# hoppMCMC: an adaptive basin-hopping Markov-chain Monte Carlo algorithm for Bayesian optimisation

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# Chapter 1

# Introduction

Bayesian methods have become increasingly popular in many disciplines of biology[16]. Advancement of computing power, accumulation of complex and noisy data together with the advantages of Bayesian methods compared to more conventional approaches foster their rapid adoption.

Canonical Markov-chain Monte Carlo (MCMC) algorithms, developed for sampling from the posterior distribution, have been extensively studied and improved[9, 8, 1, 3, 10]. A comprehensive review of the development of Bayesian computation was published in Green *et al.* 2015[7]. However, many algorithms still suffer from the choice of initial conditions, getting stuck at local minima and ineffective mixing of the chains.

Approximate Bayesian computation (ABC), specifically the methods propelled with sequential Monte Carlo (SMC)[14], offers a powerful alternative. Such algorithms are designed to deal with cases of unknown — or intractable — likelihoods. With the availability of specialised computational tools[11] they have become increasingly popular in the inference of dynamical models in epidemiology, biochemistry and systems biology[2, 17, 12]. However, despite the improvements in their efficiency[4, 6], numerical considerations still limit the size of systems such methods can deal with[12].

`hoppMCMC` circumvents the curse of dimensionality by quickly identifying the high-probability regions of the posterior and sampling locally for as long as it is permitted by computational resources. The algorithm improves mixing by adapting to the proposal distribution at certain intervals. It performs optimisation not only by varying the annealing temperature but also by applying an evolutionary concept and selecting for the optimum parameter set at regular intervals. This method can be used with a likelihood function, if available, or with an approximate Bayesian distance function.

## 1.1 Implementation

In a complex posterior distribution, there exist regions of high probability surrounded by regions of low probability. In essence, such low-probability regions prevent a Markov-chain from trespassing, and, thus, prevent sampling from the rest of the distribution. It is, therefore, important to identify these regions before attempting to sample blindly from the entire distribution.

`hoppMCMC` aims to identify and sample from the high-probability regions of a posterior with a combination of three strategies: (i) parallel MCMC[3], (ii) adaptive Gibbs sampling[10] and (iii) simulated annealing[5]. Overall, `hoppMCMC` resembles the basin-hopping algorithm of Wales and Doye, 1997[15], but is developed for a wide range of modelling approaches including stochastic models with or without time-delay.

Basin-hopping algorithm transforms the energy surface into its distinct basins of attraction to be able to jump from one basin to another and find the optimum[15]. `hoppMCMC` transforms the proximity of posterior modes the same way rendering each posterior mode achievable from another one with one or more hopp-steps, *i.e.* equivalent to basin-hopping steps. According to the Markov property, identity of the subsequent posterior mode depends only on the current, but not

