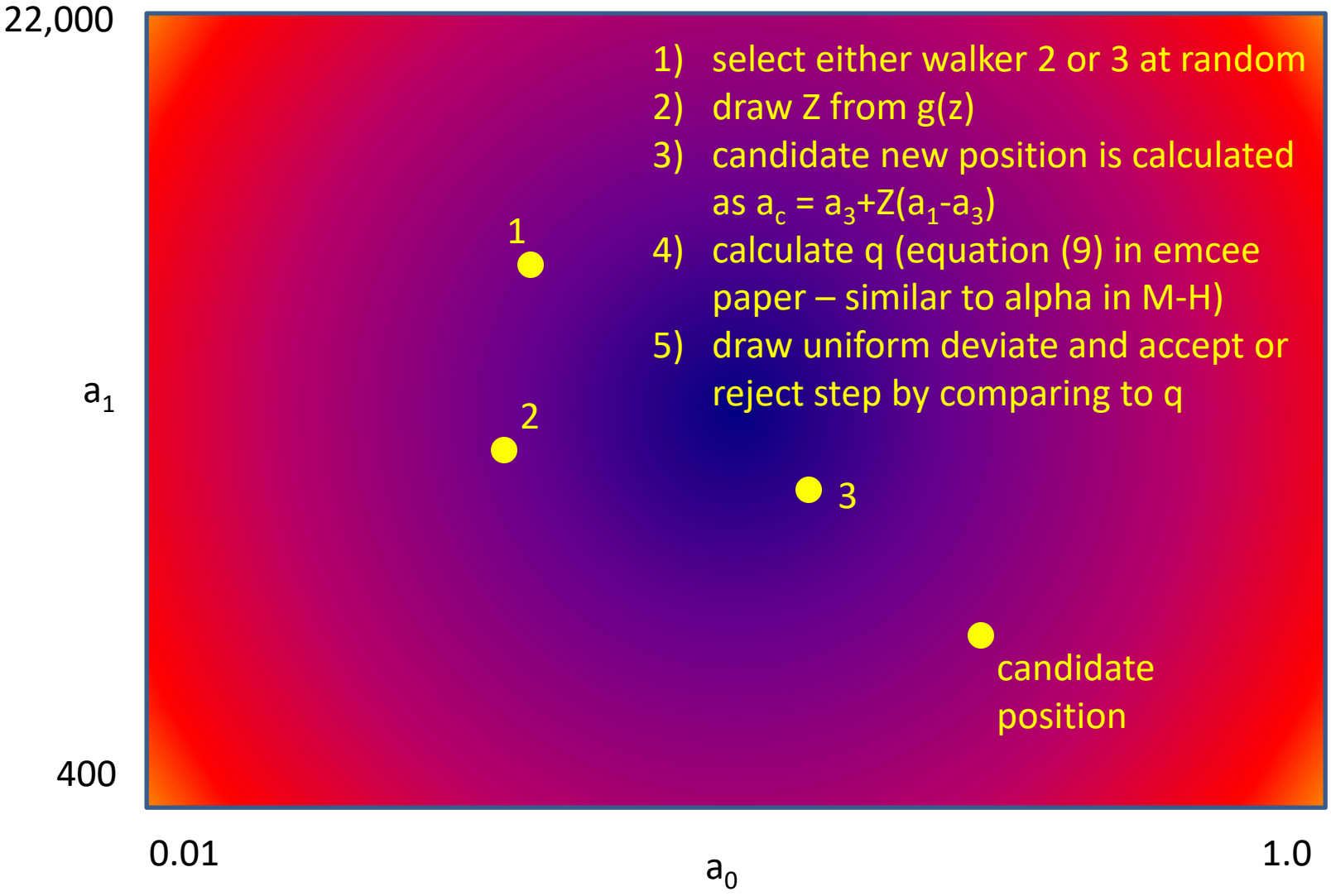

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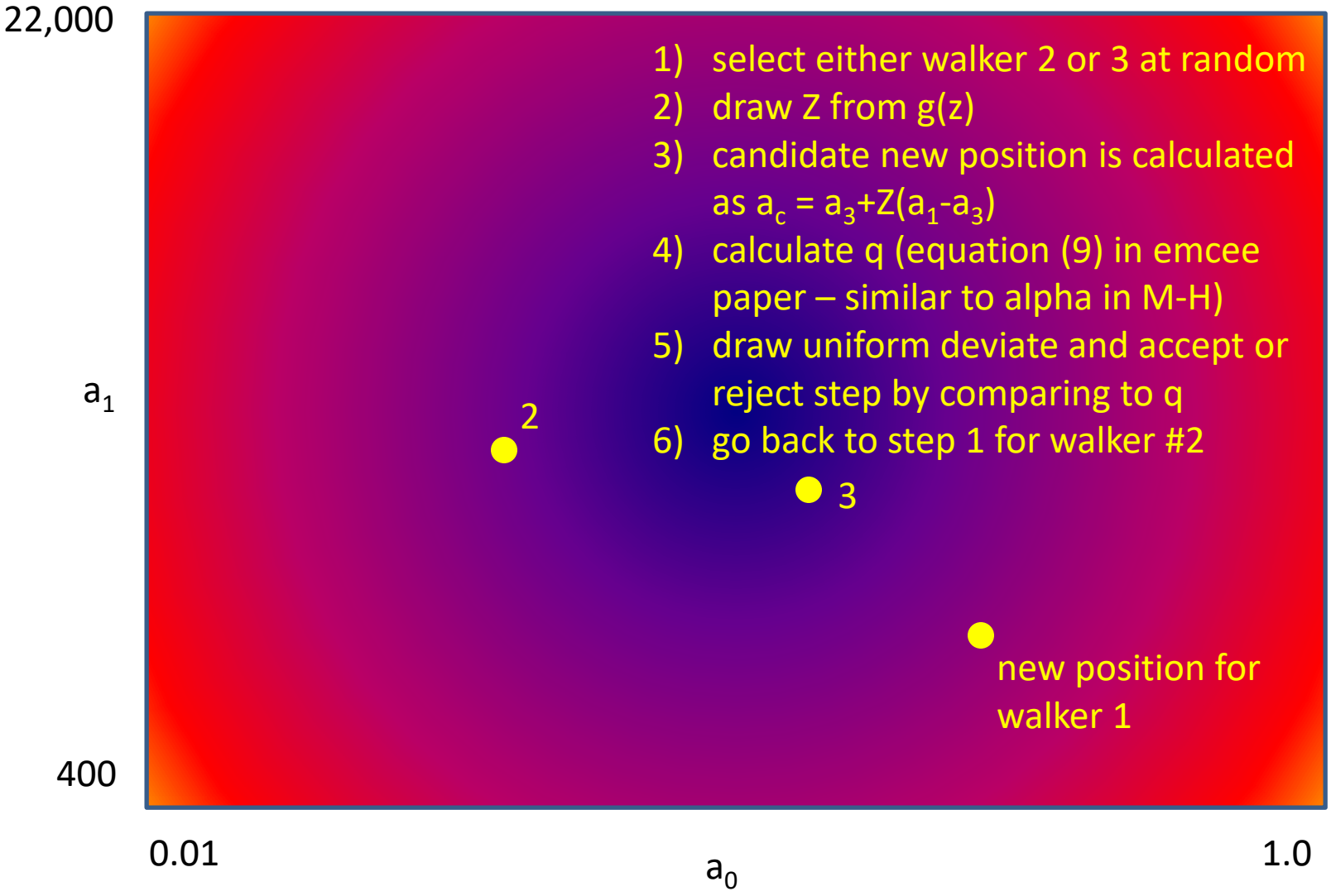

Important Points

- For detailed balance to be preserved these steps must occur in series. Deal with one walker at a time.
- Recipe is given in paper for parallelizing process.
- If things are going well, acceptance rate will be between 0.2 and 0.5.
- The technique works best with many walkers – at minimum 2x the number of free parameters (but go with something like 10x if possible)
- try downloading the emcee package with pip
  - *pip install emcee*
  - see http://dan.iel.fm/emcee/current/

Exercise #1

- Re-work the two MCMC problems from last class using the emcee package.

- Do it again using the emcee interface to lmfit