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Properties of the Parallel Tempering algorithm.

Praca magisterska
na kierunku MATEMATYKA

Praca wykonana pod kierunkiem
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Zakład Statystyki Matematycznej.

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Oświadczenie kierującego pracą

Potwierdzam, że niniejsza praca została przygotowana pod moim kierunkiem i kwalifikuje się do przedstawienia jej w postępowaniu o nadanie tytułu zawodowego.

Data Podpis kierującego pracą

Oświadczenia autora pracy

Świadom odpowiedzialności prawnej oświadczam, że niniejsza praca dyplomowa została napisana przeze mnie samodzielnie i nie zawiera treści uzyskanych w sposób niezgodny z obowiązującymi przepisami.

Oświadczam również, że przedstawiona praca nie była wcześniej przedmiotem procedur związanych z uzyskaniem tytułu zawodowego w wyższej uczelni.

Oświadczam ponadto, że niniejsza wersja pracy jest identyczna z załączoną wersją elektroniczną.

Data Podpis autora pracy

Abstract

Parallel Tempering (PT) is an extension to standard Metropolis-Hastings (MH) algorithm for simulating samples from a given distribution. The standard MH algorithm with high probability remains a local algorithm, in the sense that samples are drawn from some local probability mass cluster. This is highly problematic in case of multimodial distributions that frequently appear in applications, i.e. in bayesian hierarchical models. The PT algorithm is one of most celebrated possible solutions to that problem.

Here we present a newly developed template for running simulations written in the R statistical programming language. Being highly modular it provides a general tool for performing simulations with many user provided state-spaces.

Słowa kluczowe

Parallel Tempering, Metropolis-Hastings, Stochastic Simulations, R

Dziedzina pracy (kody wg programu Socrates-Erasmus)

11.2 Statystyka

Klasyfikacja tematyczna

ACM I.6.7.

Tytuł pracy w języku angielskim

Properties of the Parallel Tempering algorithm.

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Introduction

Parallel Tempering (PT) (also reffered to as Replica Monte Carlo Simulation) is an extension to standard Metropolis-Hastings (MH) algorithm for simulating samples from a given distribution, also called the target-distribution. The principle aim of the algorithm is to approximate the integrals

$$\mathcal{E}g(X) = \int_{\Omega} g(x) \mathrm{d}\,\Pi \tag{1}$$

where $X \sim \pi$, π is a measure, and g is some $\mathbb{L}^1(\Pi)$ function. In practical applications π has either a density function, or a probability function. The Metropolis-Hastings proceeds by creating a sequence of sample points, $\{X^{[i]}\}_{i=1}^{\mathrm{N}}$, from the limiting distribution of a certain operator, $\mathcal{Q}$, chosen so that its invariant distribution exists, is unique, and coincides with π. The approximation is then taken to be simply

$$\mathcal{E}g(X) \approx \frac{1}{\mathrm{N}} \sum_{i=1}^{\mathrm{N}} g(X^{[i]}).$$

The problem with the usual Metropolis-Hastings is that it has poor mixing abilities, so that the above approximations may be biased when π is multimodial. The Parallel Tempering provides a potential solution to this problem by enlarging the state space. Several copies of progressively modified operators are run on this space, the differences between them depending on one parameter only[1]. This parameter is traditionally called *the temperature*, because of the physical interpretion it had in the seminal work of Swendsen and Wang (1986).

The sample points created by individual operators are sometimes refered to as chains. The idea of simultaneous simulations is the first of two consituents of the Parallel Tempering, the other being that of interlacing results from different chains. The new distributions have their probability mass spread in regions around the clusters of probability of the target-measure in a less and less concentrated way. Consequently, simulations from these distributions explore more of the state-space at the cost of higher variance. The subsequent random interchange between samples generated from different chains enables the base-level chain, corresponding to the target distribution, to explore most of its structure resulting in simulations better estimates.

The applicability of the Parallel Tempering stems from the more and more widespread use of the Bayesian modeling. In fact, it is the need of calculating some the a posteriori distributions that in many cases has driven scientists to develop efficient sampling techniques in the first place. Nowadays the use of Bayesian models spreads from meteorology, to chemistry, from OCRs, to biogenetics. And in all of these fields it is very natural for the multimodial distributions at some point to appear.

[1] There are many similarities with the homotopy theory in this regard.

Chapter 1

Motivation

In this Chapter we motivate the use of the Parallel Tempering making use of an example widely-cited in the literature,see Baragatti *et al.* (2013) and Liang and Wong (2001).