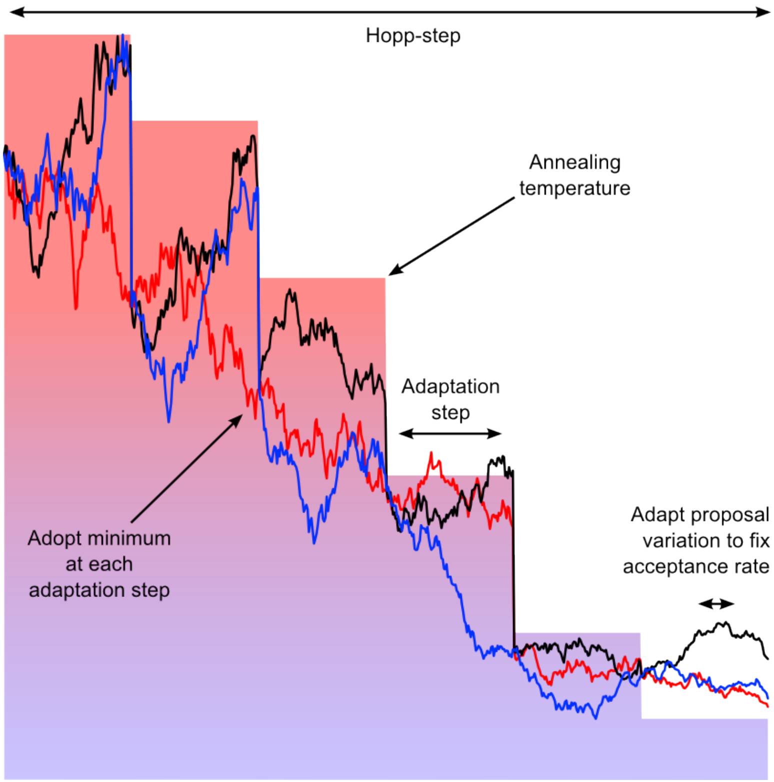

Hopp-step
Annealing temperature
Adaptation step
Adopt minimum at each adaptation step
Adapt proposal variation to fix acceptance rate

Figure 1.1: **Summary of the `hoppMCMC` algorithm.**

the previous ones.

A hopp-step is composed of a number of adaptation steps each with a specific annealing temperature, $T_i = \{T_0, \ldots, T_f\}$. The following algorithm describes an adaptation step, which comprises a single round of parallel iteration of $N$ independent MCMC chains, $\zeta$, with fixed annealing temperature. The essence of the `hoppMCMC` algorithm is also given in Figure 1.1.

1. `Initiate` $N$ `independent MCMC chains,` $\{\zeta_0, \ldots, \zeta_N\}$`, with the following configuration:`
   - `Initial value (`$\zeta_{\cdot 0}$`):` $x$
   - `Proposal variance:` $\sigma^2\Sigma$ `where` $\sigma^2 = 1$
   - `Annealing temperature:` $T = T_h$
2. `Iterate each chain for` $n$ `iterations maintaining an acceptance rate of` $1/2$ `by updating` $\sigma^2$ `in set intervals:`
   - `Acceptance probability:` $\text{Pr}(x, x', T)$
3. `Update the proposal distribution according to the following:`
   - $x = \texttt{min}\{\zeta_{\cdot n}\}$
   - $\Sigma = \texttt{var}\{\zeta_{\cdot n}\}$
   - $T = T_{h+1}$

The acceptance probability is defined as

$$\text{Pr}(x, x', T) = \min\left(1, \quad \exp\left\{\frac{f(x) - f(x')}{T}\right\}\right), \tag{1.1}$$

where $x'$ is the proposed value and $f$ is the objective function. In a Bayesian context, $f$ is defined as

$$f(x) = -\ln \text{Pr}(x), \tag{1.2}$$

where $\Pr(x)$ is the posterior probability of parameter $x$. Please note that when $\Pr(x)$ is Gaussian, $T$ acts as a scaling factor for standard deviation.

By default, `hoppMCMC` adopts an adaptive Gibbs sampling strategy where each chain is iterated sequentially along each parameter axis. Iterative Gibbs sampling could be numerically more stable than Metropolis-Hastings sampling especially for large number of parameters. Accordingly, a one-dimensional Gaussian distribution with variance $\sigma_i^2\Sigma_{ii}$ is used for each parameter axis $i$, and $\sigma_i^2$ is varied to regulate acceptance rate along each axis. When all the chains are iterated $n$ steps, $\Sigma$ is updated based on the variability across the final states of the chains. In essence, a two-step adaptation process is employed where $\sigma^2$ is updated within an adaptation step and $\Sigma$ at the end of it.

At the end of an adaptation step, annealing temperature is also updated and all chains are reset to begin with the parameter value minimising posterior probability in the last iteration. We observed that selecting for the single best parameter value aids in mixing of the chains in subsequent iterations. However, different evolutionary sampling strategies can also be employed.

`hoppMCMC` employs a sigmoidal cooling schedule where annealing temperature is updated according to the rule

$$T_{\text{low}} + (T_{\text{hi}} - T_{\text{low}}) \left(1 - \frac{1}{1 + e^{-\frac{12.5}{n}(x - 0.5\,n)}}\right). \tag{1.3}$$

In this equation, $T_{\text{low}}$ and $T_{\text{hi}}$ are the lower and higher bounds of annealing temperature, respectively, and $x$ is the chain length. This provides two important plateaus in temperature, one at the beginning and one at the end of each adaptation step. It allows sufficient time for adaptation of proposal distribution before and after cooling takes place.

