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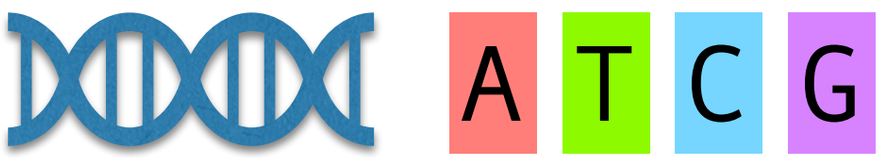

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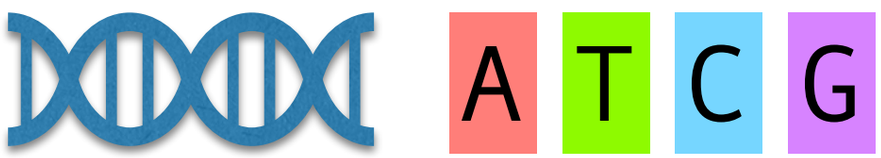

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P(purine) = 0.25 + 0.25 = 0.5

Bayes theorem

Likelihood Prior probability

Posterior probability

$$P(\alpha|x) = \frac{P(x|\alpha) \times P(\alpha)}{P(x)}$$

probability of the data a.k.a.
marginal likelihood, normalizing
constant or evidence

alpha = unknown parameters of a model *M* (alpha is usually what we are after)

x = data (e.g. a set of measurements, molecular sequences, etc.)

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M = model (more about this later)

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Likelihood: probability of observing the data you observe given a model and its parameters

Prior: probability of the parameter values based on some prior knowledge about them

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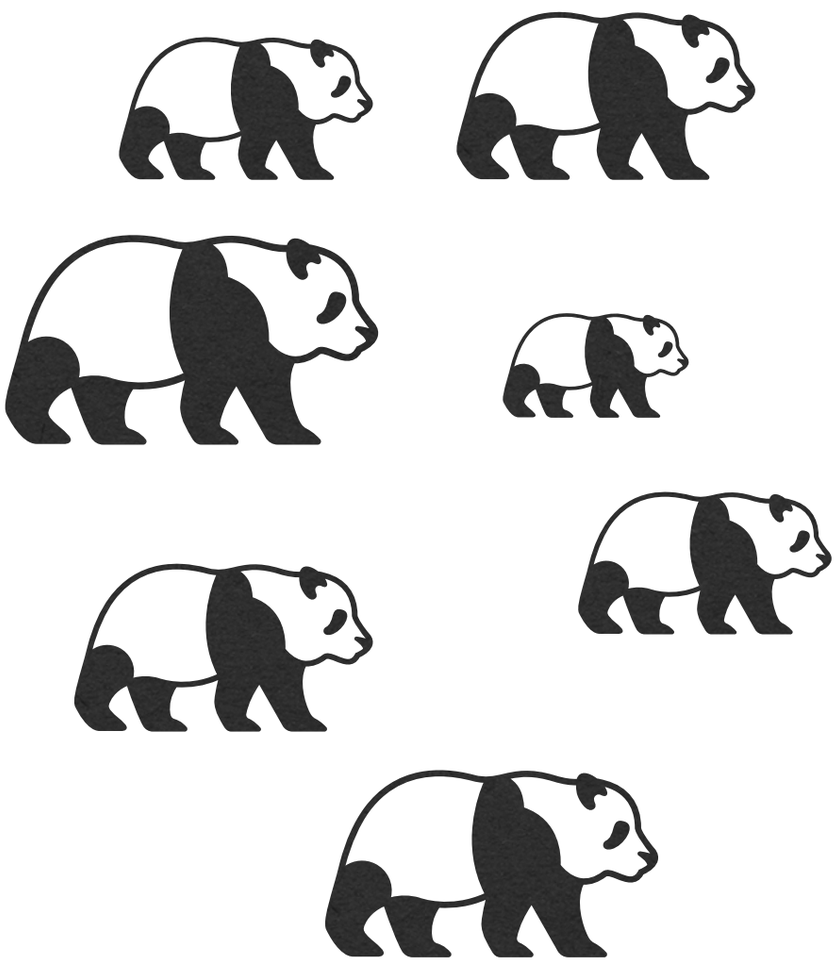
probability of the data a.k.a. marginal likelihood, normalizing constant or evidence

the three components:

data **model** **parameters**

Data

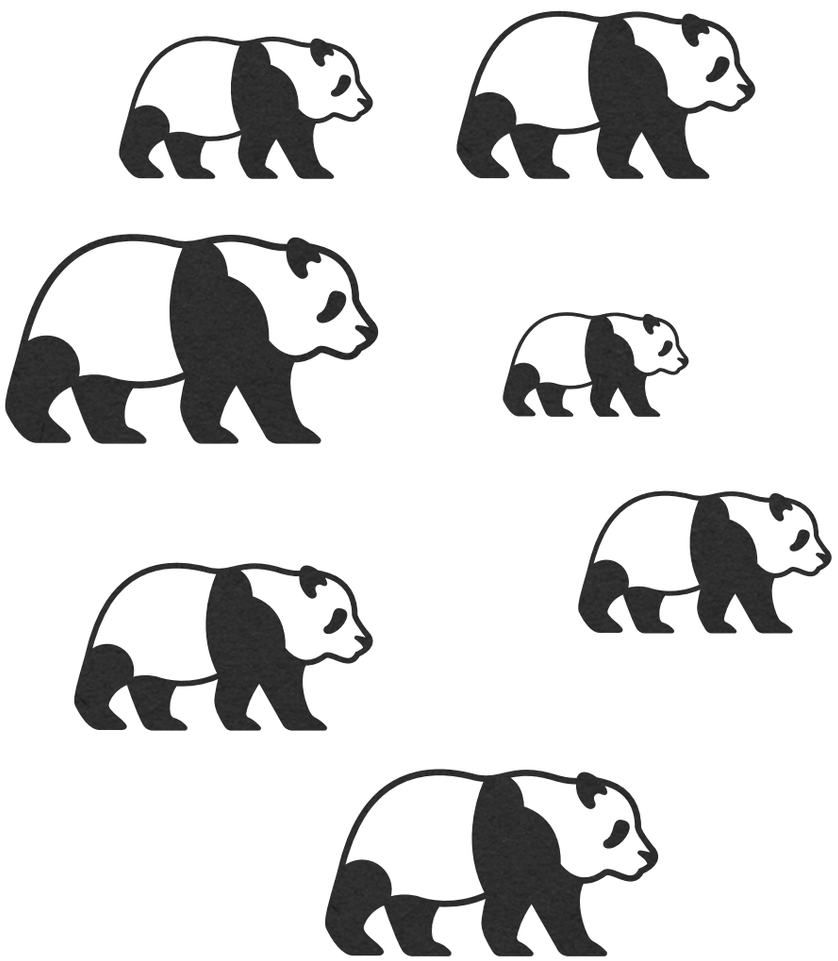
a panda population: several individuals of different sizes



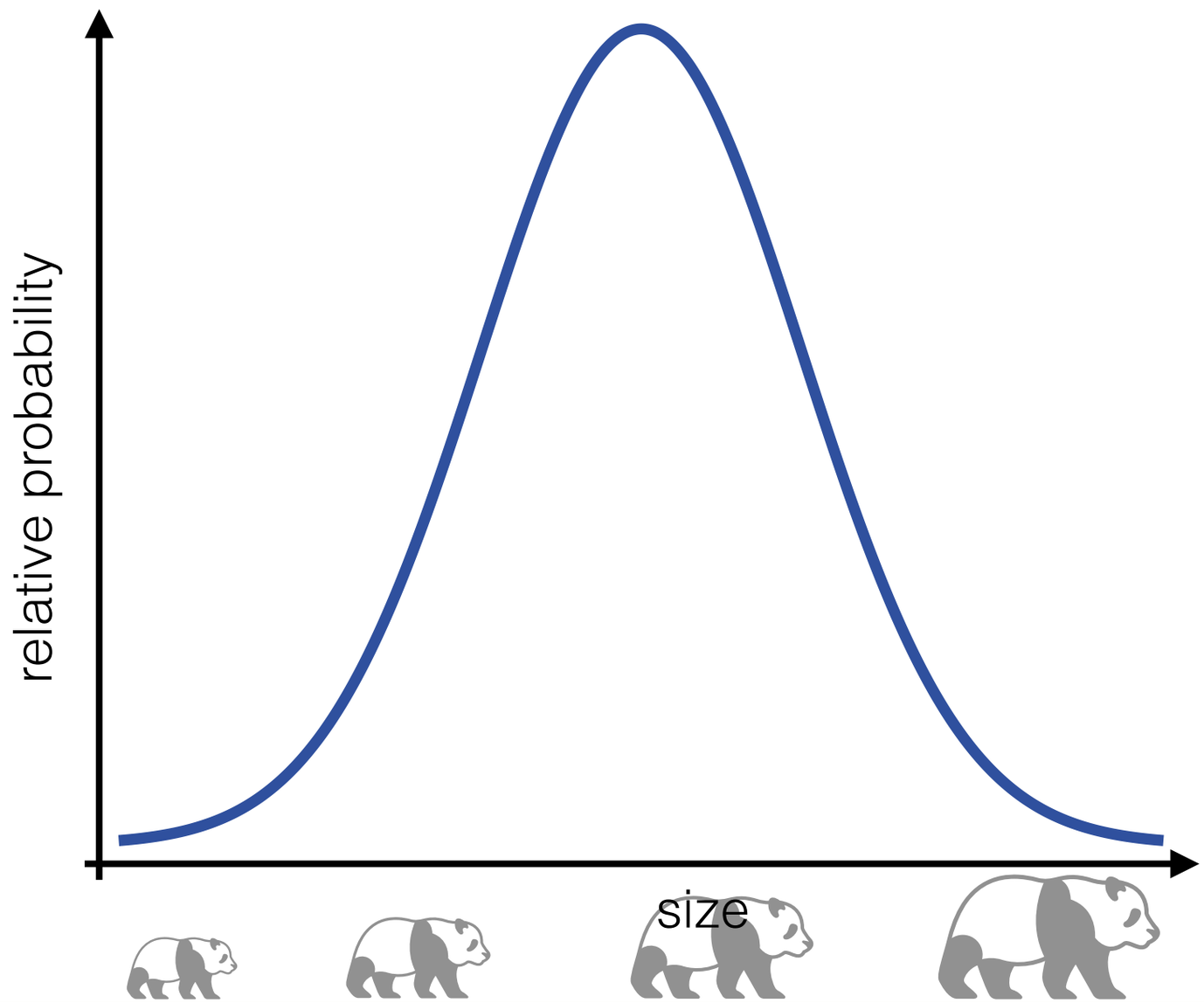
Model

The model should reflect the question we are after.

For instance: What are mean and variance of panda's sizes in a population?

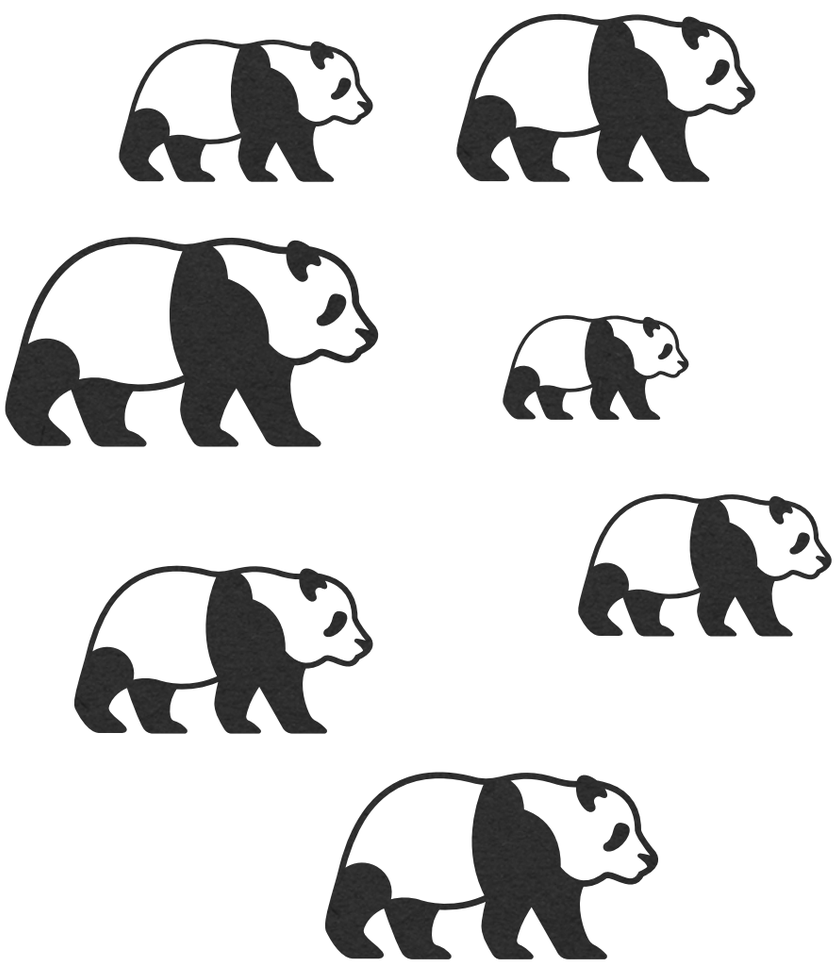


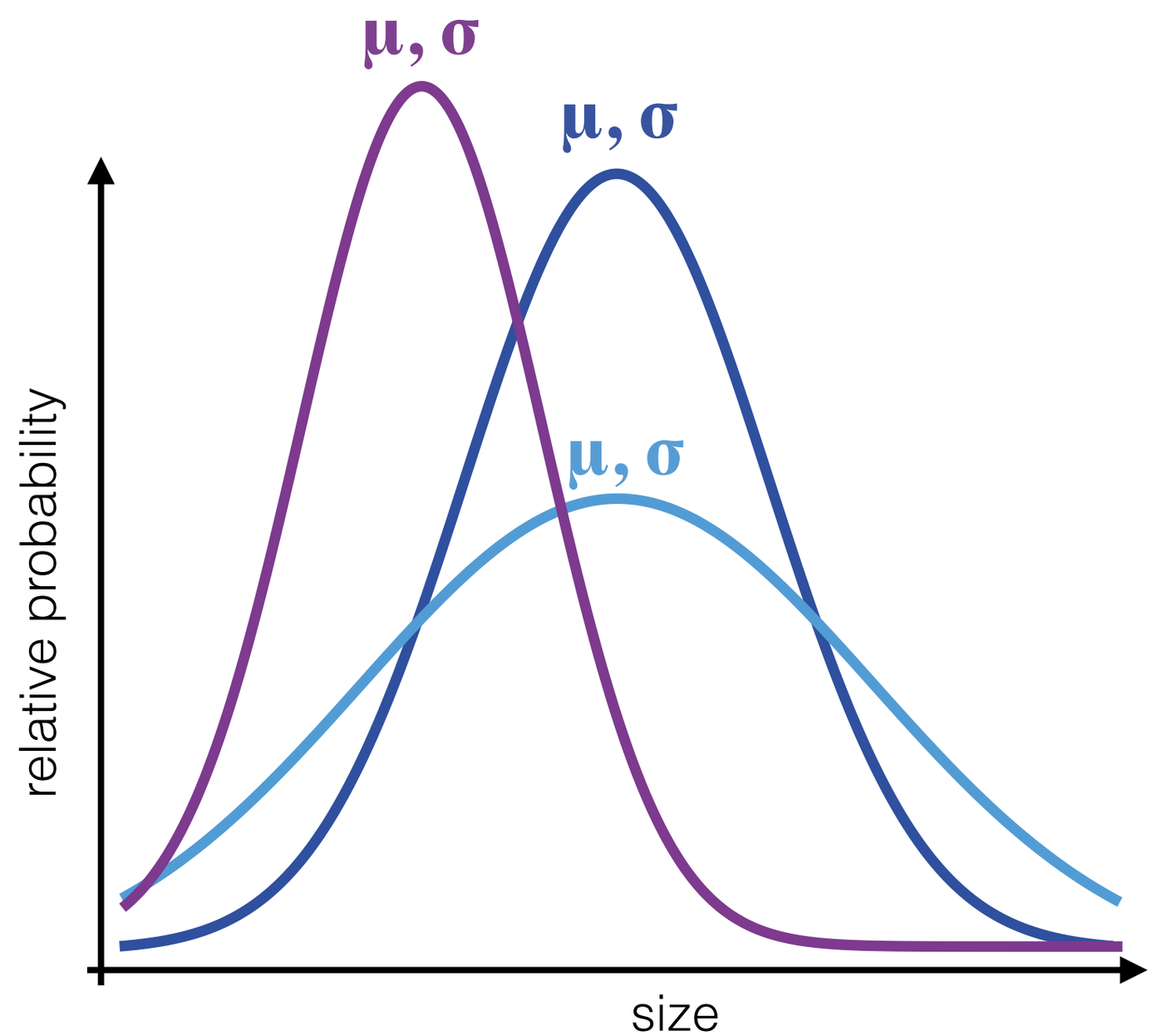
A simple example of a model is a distribution (e.g. a normal distribution)



Parameters

A model is defined by its parameters, e.g. mean and variance of a normal distribution





Bayes theorem for pandas

$$P(\alpha|x, M) = \frac{P(x|\alpha, M) \times P(\alpha|M)}{P(x|M)}$$

alpha = parameters

x = data

M = model

Posterior probability

Likelihood

Prior probability

$$P(\mu, \sigma|🐼, \mathcal{N}) = \frac{P(🐼|\mu, \sigma, \mathcal{N}) \times P(\mu, \sigma)}{P(🐼|\mathcal{N})}$$

Marginal likelihood

Bayes theorem for pandas

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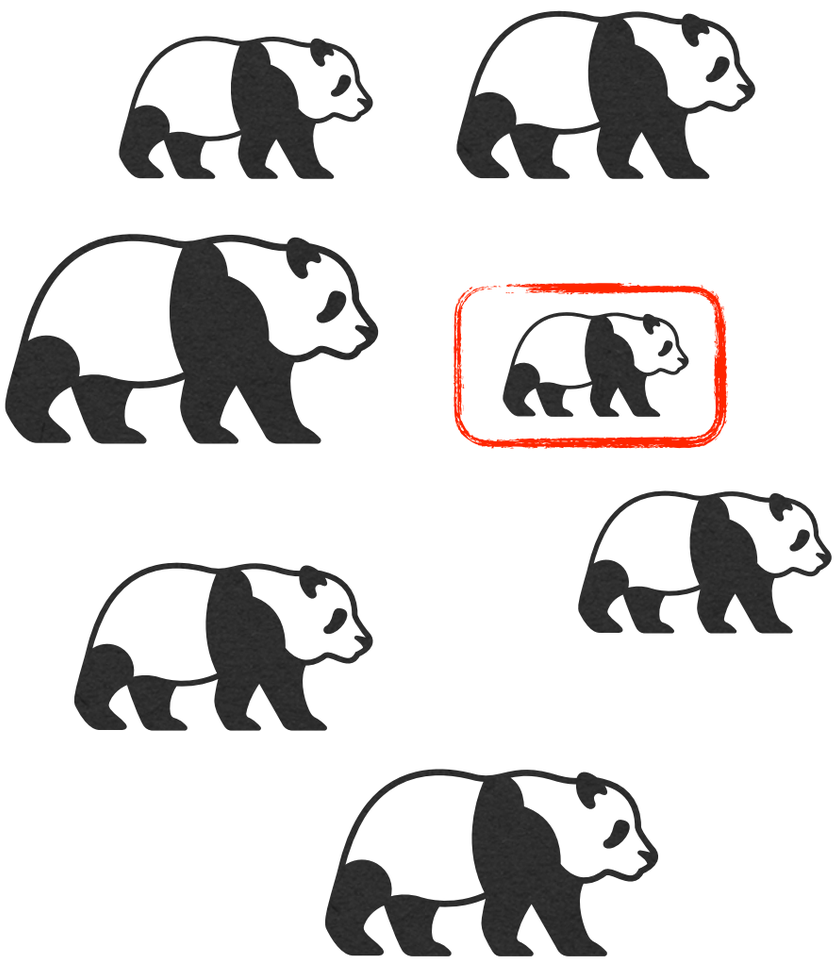
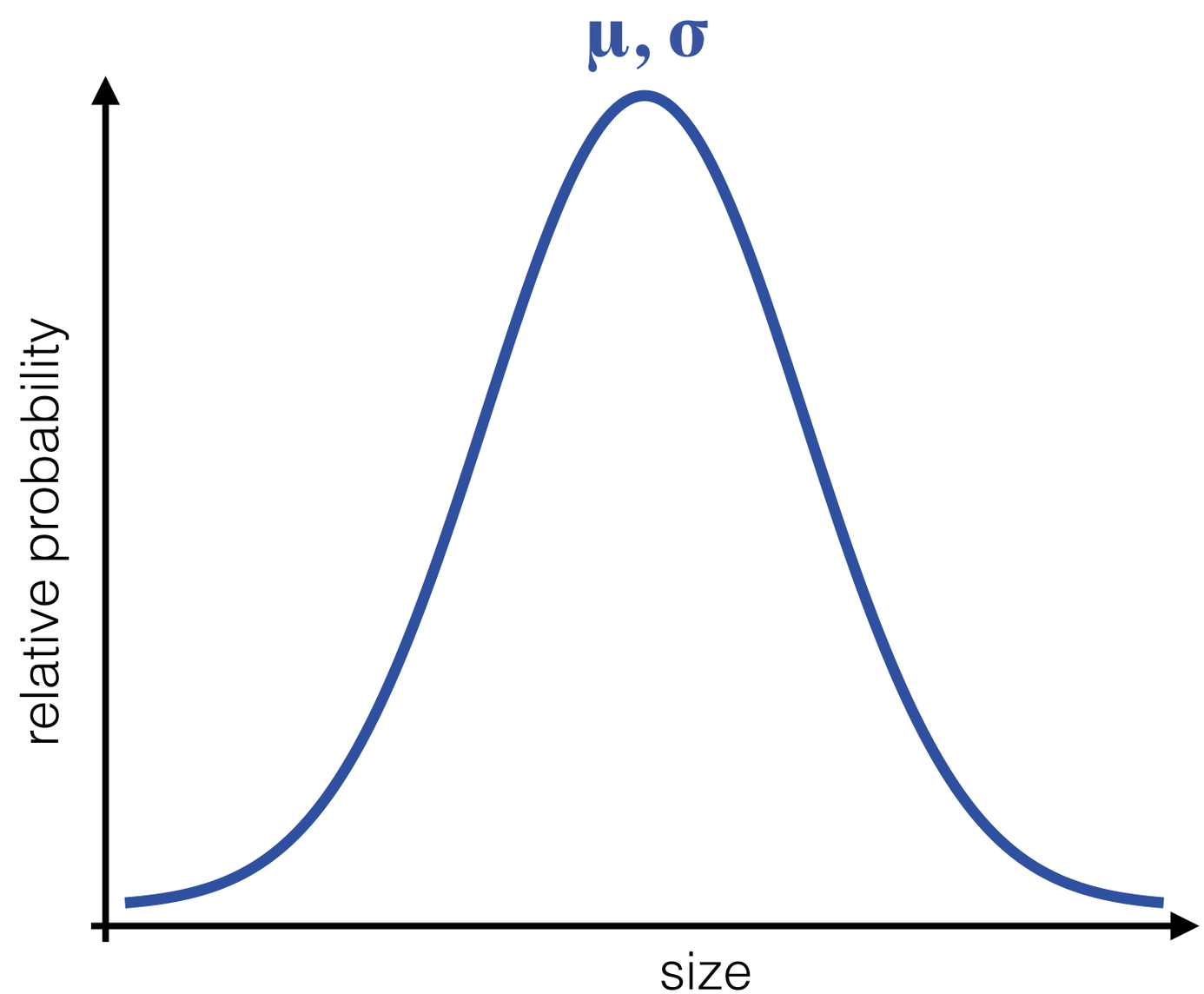
Marginal likelihood

Warning: always avoid emojis in equations, if you can.

Calculating the likelihood: $P(🐼|\mu, \sigma, \mathcal{N})$

Likelihood: probability of observing the data you observe given a model and its parameters





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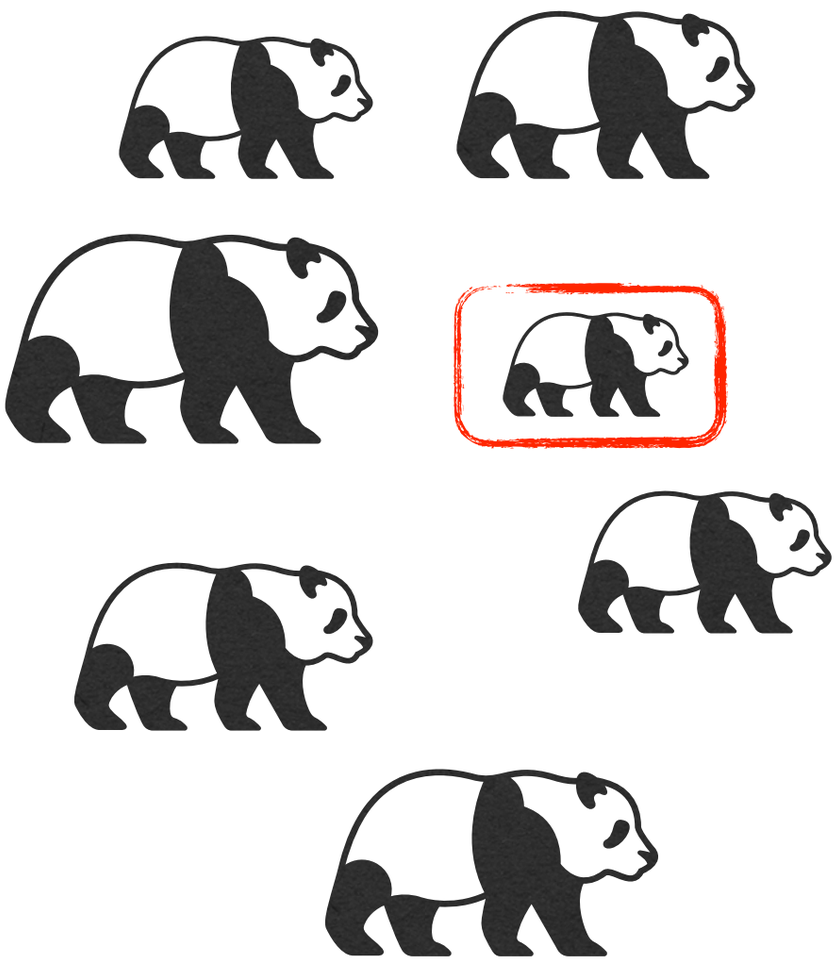

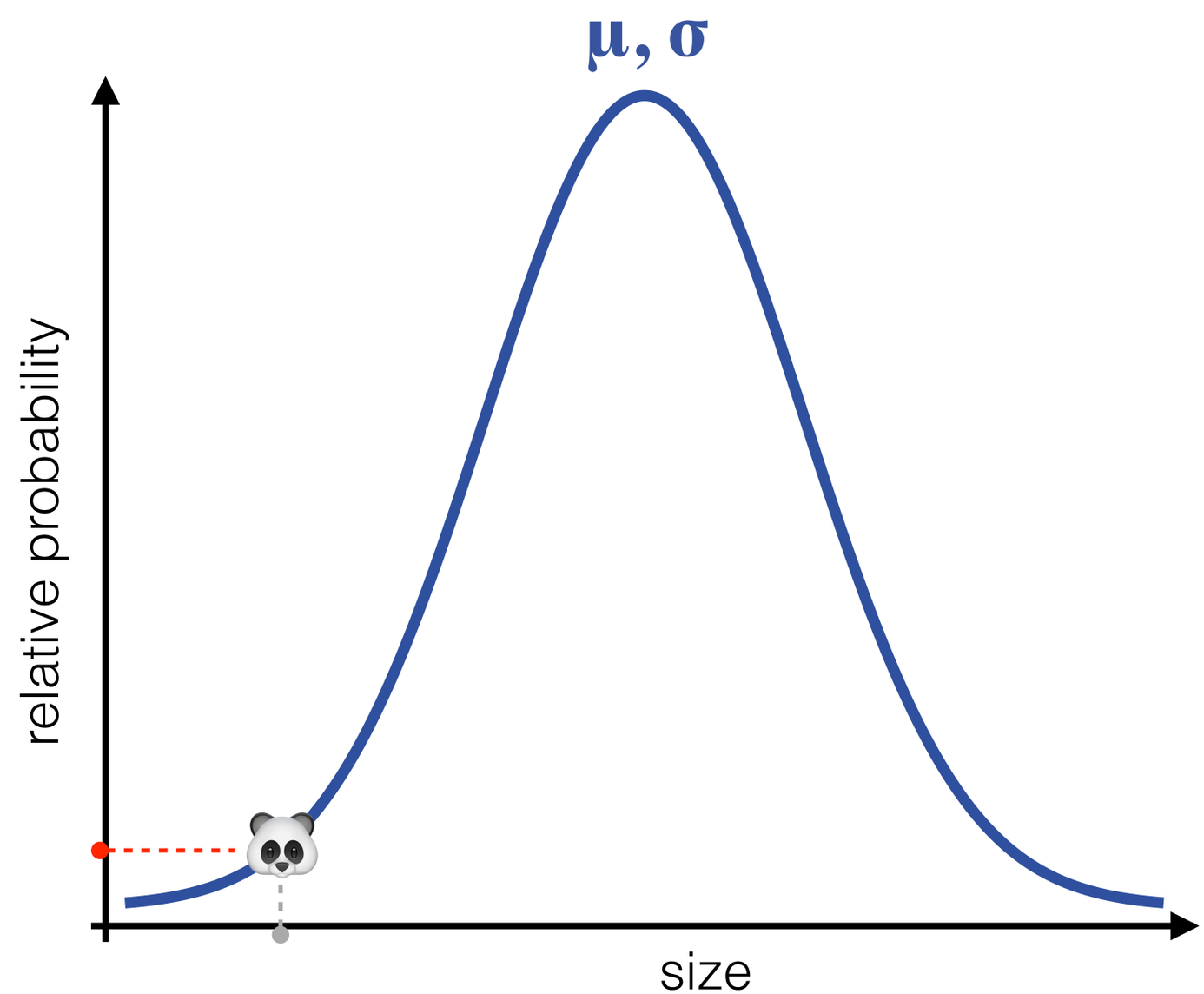

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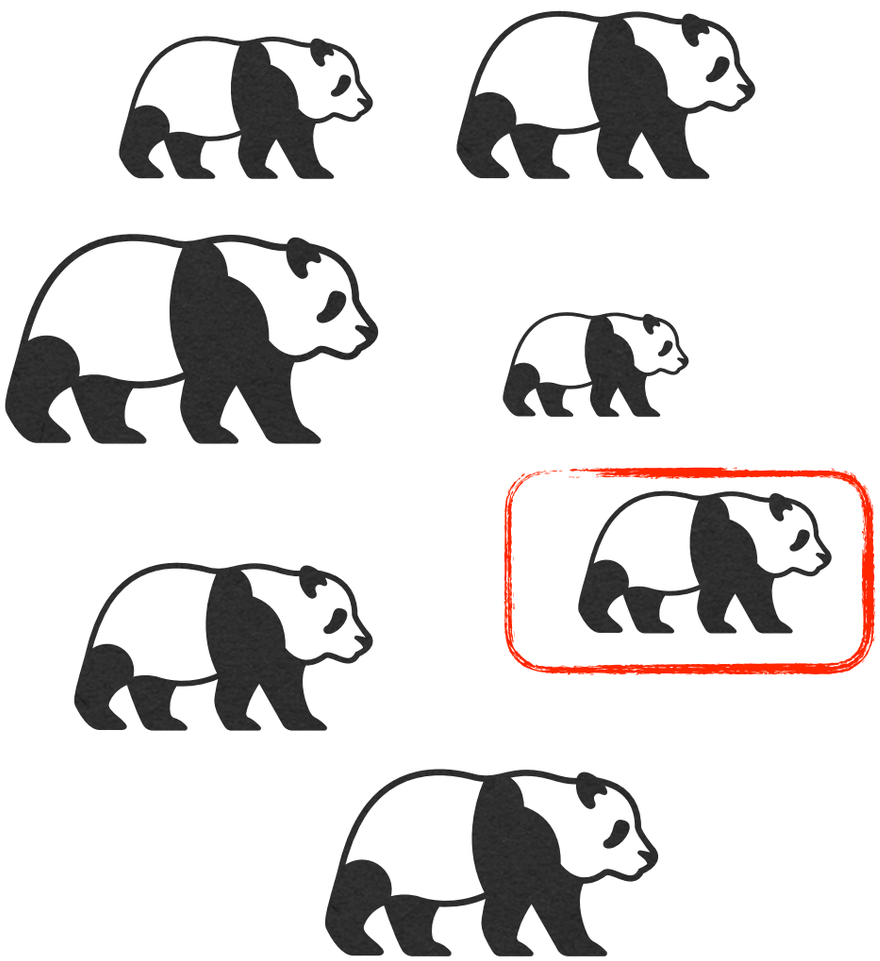

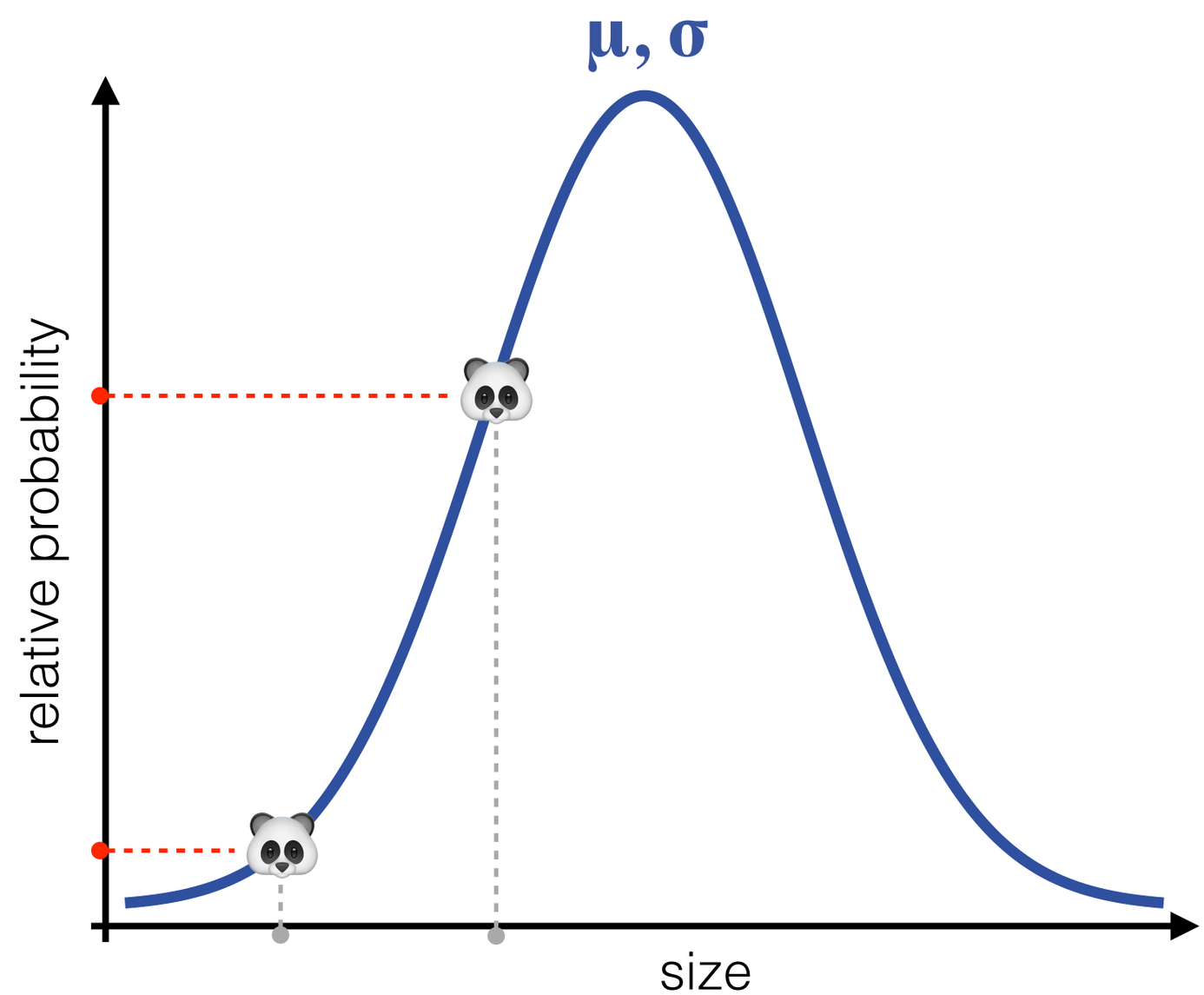

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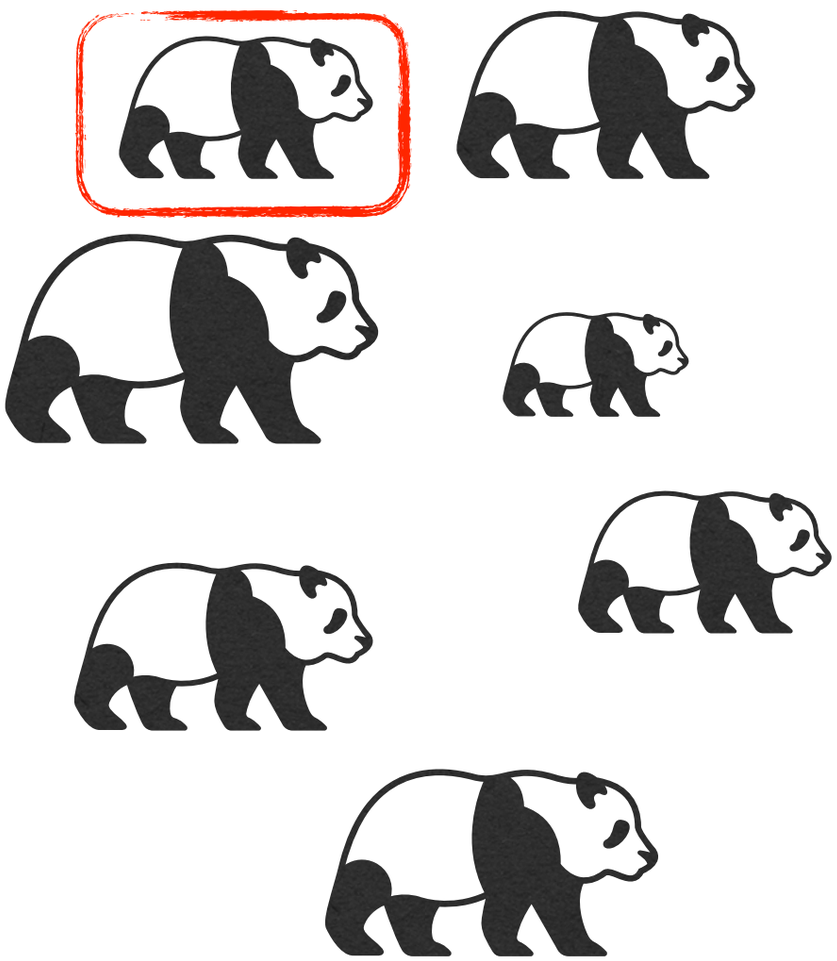

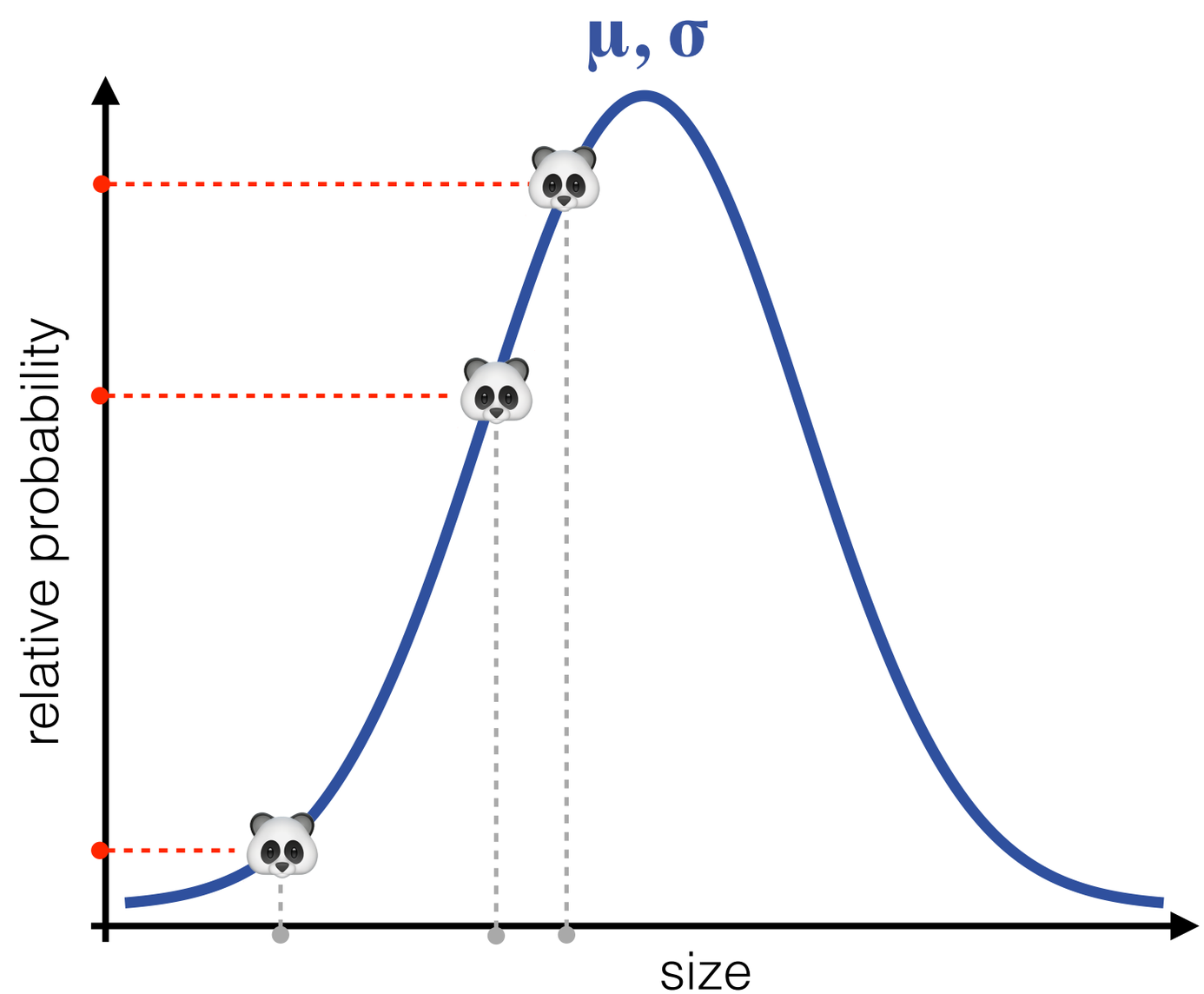

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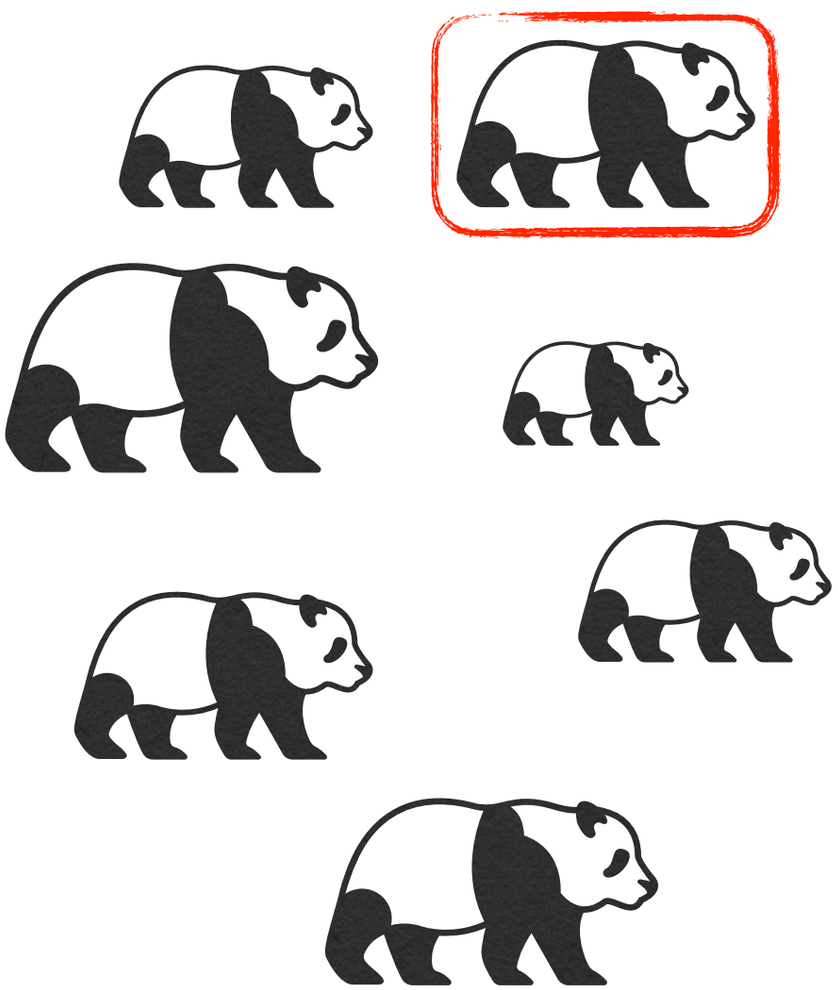