As pointed out in the Introduction, the reason for using the Parallel Tempering is the multimodiality of the distribution of interest, π. In our simulations we assume to know the density function of π to be the following mixture of normal densities:

$$f(x) = \sum_{i=1}^{20} \frac{\omega_i}{\sigma_i \sqrt{2\pi}} \exp\Big(- \frac{(x-\mu_i)^{\mathrm{t}}(x-\mu_i)}{2\sigma_i^2} \Big), \tag{1.1}$$

where $\sigma_1 = \cdots = \sigma_{20} = 0.1$, $\omega_1 = \cdots = \omega_{20} = 0.05$, and where the means μ_i are given by

μ_1	μ_2	μ_3	μ_4	μ_5	μ_6	μ_7	μ_8	μ_9	μ_{10}
2.18	8.67	4.24	8.41	3.93	3.25	1.70	4.59	6.91	6.87
5.76	9.59	8.48	1.68	8.82	3.47	0.50	5.60	5.81	5.40

and

μ_{11}	μ_{12}	μ_{13}	μ_{14}	μ_{15}	μ_{16}	μ_{17}	μ_{18}	μ_{19}	μ_{20}
5.41	2.70	4.98	1.14	8.33	4.93	1.83	2.26	5.54	1.69
2.65	7.88	3.70	2.39	9.50	1.50	0.09	0.31	6.86	8.11

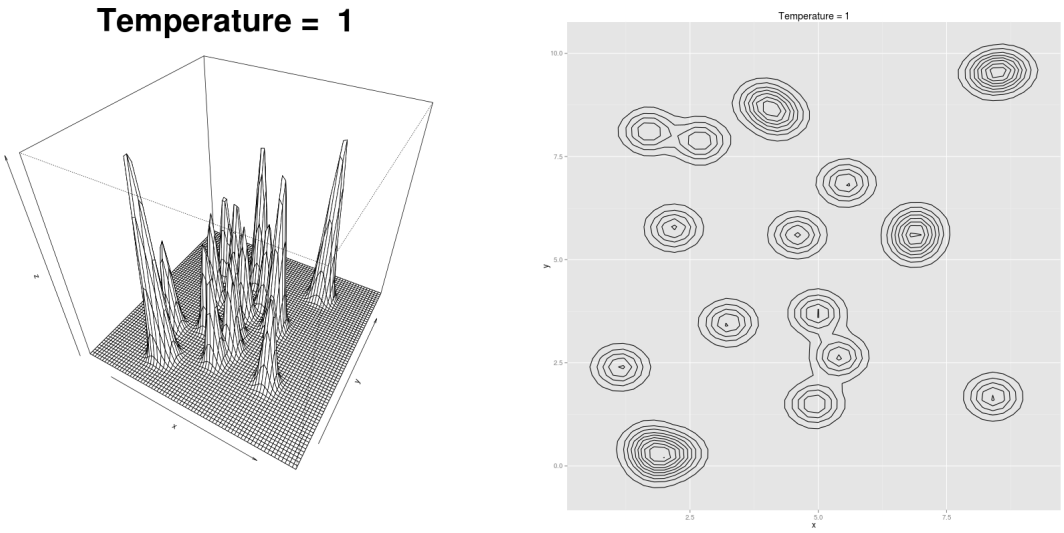
Figure 1.1 inspects visually the density. One notices easily that different peaks get intermingled, as only 15 out of 20 peaks are clearly visible.

The Metropolis-Hastings is known to be a local algorithm and the reasons for it will be exposed in Chapter 2. To motivate the use of the Parallel Tempering it is enough to say for now that sample points generated by the usual Metropolis-Hastings[1] will be more often drawn from the vicinity of modes. This in turn might give the impression that most of the probability is concentrated somewhere next to the starting points[2]. We shall refer to the percentages of iterations in the vicinity of a particular mode its sojourn time, without giving its full definition right now.

In theory, by the ergodic theory, the sojourn times for each mode should converge to the probabilities of the modes' vicinity areas. However, in practical terms, this convergence might be prohibitively long, especially to what a typical user would consider to be a fortunate amount of computation time. This is clearly a big problem, since in practical applications, as mentioned in the

[1]For introduction to the theory behind the Metropolis-Hastings algorithm consider Geyer (2012).