The algorithm is iterated for an arbitrary number of hopp-steps to allow jumping from one posterior mode to another. At the end of each hopp-step, all chains relocate to a different mode or stay in place.

The probability that the current mode is accepted compared to the previous one is

$$\alpha = \frac{\Pr(\mu_2|\mathcal{D})}{\Pr(\mu_1|\mathcal{D})},$$

where $\mathcal{D}$ represents observation, and $\mu_i$ represents model $\mathcal{M}$ with parameters sampled around the $i^{\text{th}}$ posterior mode. If accepted, all chains retain their current configuration; otherwise, they are reversed to the previous state for the next hopp-step.

Although hopp-steps are likely to settle on posterior modes, they will not generate proper posterior samples. The following approximation is used to estimate the probability of retaining the current state or reversing back to the previous posterior mode.

$$\Pr(\mu_i|\mathcal{D}) = \Pr(\mathcal{M}_{\theta_i}|\mathcal{D}) \approx \frac{1}{n}\sum_{j=1}^{n} \frac{\Pr(\mathcal{M}_{\theta_{ij}}|\mathcal{D}, T_{\mathcal{M}})}{\Pr(\mathcal{M}_{\theta_{ij}})}, \tag{1.4}$$

where $n$ is the number of chains, and $\mathcal{M}_{\theta_{ij}}$ represents model $\mathcal{M}$ with parameter $\theta_{ij}$ from the $i^{\text{th}}$ hopp-step of the $j^{\text{th}}$ chain. $\Pr(\mathcal{M}_{\theta_{ij}}|\mathcal{D}, T_{\mathcal{M}})$ refers to the posterior probability calculated at temperature $T_{\mathcal{M}}$. This allows introducing an arbitrary tolerance for sampling posterior modes with low probabilities. In coherence with Eqn. 1.1, this probability is defined as

$$\Pr(\mathcal{M}_{\theta_{ij}}|\mathcal{D}, T_{\mathcal{M}}) = \exp\left\{-\frac{f(\mathcal{M}_{\theta_{ij}}|\mathcal{D})}{T_{\mathcal{M}}}\right\} = \exp\left\{\frac{\ln\Pr(\mathcal{M}_{\theta_{ij}}|\mathcal{D})}{T_{\mathcal{M}}}\right\}.$$

In Equation 1.4, $\Pr(\mathcal{M}_{\theta_{ij}})$ is the probability of the $j^{\text{th}}$ model-parameter combination with respect to the other chains. Gaussian kernel density estimator is used, from the scipy package, to arrive at an estimate for $\Pr(\mathcal{M}_{\theta_{ij}})$.

# Chapter 2

# Examples

To demonstrate the `hoppMCMC` algorithm we selected the Langermann's function and the drop wave function from the exhaustive list presented in Molga *et al.* 2005[13]. Despite having only two dimensions, $x$ and $y$, these functions provide multiple modes and different topological features.

We used the following Langermann's function,

$$f(x,y) = 4\left(6 + \sum_{i=1}^{m} c_i \exp\left\{-\frac{1}{\pi}(x-\alpha_i)^2 - \frac{1}{\pi}(y-\beta_i)^2\right\} \cos\left\{\pi(x-\alpha_i)^2 + \pi(y-\beta_i)^2\right\}\right),$$

where $m = 5$, $c = [1,2,5,3,5]$, $\alpha = [3,5,2,1,7]$, and $\beta = [5,2,1,4,9]$, and the following drop wave function,