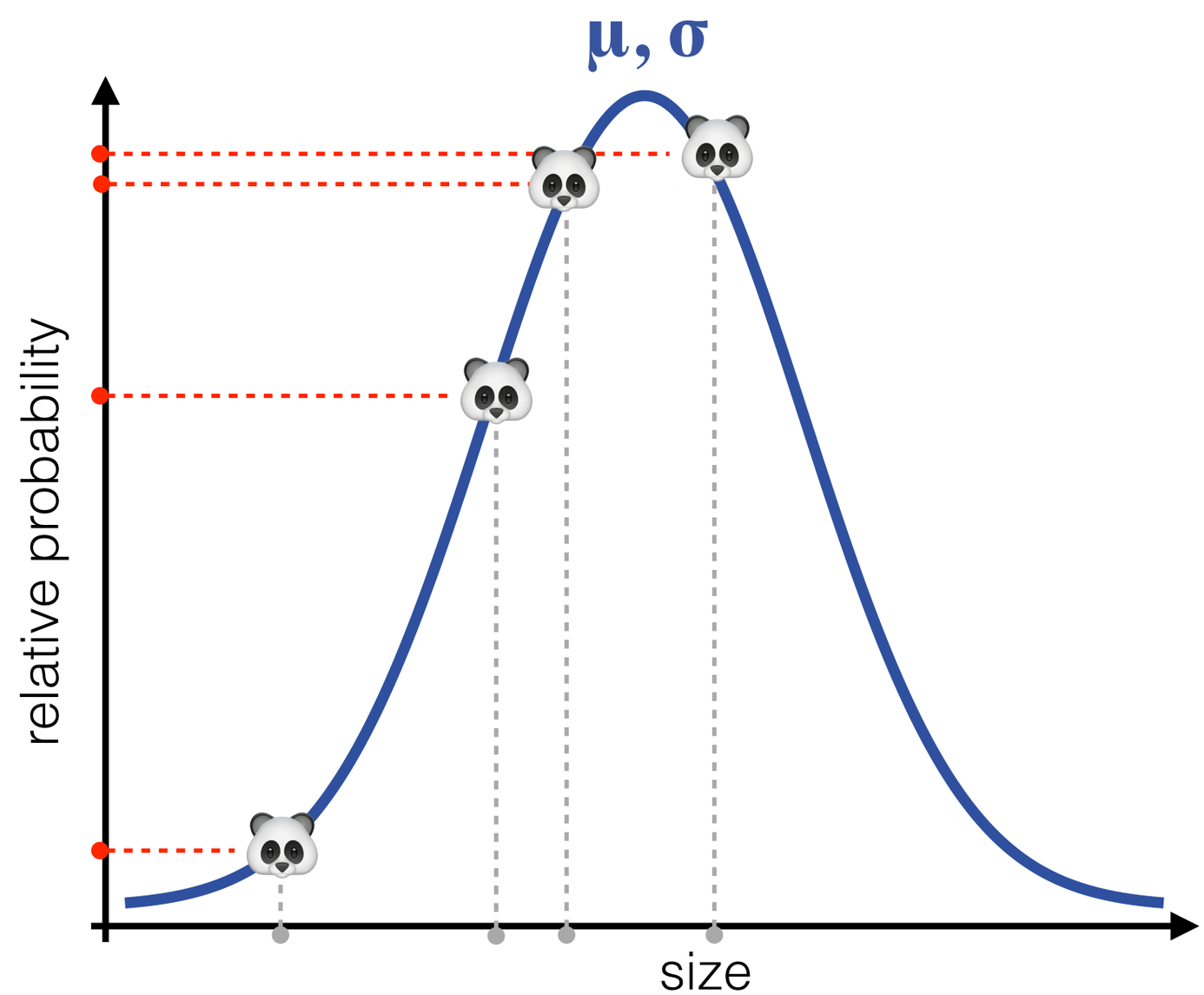

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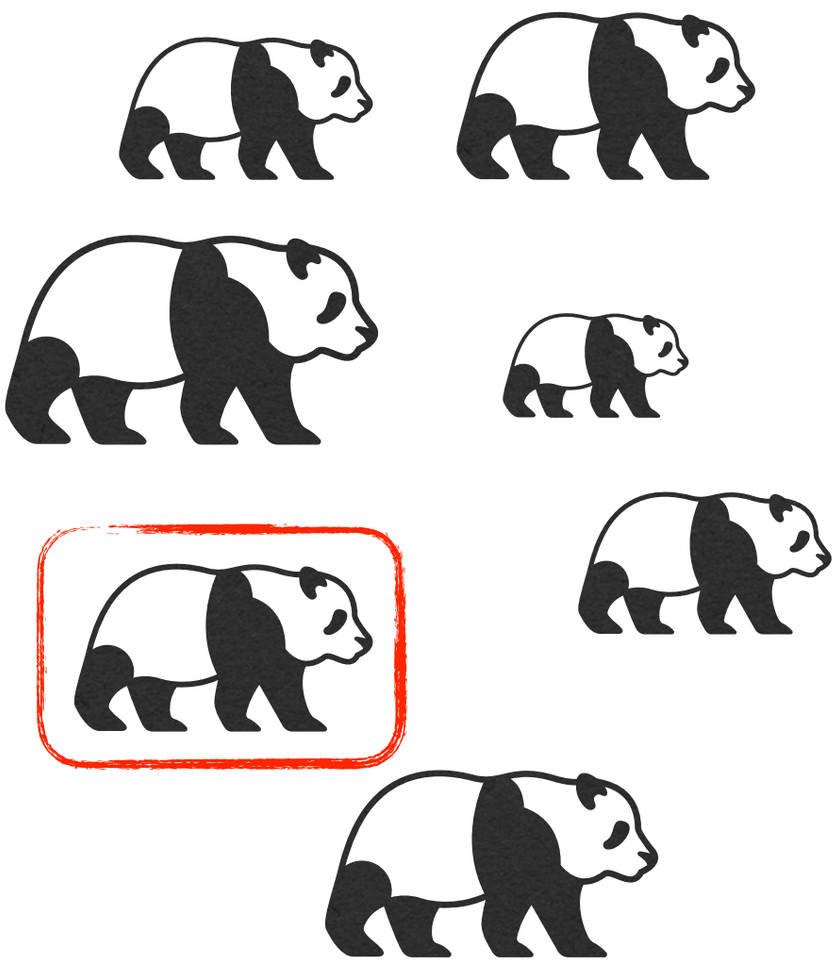

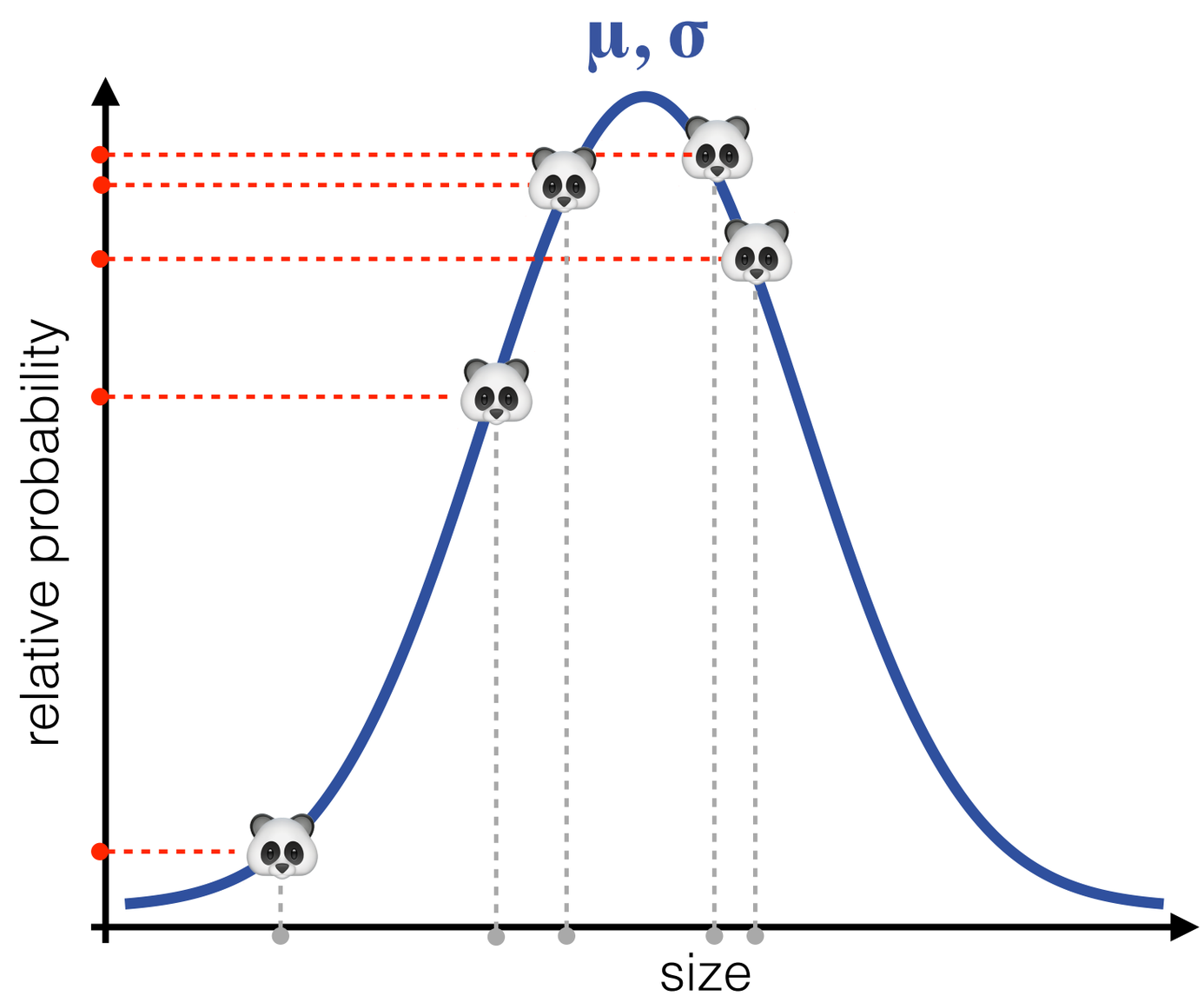

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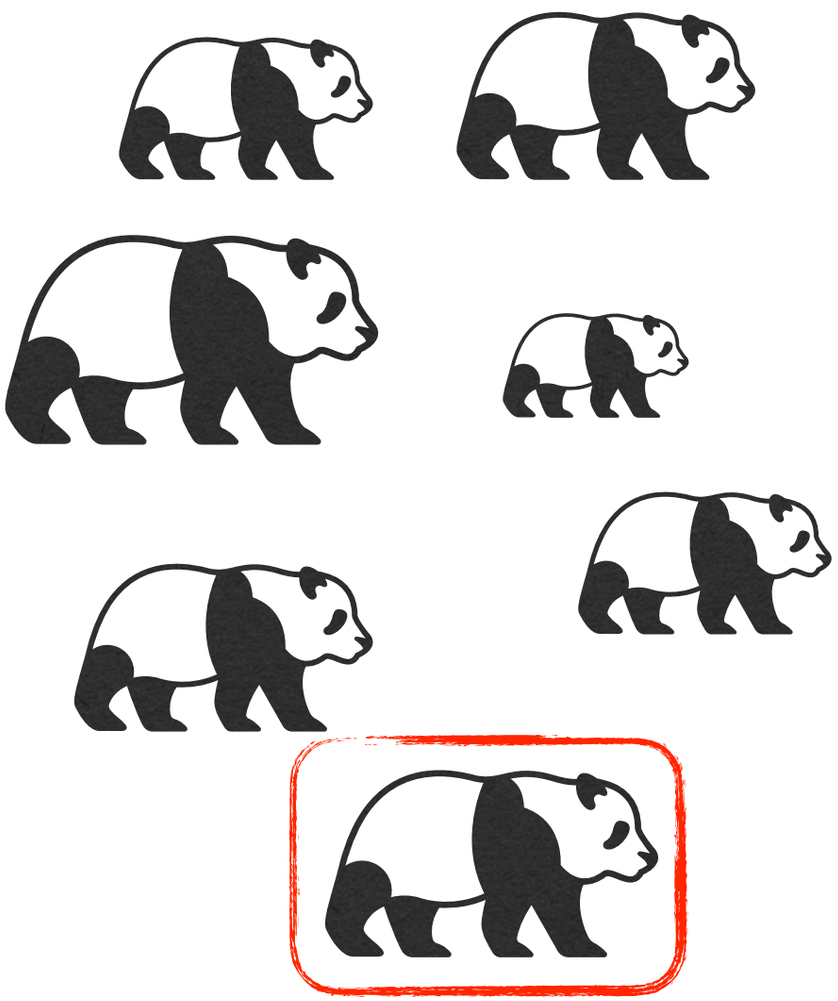

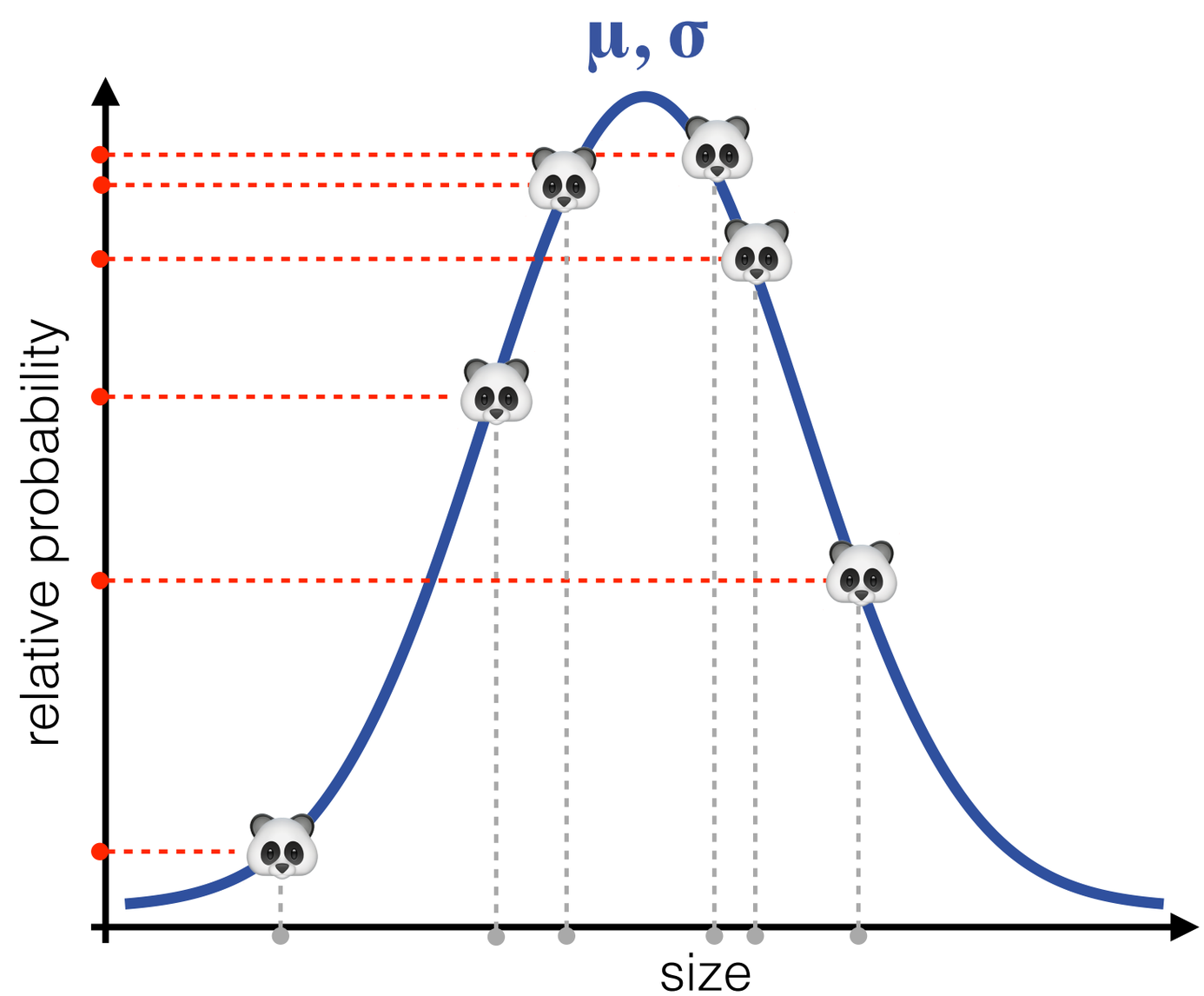

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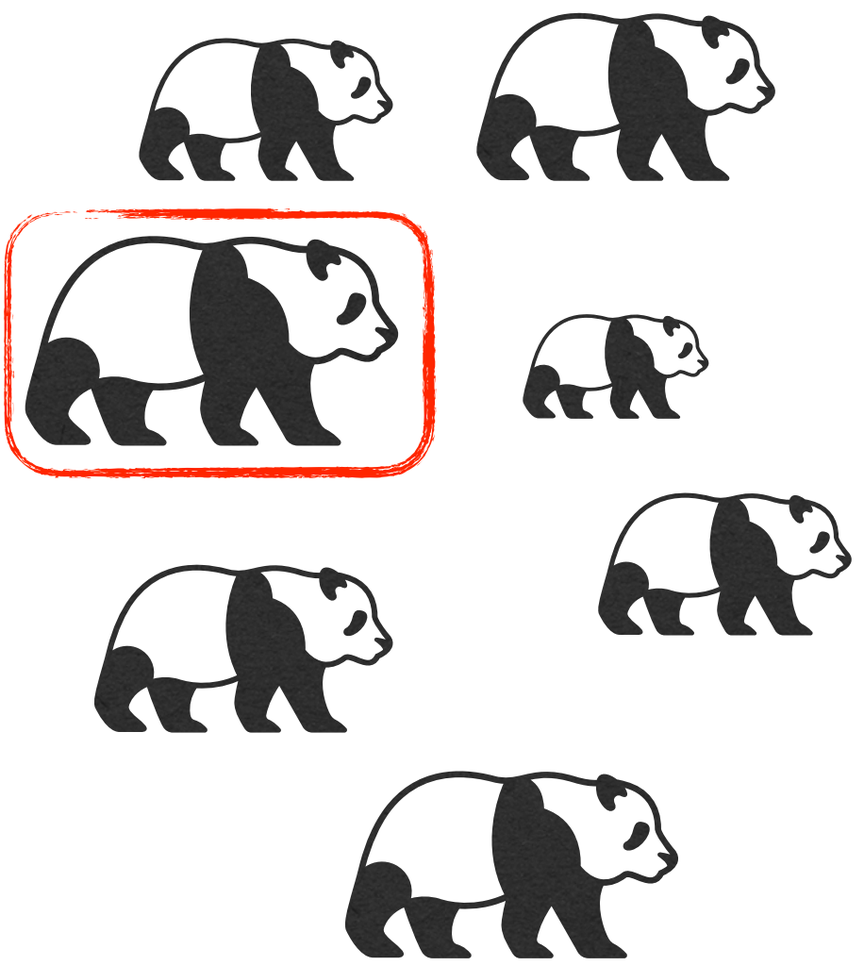

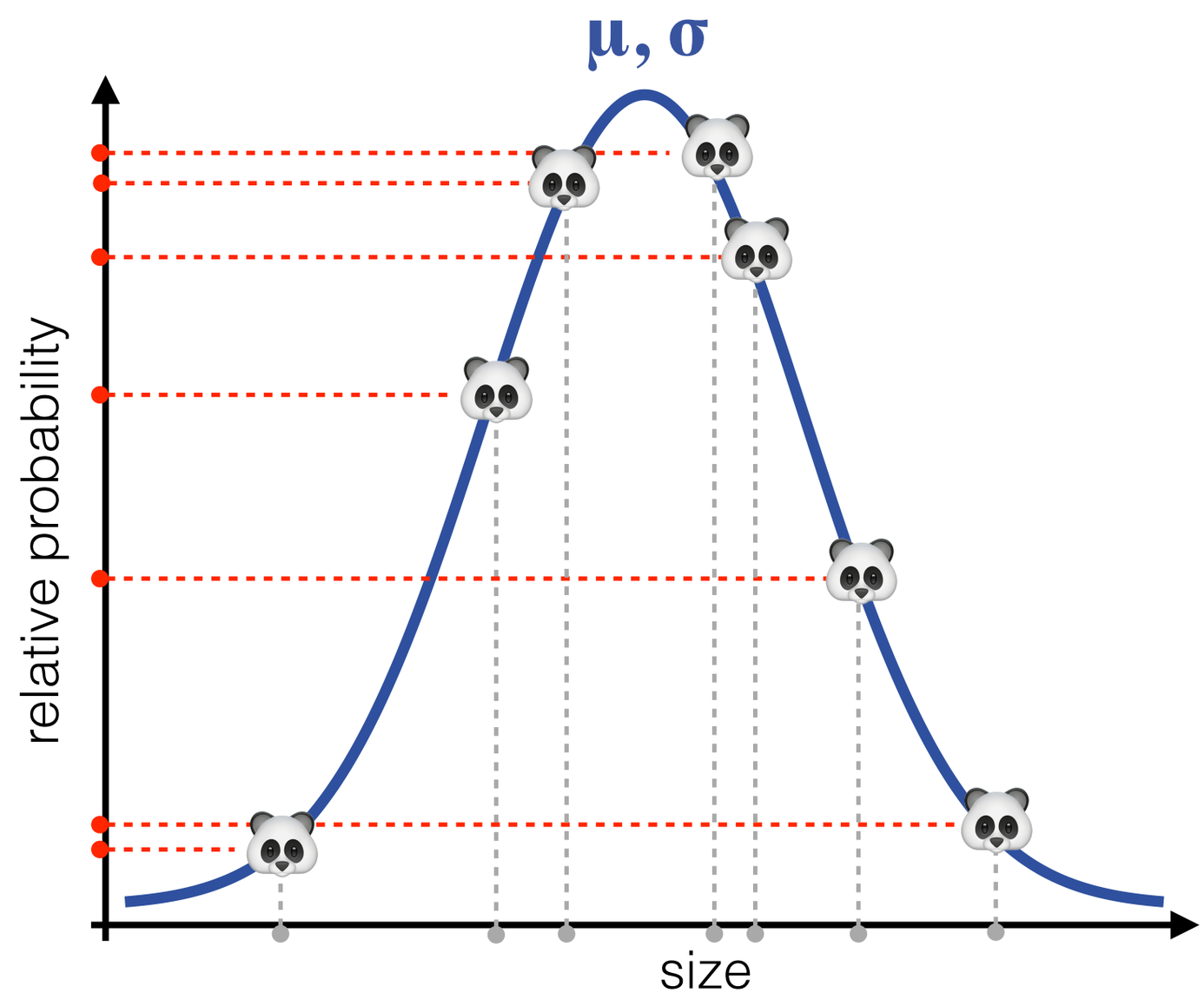

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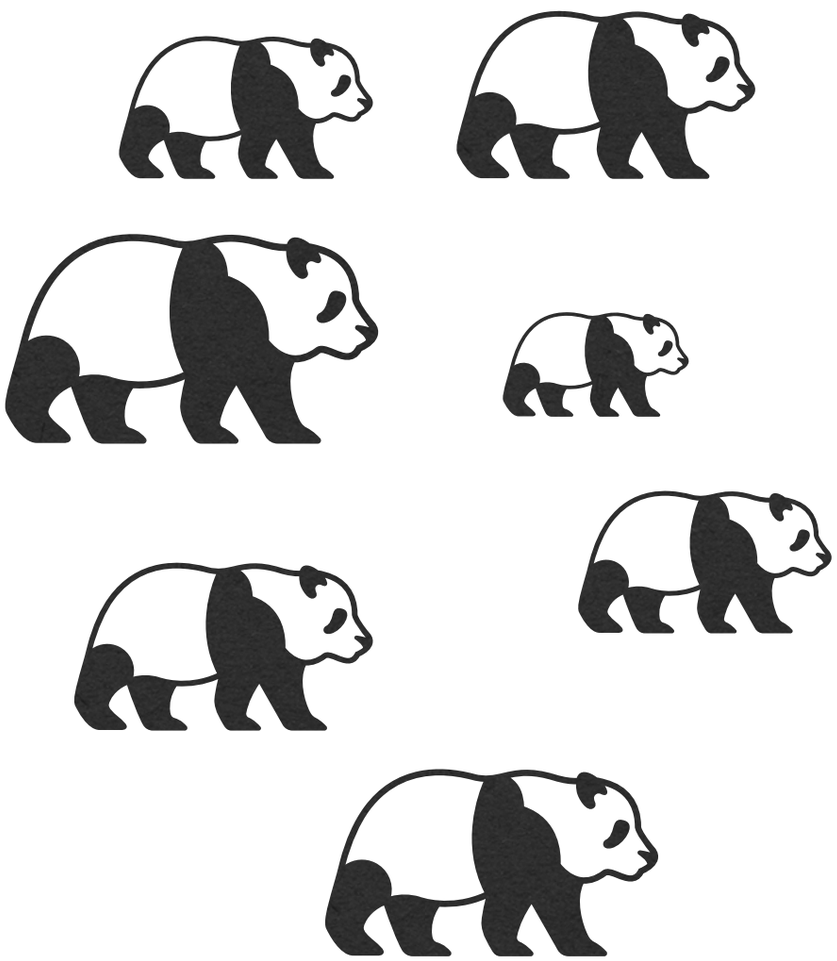

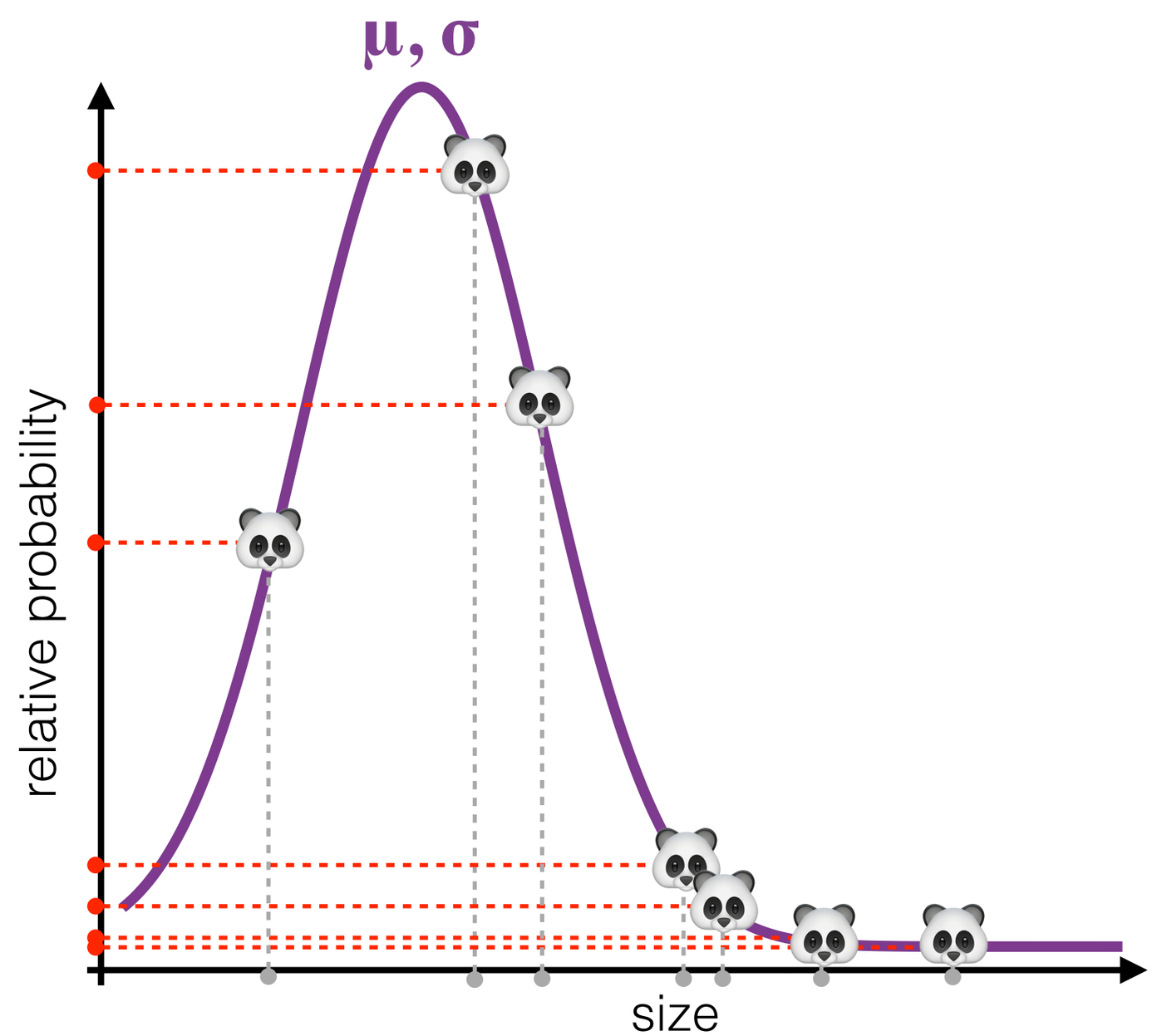

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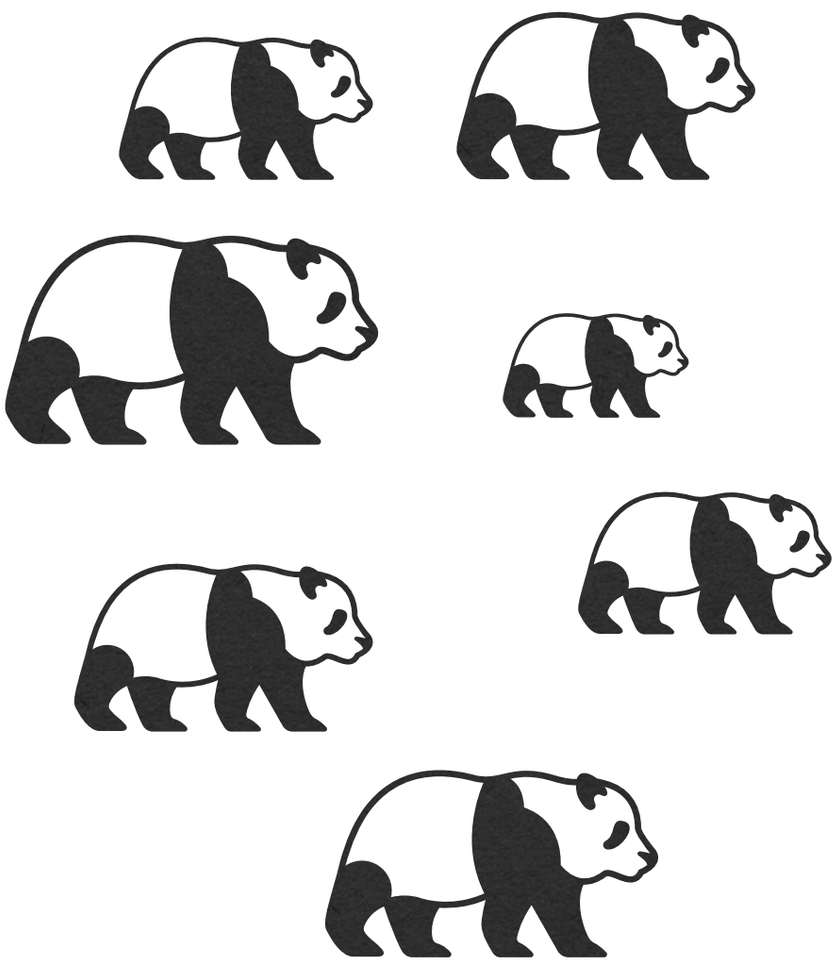

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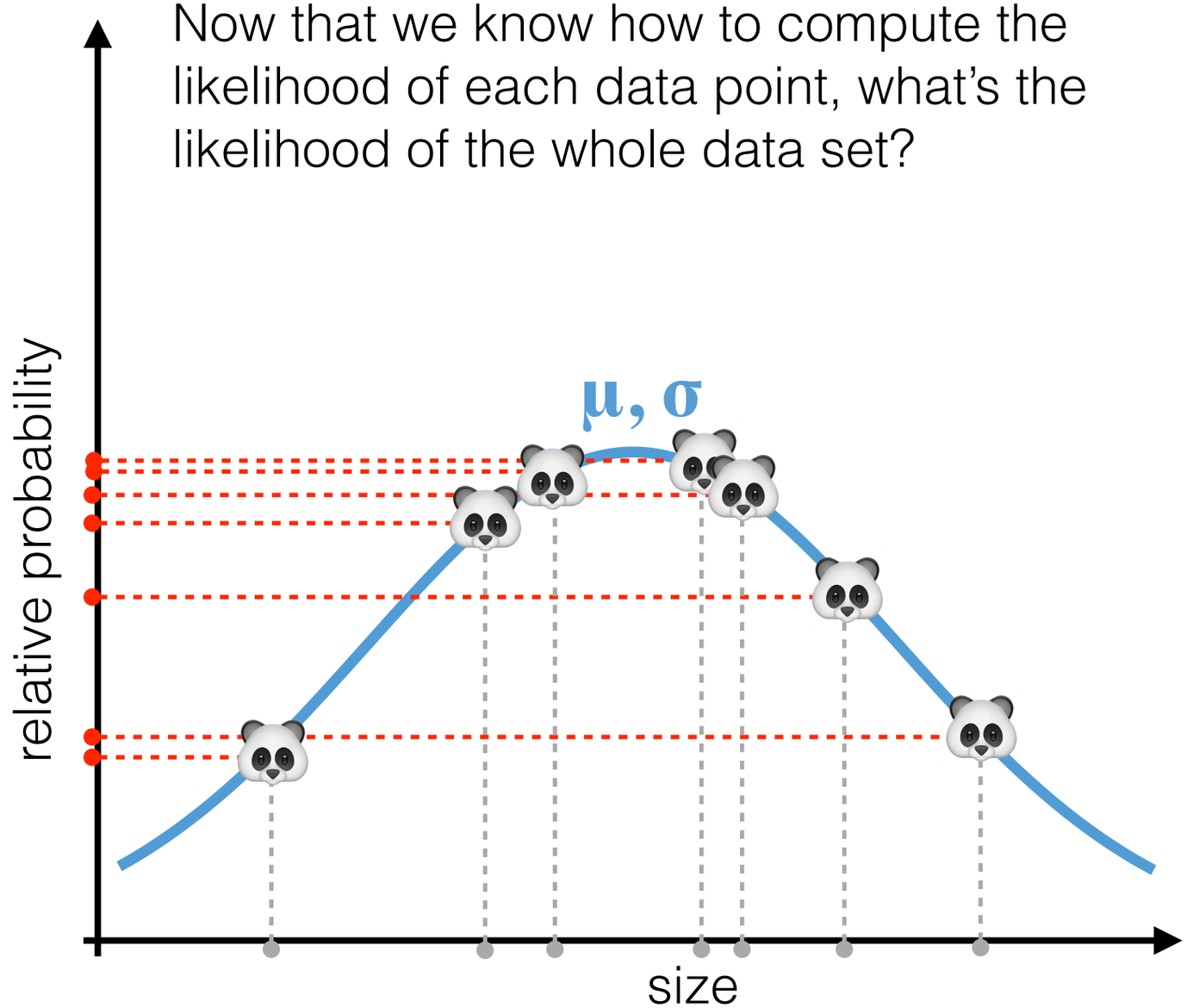
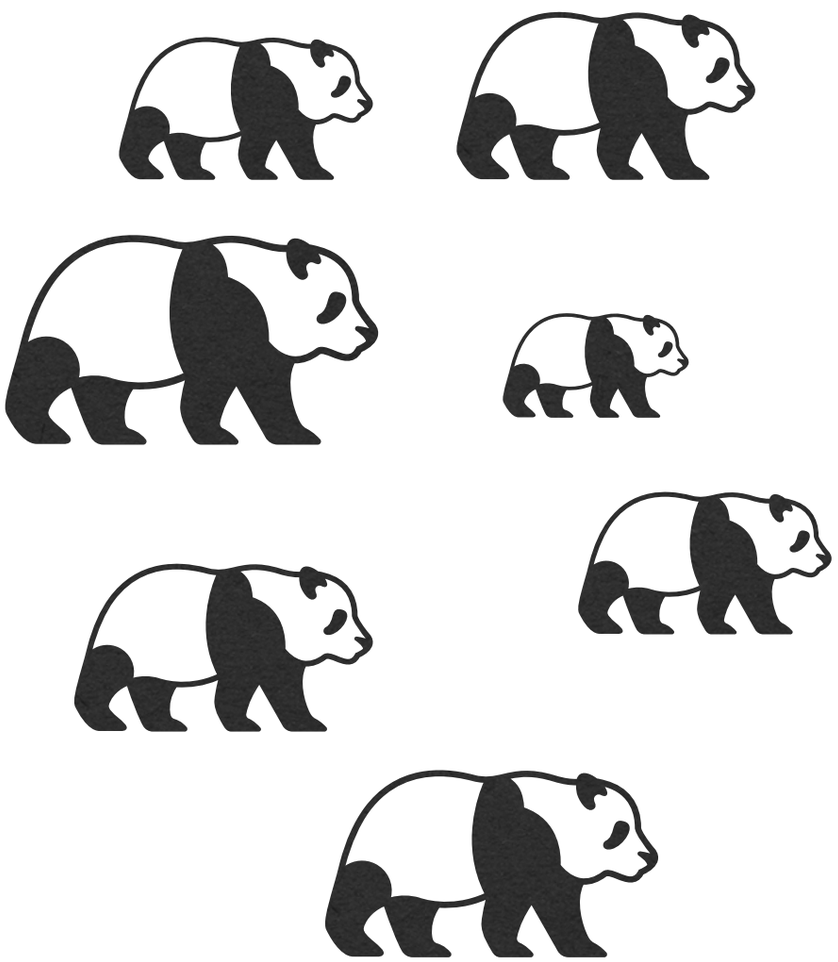


Calculating the likelihood: $P(🐼|\mu, \sigma, \mathcal{N})$

$$P(🐼_1, \ldots, 🐼_7|\mu, \sigma, \mathcal{N}) = \prod_{i=1}^{7} P(🐼_i|\mu, \sigma, \mathcal{N})$$



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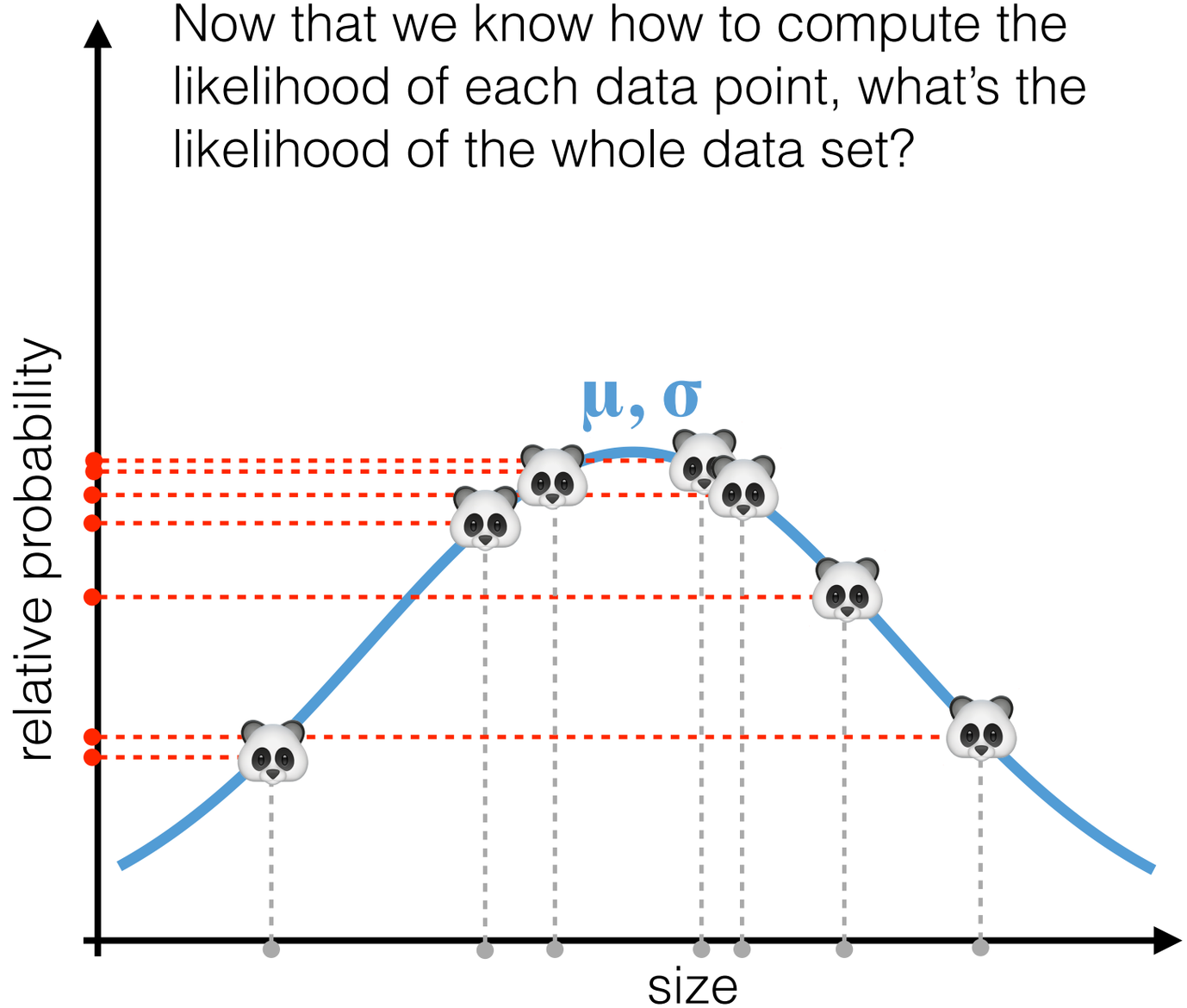

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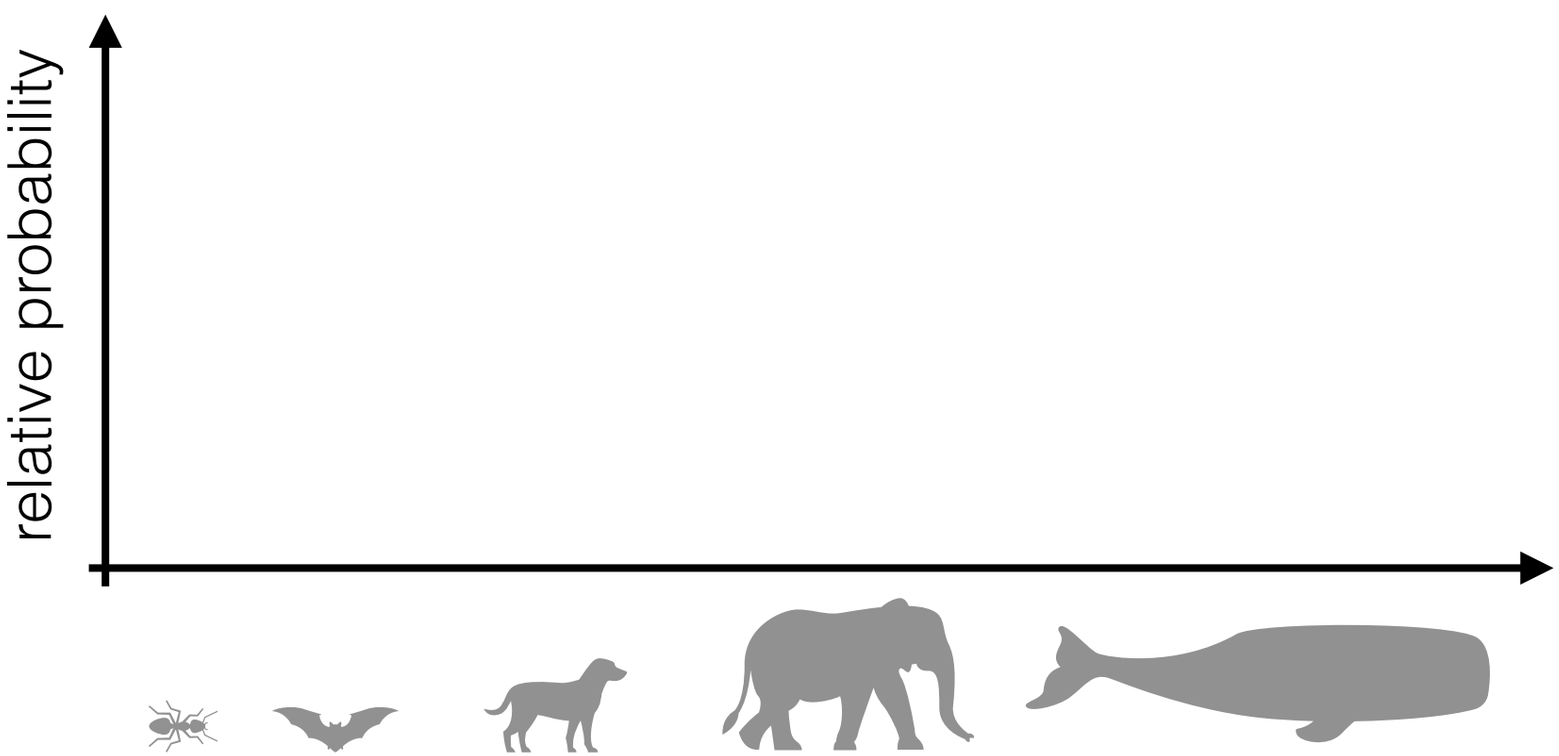
Calculating the prior: $P(\mu, \sigma)$

Prior: probability of the estimated parameter values μ and σ

$$P(\mu) = ?$$

What do we know a priori about
the parameter μ ?