[2]We choose the starting points at random



(a) Perspective view

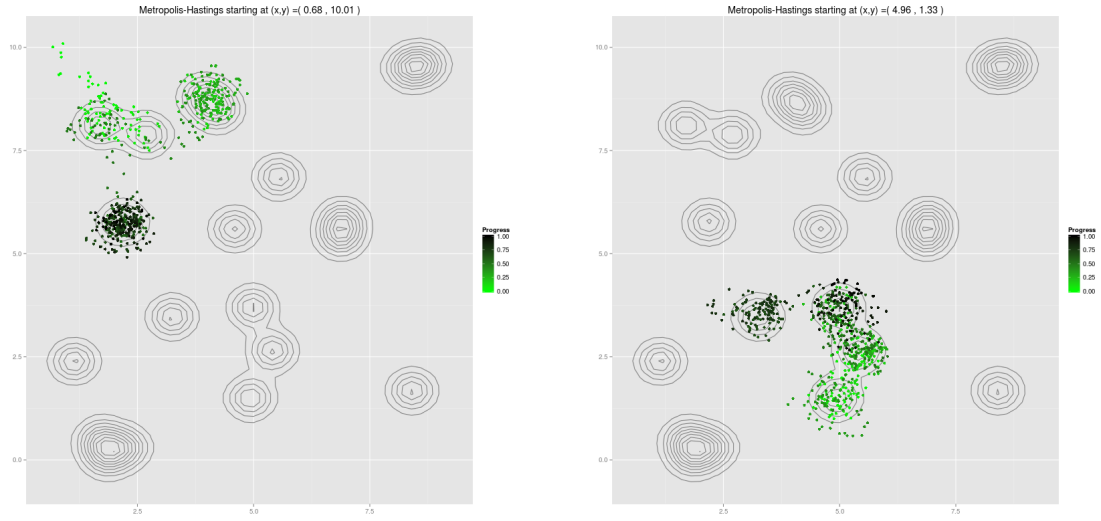
(b) Level-set view

Figure 1.1: Toy-example density.

Introduction, one considers the approximation of the needed integral to be simply the mean evaluation of a function on the generated sample point and these approximations cannot possibly be good if we cut the procedures too quickly.

To investigate the Metropolis-Hastings's localness, we have run the Metropolis routine choosing the State Space to be Real-Tempered. Figures 1.2 and 1.3 show that the localness of the algorithm is persistent even with longer runs of the Metropolis-Hastings.

Everything changes when one considers the Parallel Tempering instead, as seen in Figures 1.4 and 1.5.



(a) Thousand steps…

(b) …that lead nowhere.

Figure 1.2: Thousand Iterations of Metropolis-Hastings - about 250 different points generated. Colour intensity increases as points get generated in more advanced stages of the algorithm. One notices easily that short runs of the algorithm do not explore the whole State Space.