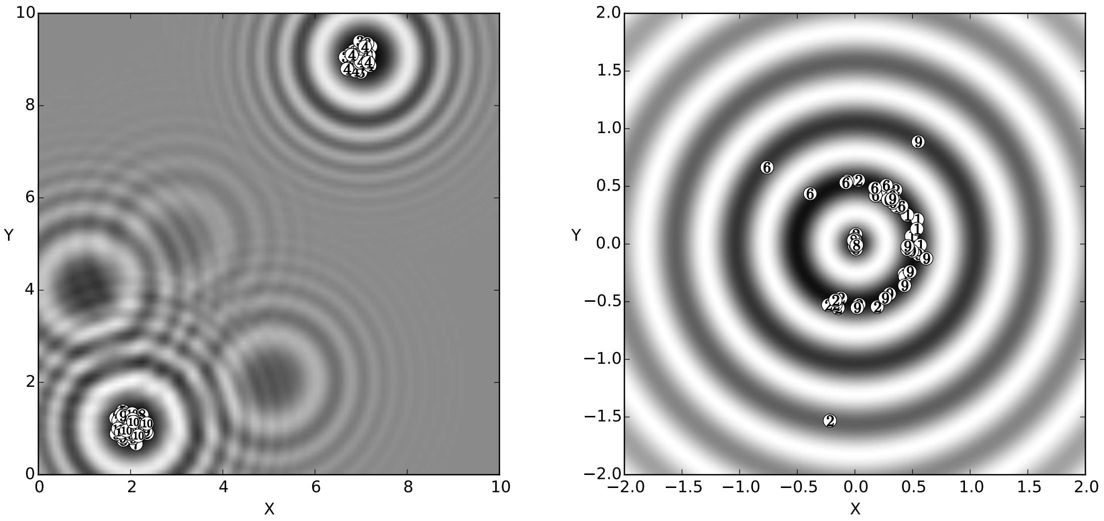
$$f(x,y) = 10\left(1 - \frac{1 + \cos\left(12\sqrt{(x^2+y^2)}\right)}{0.5\,(x^2+y^2) + 2}\right).$$

We assumed that these are proportional to the negative logarithm of posterior probability (Eqn. 1.2). We performed inference for $x$ and $y$ within the domain of $[0,10]$ for the Langermann's function and $[-5.12, 5.12]$ for the drop wave function. We iterated 12 parallel chains for 10 hopp-steps, while each hopp-step comprised 50 adaptation steps. During each adaptation step we allowed annealing temperature to drop from 10 to 1 (Eqn 1.3), and set $T_{\mathcal{M}} = 10$. In each adaptation step, we iterated the chains for 50 steps allowing $\sigma^2$ adaptation at every 10th step. This procedure sums up to a total of $3 \times 10^5$ steps. It is important to note, however, that each step of a chain comprises of 2 model simulations in accordance with the Gibbs sampling procedure. Therefore, at the end of all hopp-steps, a total of $6 \times 10^5$ function calls were performed.

As a result, the `hoppMCMC` algorithm successfully sampled from different local minima and identified the global minimum in both cases (Fig. 2.1). In Figure 2.1(a), we see that the two major modes of equal probability of the Langermann's equation were sampled, however, the remaining three with lesser probabilities were skipped. The reason for not sampling from these low-probability modes were their proximity to one of the high-probability modes and their relatively weak boundaries. During the annealing process, chains moved quickly to one of the major modes before further mode switches were prohibited by low annealing temperatures.

In Figure 2.1(b), we see that the algorithm performs equally well with circular posterior modes. As a result, the global minimum of the drop wave function and the circular local minimum immediately surrounding it were successfully identified.

Code is available in the `examples` directory to demonstrate the use of the package and to run the `hoppMCMC` algorithm with the selected objective functions.



(a) Langermann's function

(b) Drop wave function

Figure 2.1: **Testing the algorithm on multimodal score functions.** In (a) the Langermann's function and in (b) the drop wave function are given where the intensity of grey indicates low values, *i.e.* high probabilities. Points with numbers, $i$, indicate values of inferred parameters, $x$ and $y$, at the end of the $i^{th}$ hopp-step (see text).

# Chapter 3

# Conclusion

`hoppMCMC` is an algorithm for global optimisation, which is applicable for various modelling approaches frequently used in systems biology. With this algorithm, it is possible to effectively identify the maximum *a posteriori* estimate and avoid getting stuck at posterior modes with lower probabilities. The algorithm aims to sample from multiple high-probability posterior modes, but not to sample from the entire posterior distribution. This strategy, and the `hoppMCMC` algorithm, is effective in discovering the high-probability regions of the posterior to aid in subsequent analyses.

## 3.1 Acknowledgements

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