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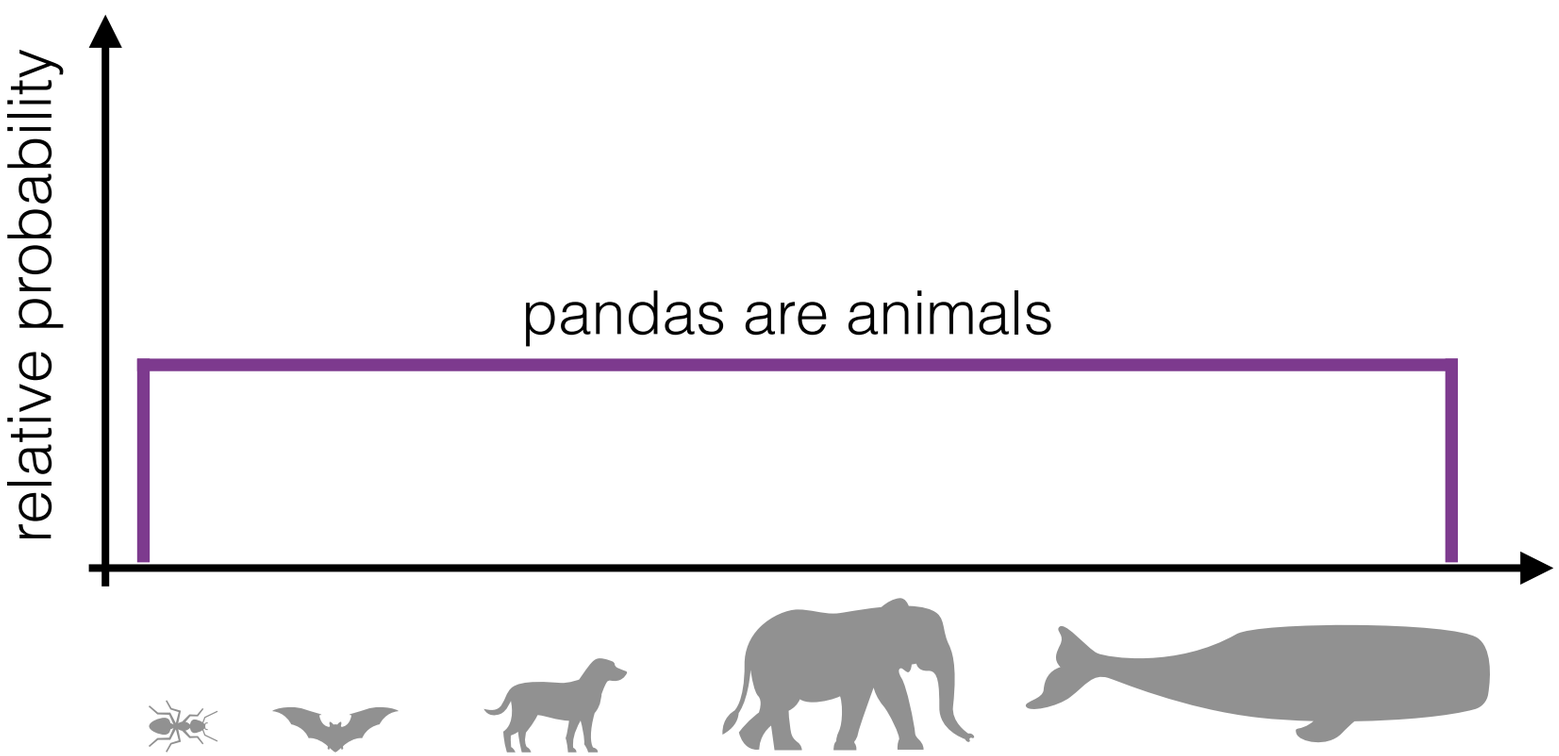

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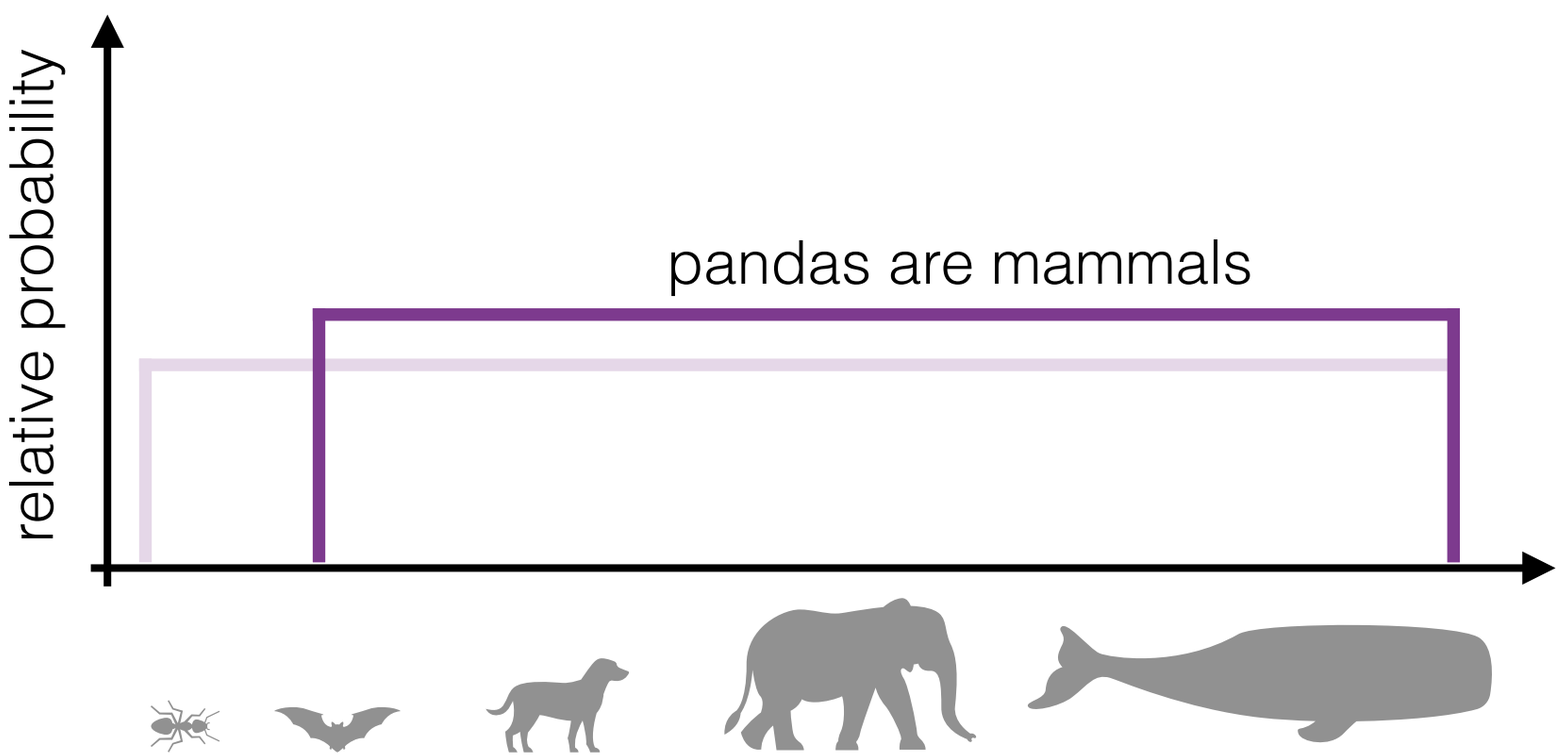

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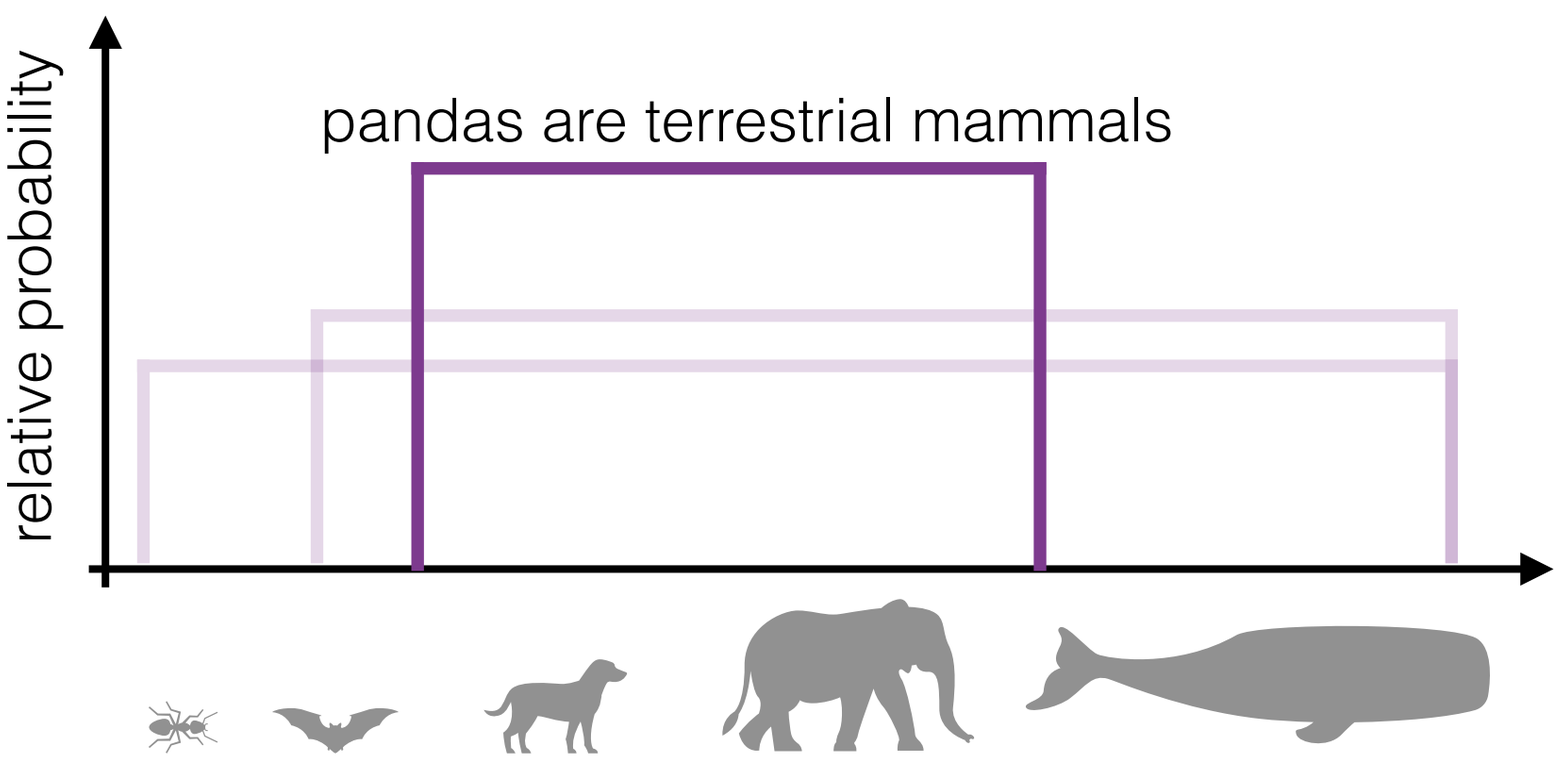

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Prior: probability of the estimated parameter values μ and σ

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$$P(\sigma) = ?$$

What do we know a priori about the parameter σ ?

Calculating the prior: $P(\mu, \sigma)$

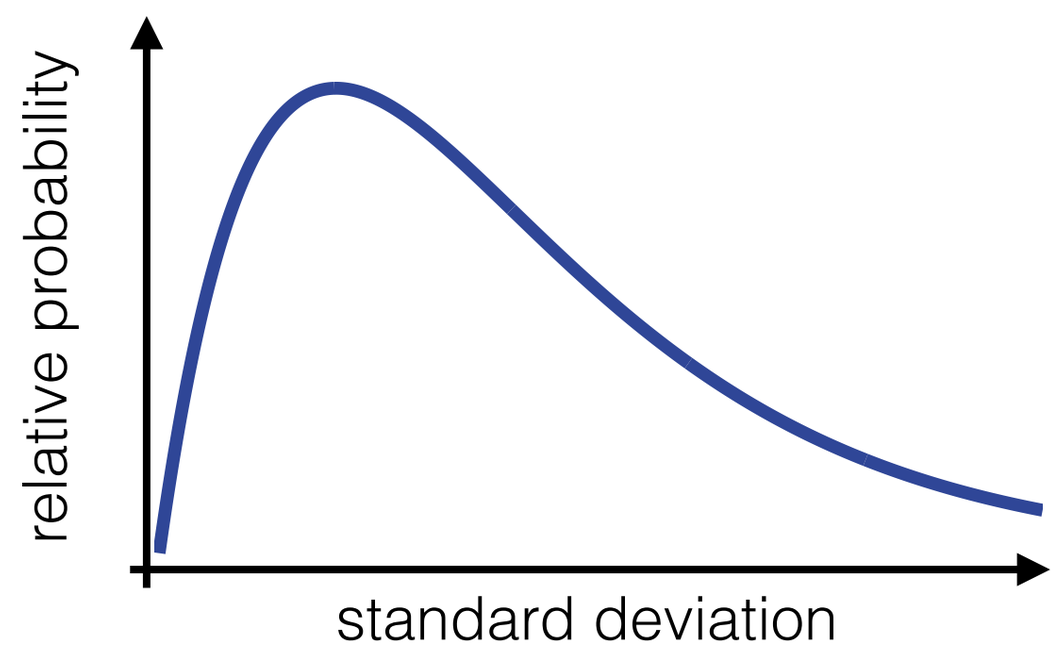
Prior: probability of the estimated parameter values μ and σ

$P(\mu) \sim \mathcal{U}($🐭, 🐘$)$

$P(\sigma) \sim \Gamma(\alpha, \beta)$

What do we know a priori about the parameter σ ?

it must be positive, it is unlikely to be infinite



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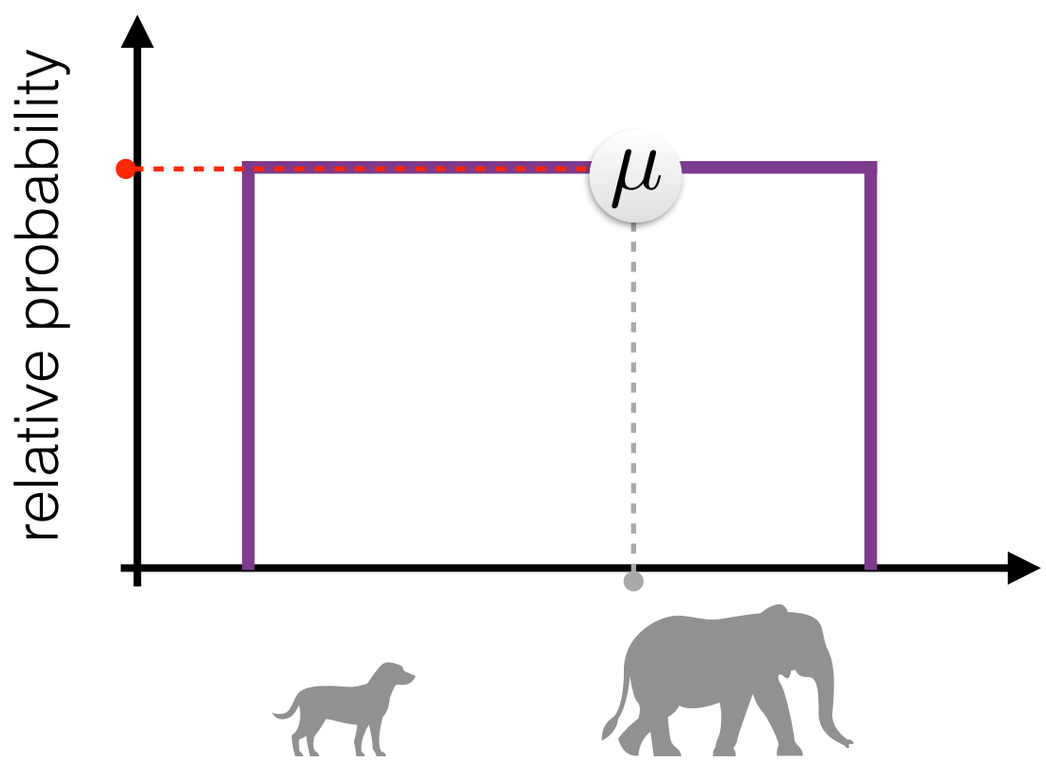
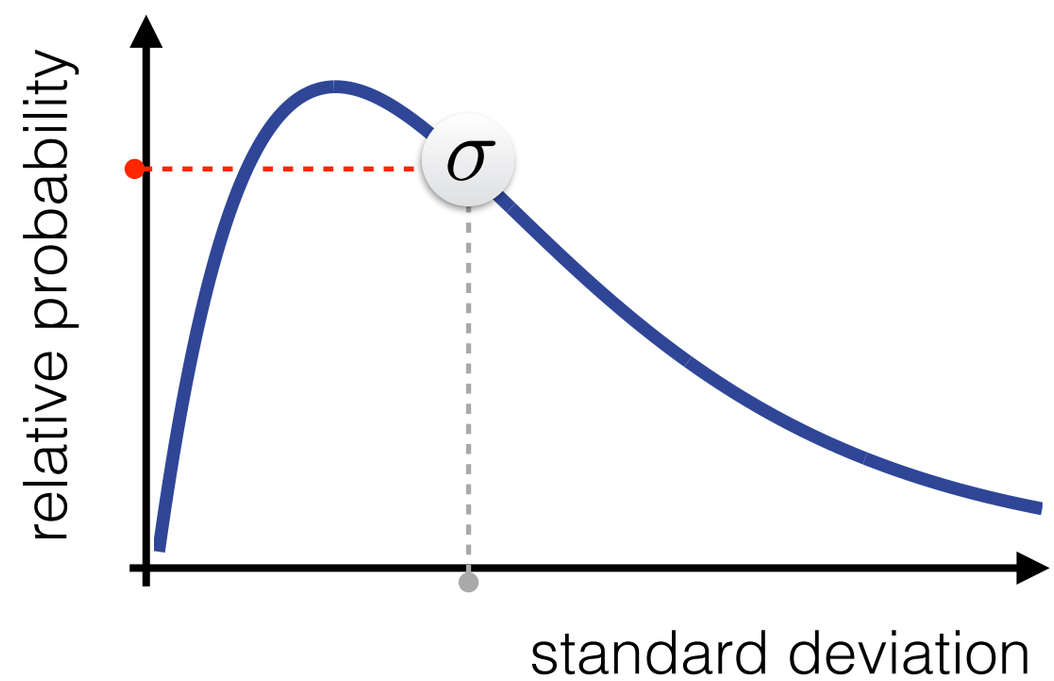
$$P(\mu, \sigma) = P(\mu | 🐭, 🐘, \mathcal{U}) \times P(\sigma | \alpha, \beta, \Gamma)$$





Bayes theorem

Likelihood Prior probability

Posterior probability

$$P(\mu, \sigma | 🐼, \mathcal{N}) = \frac{P(🐼 | \mu, \sigma, \mathcal{N}) \times P(\mu, \sigma)}{P(🐼 | \mathcal{N})}$$

Marginal likelihood

Likelihood: probability of observing the data you observe given a model and its parameters

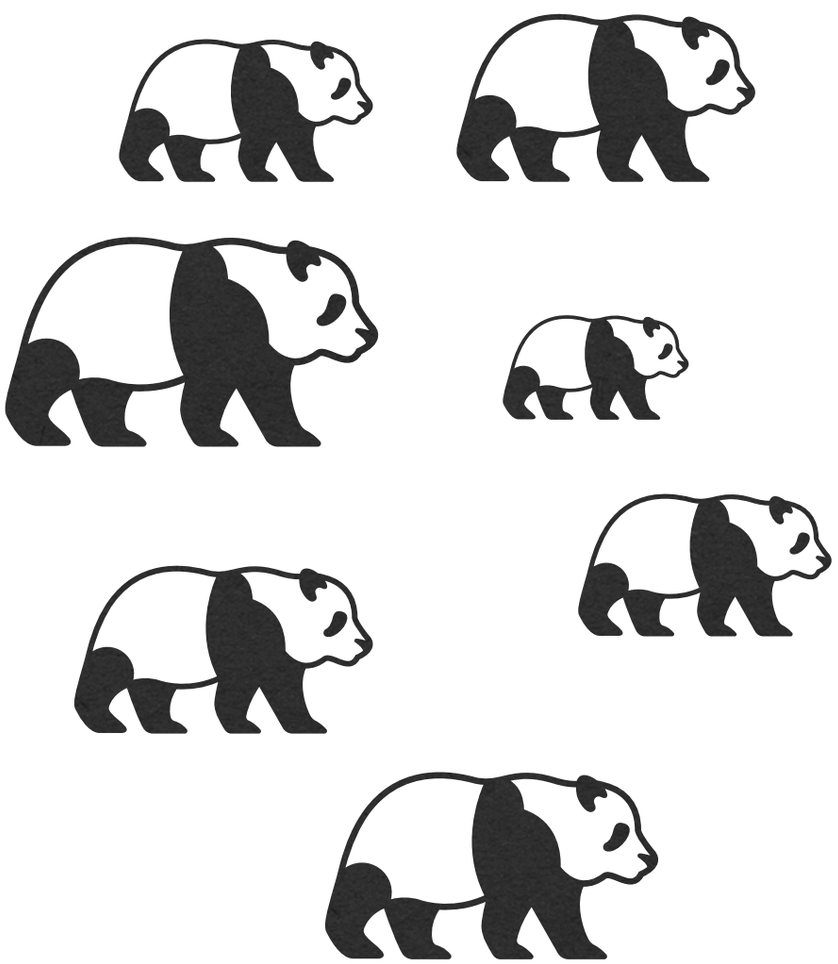
Prior: probability of the parameter values based on some prior knowledge about them

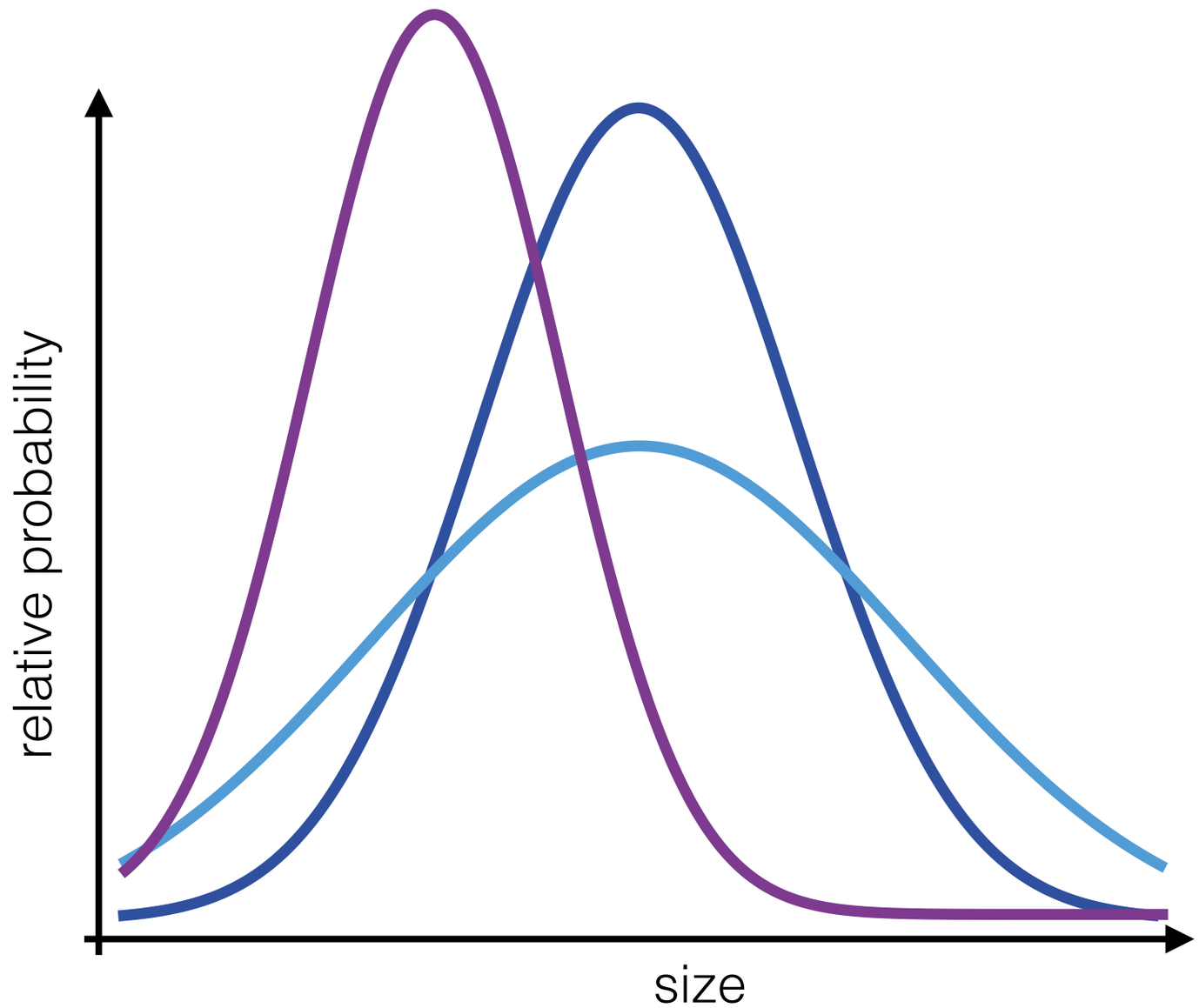
Marginal likelihood: probability of observing the data you observe given a model and all possible parameter values

Probability of the data: $P(🐼|\mathcal{N})$

Probability of the data given the model, integrating all possible parameter values

$$P(🐼|\mathcal{N}) = \int_\mu \int_\sigma P(🐼|\mu, \sigma, \mathcal{N}) \times P(\mu, \sigma|\mathcal{N})\ d\mu\ d\sigma$$

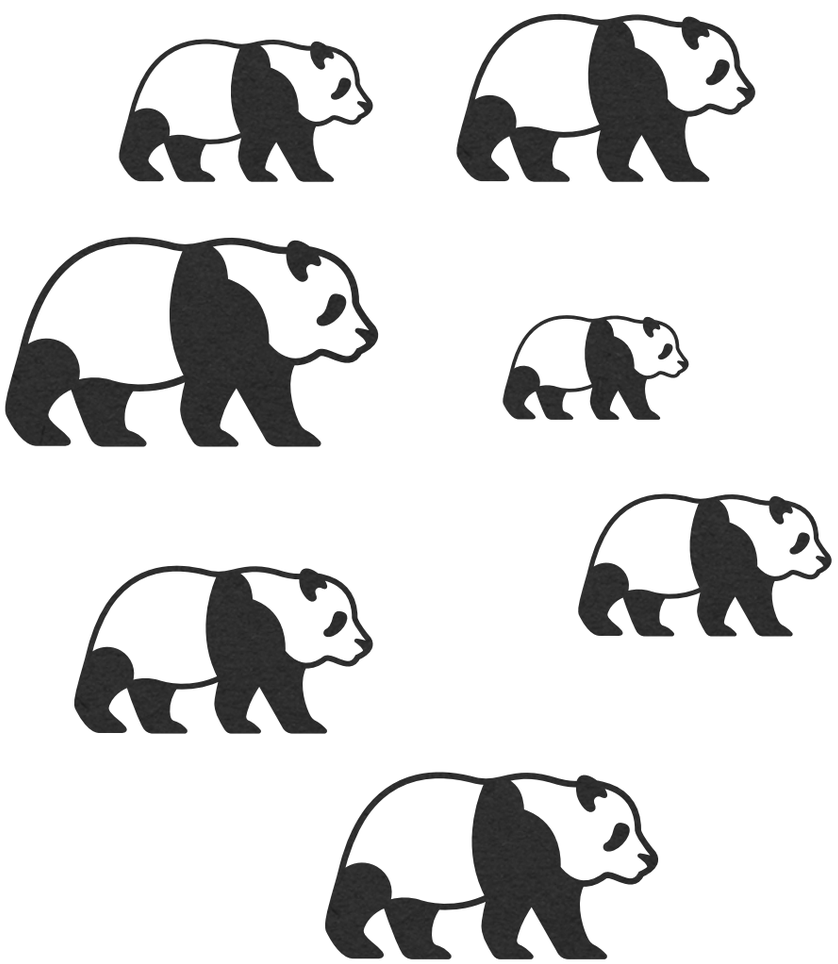


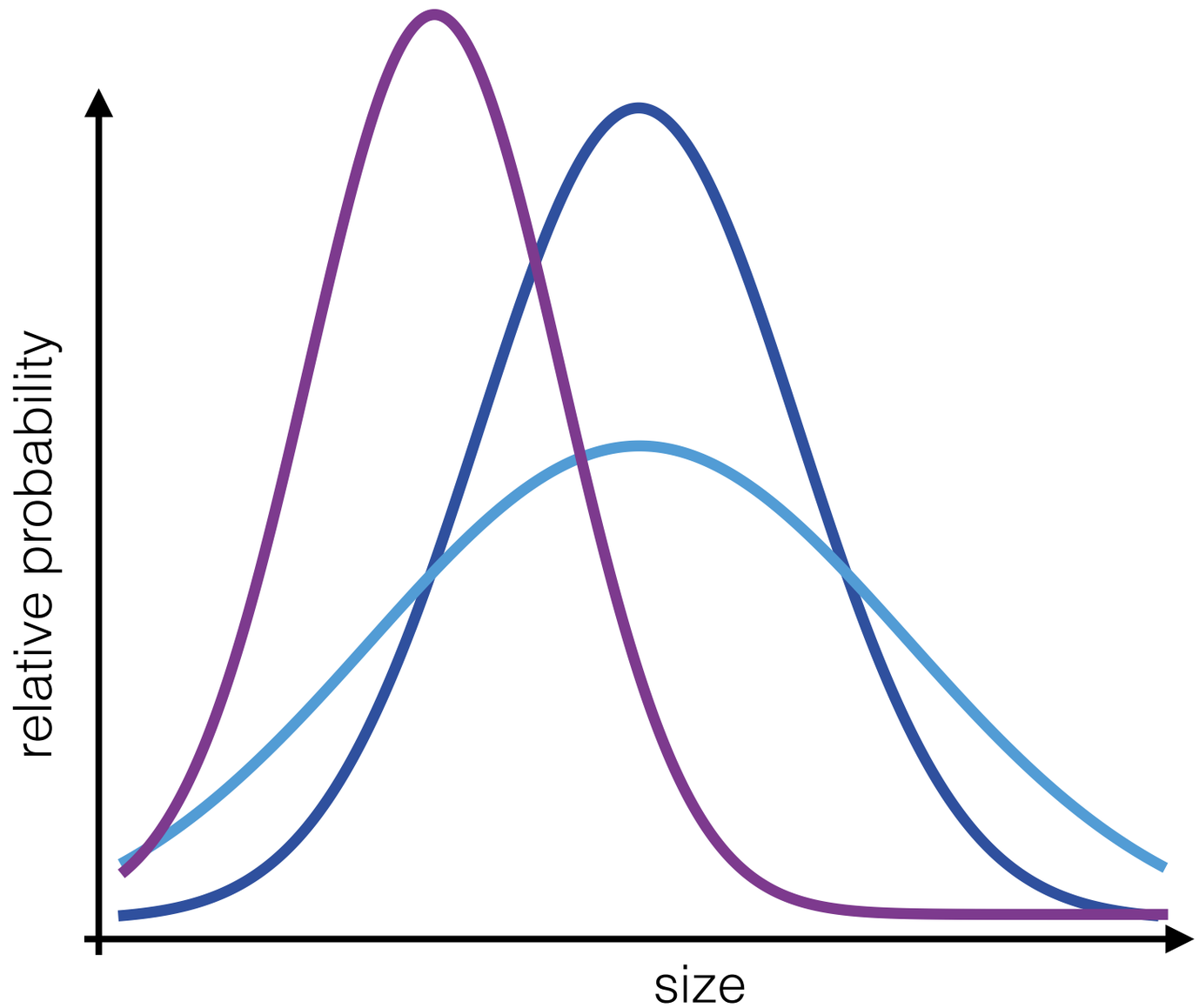


Probability of the data: $P(🐼|\mathcal{N})$

Probability of the data given the model, integrating all possible parameter values

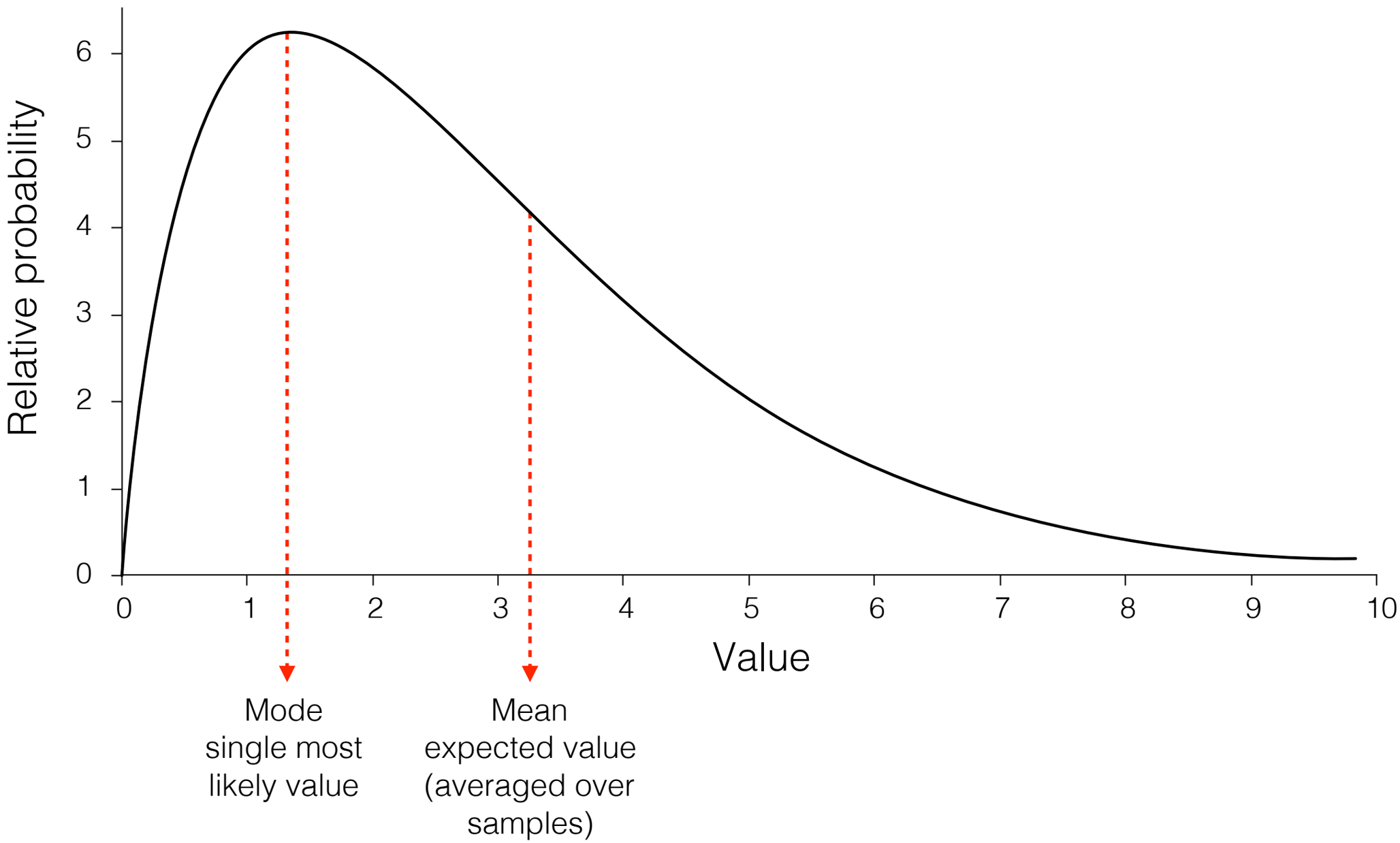
$$P(🐼|\mathcal{N}) = \text{constant}$$



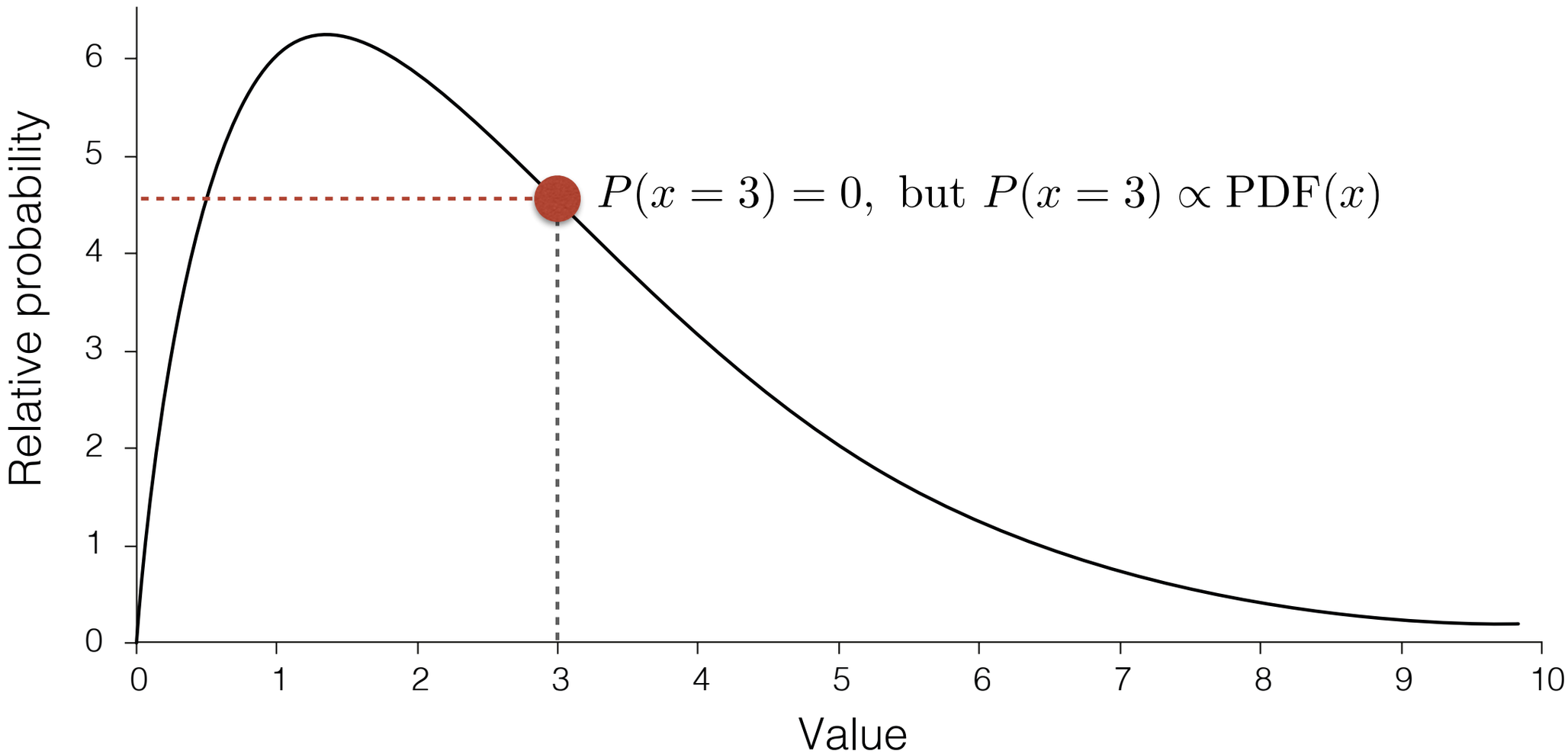


Probability density functions

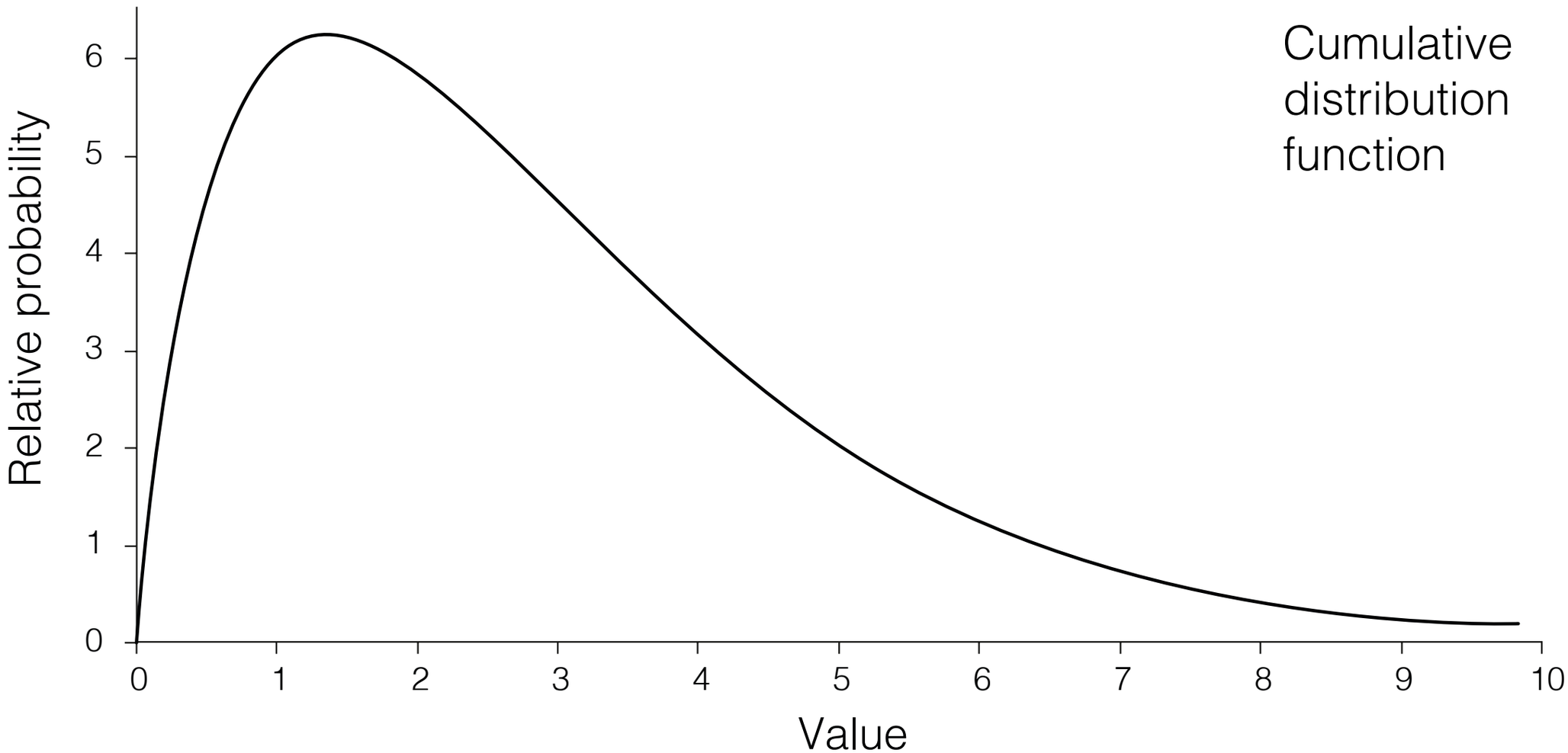
PDF $\neq$



Properties of a PDF



Properties of a PDF

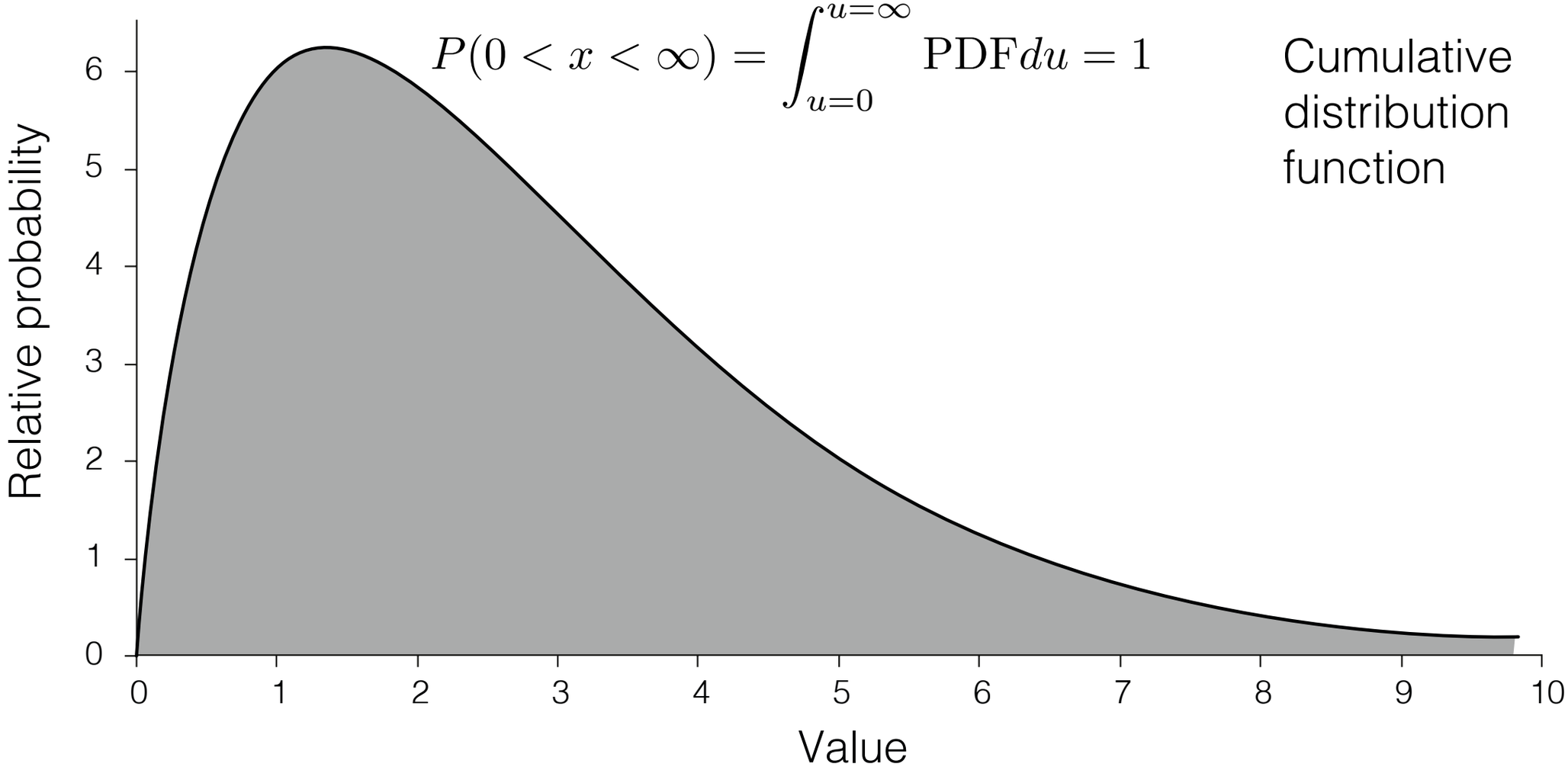


Cumulative distribution function

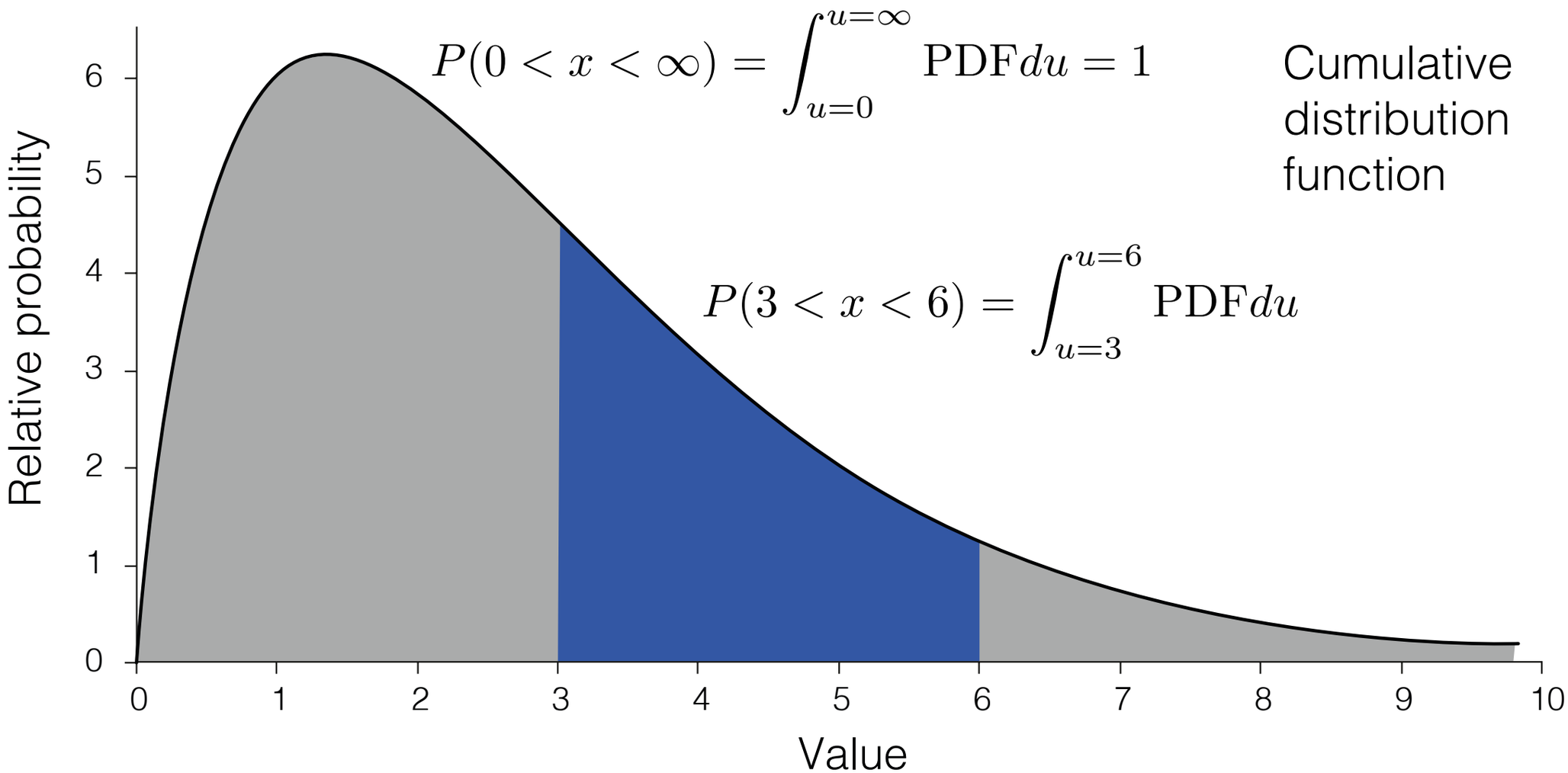
Properties of a PDF

$$P(0 < x < \infty) = \int_{u=0}^{u=\infty} \mathrm{PDF} du = 1$$

Cumulative distribution function



Properties of a PDF



Cumulative distribution function

Why using log-probabilities and log-likelihoods?

$P(A) = 0.25$

Why using log-probabilities and log-likelihoods?

P(A) = 0.25

P(ACGTT)= ?

Why using log-probabilities and log-likelihoods?

$$P(A) = 0.25$$

$$P(ACGTT) = P(A)P(C)P(G)P(T)P(T) = 0.001$$

Why using log-probabilities and log-likelihoods?

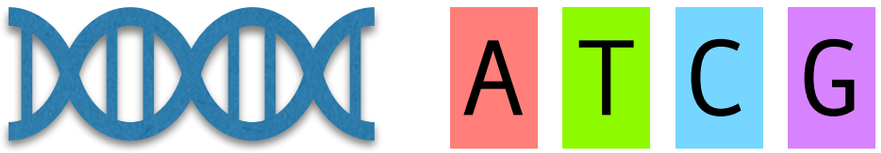
$P(A) = 0.25$

$P(ACGTT) = P(A)P(C)P(G)P(T)P(T) = 0.001$

$P($ $) = 0$

1,000 b

Why using log-probabilities and log-likelihoods?



$P(A) = 0.25$

$P(ACGTT) = P(A)P(C)P(G)P(T)P(T) = 0.001$

$P($ $) =$

1,000 b

Why using log-probabilities and log-likelihoods?

$P(A) = 0.25$

$P(ACGTT) = P(A)P(C)P(G)P(T)P(T) = 0.001$

$P($ $) =$

1,000 b

$\log P($ $) = ?$

1,000 b

Why using log-probabilities and log-likelihoods?

P(A) = 0.25

P(ACGTT) = P(A)P(C)P(G)P(T)P(T) = 0.001

P( ) =

1,000 b

logP( ) = -1386

1,000 b

Exercise: log-transform these operations

```
a+b
a-b
a*b
a/b
sqrt(a)
a^b
a!
exp(a)
```

Exercise: log-transform these operations

`a+b`	`log(a+b)`
`a-b`	`log(a-b)`
`a*b`	`log(a) + log(b)`
`a/b`	`log(a) - log(b)`
`sqrt(a)`	`0.5 * log(a)`
`a^b`	`b * log(a)`
`a!`	`sum(log(range(1,a)))`
`exp(a)`	`a`

Bayesian inference

Likelihood Prior probability

Posterior probability

$$P(\alpha|x, M) = \frac{P(x|\alpha, M) \times P(\alpha|M)}{P(x|M)}$$

Probability of the data

Bayesian inference

Likelihood Prior probability

Posterior probability

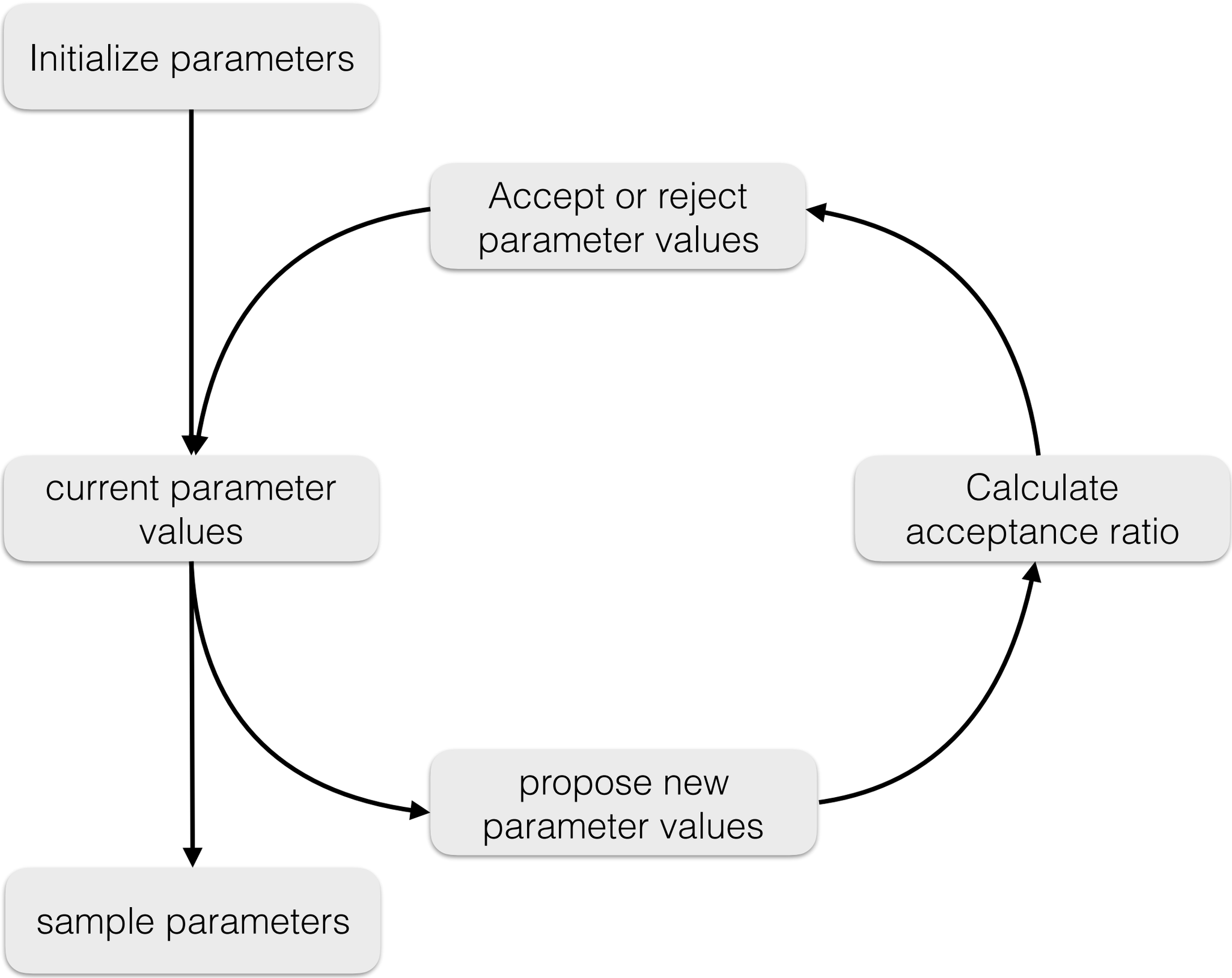
$$P(\alpha|x, M) = \frac{P(x|\alpha, M) \times P(\alpha|M)}{P(x|M)}$$

Probability of the data

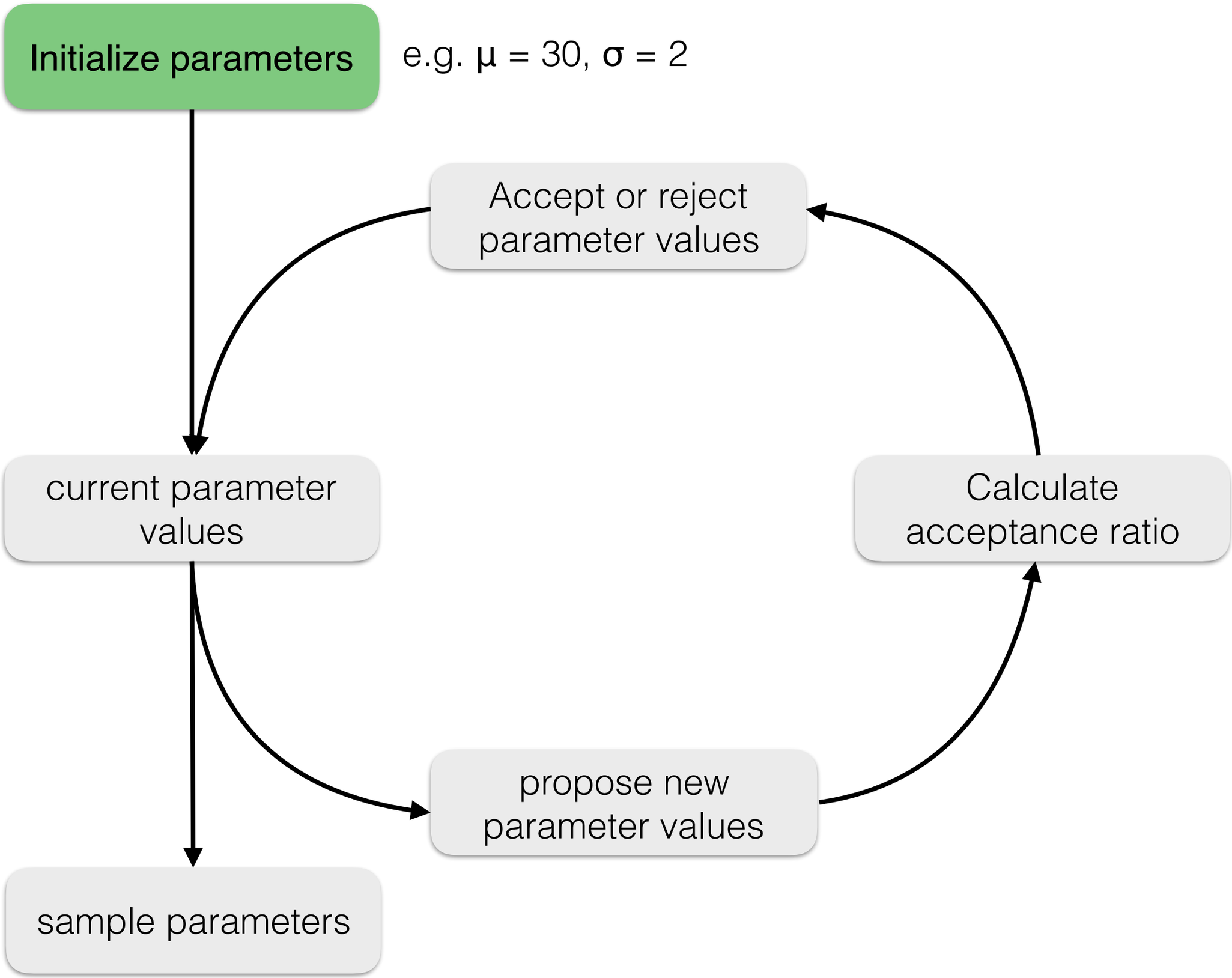
$$P(\alpha|x, M) \propto P(x|\alpha, M) \times P(\alpha|M)$$

Posterior probability is proportional to the product of likelihood and prior

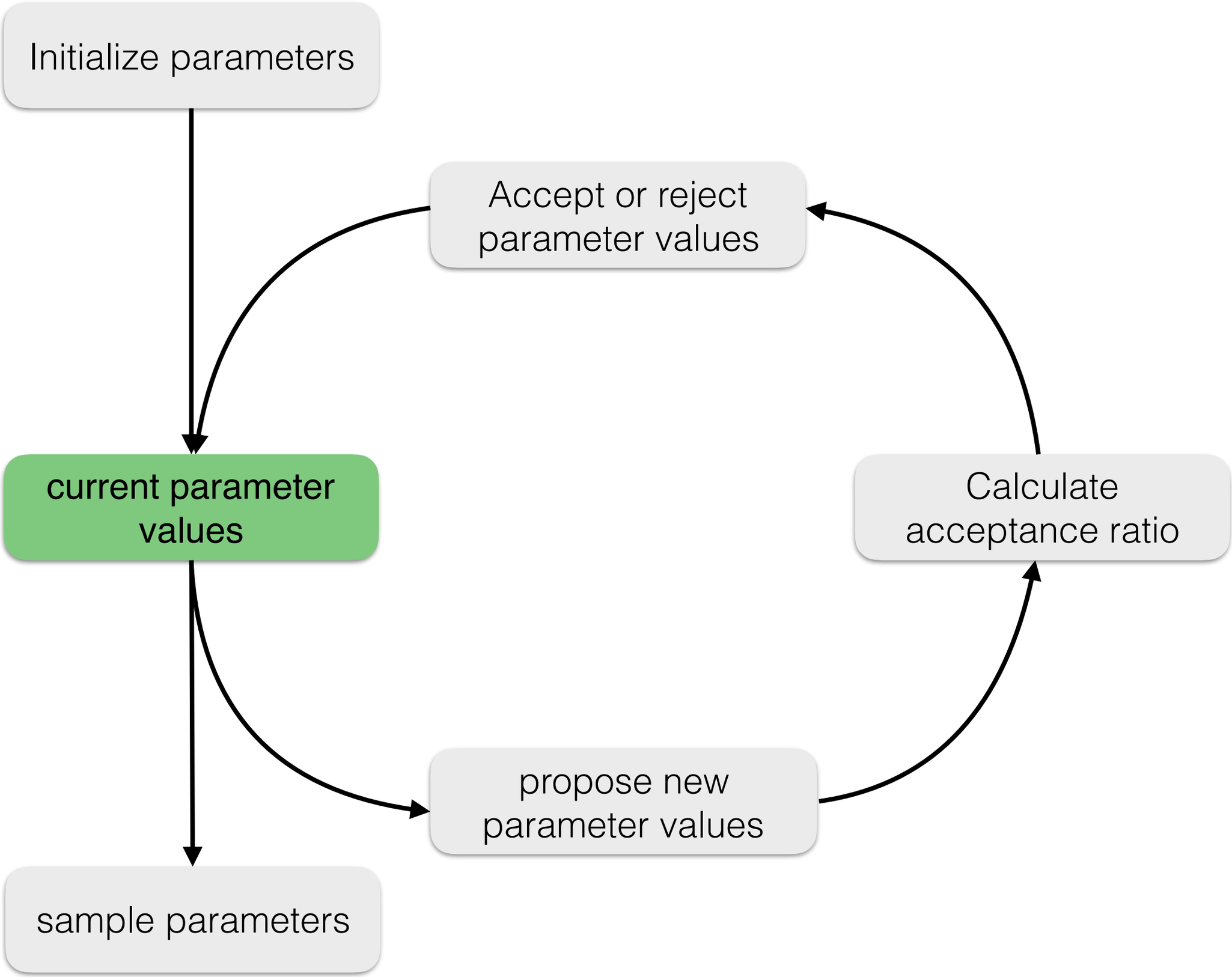
Metropolis-Hastings MCMC



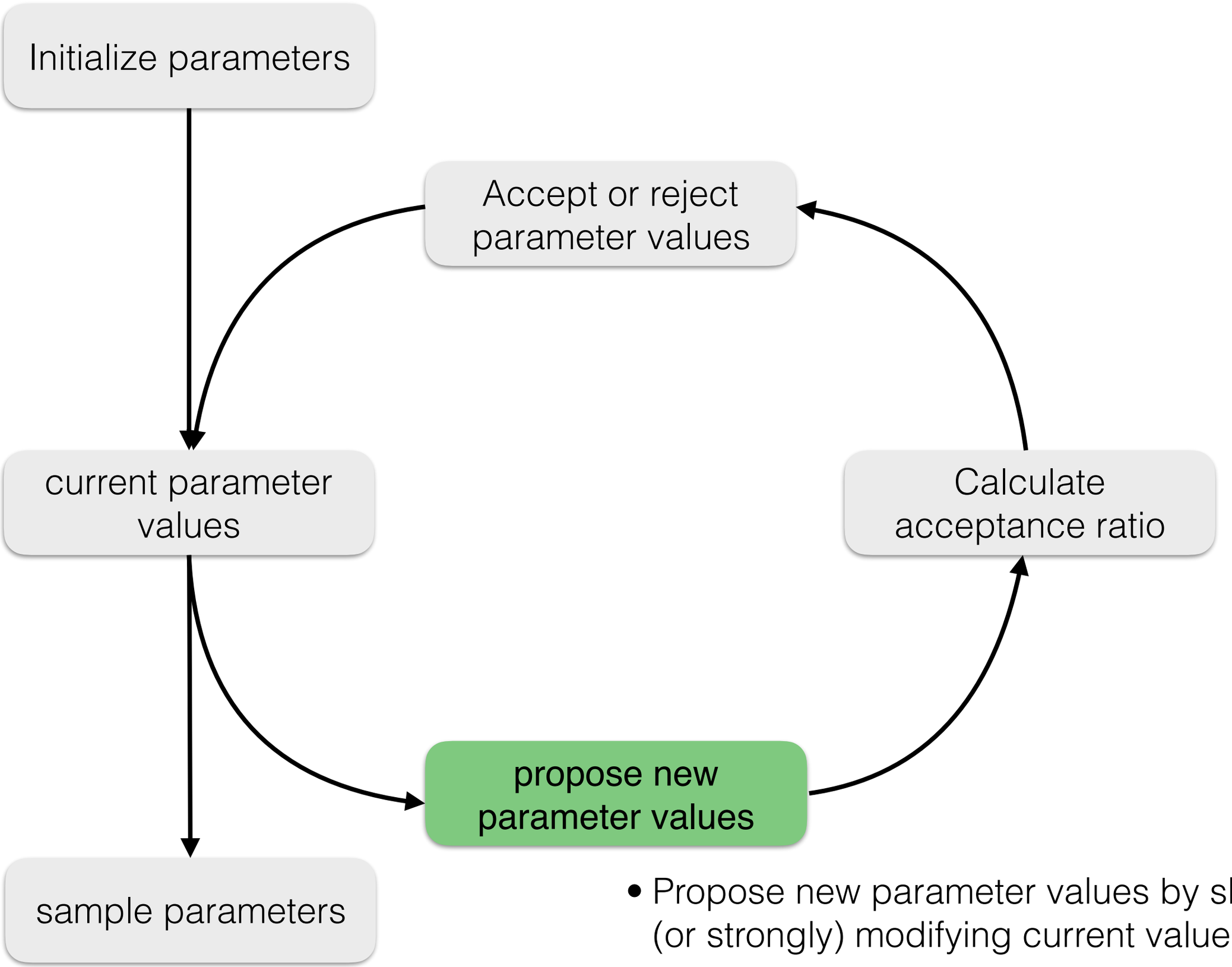
Metropolis-Hastings MCMC



Metropolis-Hastings MCMC



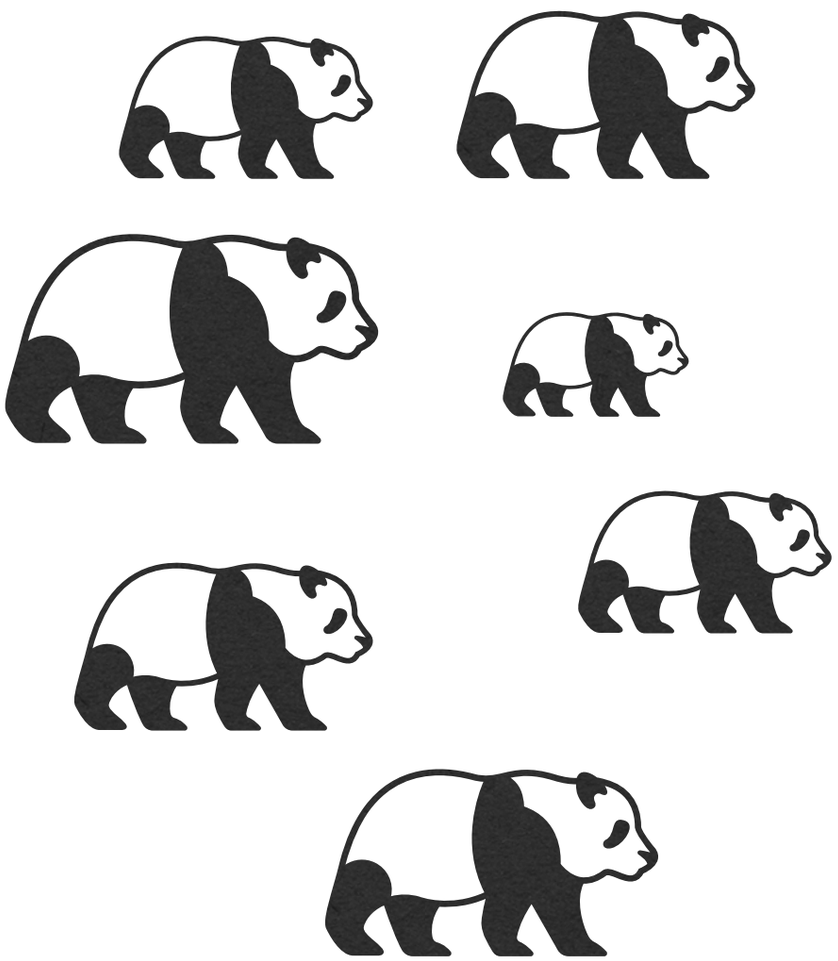
Metropolis-Hastings MCMC

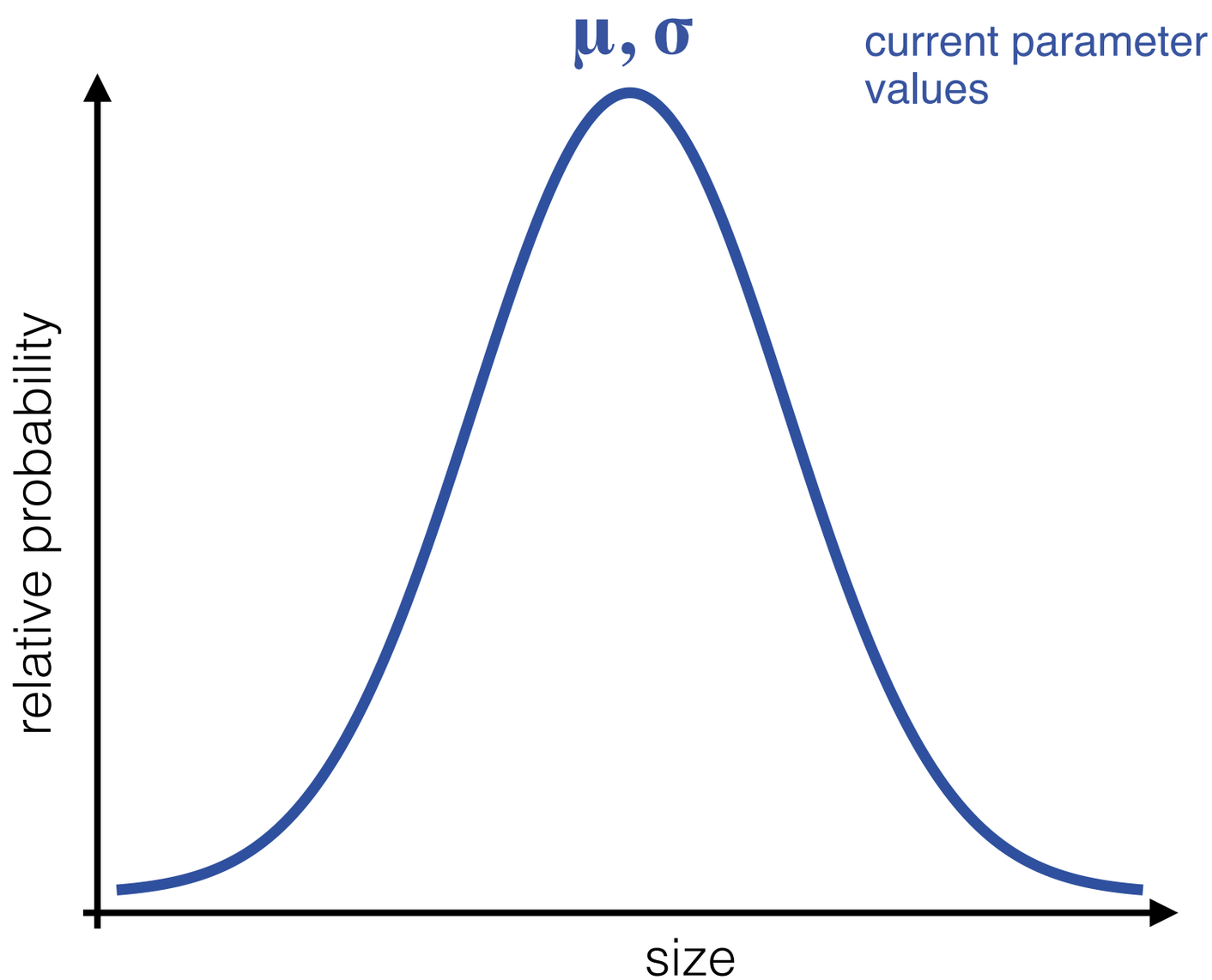


- Propose new parameter values by slightly (or strongly) modifying current values

Propose new parameter values

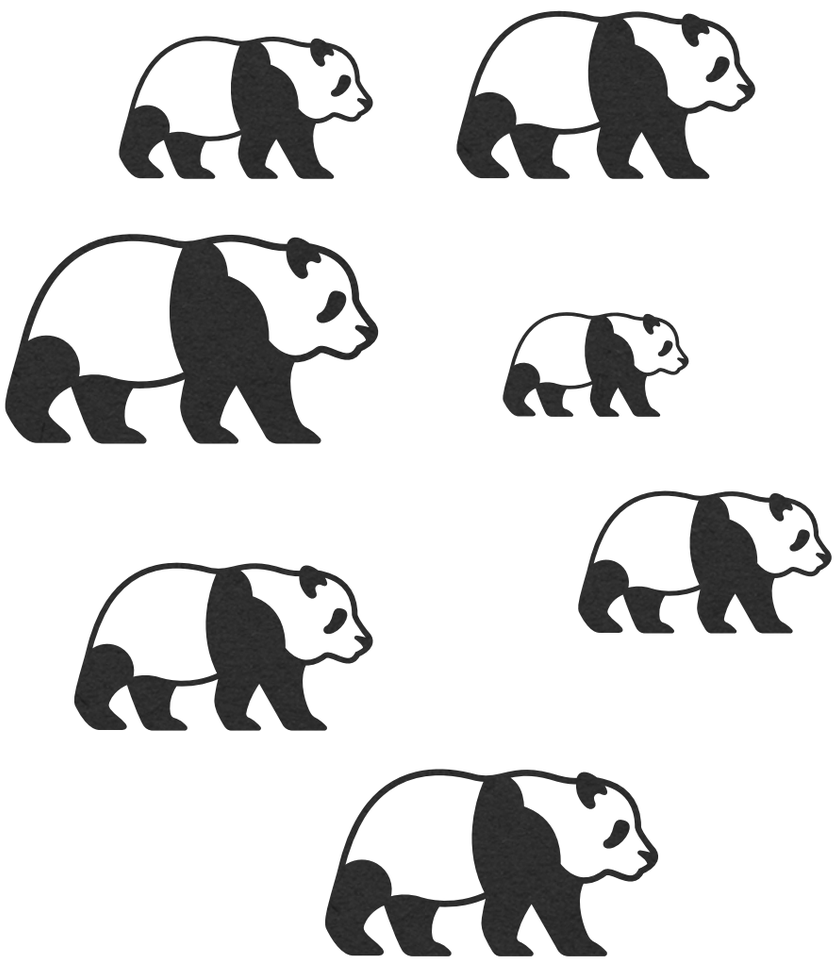
E.g. propose a new standard deviation

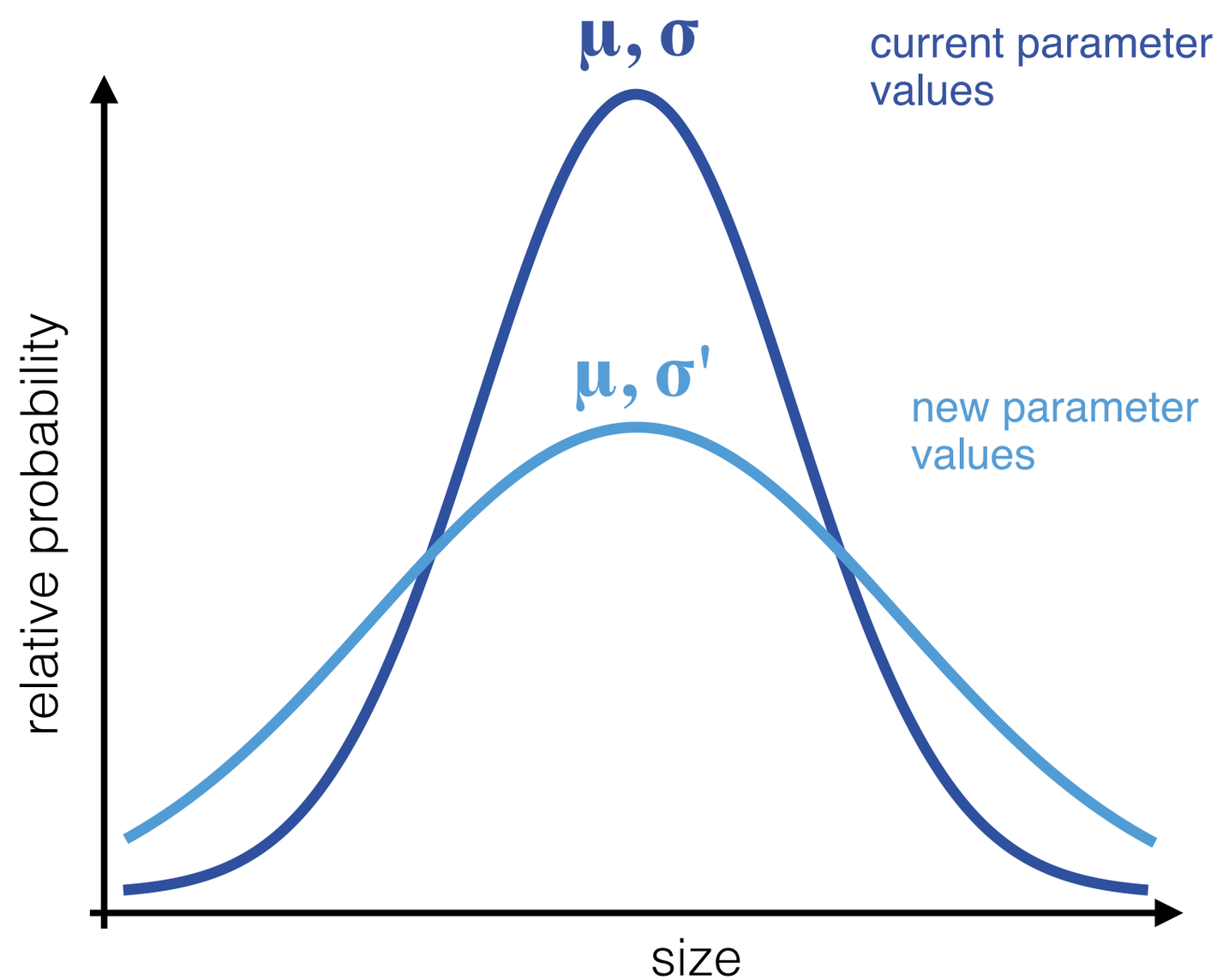




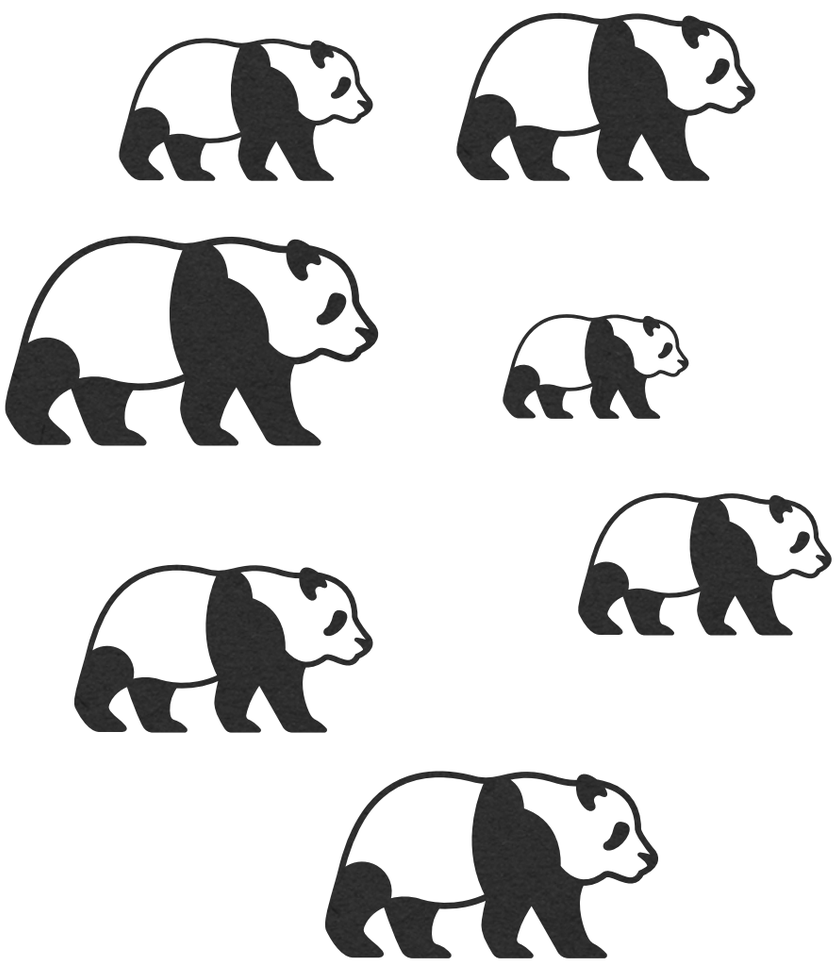
Propose new parameter values

E.g. propose a new standard deviation

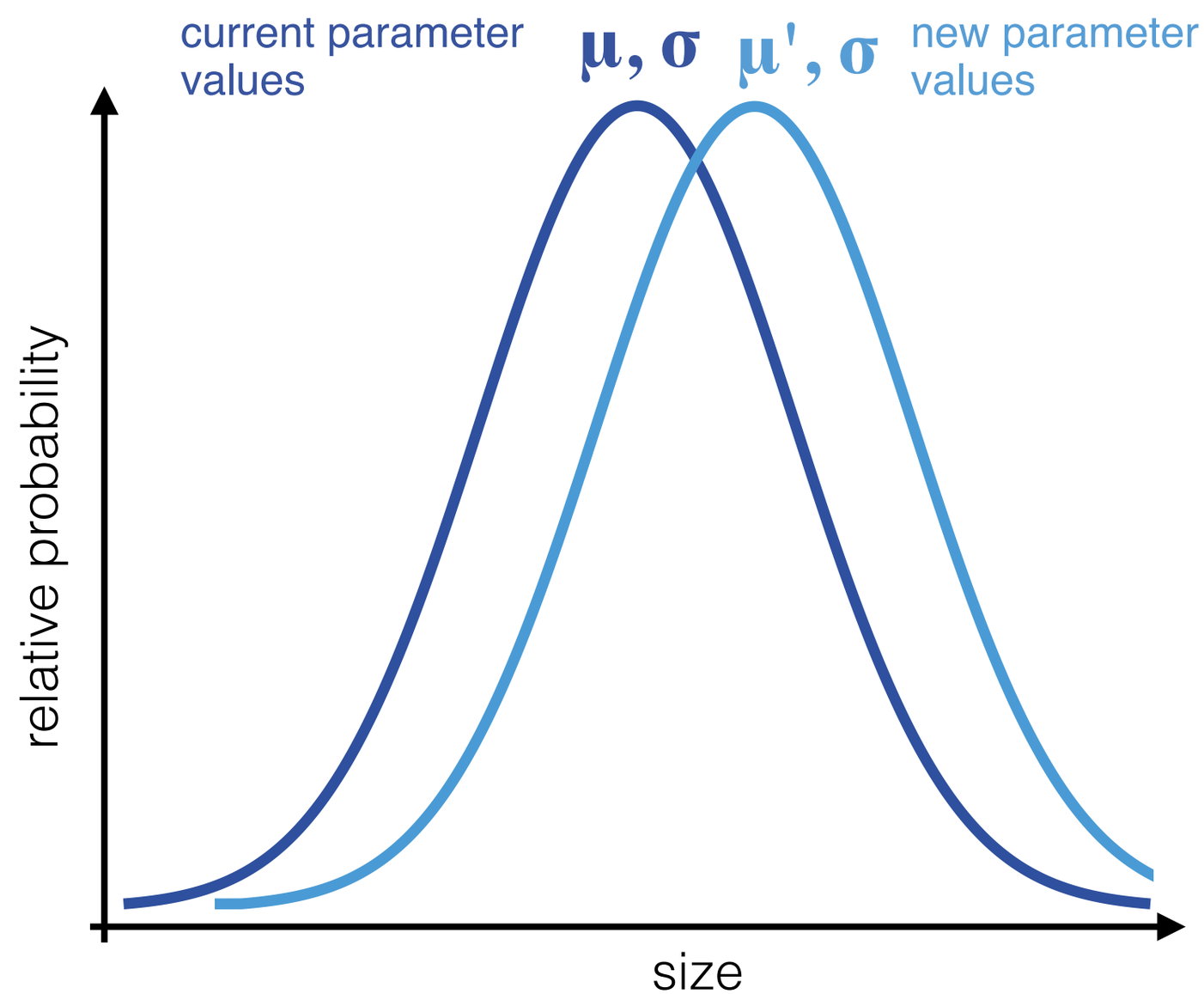




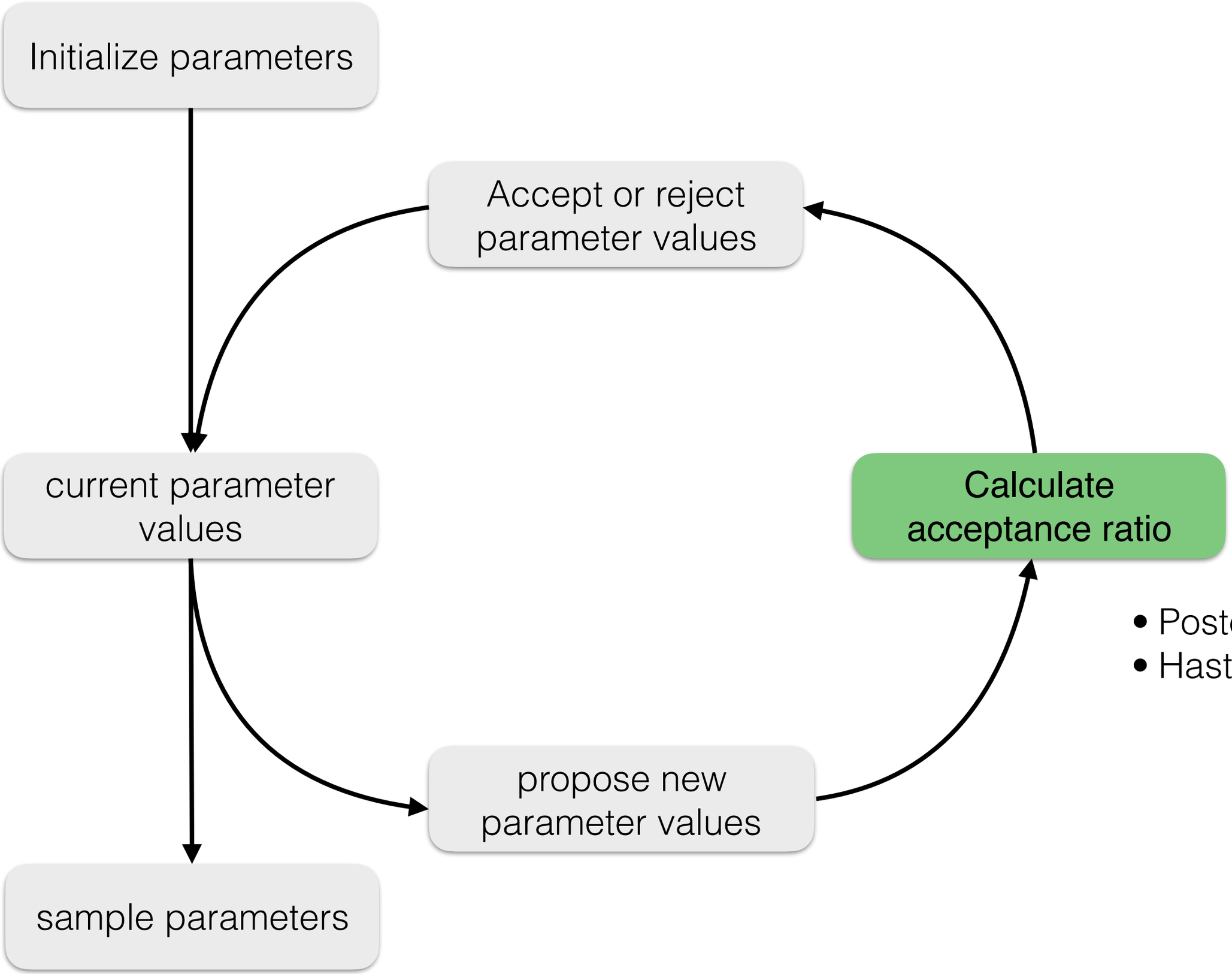
Propose new parameter values



E.g. propose a new mean



Metropolis-Hastings MCMC



- Posterior ratio
- Hastings ratio

Acceptance ratio

Comparing the new state against the old state

Posterior ratio

$$\frac{P(\alpha'|x, M)}{P(\alpha|x, M)}$$

Hastings ratio

Acceptance ratio

Comparing the new state against the old state

Posterior ratio

$$\frac{P(\alpha'|x,M)}{P(\alpha|x,M)} = \frac{\dfrac{P(x|\alpha',M)\times P(\alpha'|M)}{P(x|M)}}{\dfrac{P(x|\alpha,M)\times P(\alpha|M)}{P(x|M)}}$$

Hastings ratio

Acceptance ratio

Comparing the new state against the old state

Posterior ratio

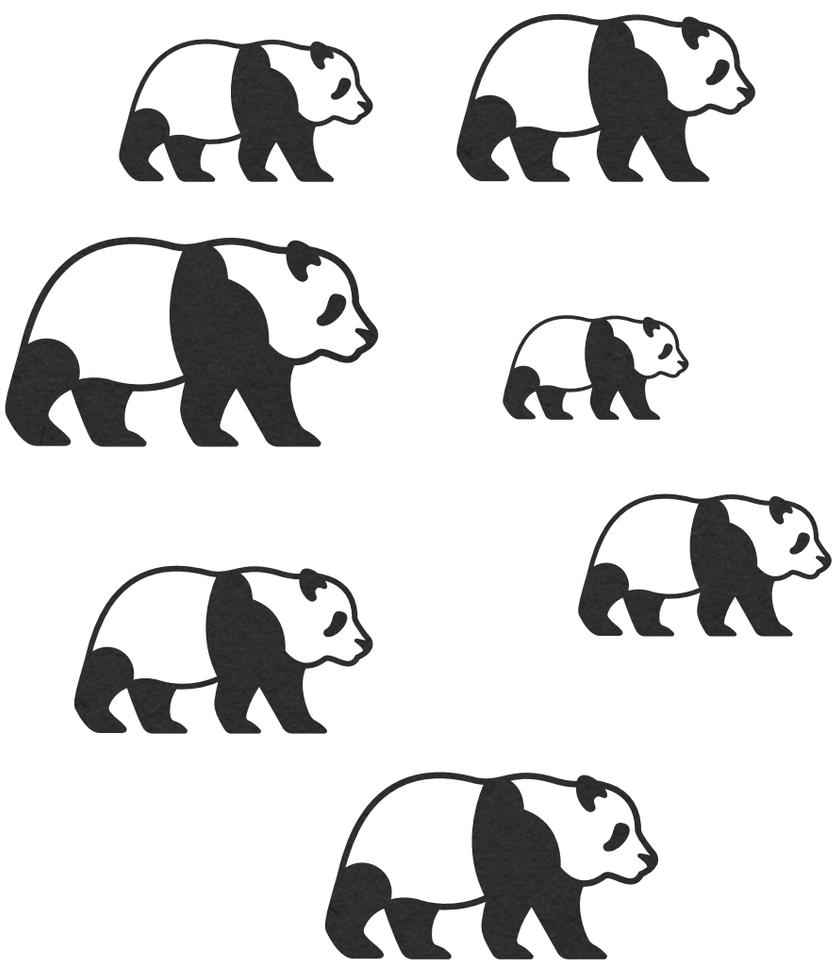
$$\frac{P(\alpha'|x,M)}{P(\alpha|x,M)} = \frac{\dfrac{P(x|\alpha',M)\times P(\alpha'|M)}{P(x|M)}}{\dfrac{P(x|\alpha,M)\times P(\alpha|M)}{P(x|M)}}$$

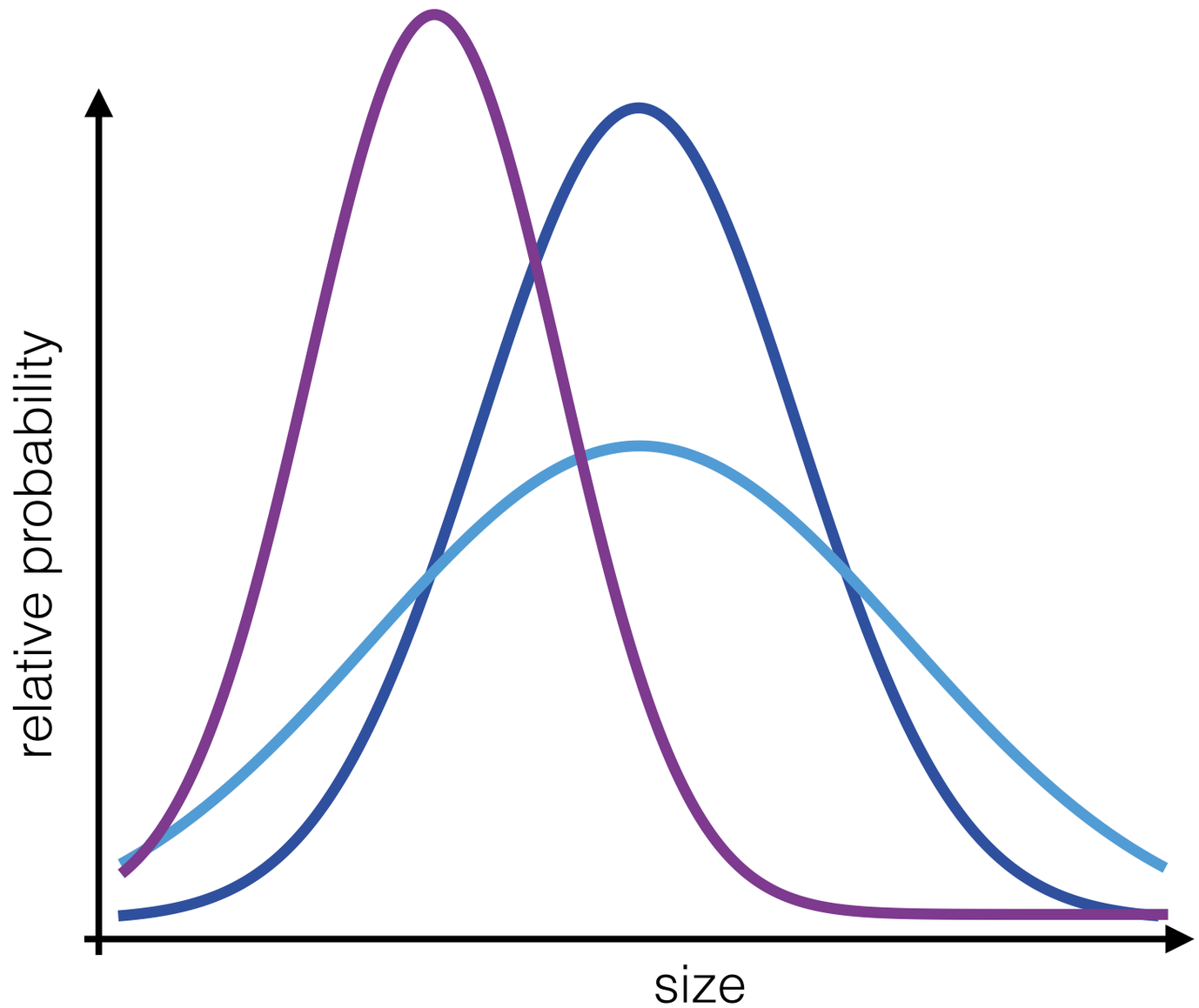
Hastings ratio

Probability of the data: $P(🐼|\mathcal{N})$

Probability of the data given the model

$$P(🐼|\mathcal{N}) = \text{constant}$$





Acceptance ratio

Comparing the new state against the old state

Posterior ratio

$$\frac{P(\alpha'|x,M)}{P(\alpha|x,M)} = \frac{\dfrac{P(x|\alpha',M)\times P(\alpha'|M)}{\cancel{P(x|M)}}}{\dfrac{P(x|\alpha,M)\times P(\alpha|M)}{\cancel{P(x|M)}}}$$

Hastings ratio

Acceptance ratio

Comparing the new state against the old state

Posterior ratio

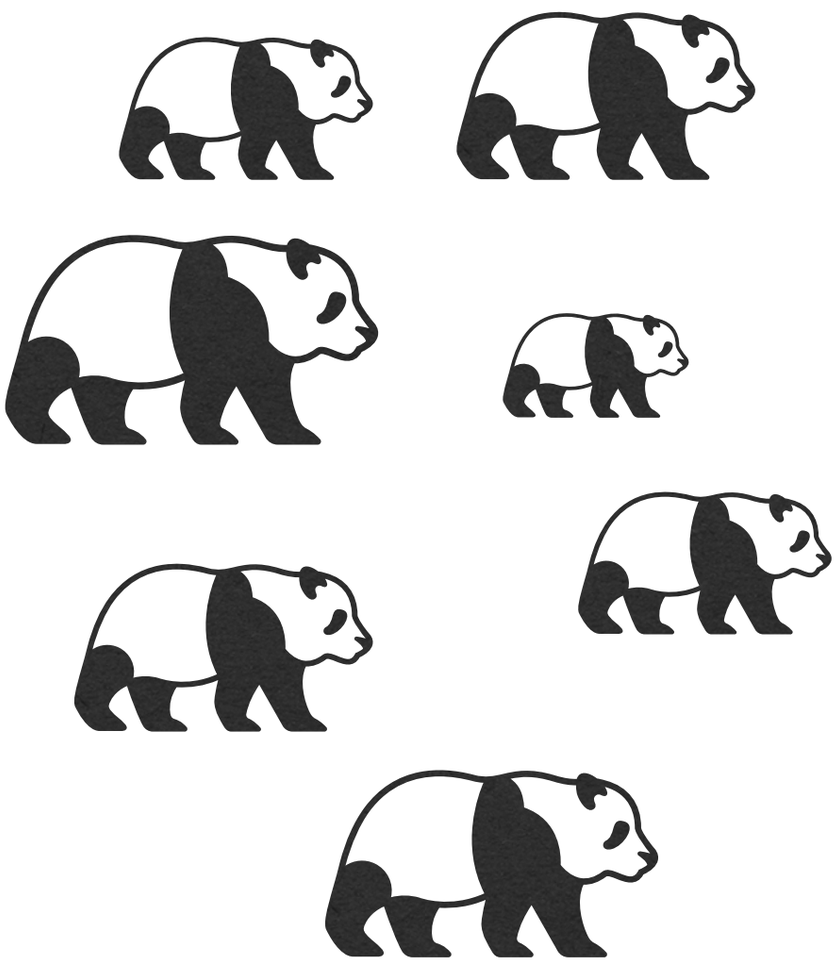
$$\frac{P(\alpha'|x,M)}{P(\alpha|x,M)} = \frac{\dfrac{P(x|\alpha',M)\times P(\alpha'|M)}{\cancel{P(x|M)}}}{\dfrac{P(x|\alpha,M)\times P(\alpha|M)}{\cancel{P(x|M)}}} = \underbrace{\frac{P(x|\alpha',M)}{P(x|\alpha,M)}}_{\text{Likelihood ratio}} \times \underbrace{\frac{P(\alpha'|M)}{P(\alpha|M)}}_{\text{Prior ratio}}$$

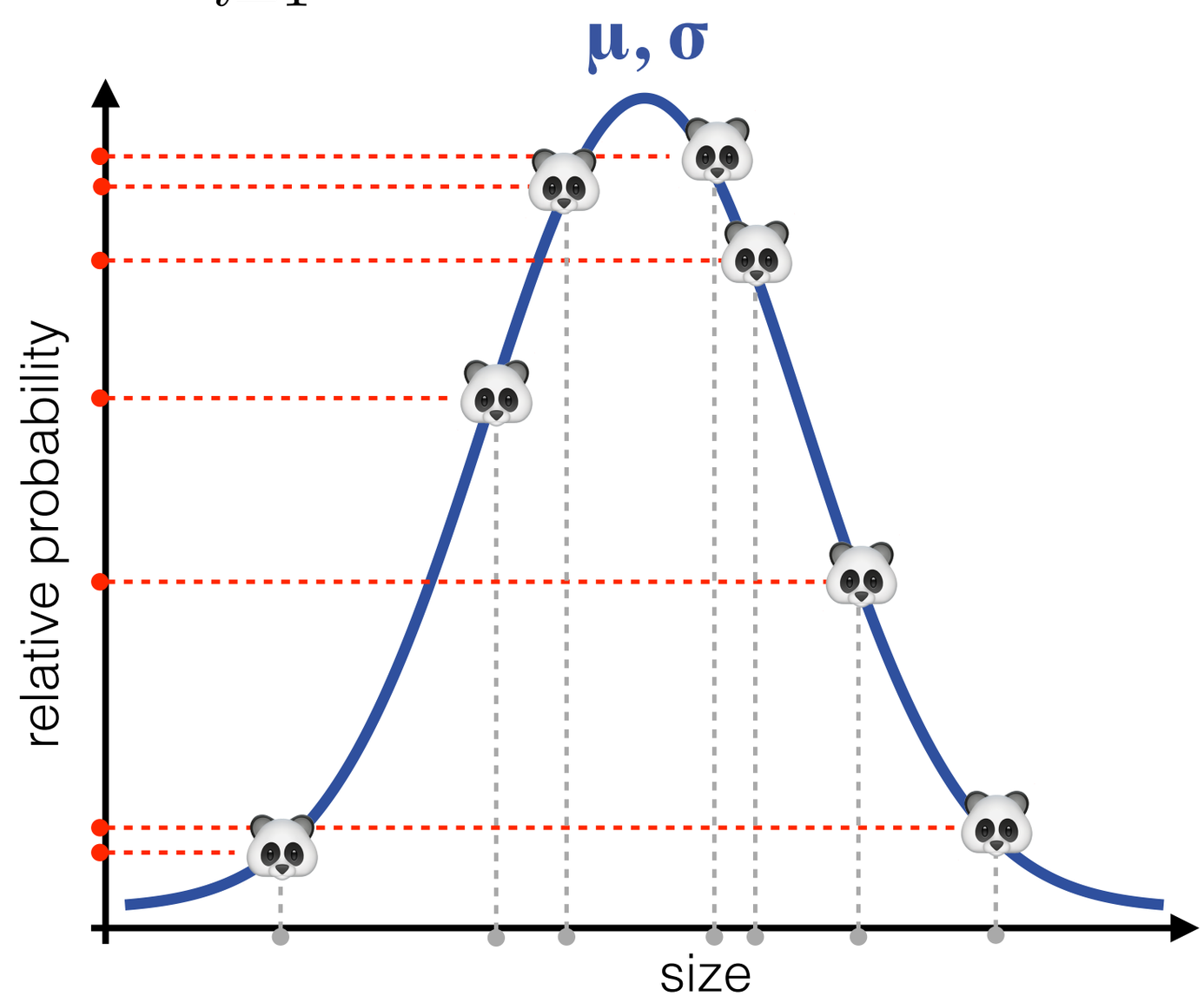
Hastings ratio

Calculating the likelihood: $P(🐼|\mu, \sigma, \mathcal{N})$

Likelihood: probability of observing the data you observe given a model and its parameters

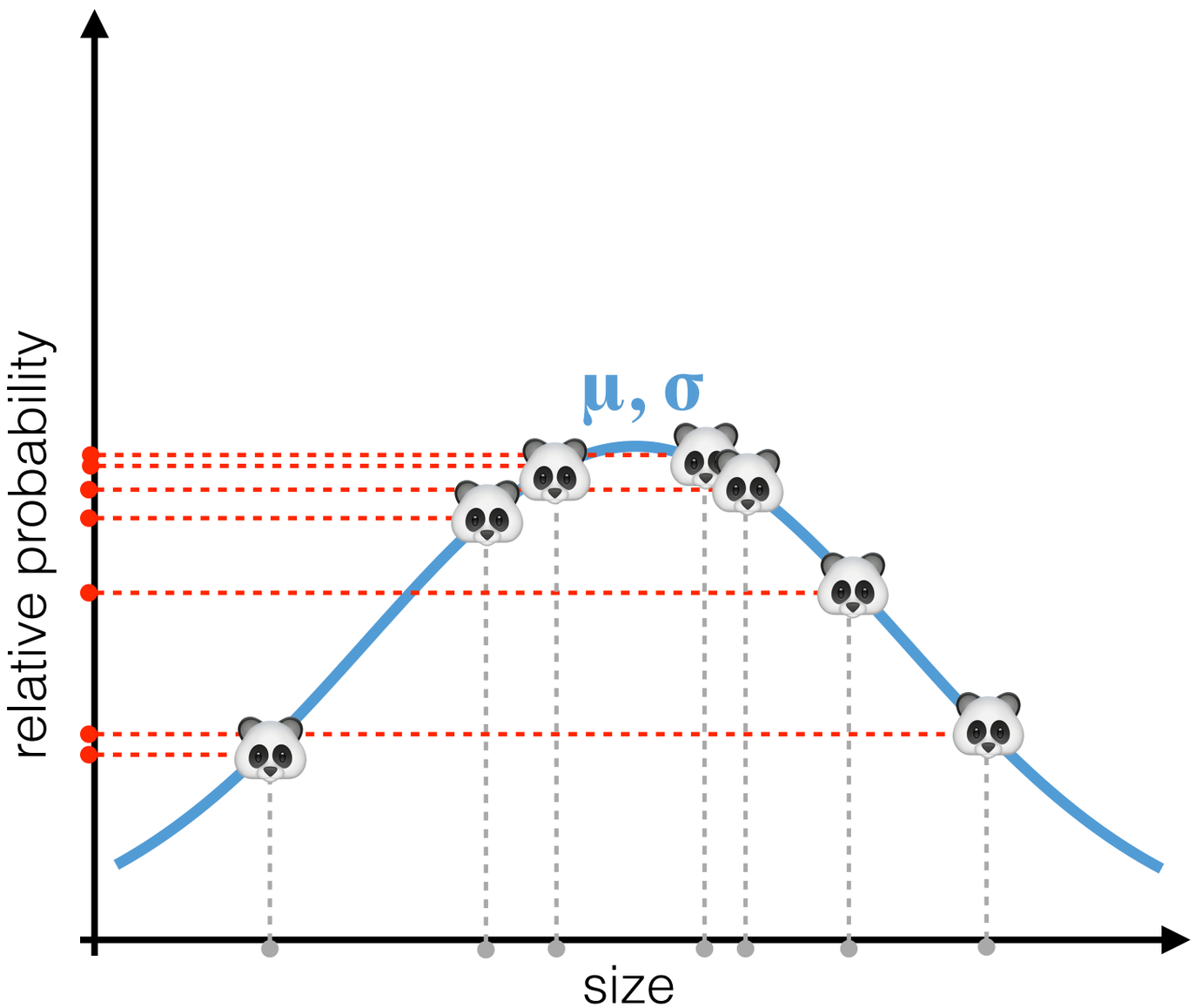
$$P(🐼_1, ..., 🐼_7|\mu, \sigma, \mathcal{N}) = \prod_{i=1}^{7} P(🐼_i|\mu, \sigma, \mathcal{N})$$



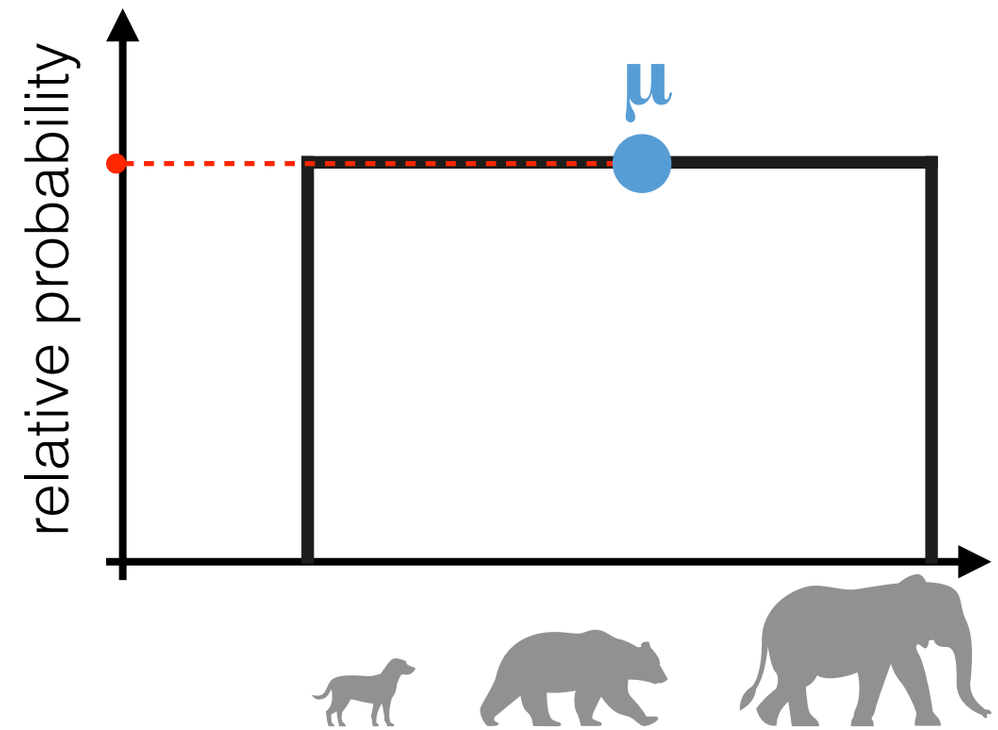


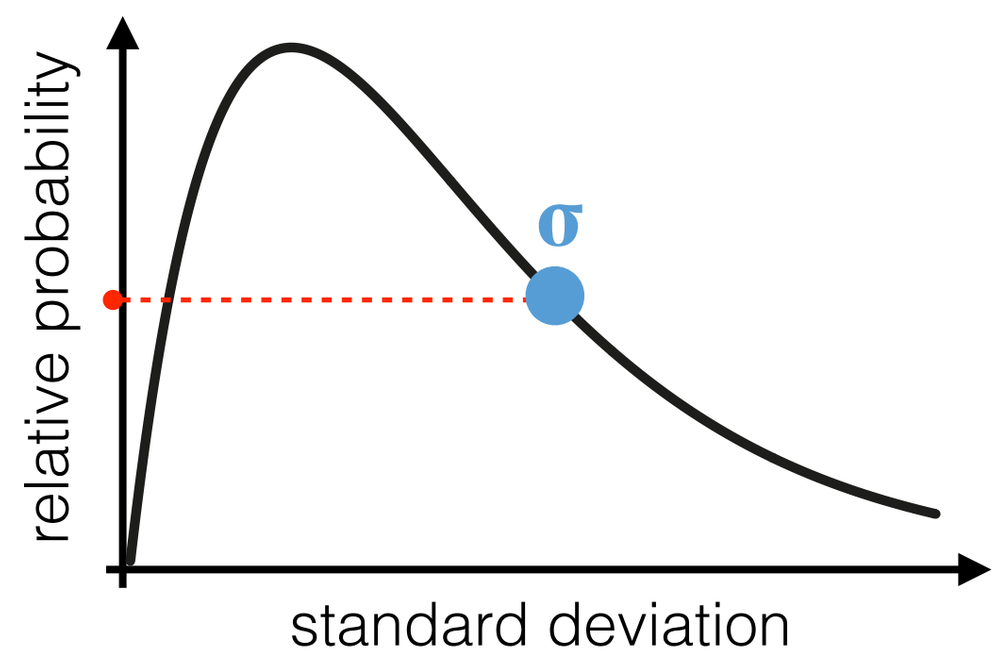
Calculating the posterior: $P(\mu, \sigma | 🐼, \mathcal{N})$

Likelihood



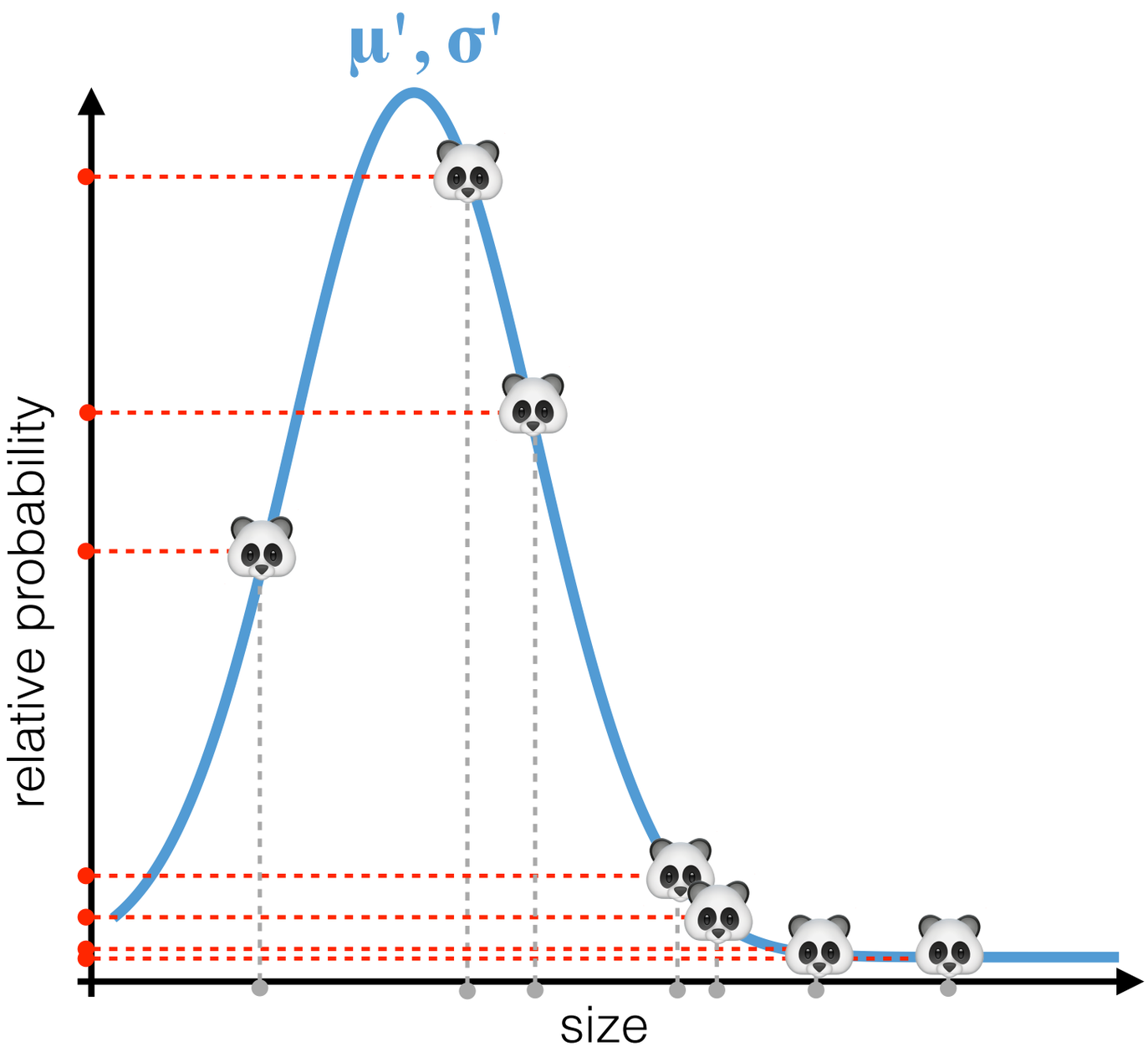
Priors



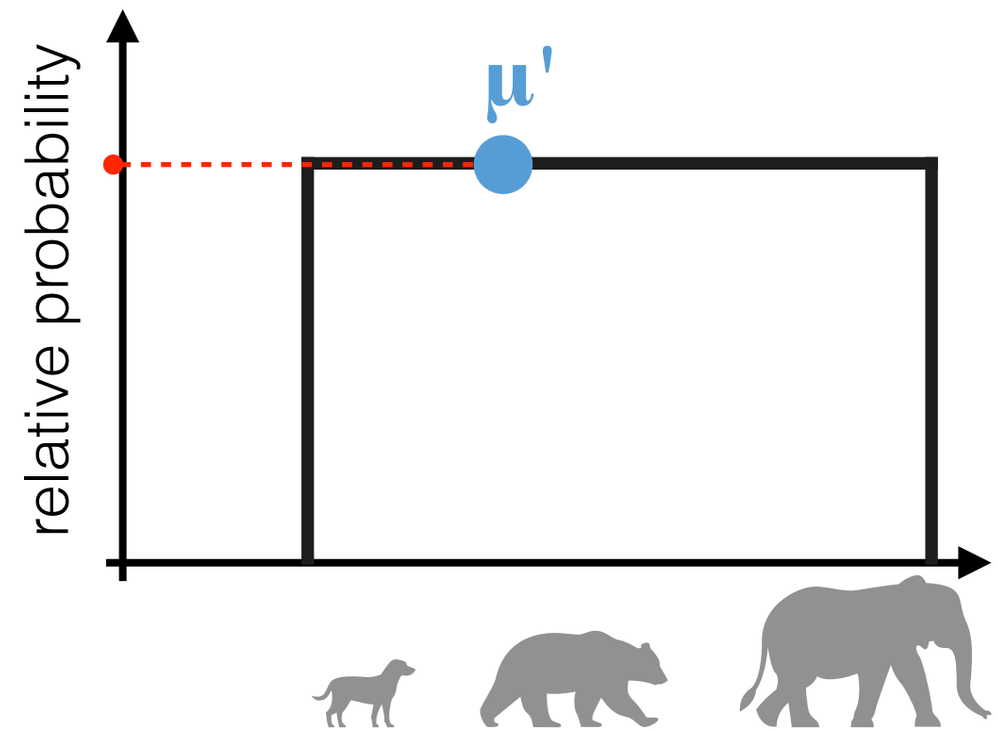


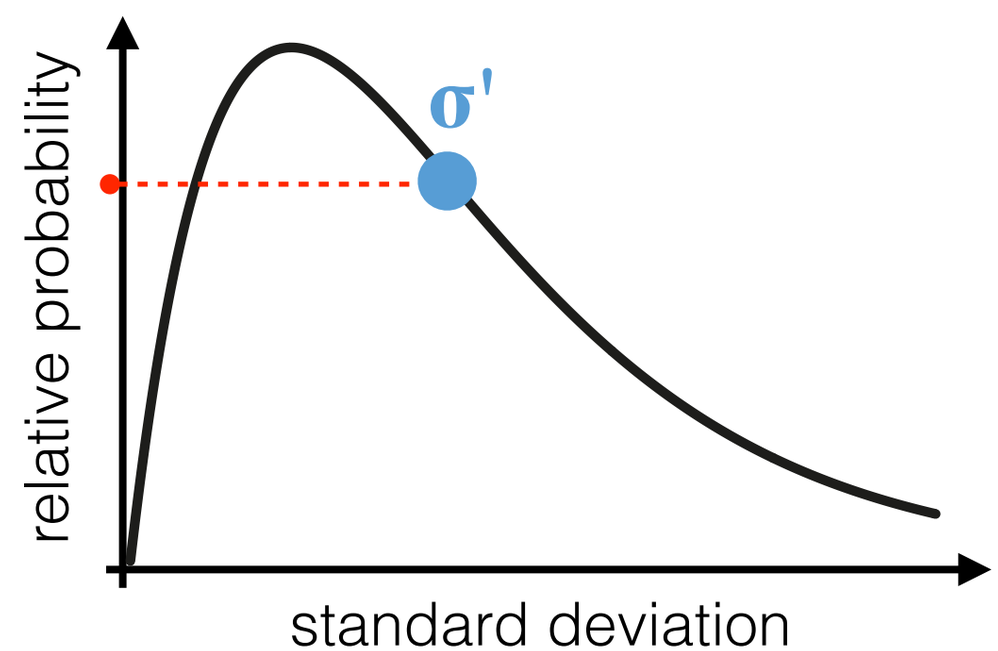
Calculating the posterior: $P(\mu', \sigma' | 🐼, \mathcal{N})$

Likelihood



Priors





Acceptance ratio

Comparing the new state against the old state

Posterior ratio

$$\frac{P(\alpha'|x,M)}{P(\alpha|x,M)} = \underbrace{\frac{P(x|\alpha',M)}{P(x|\alpha,M)}}_{\text{Likelihood ratio}} \times \underbrace{\frac{P(\alpha'|M)}{P(\alpha|M)}}_{\text{Prior ratio}}$$

Hastings ratio

$$\frac{P(\alpha|\alpha')}{P(\alpha'|\alpha)}$$

Probability of going back to previous state

Probability of proposing new state from previous

Acceptance ratio

Comparing the new state against the old state

Posterior ratio

$$\frac{P(\alpha'|x,M)}{P(\alpha|x,M)} = \underbrace{\frac{P(x|\alpha',M)}{P(x|\alpha,M)}}_{\text{Likelihood ratio}} \times \underbrace{\frac{P(\alpha'|M)}{P(\alpha|M)}}_{\text{Prior ratio}}$$

Hastings ratio

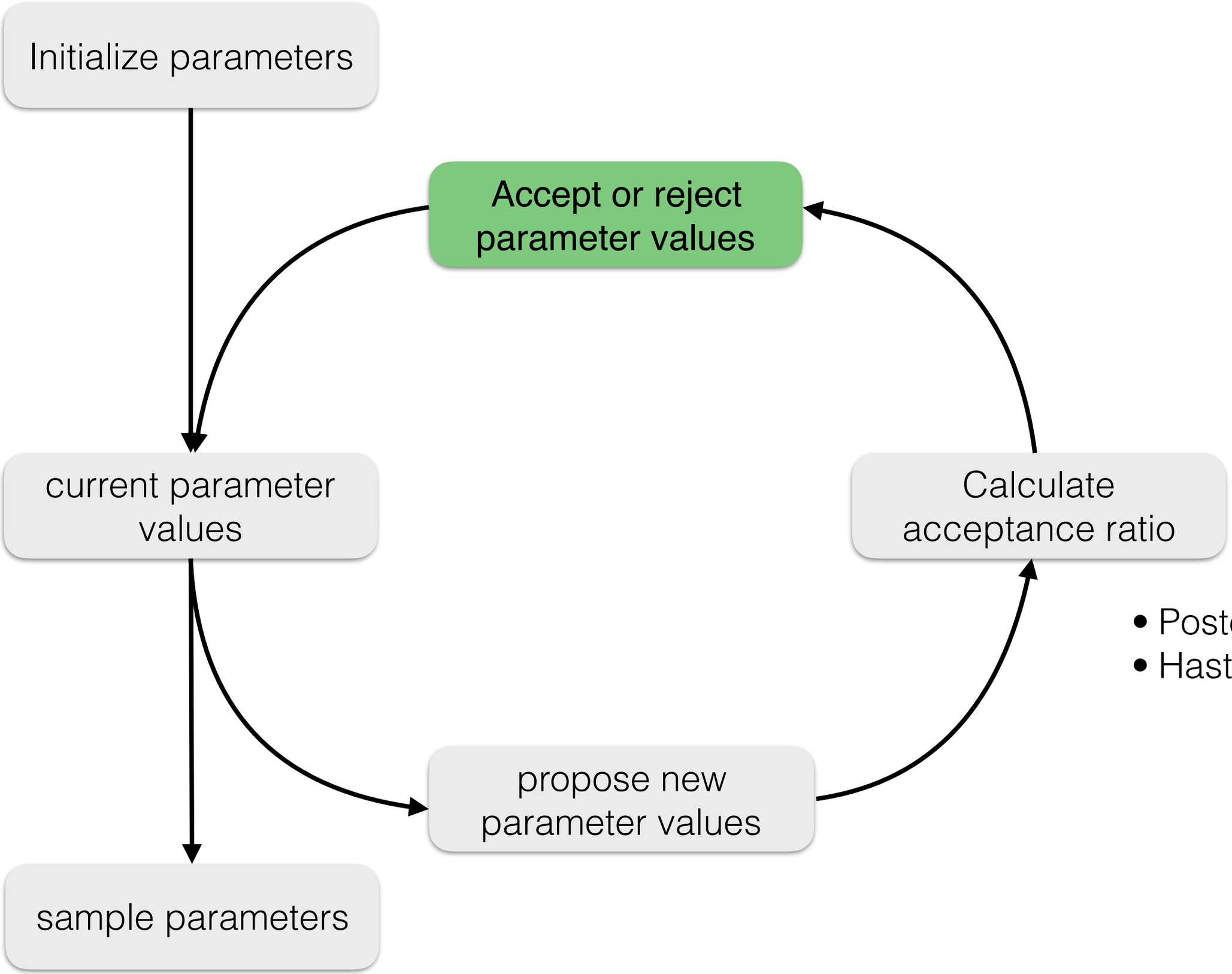
$$\frac{\cancel{P(\alpha|\alpha')}}{\cancel{P(\alpha'|\alpha)}}$$

Probability of going back to previous state

Probability of proposing new state from previous

For now let's assume it's constant (it is in most cases)

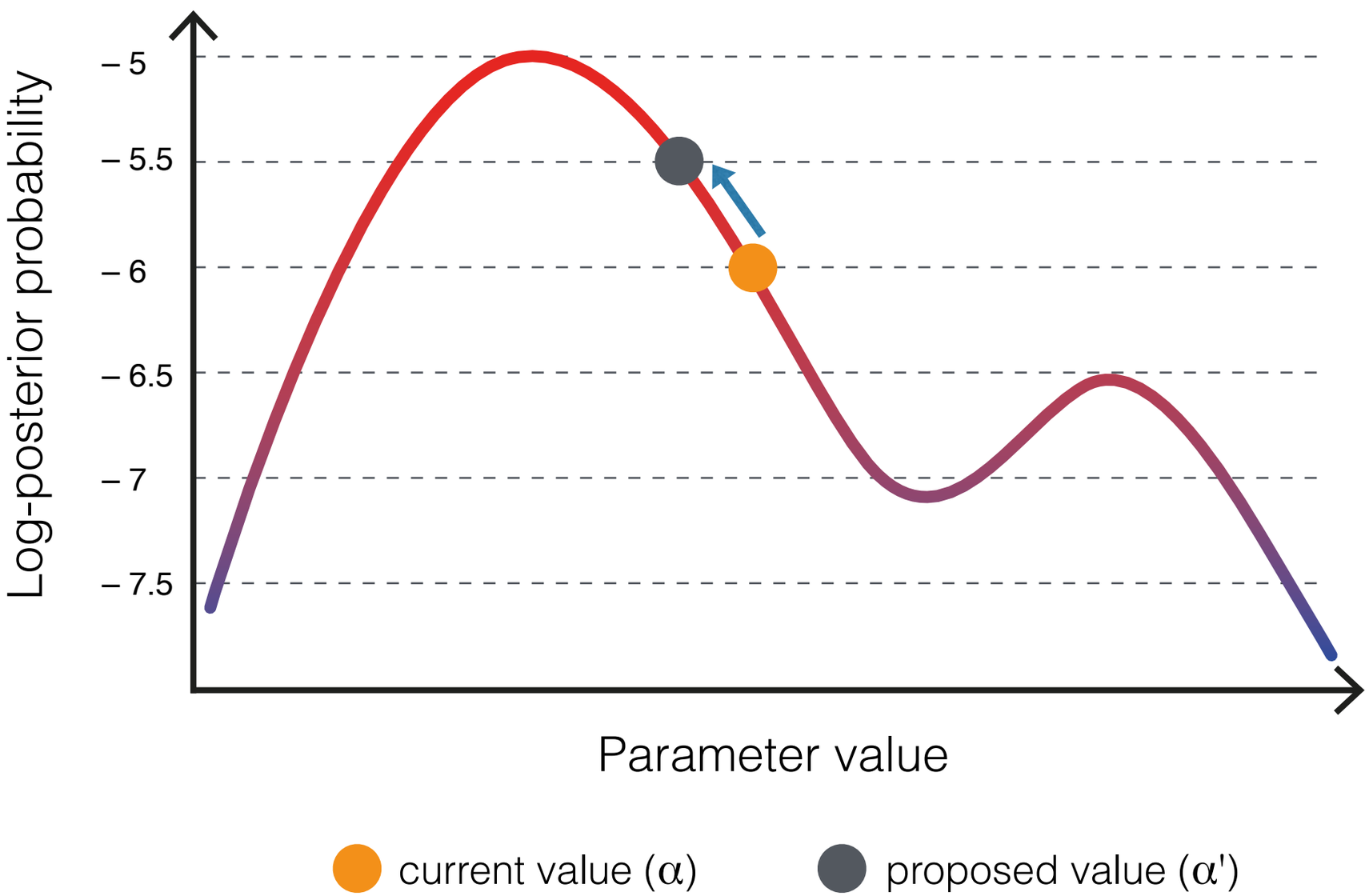
Metropolis-Hastings MCMC



- Posterior ratio
- Hastings ratio

Acceptance probability

$$r = \min\left\{1, \underbrace{\frac{P(\alpha'|x,M)}{P(\alpha|x,M)}}_{\text{Posterior ratio}} \times \underbrace{\frac{\cancel{P(\alpha|\alpha')}}{\cancel{P(\alpha'|\alpha)}}}_{\text{Hastings ratio}}\right\}$$

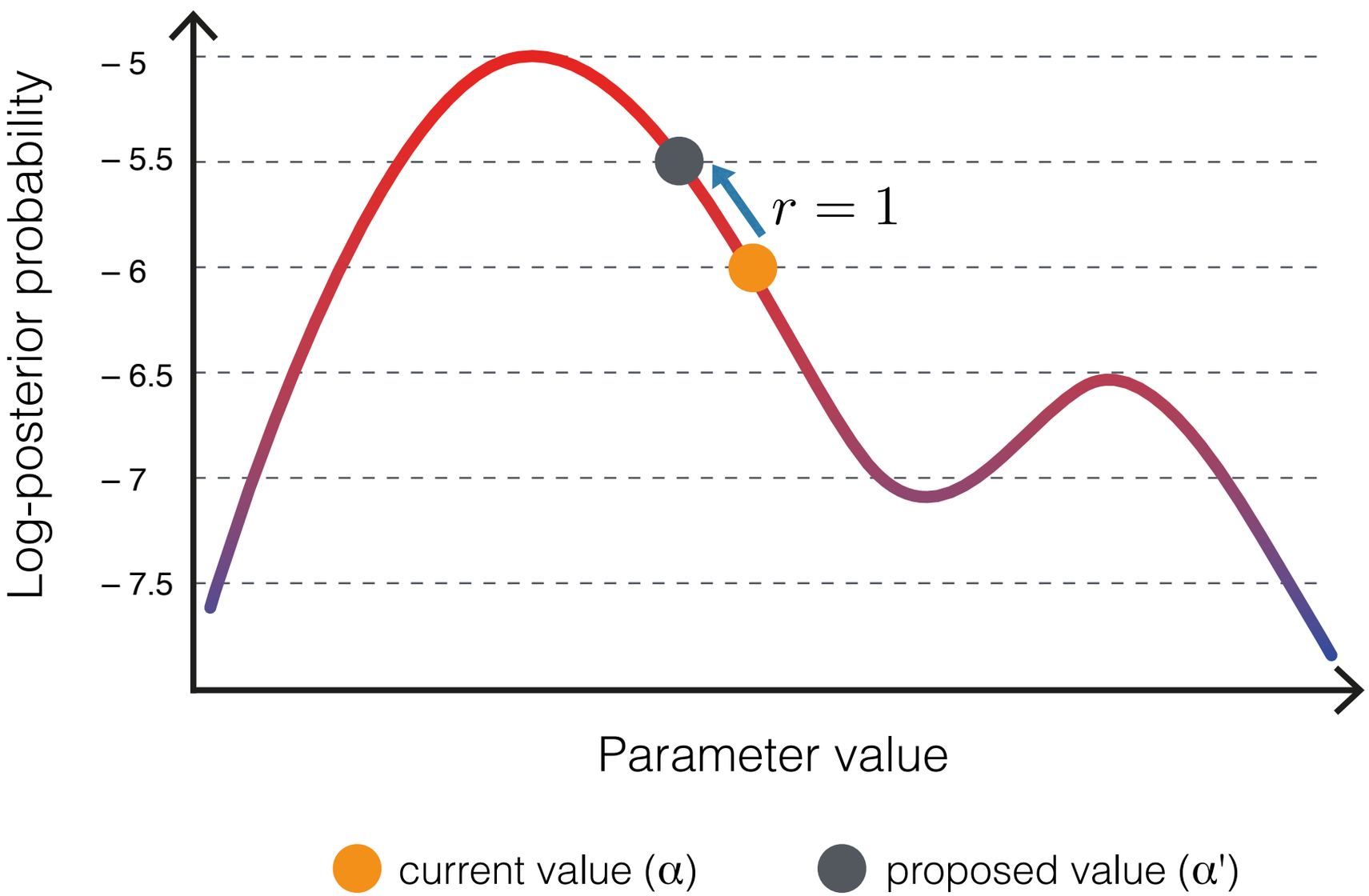


$\log P(\bullet|x,M) = -5.5$

$\log P(\bullet|x,M) = -6$

Acceptance probability

$$r = \min\left\{1, \underbrace{\frac{P(\alpha'|x,M)}{P(\alpha|x,M)}}_{\text{Posterior ratio}} \times \underbrace{\frac{\cancel{P(\alpha|\alpha')}}{\cancel{P(\alpha'|\alpha)}}}_{\text{Hastings ratio}}\right\}$$

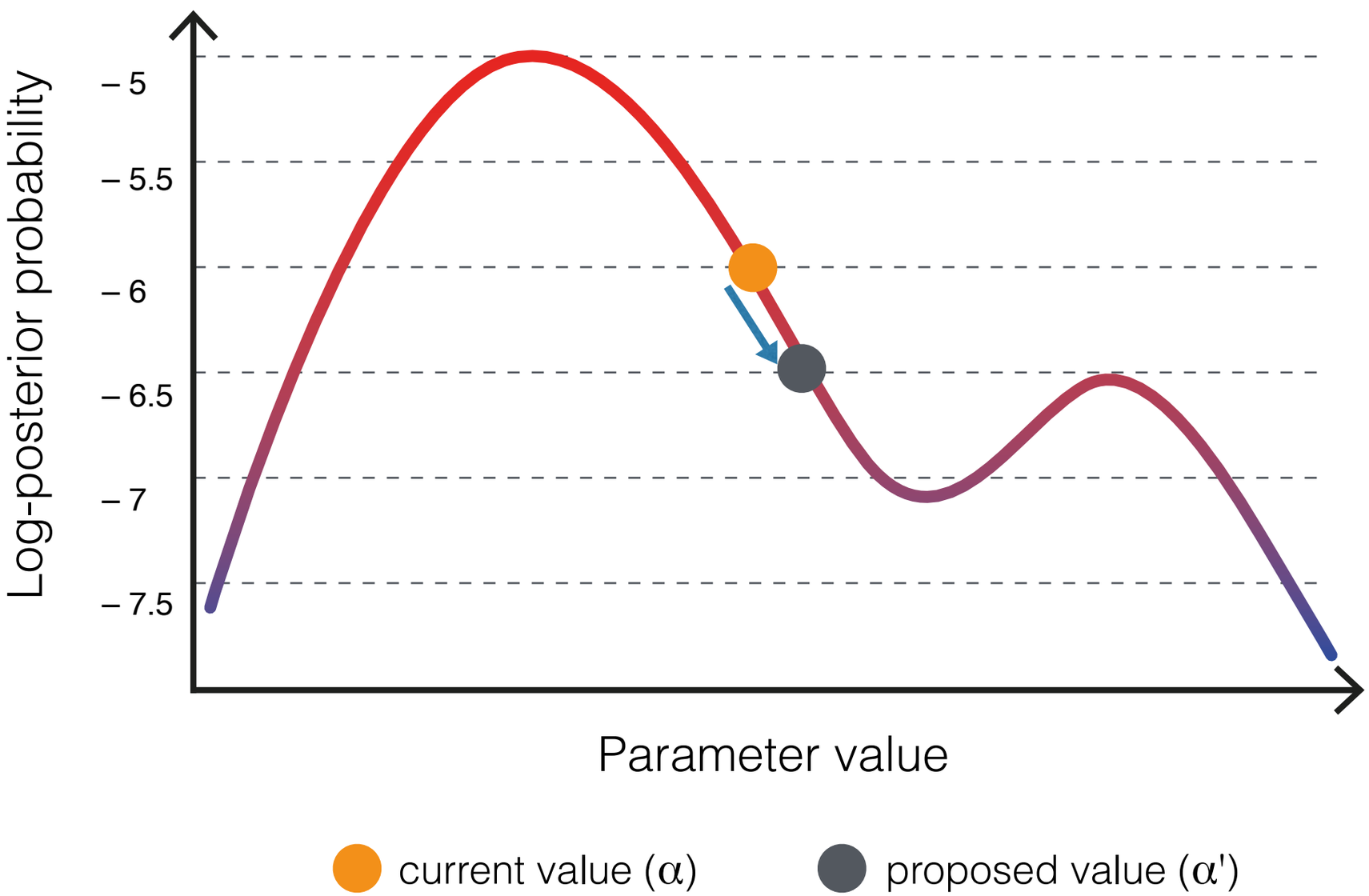


$\log P(\bullet|x, M) = -5.5$

$\log P(\bullet|x, M) = -6$

Acceptance probability

$$r = \min\left\{1, \underbrace{\frac{P(\alpha'|x,M)}{P(\alpha|x,M)}}_{\text{Posterior ratio}} \times \underbrace{\frac{\cancel{P(\alpha|\alpha')}}{\cancel{P(\alpha'|\alpha)}}}_{\text{Hastings ratio}}\right\}$$

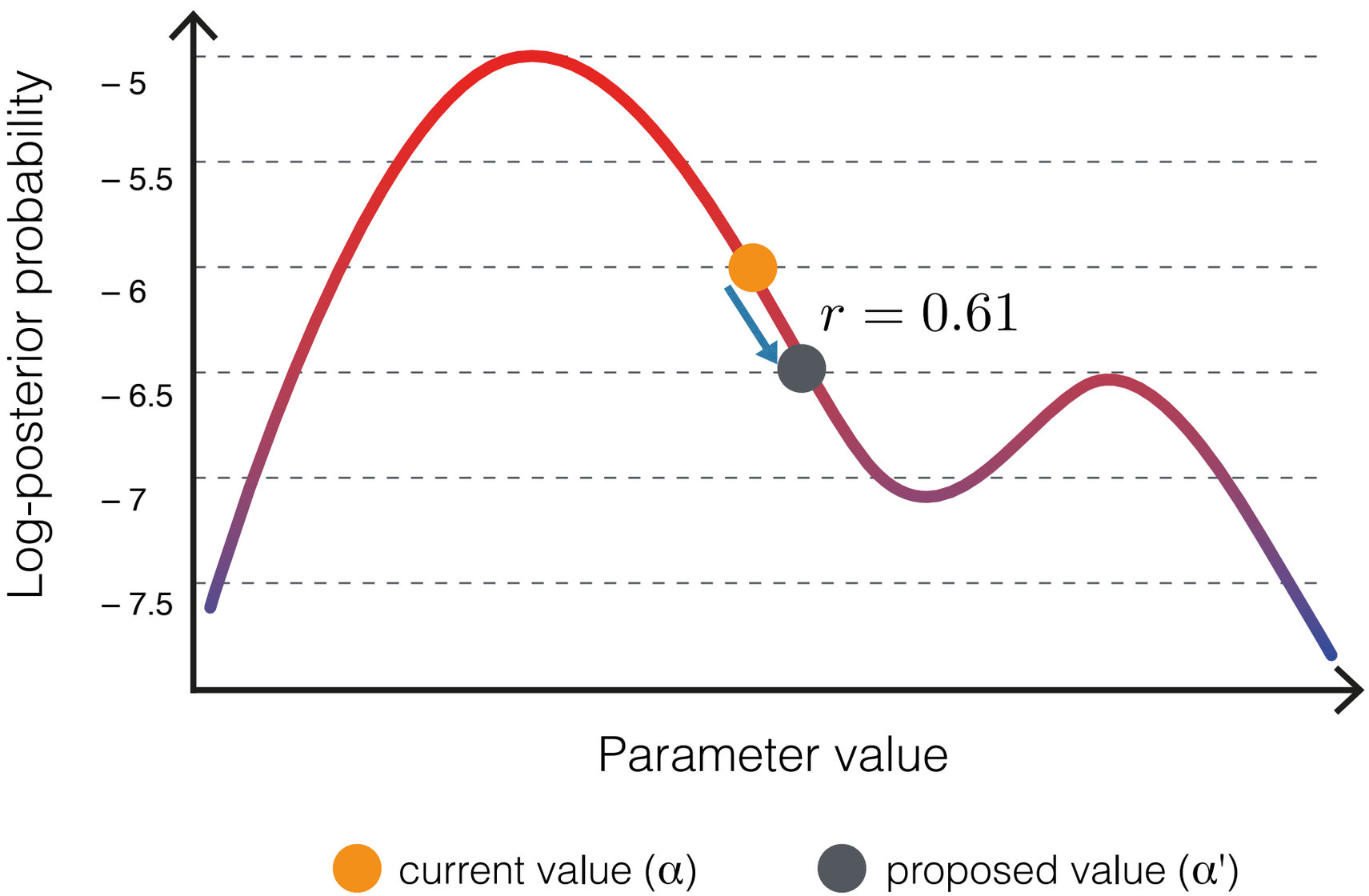


$\log P(\bullet|x,M) = -6$

$\log P(\bullet|x,M) = -6.5$

Acceptance probability

$$r = \min\left\{1, \underbrace{\frac{P(\alpha'|x,M)}{P(\alpha|x,M)}}_{\text{Posterior ratio}} \times \underbrace{\frac{\cancel{P(\alpha|\alpha')}}{\cancel{P(\alpha'|\alpha)}}}_{\text{Hastings ratio}}\right\}$$

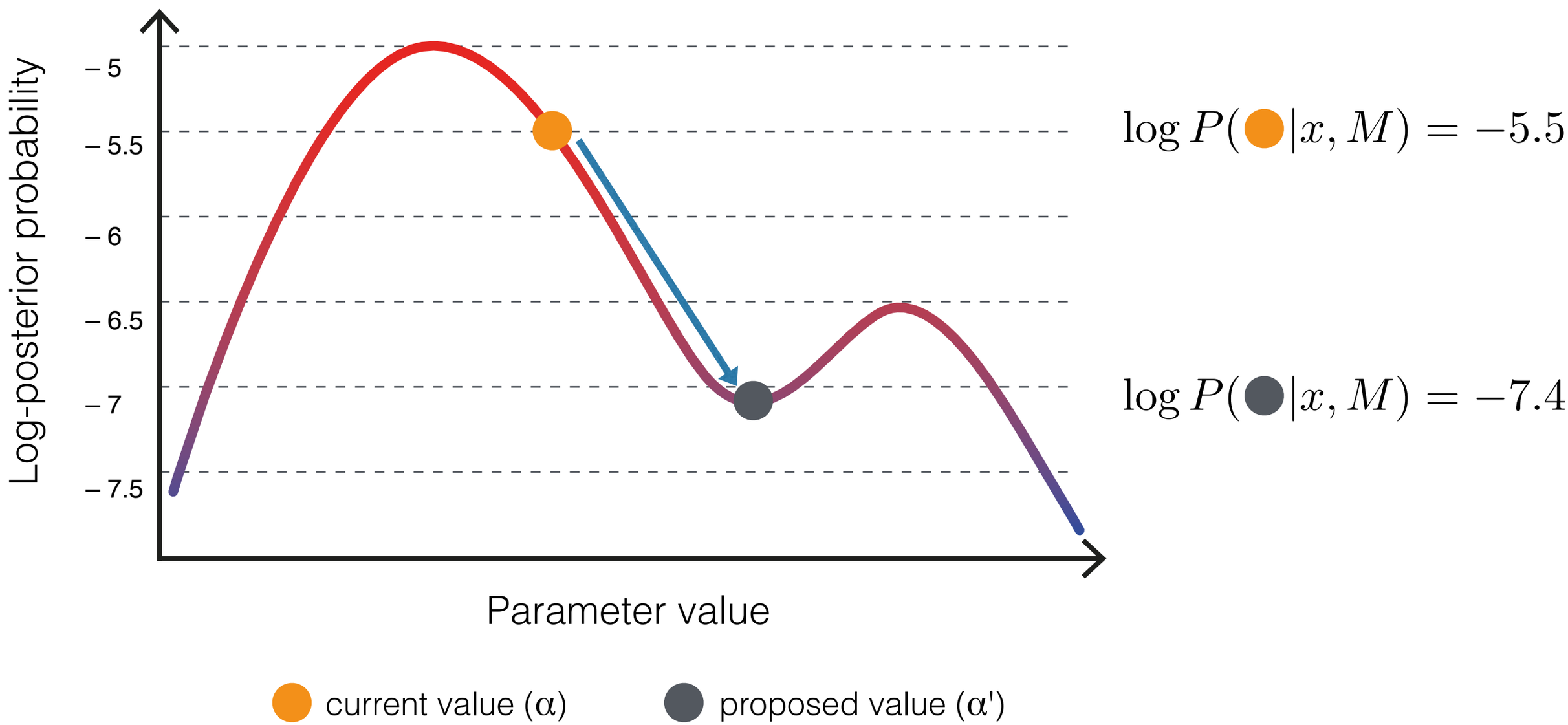


$\log P(\bullet|x,M) = -6$

$\log P(\bullet|x,M) = -6.5$

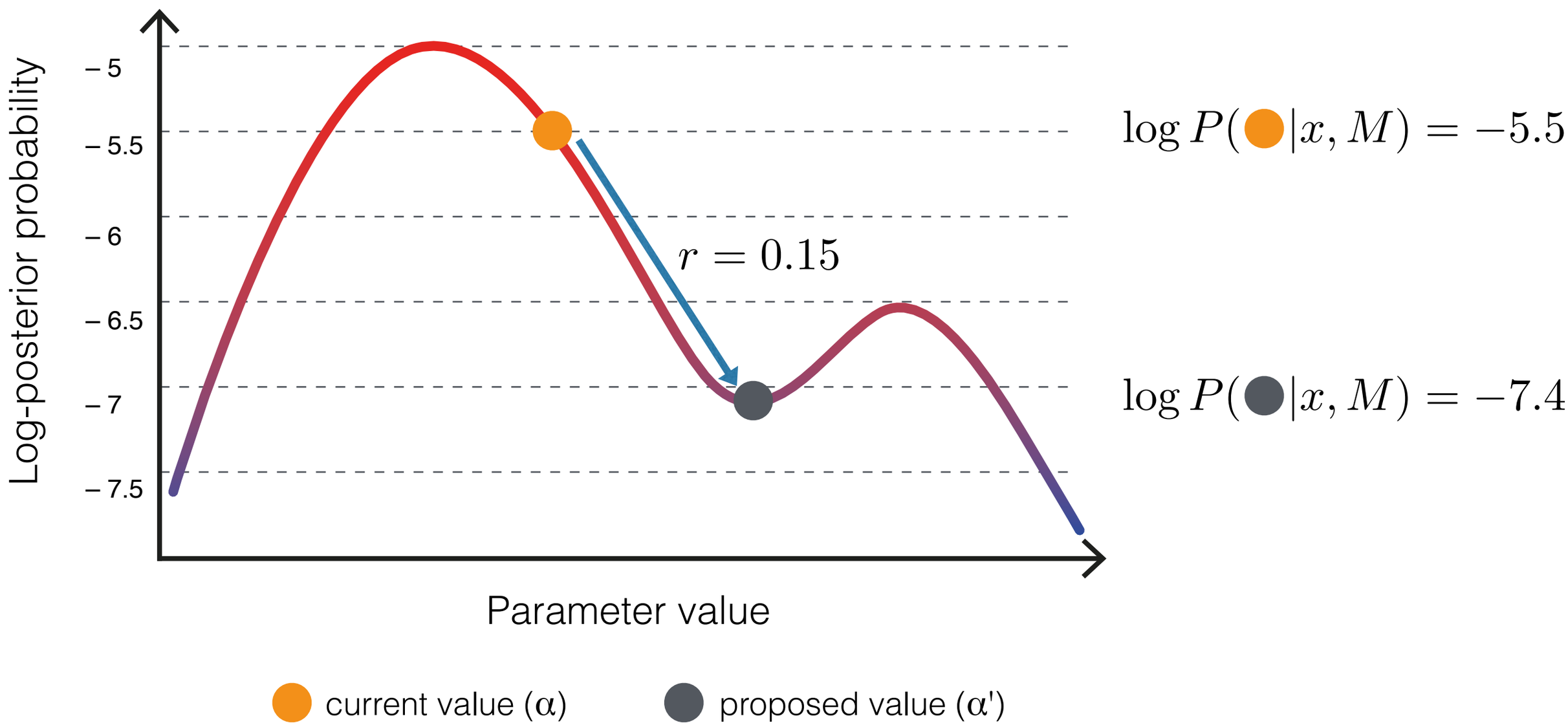
Acceptance probability

$$r = \min\left\{1, \underbrace{\frac{P(\alpha'|x,M)}{P(\alpha|x,M)}}_{\text{Posterior ratio}} \times \underbrace{\frac{\cancel{P(\alpha|\alpha')}}{\cancel{P(\alpha'|\alpha)}}}_{\text{Hastings ratio}}\right\}$$

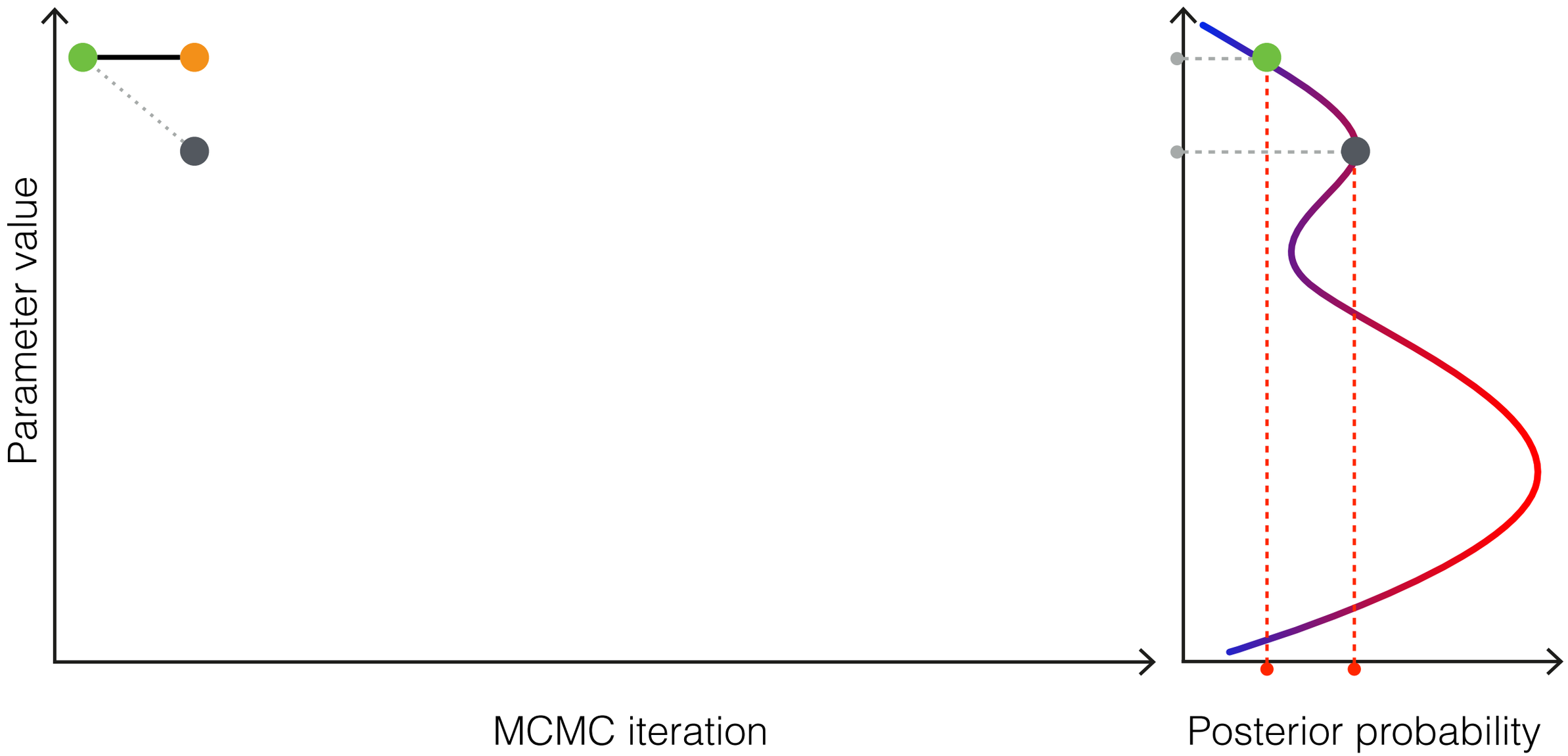


Acceptance probability

$$r = \min\left\{1, \underbrace{\frac{P(\alpha'|x,M)}{P(\alpha|x,M)}}_{\text{Posterior ratio}} \times \underbrace{\frac{\cancel{P(\alpha|\alpha')}}{\cancel{P(\alpha'|\alpha)}}}_{\text{Hastings ratio}}\right\}$$

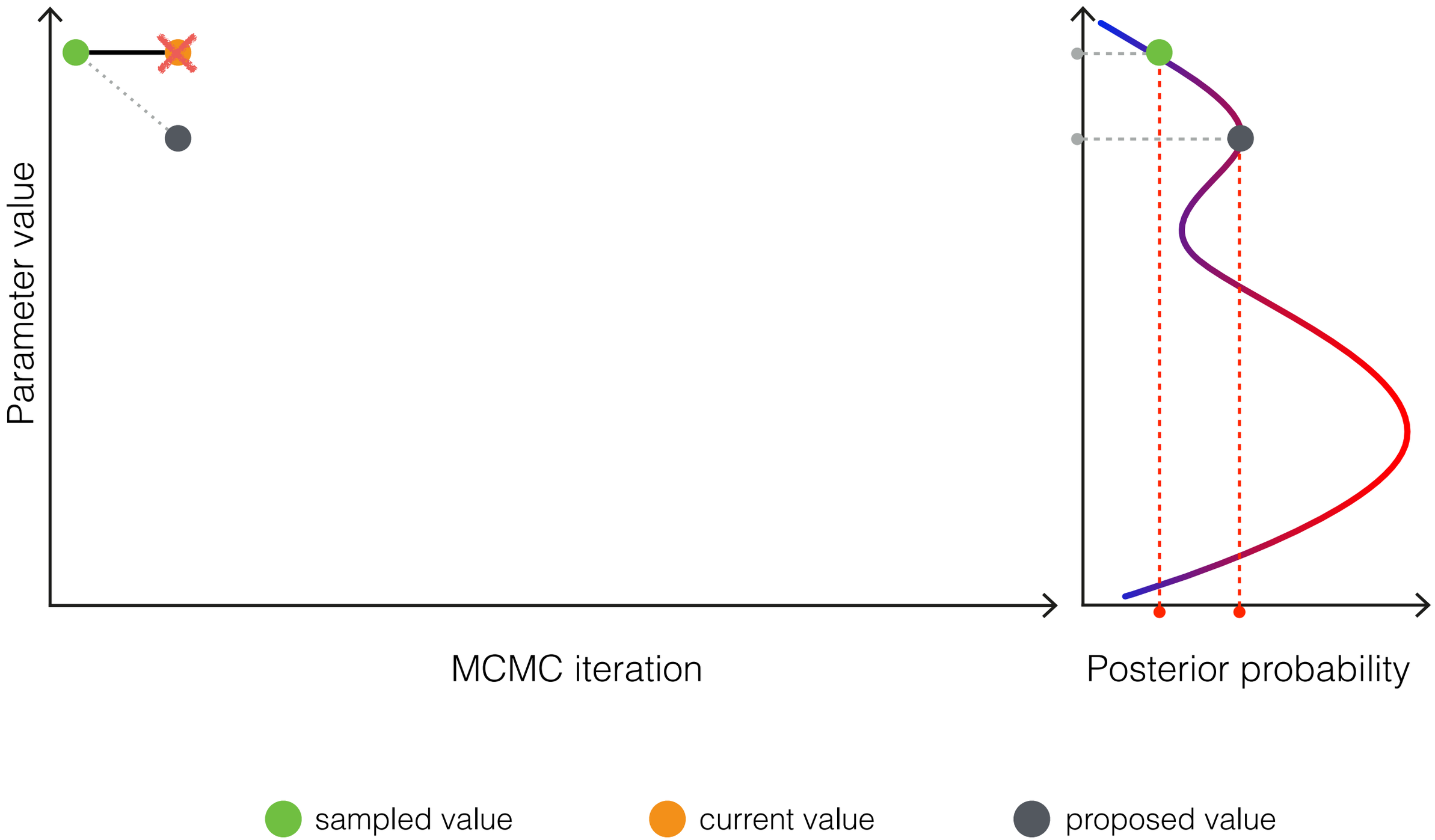


Sampling from the posterior using MCMC

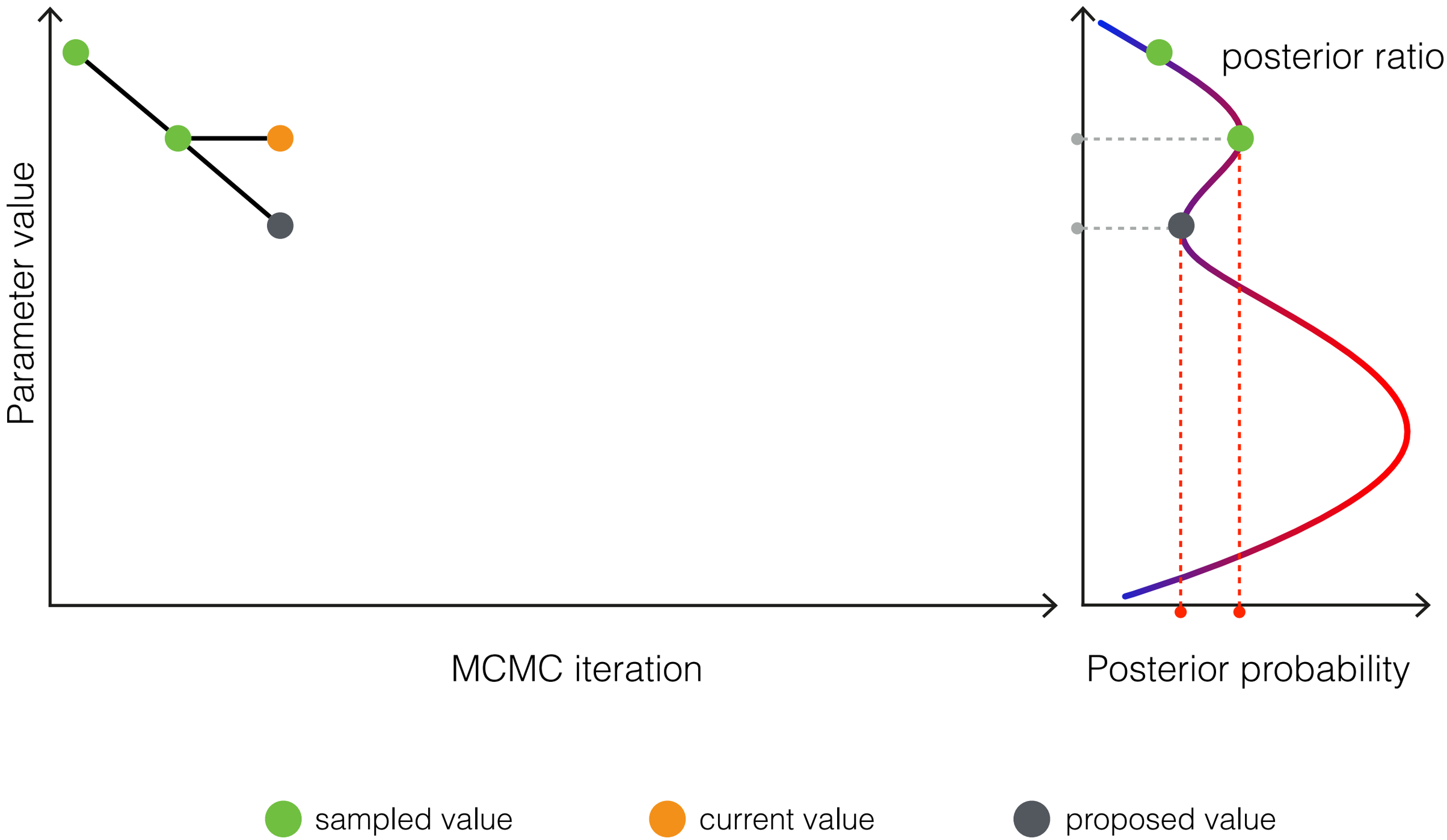


sampled value current value proposed value

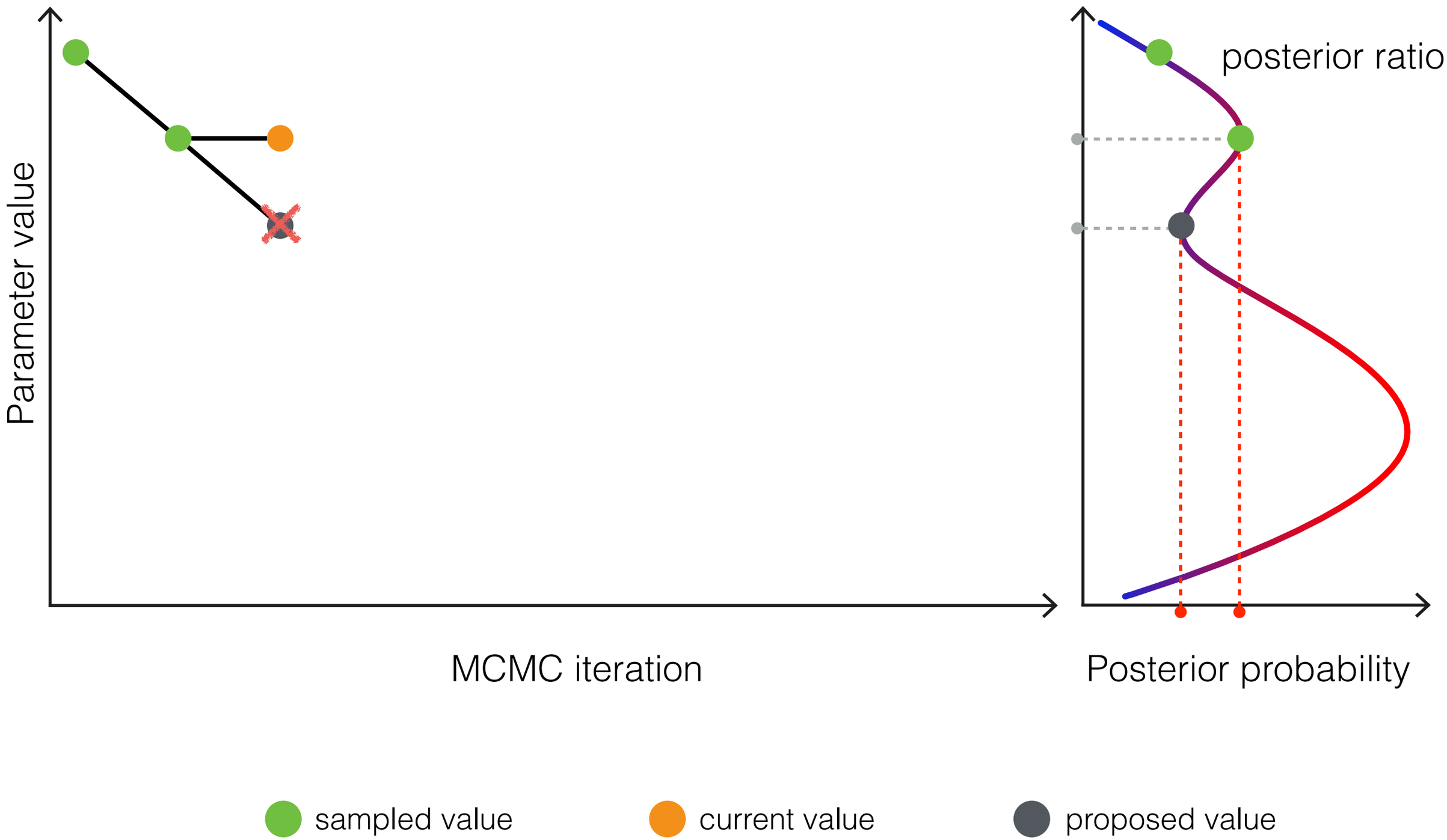
Sampling from the posterior using MCMC



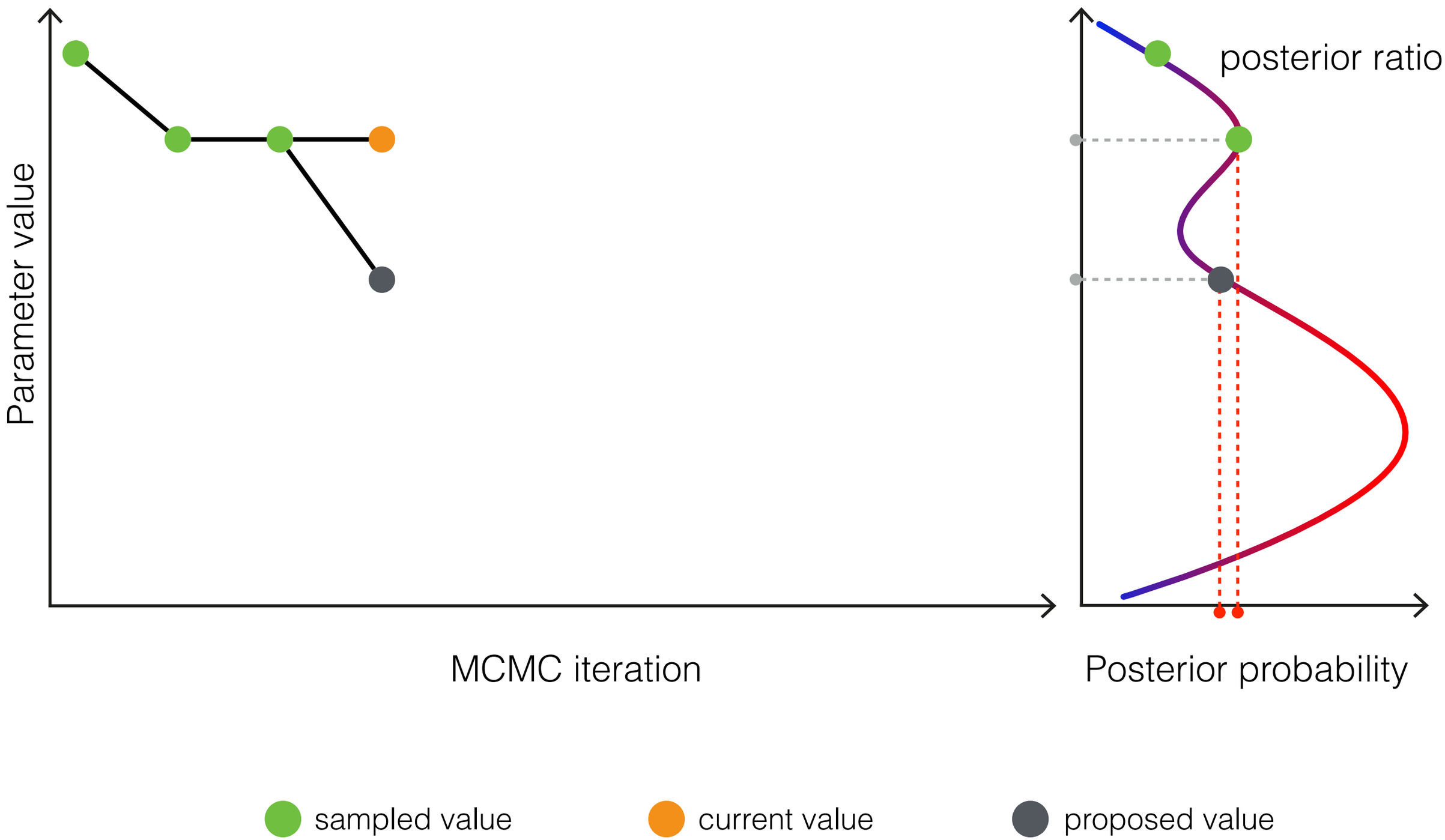
Sampling from the posterior using MCMC



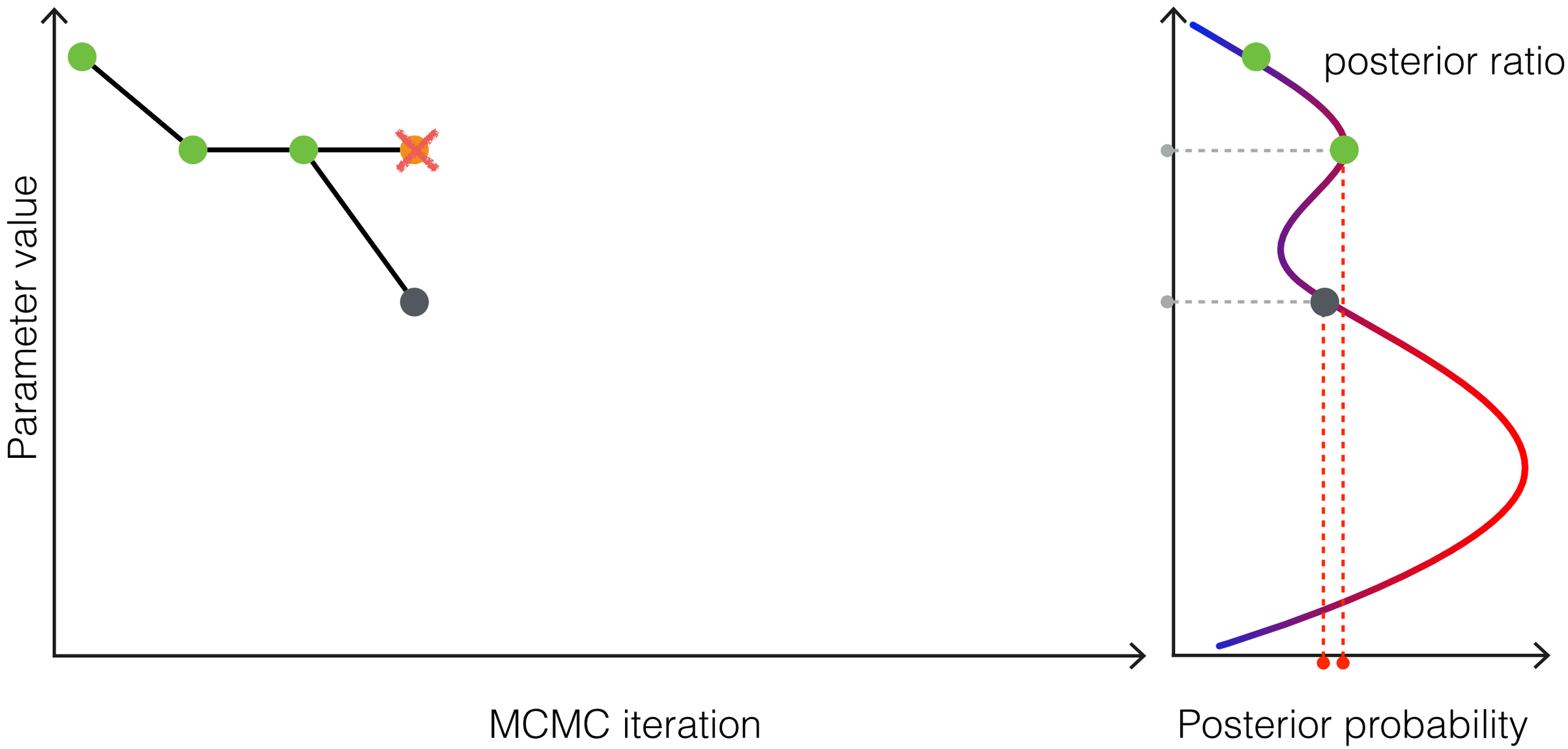
Sampling from the posterior using MCMC



Sampling from the posterior using MCMC

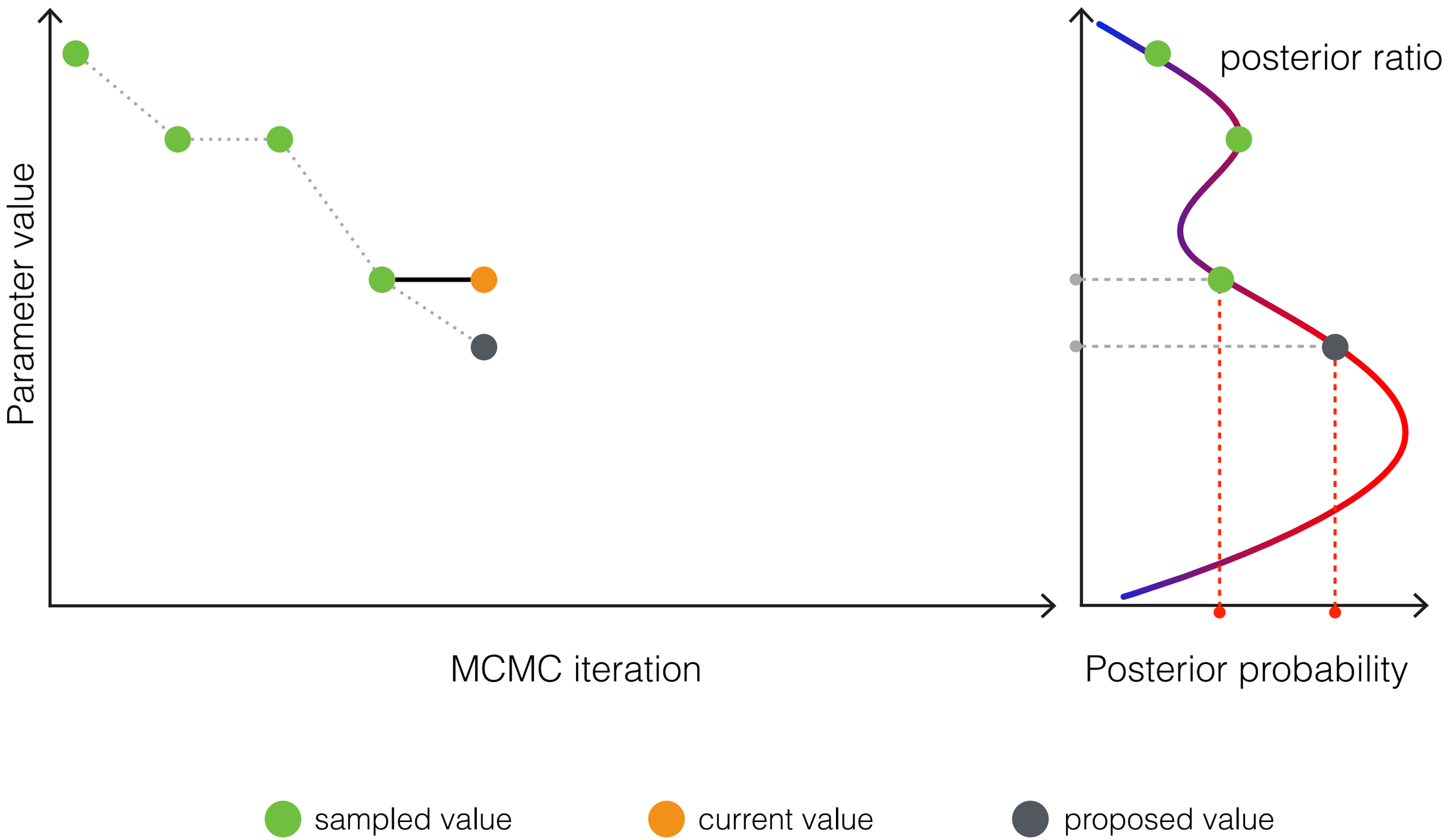


Sampling from the posterior using MCMC

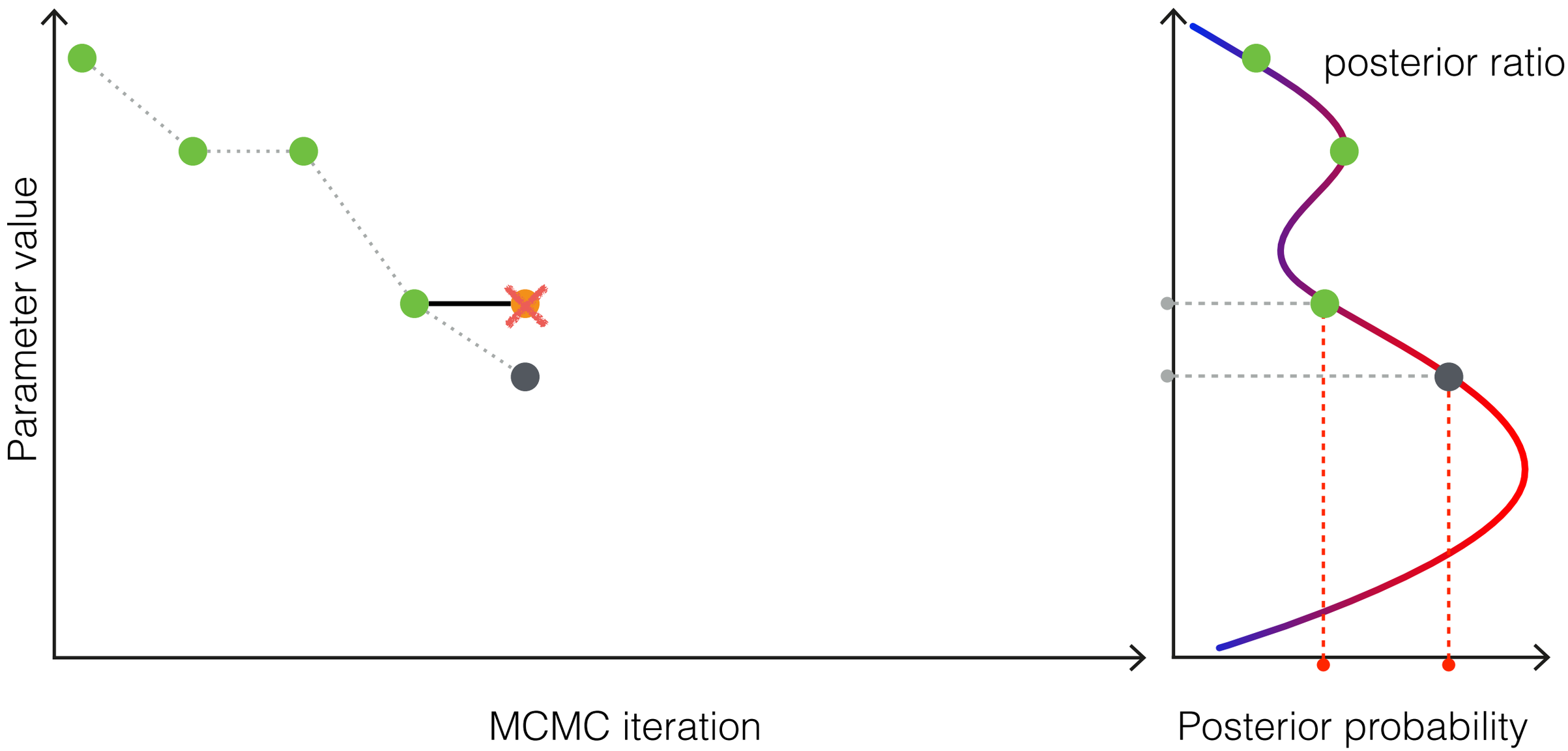


sampled value current value proposed value

Sampling from the posterior using MCMC

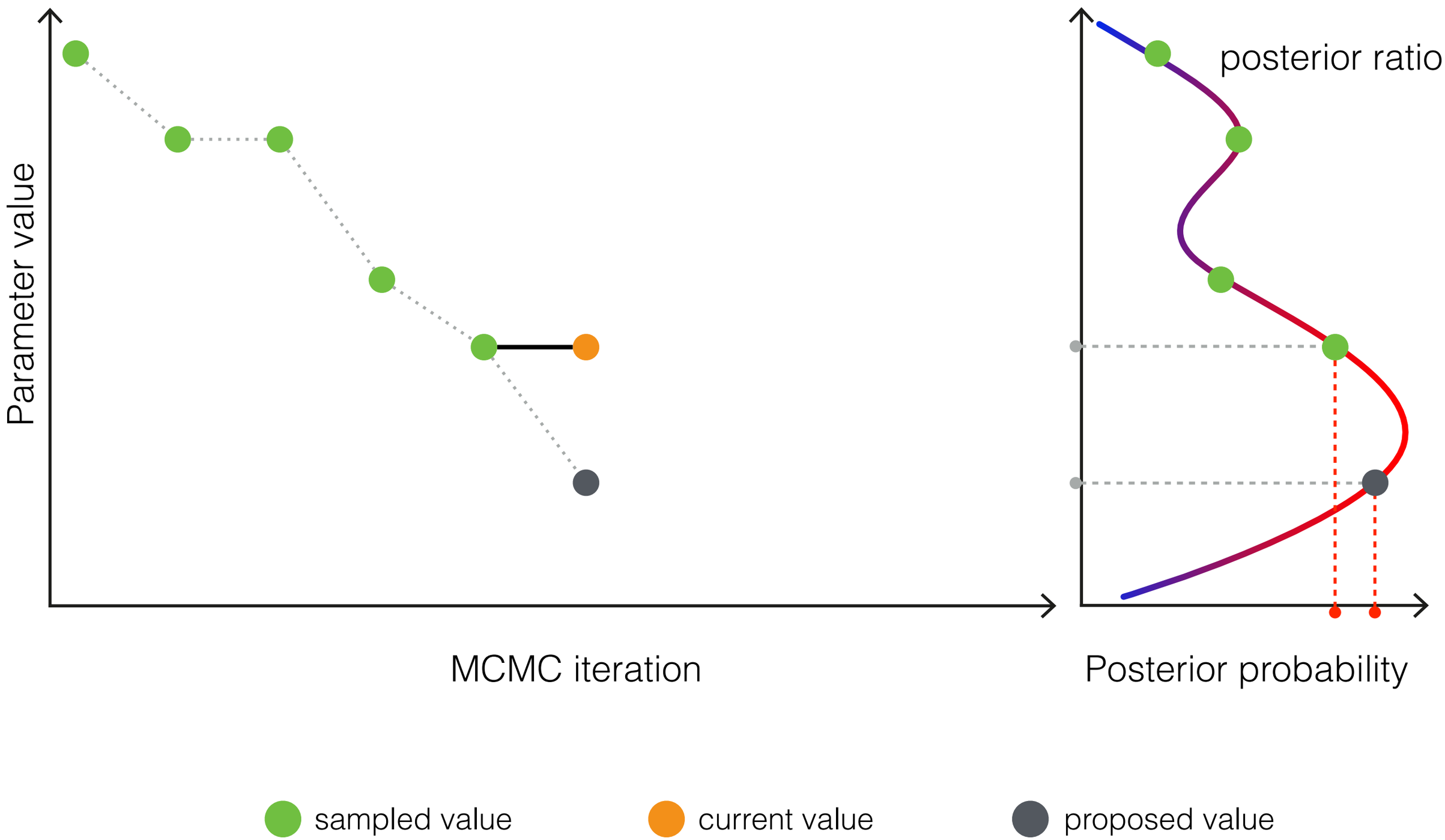


Sampling from the posterior using MCMC

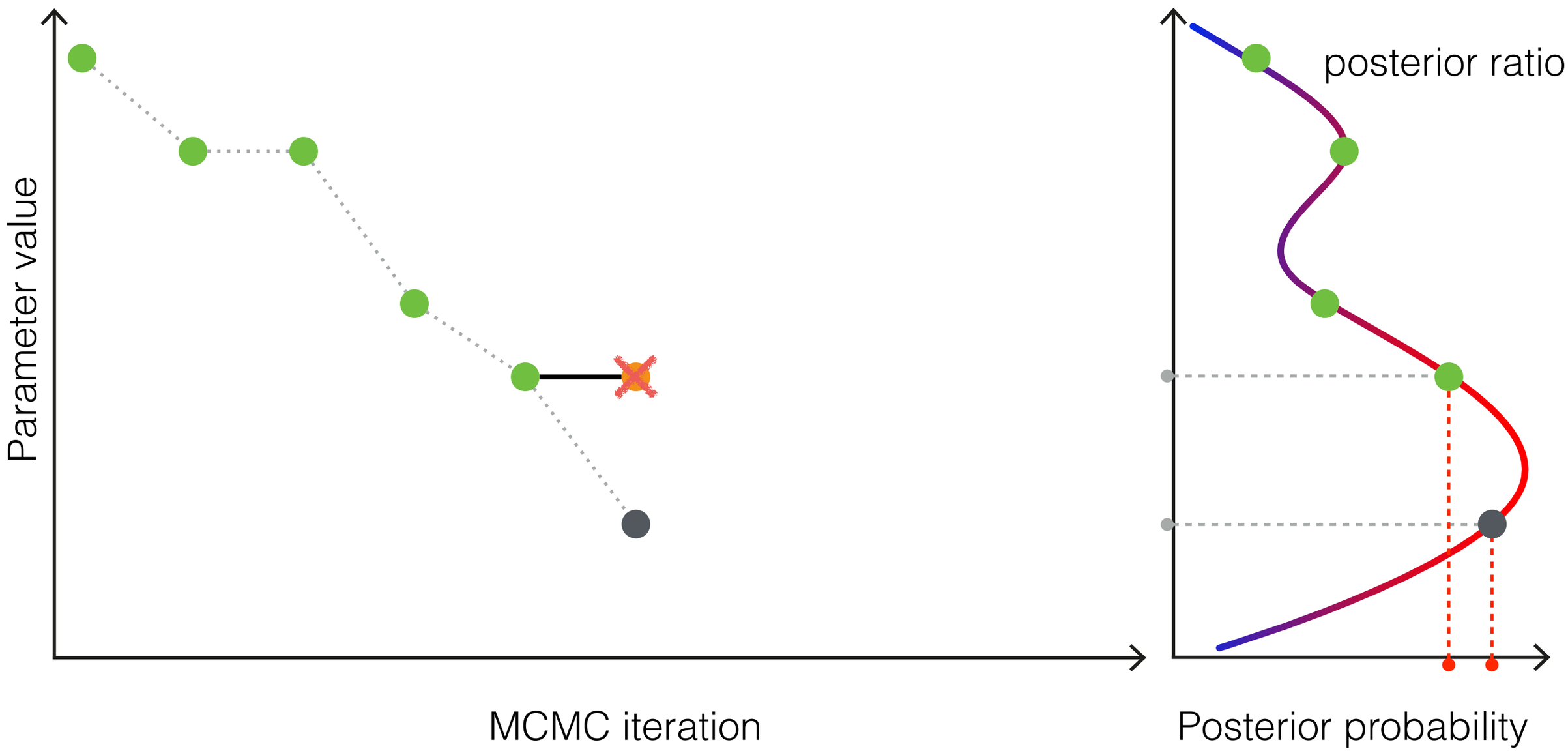


sampled value current value proposed value

Sampling from the posterior using MCMC

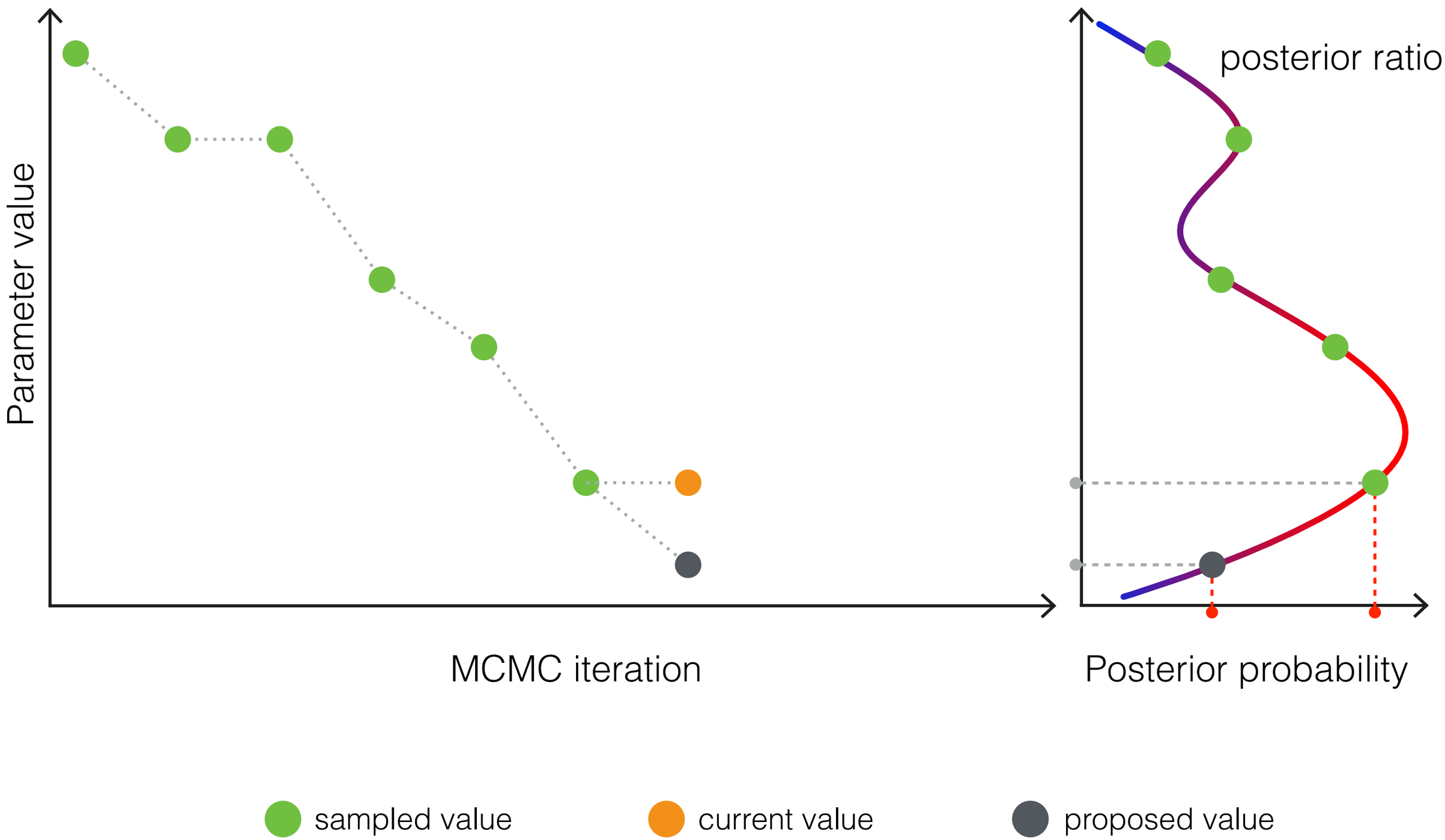


Sampling from the posterior using MCMC

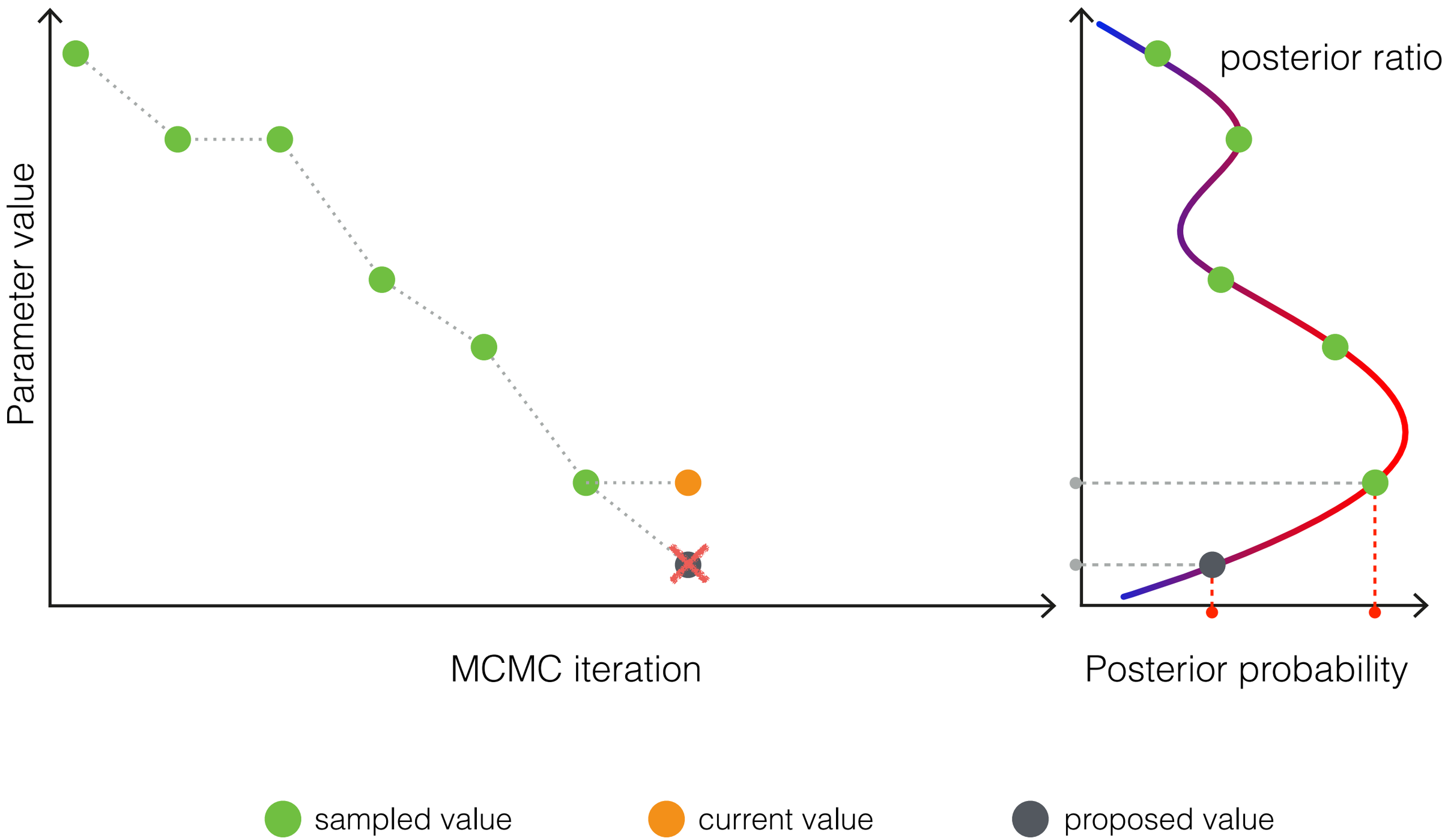


sampled value current value proposed value

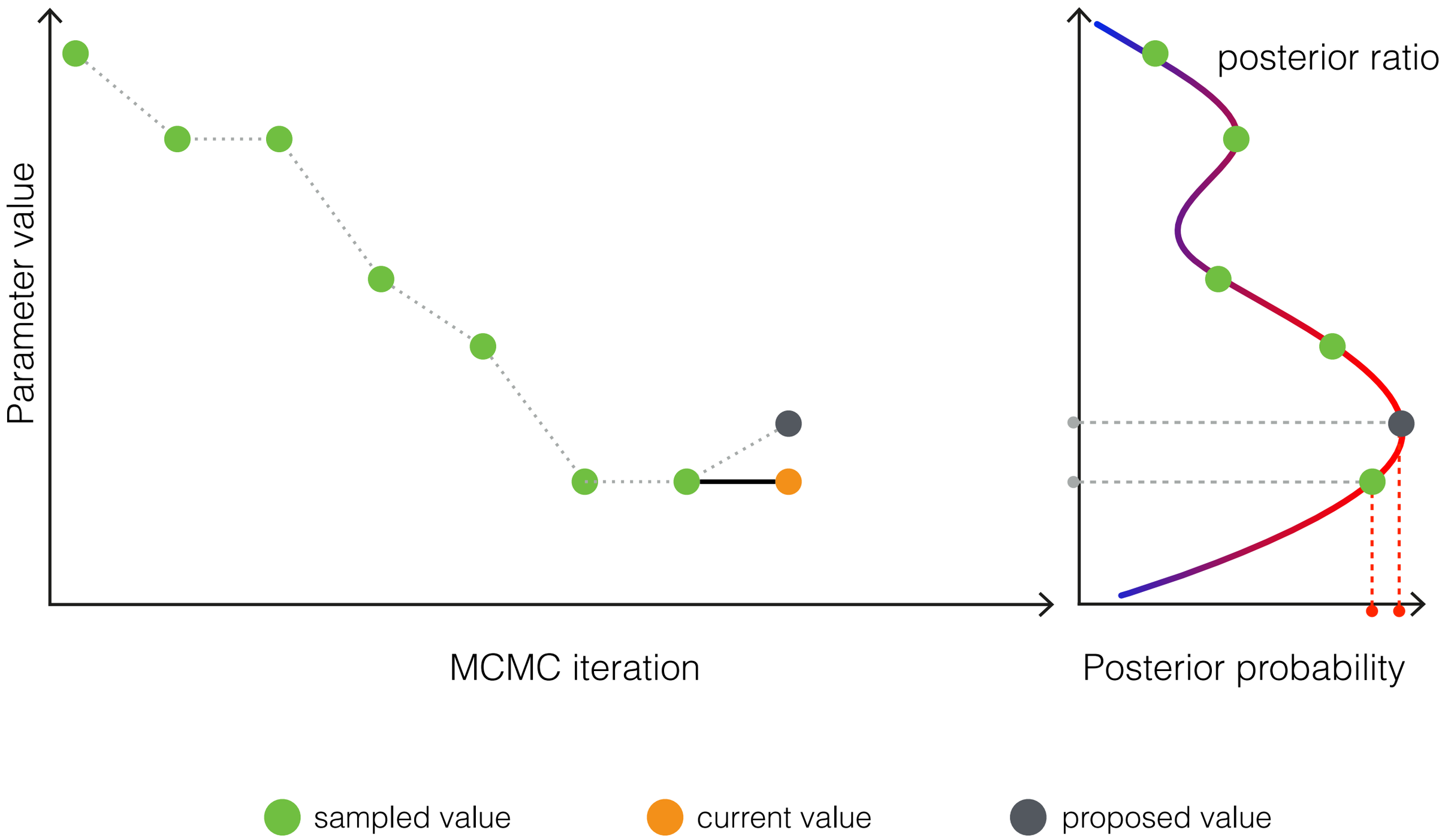
Sampling from the posterior using MCMC



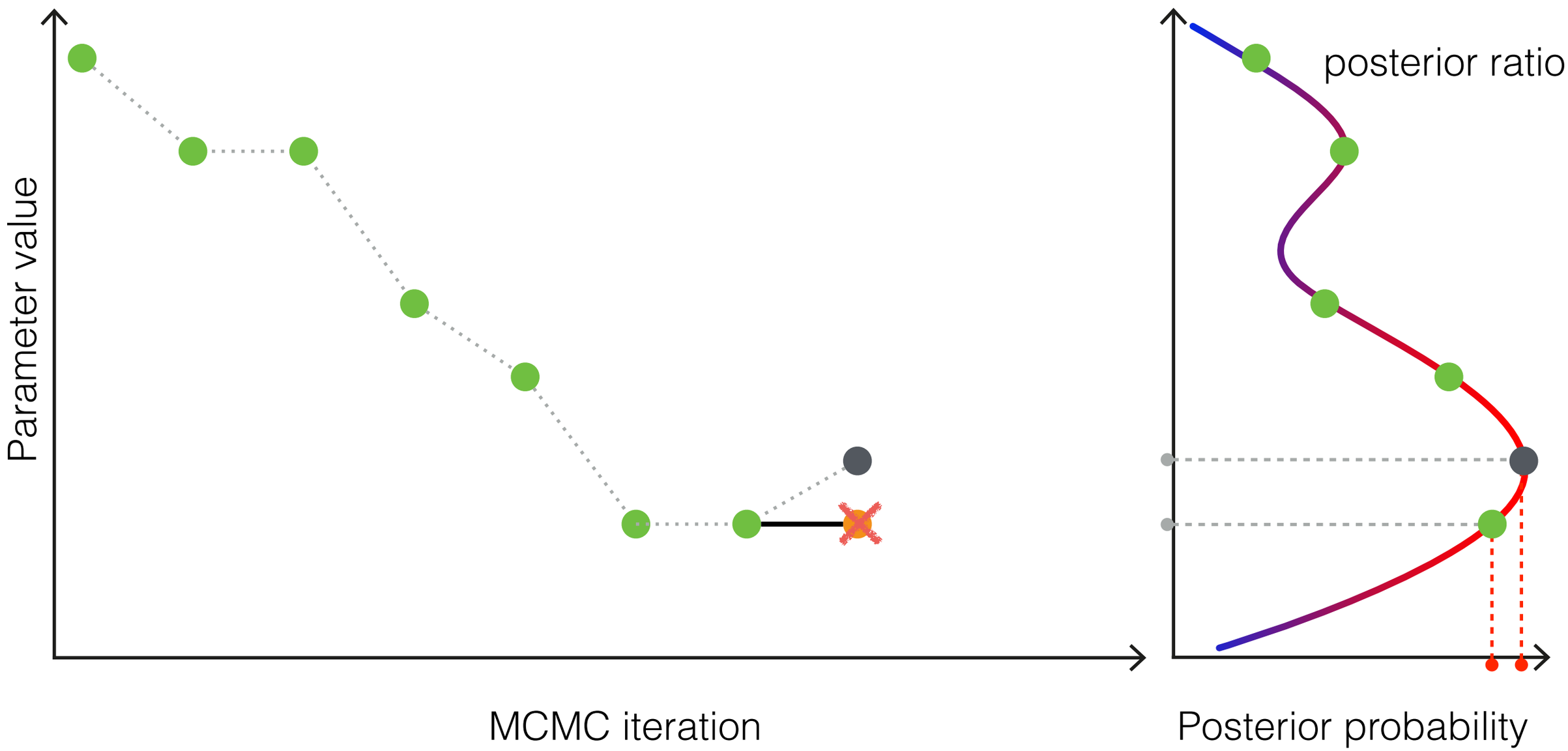
Sampling from the posterior using MCMC



Sampling from the posterior using MCMC

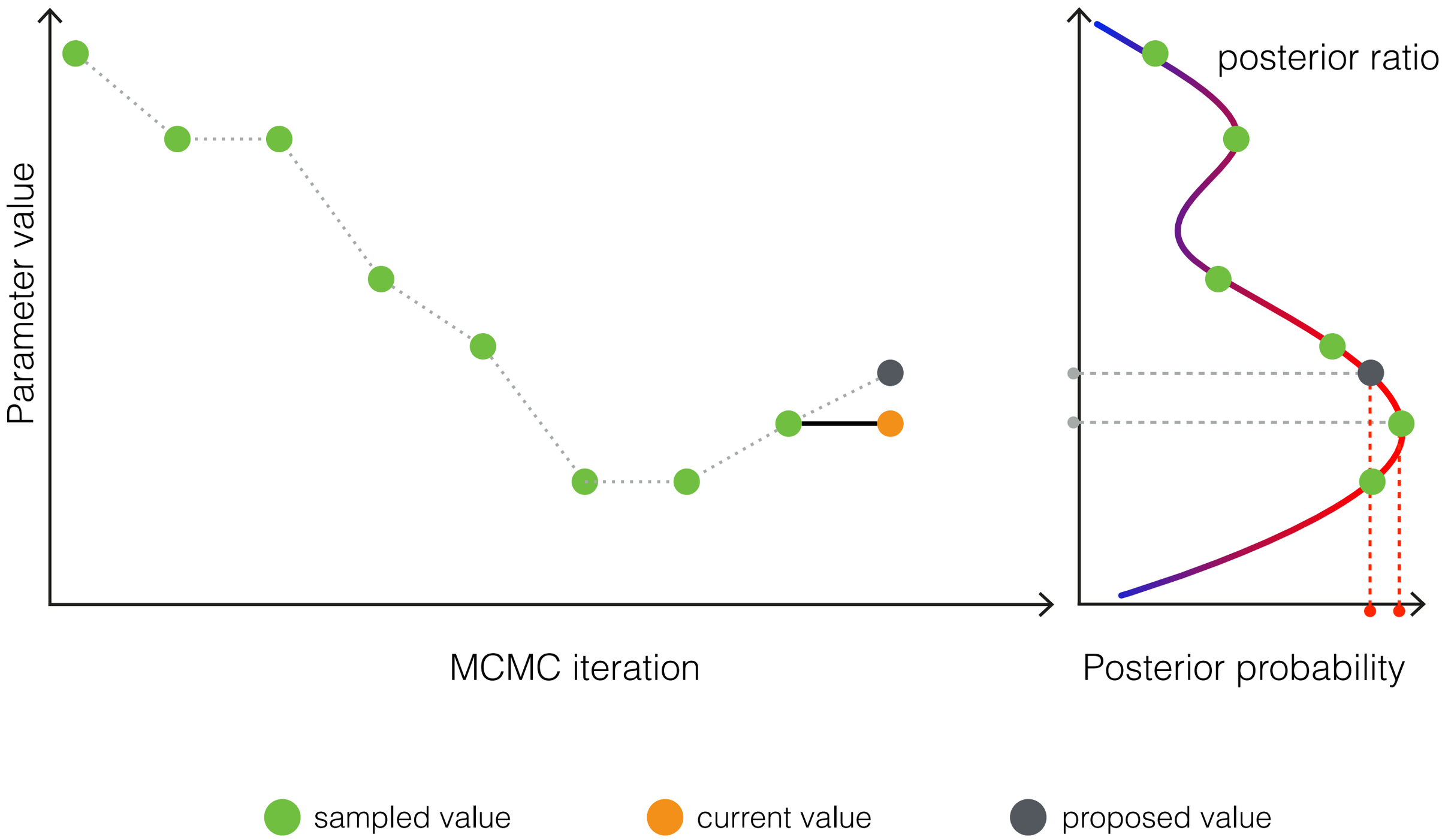


Sampling from the posterior using MCMC

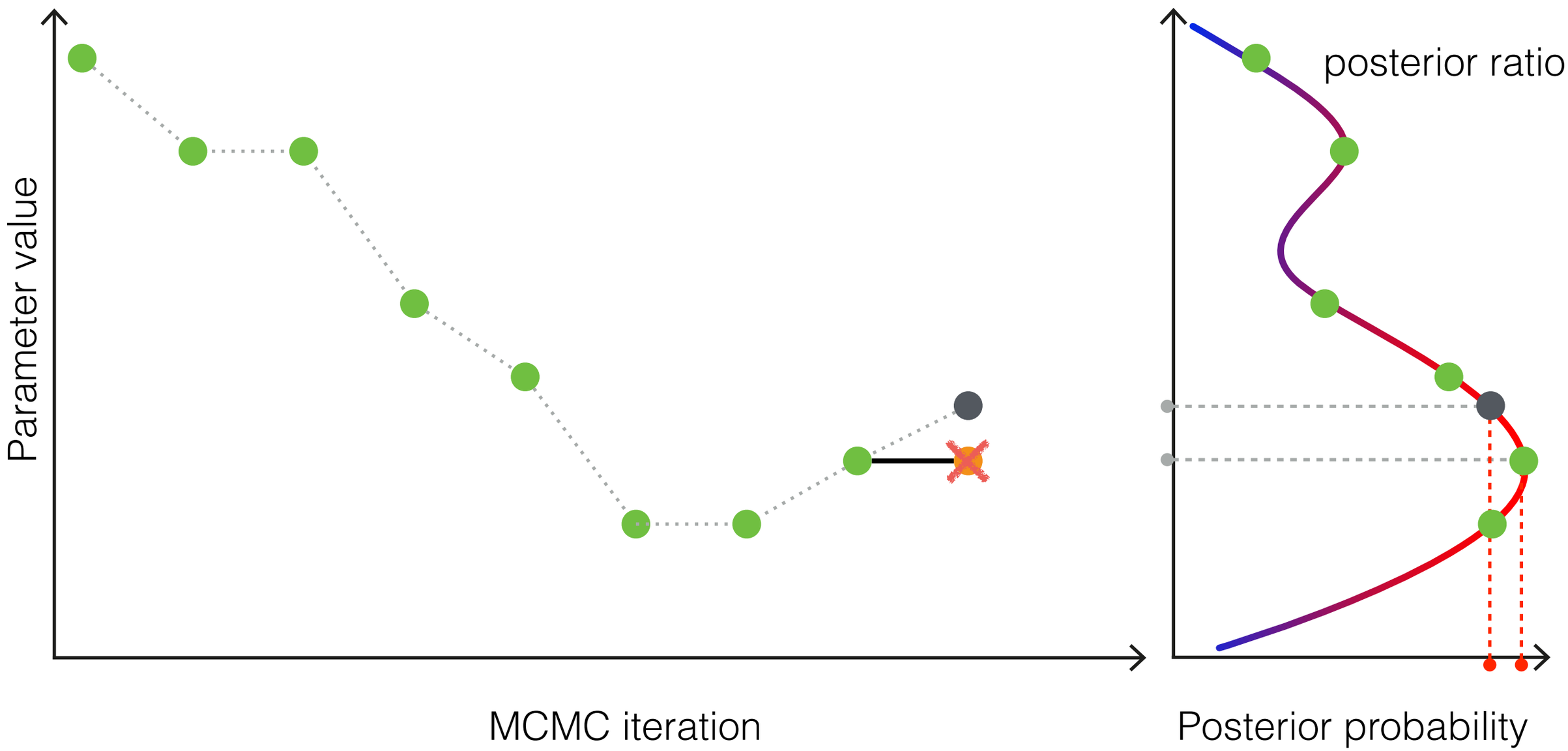


sampled value current value proposed value

Sampling from the posterior using MCMC

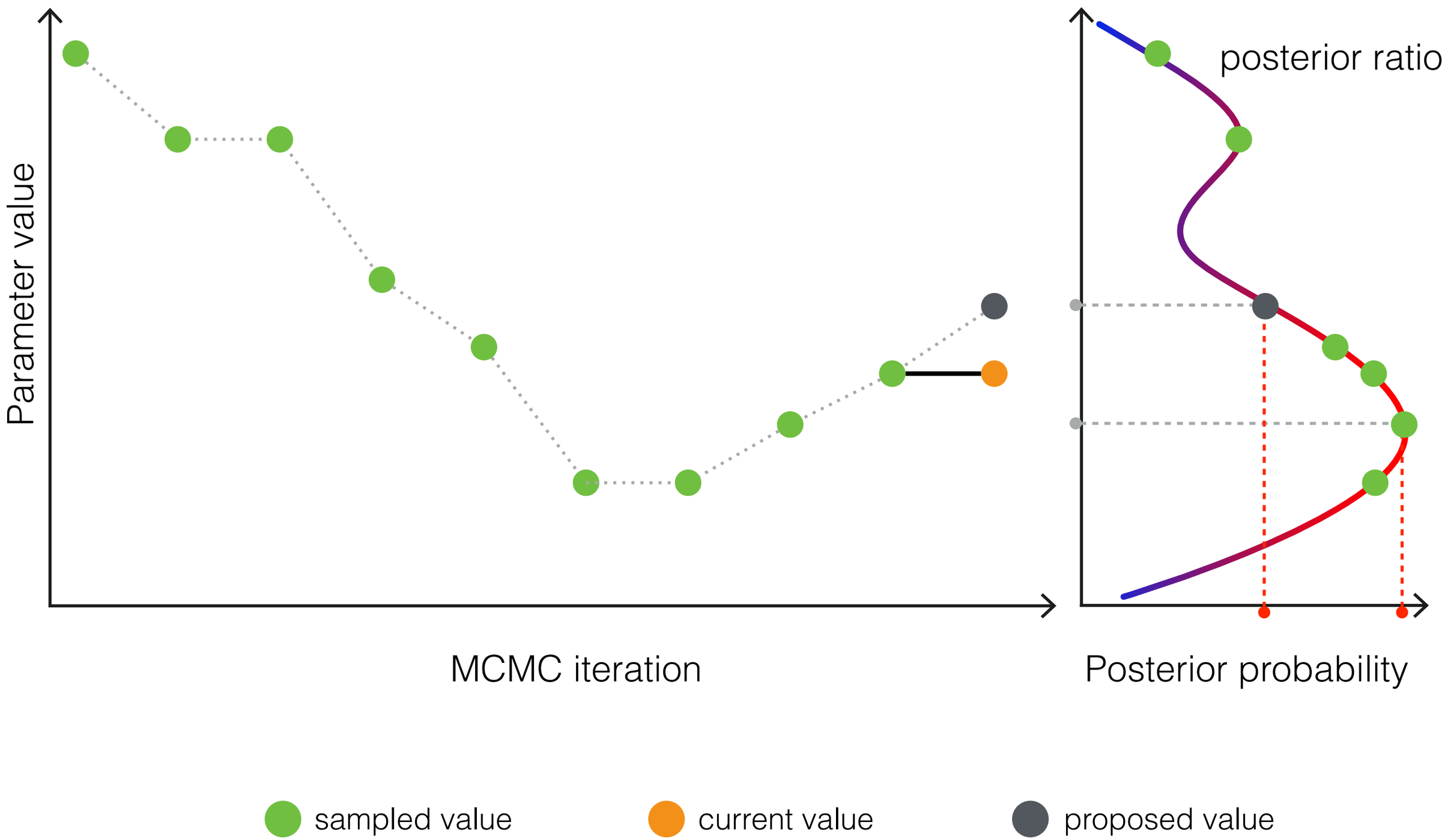


Sampling from the posterior using MCMC

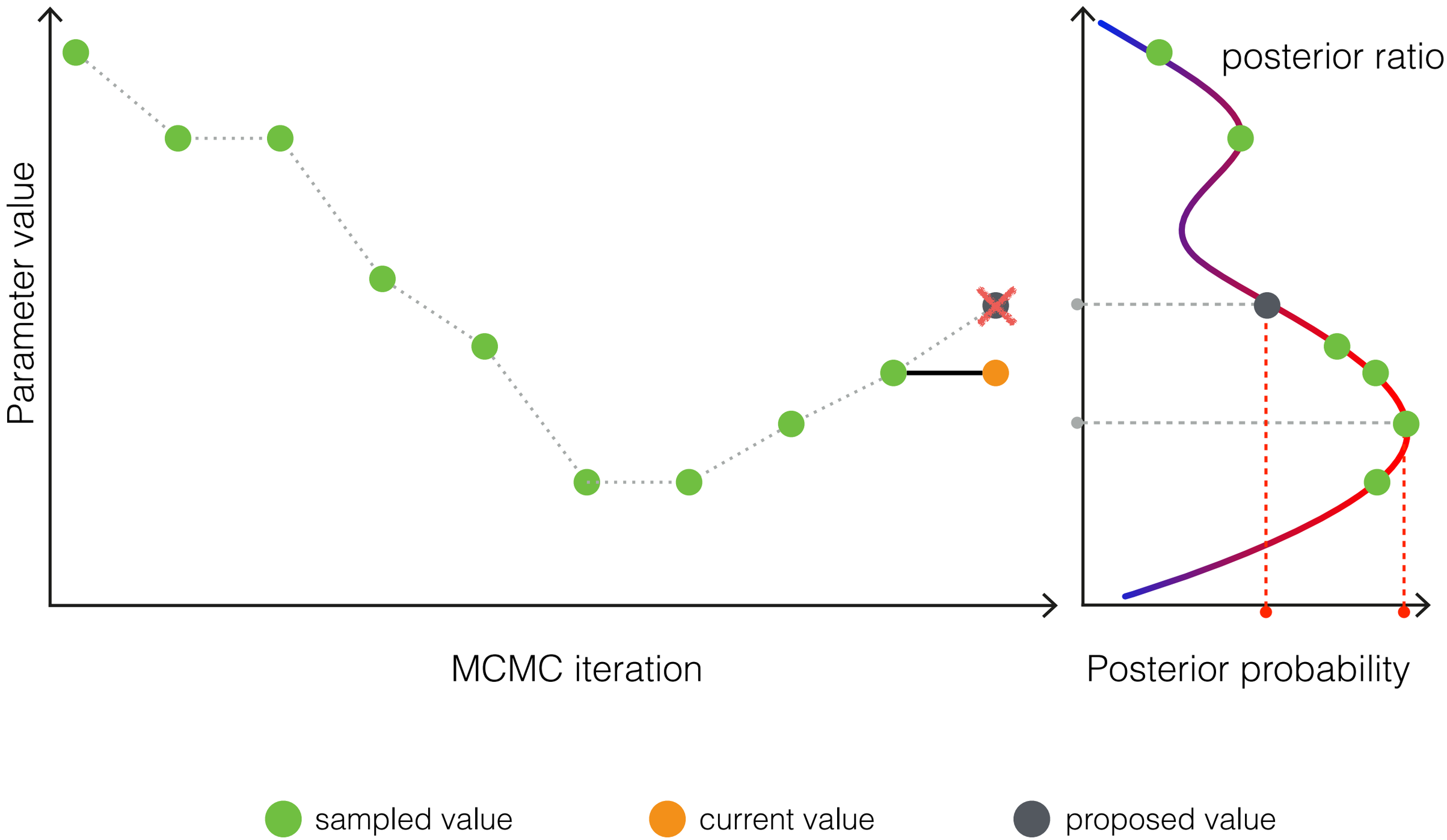


sampled value current value proposed value

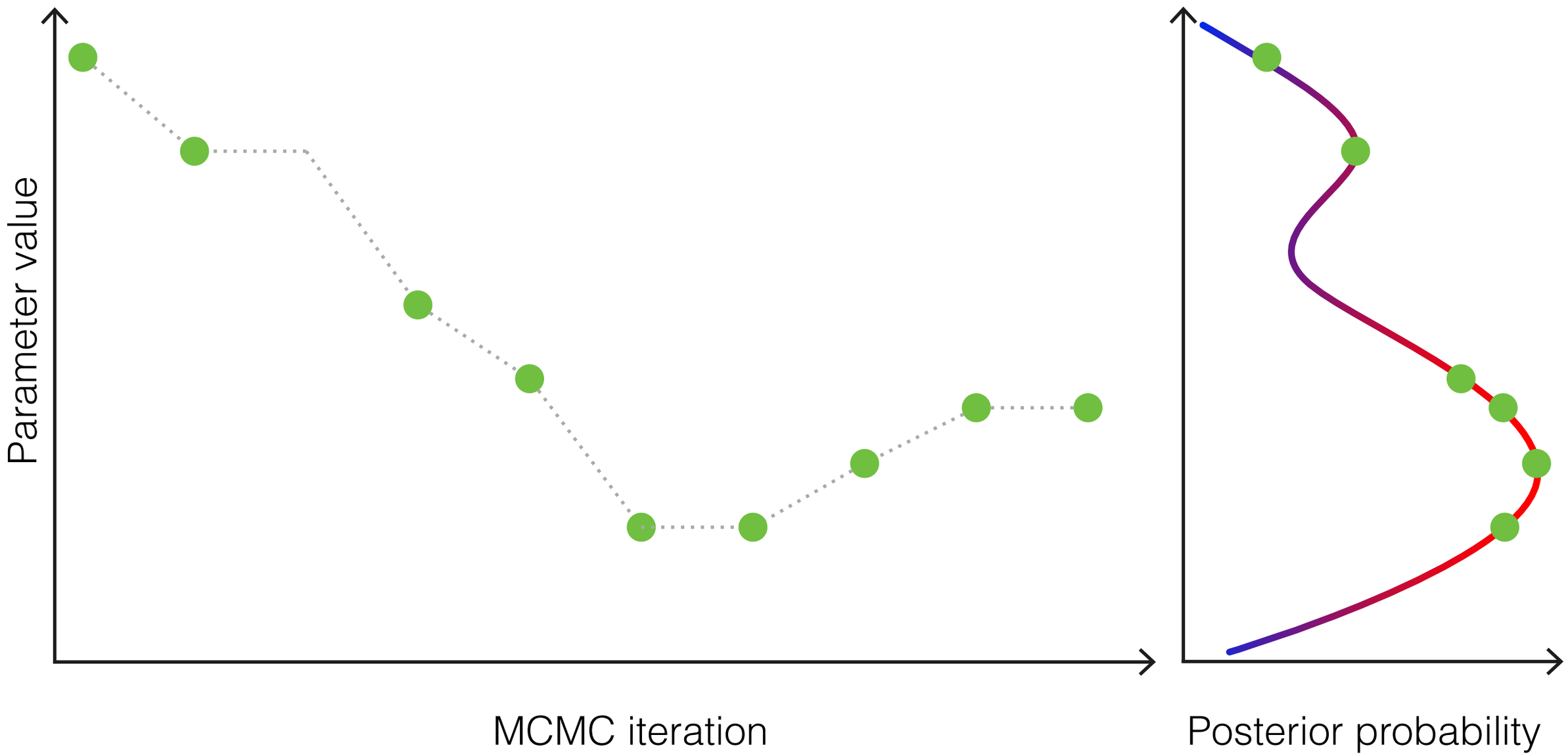
Sampling from the posterior using MCMC



Sampling from the posterior using MCMC

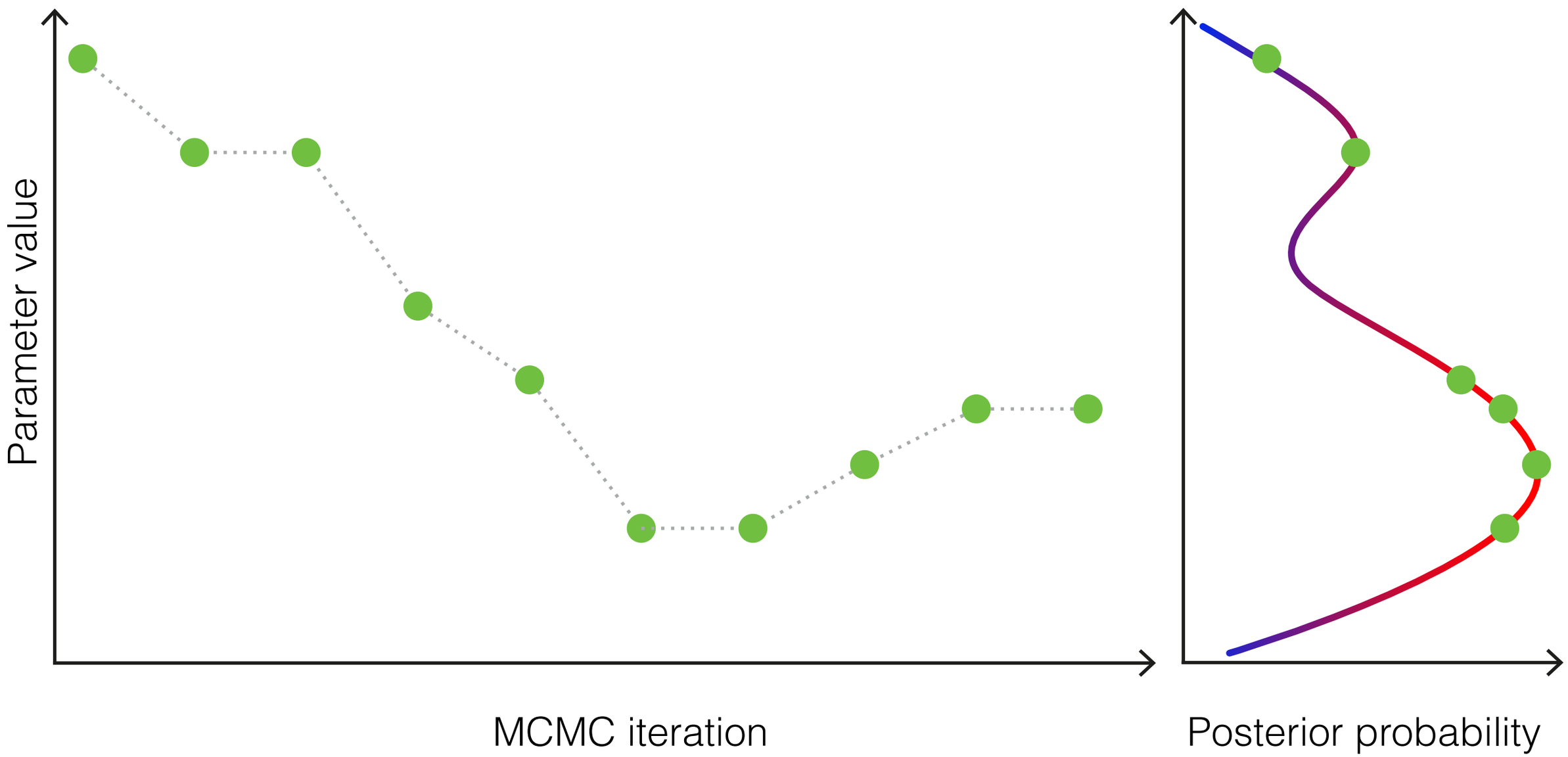


Sampling from the posterior using MCMC



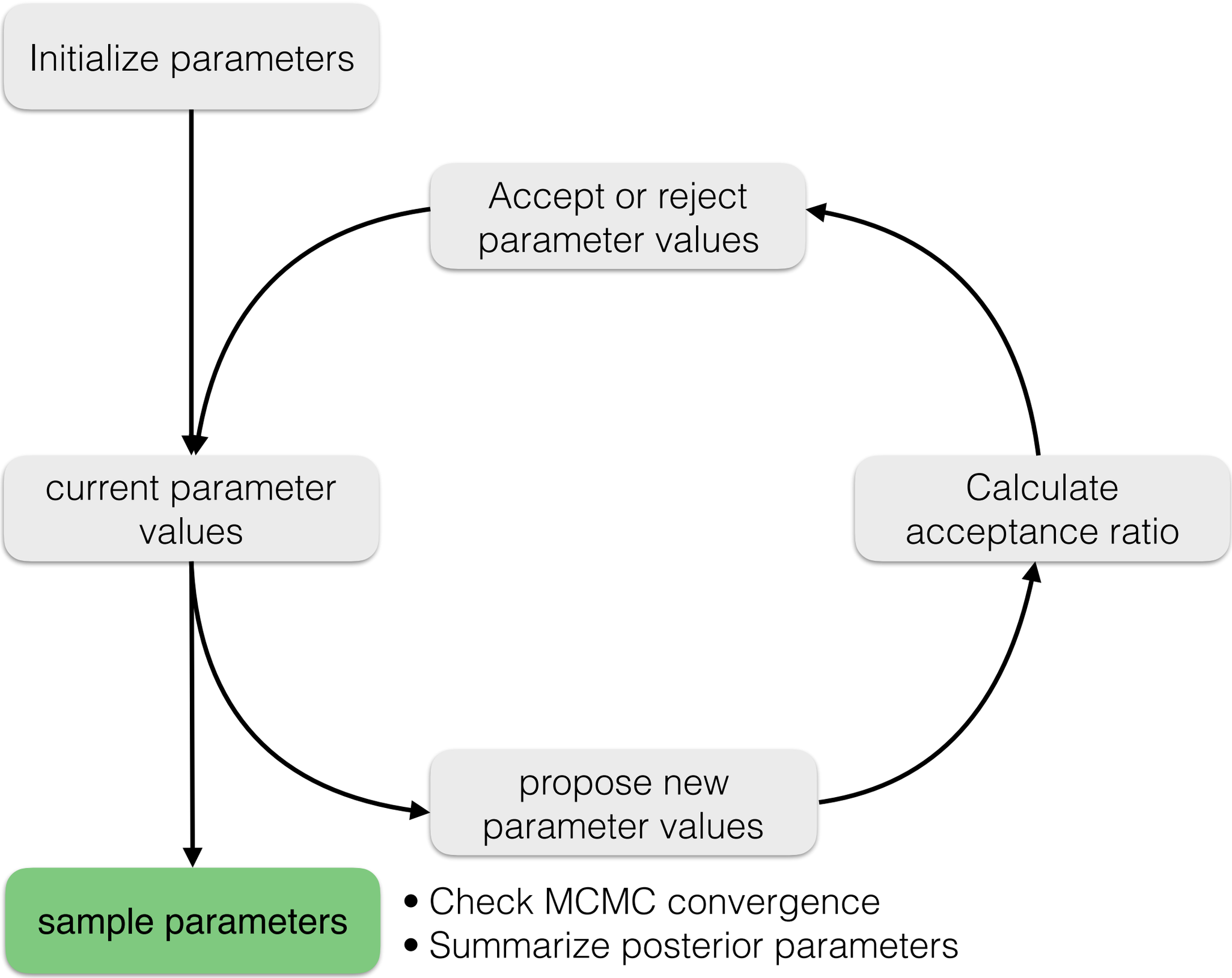
sampled value current value proposed value

Sampling from the posterior using MCMC



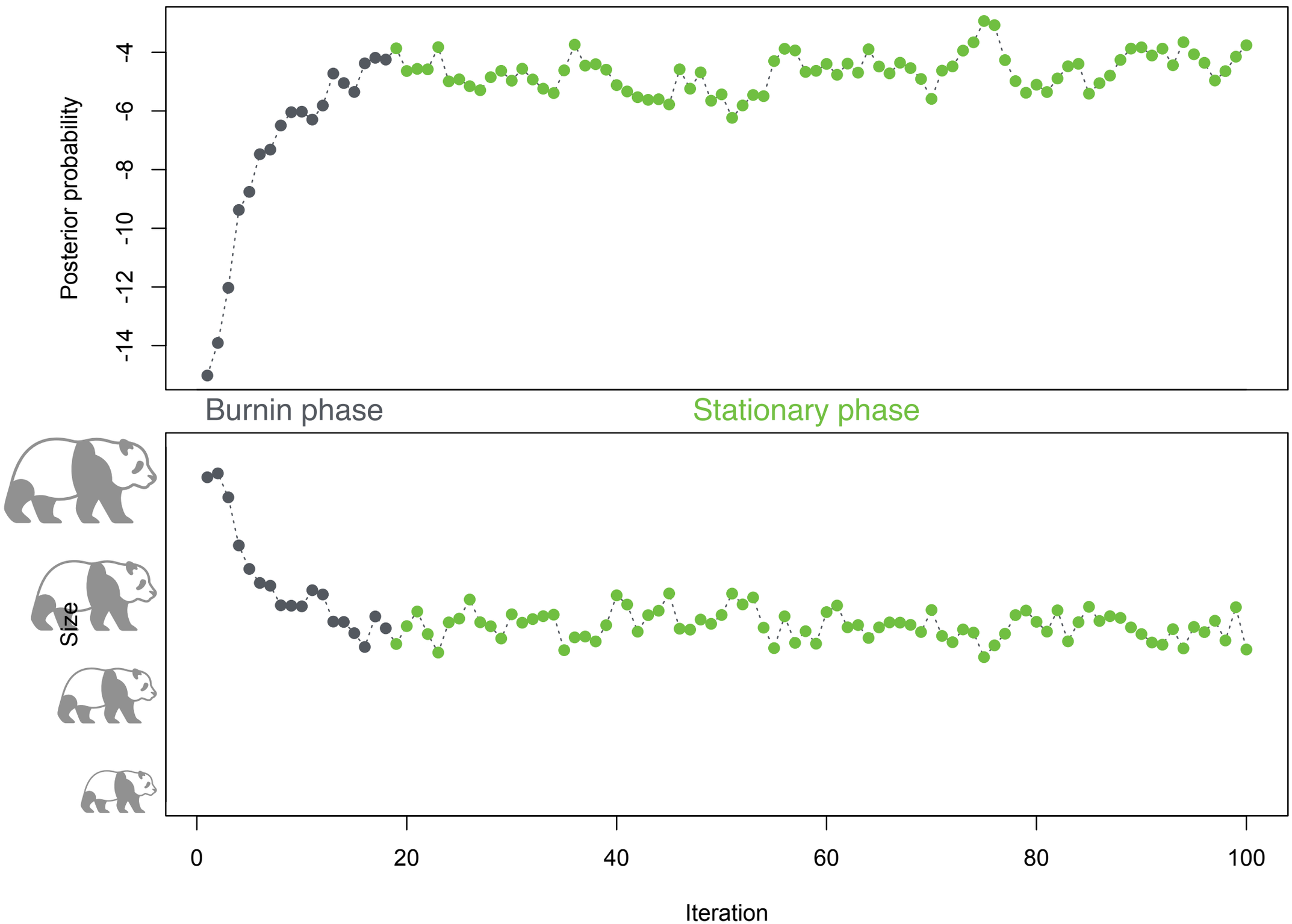
sampled value current value proposed value

Metropolis-Hastings MCMC

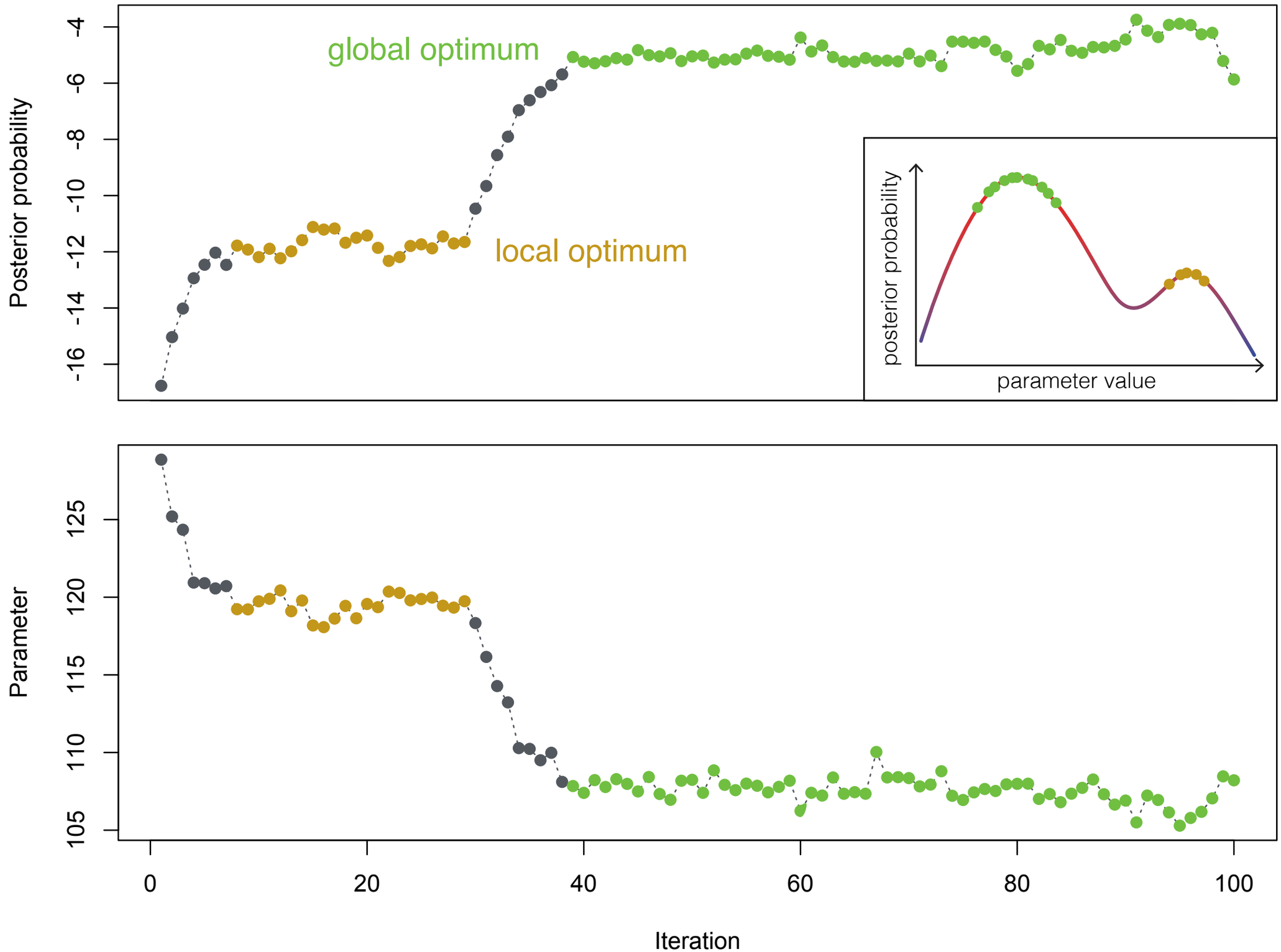


- Check MCMC convergence
- Summarize posterior parameters

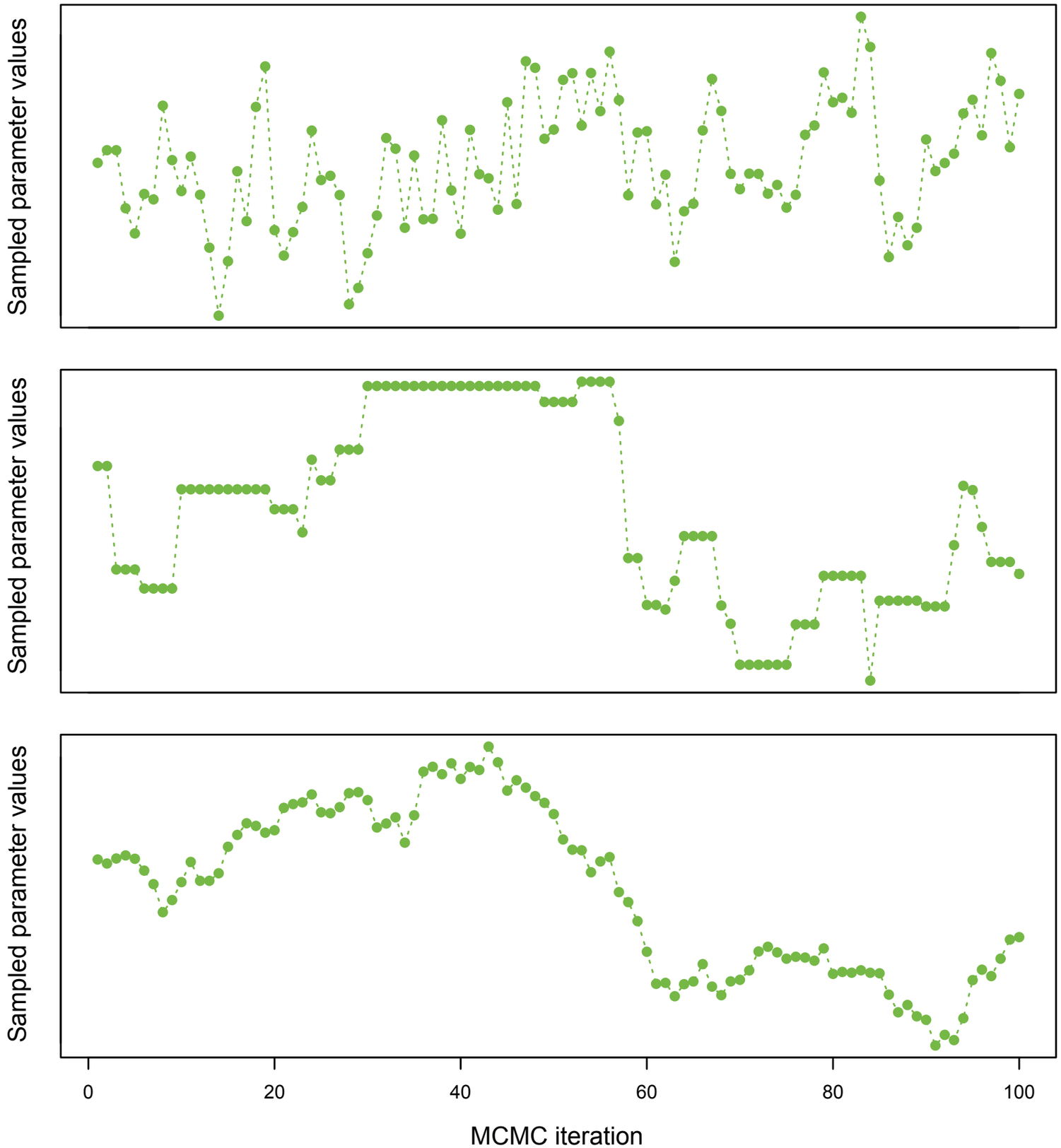
Burn-in and MCMC convergence



Burn-in and MCMC convergence



Posterior samples: Effective Sample Size (ESS)

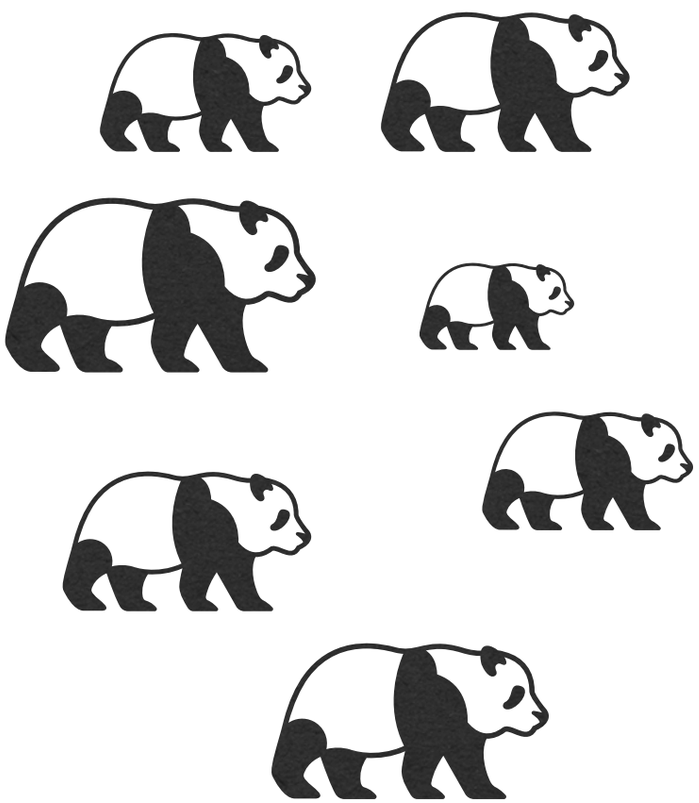


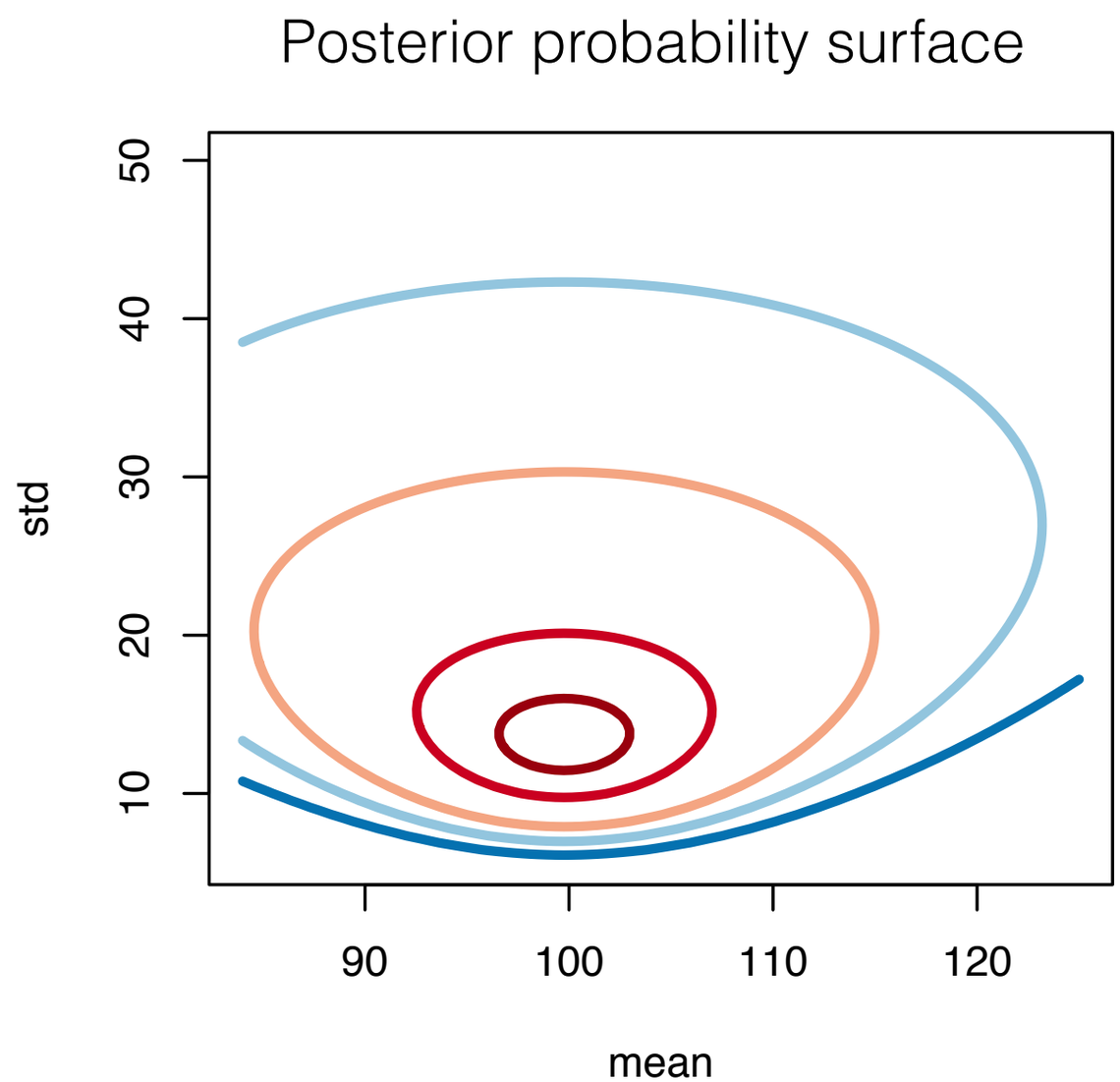
High ESS

Low ESS

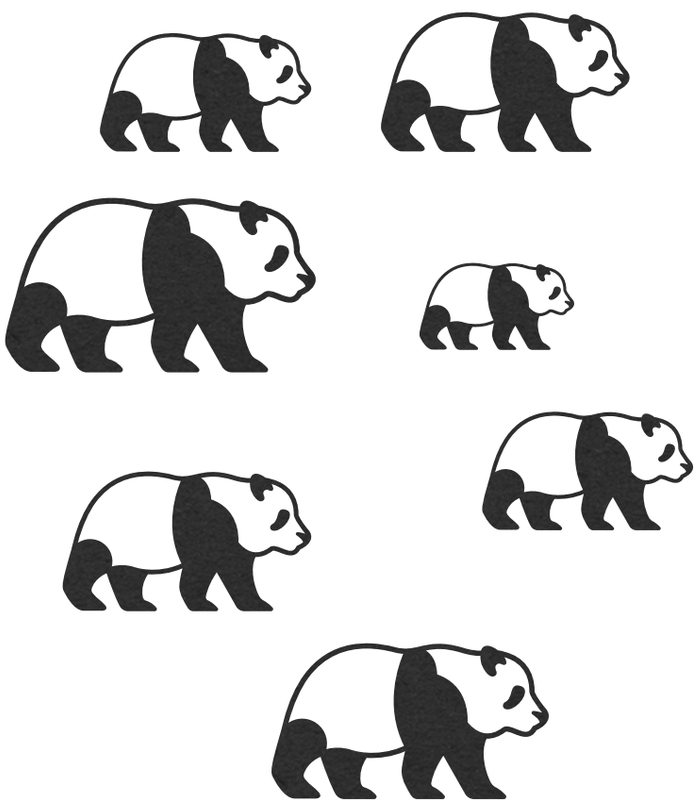
Low ESS

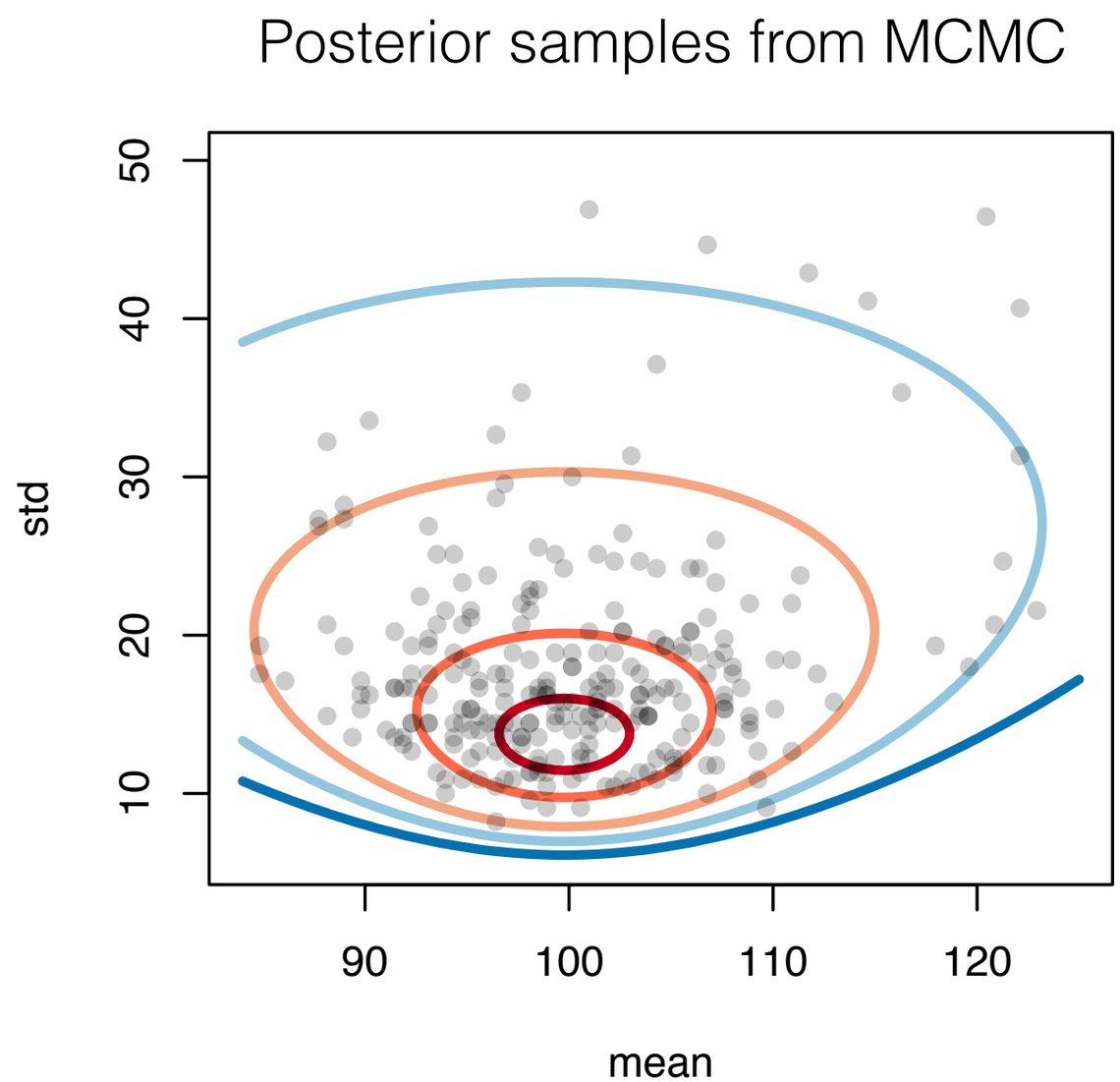
Summarizing MCMC samples



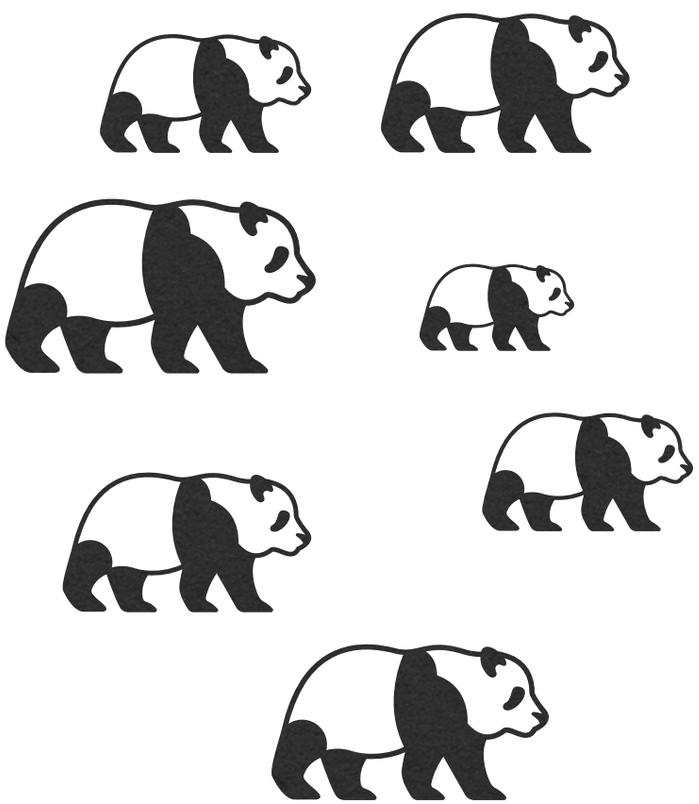


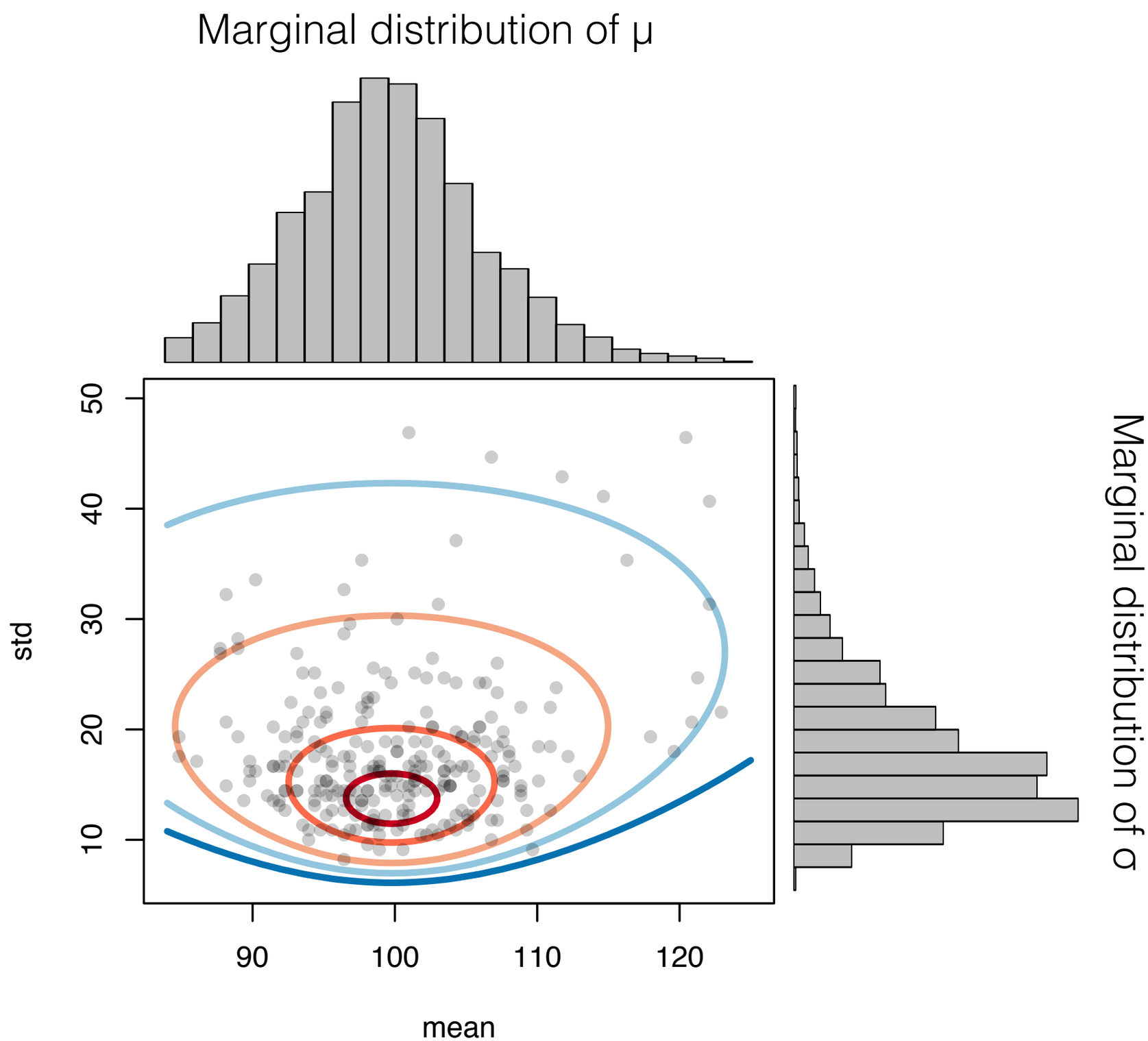
Summarizing MCMC samples



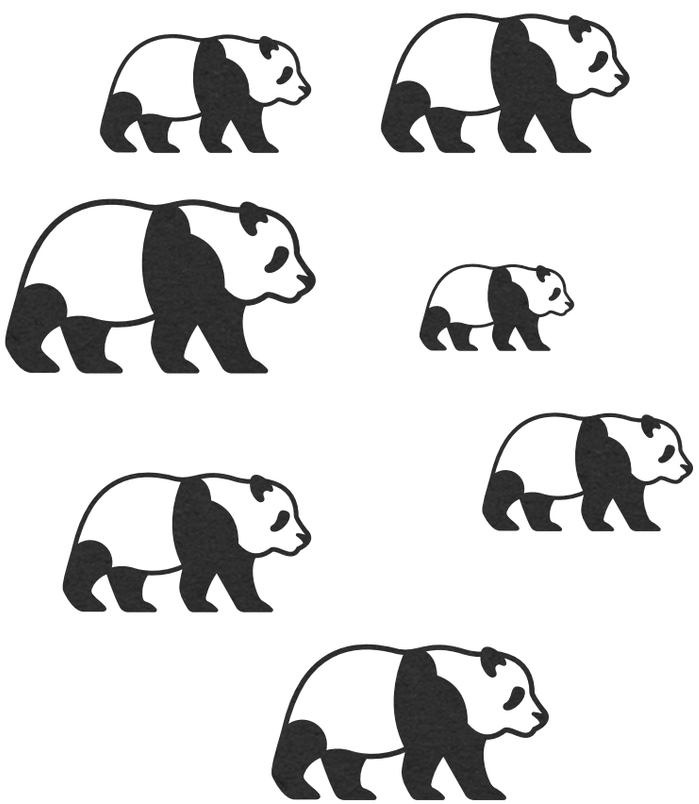
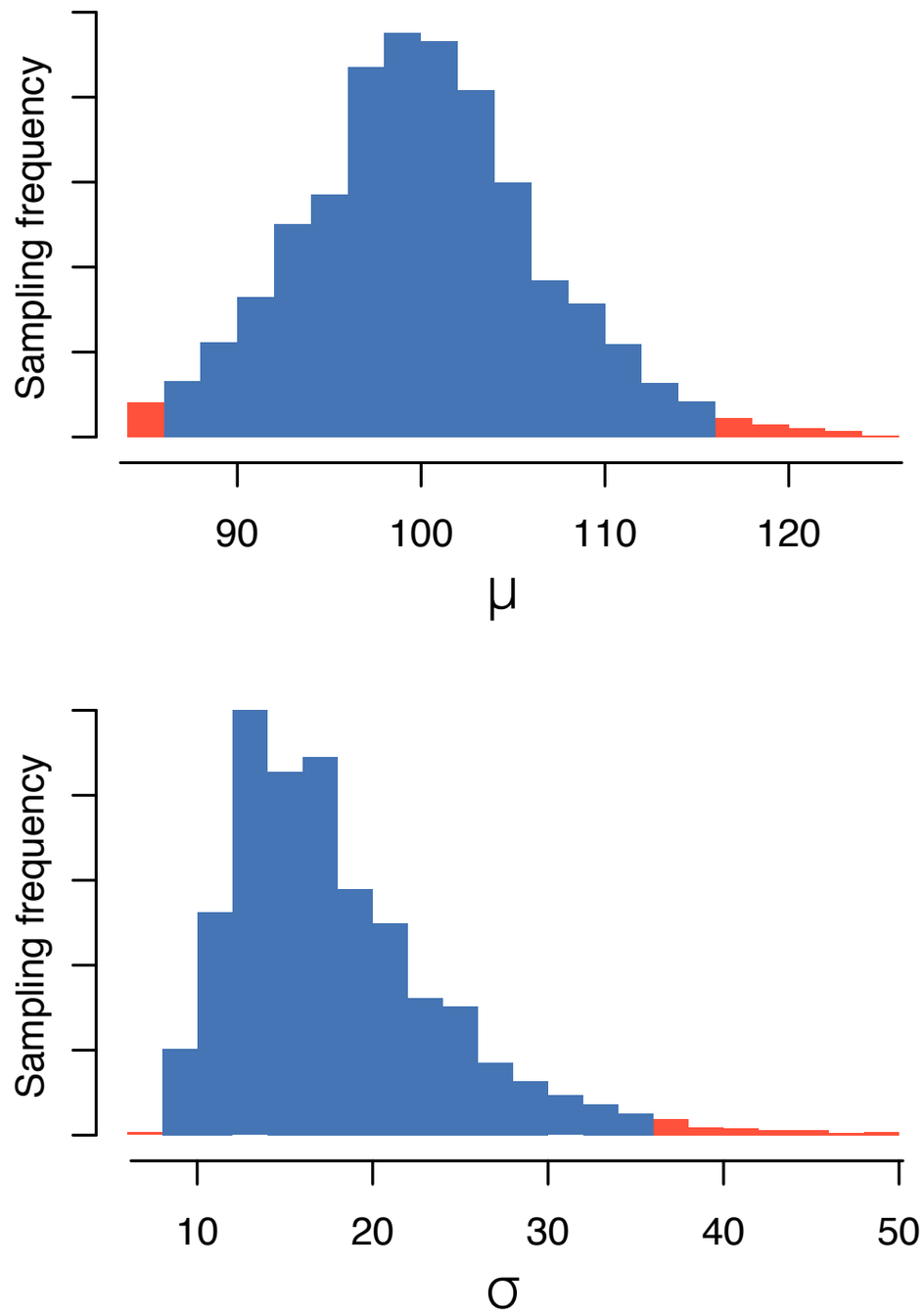


Summarizing MCMC samples





Summarizing MCMC samples

Posterior estimate: mean of MCMC samples

95% Credible intervals