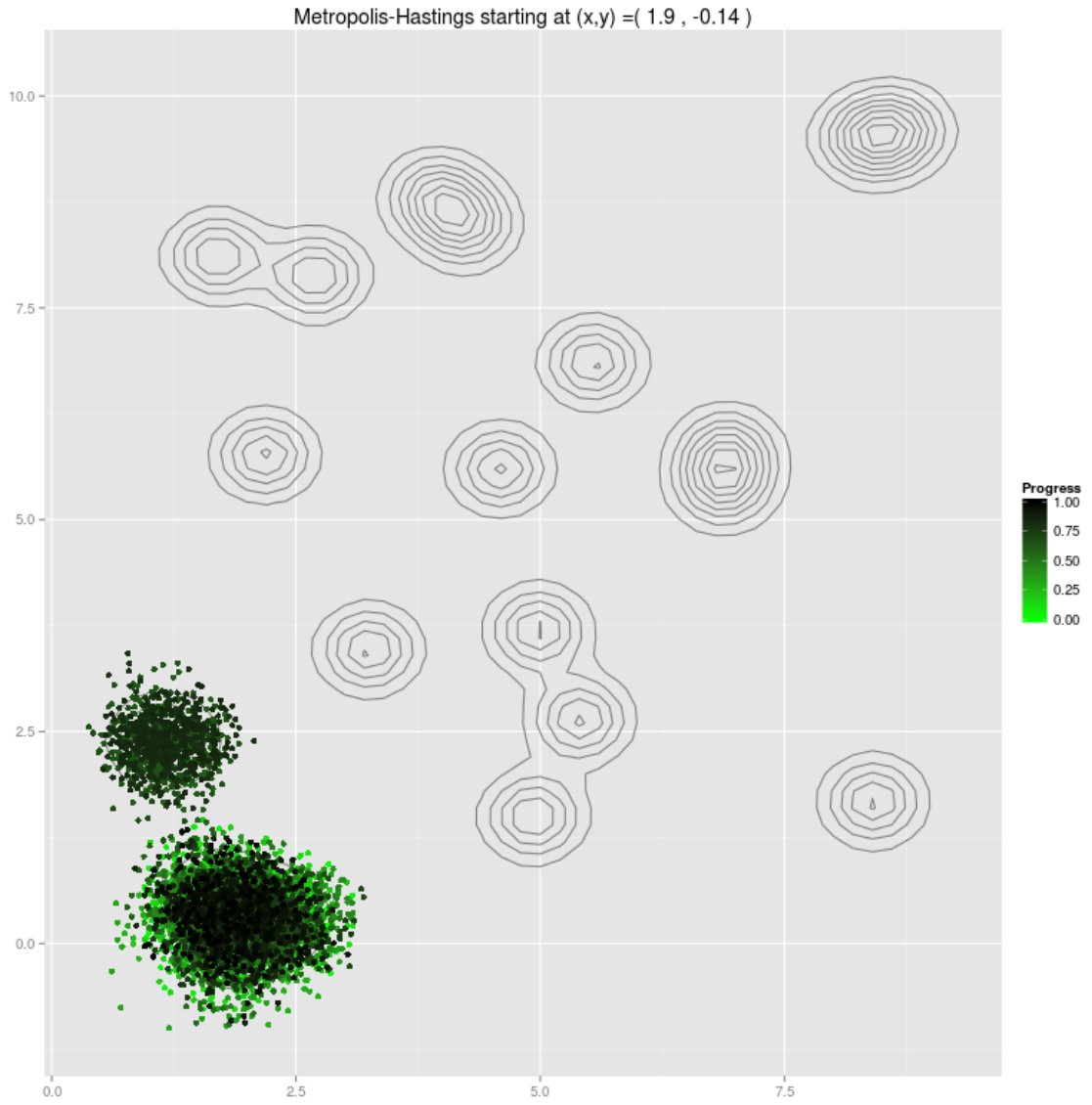
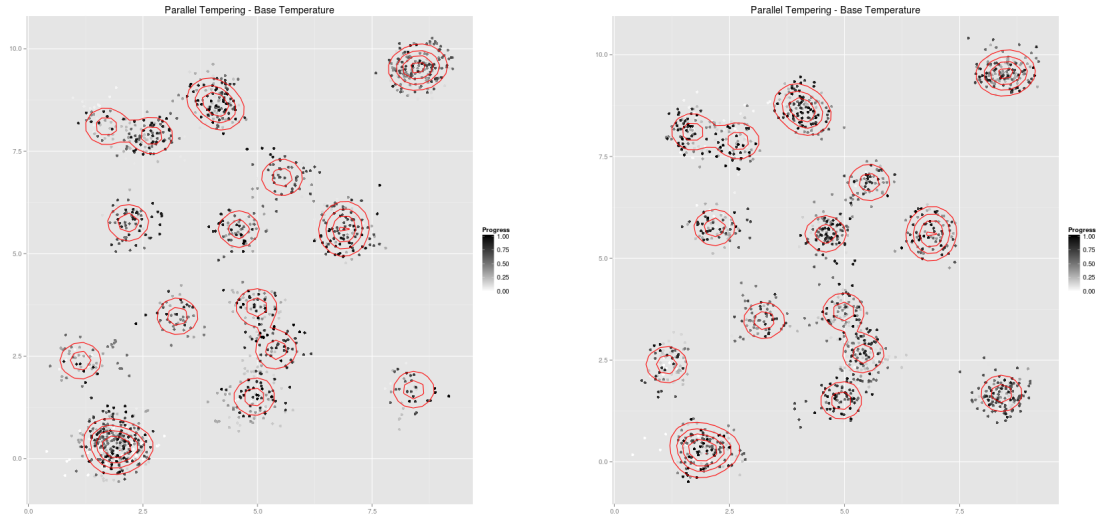


Figure 1.3: Ten Thousand Iterations of Metropolis-Hastings - about a quarter of which resulted in different points. Again the Metropolis-Hastings failed at exploring the whole State Space.



(a) Two thousand steps under Strategy 1....

(b) Two thousand steps under Strategy 2.

Figure 1.4: Results of the Parallel Tempering when and Strategy 2 from Chapter 2 are applied. One notices immediately the qualitative difference between these examples and the Metropolis-Hastings results, as the State Space is explored more thouroughly. The results are obtainable under a minute on a modern computer.

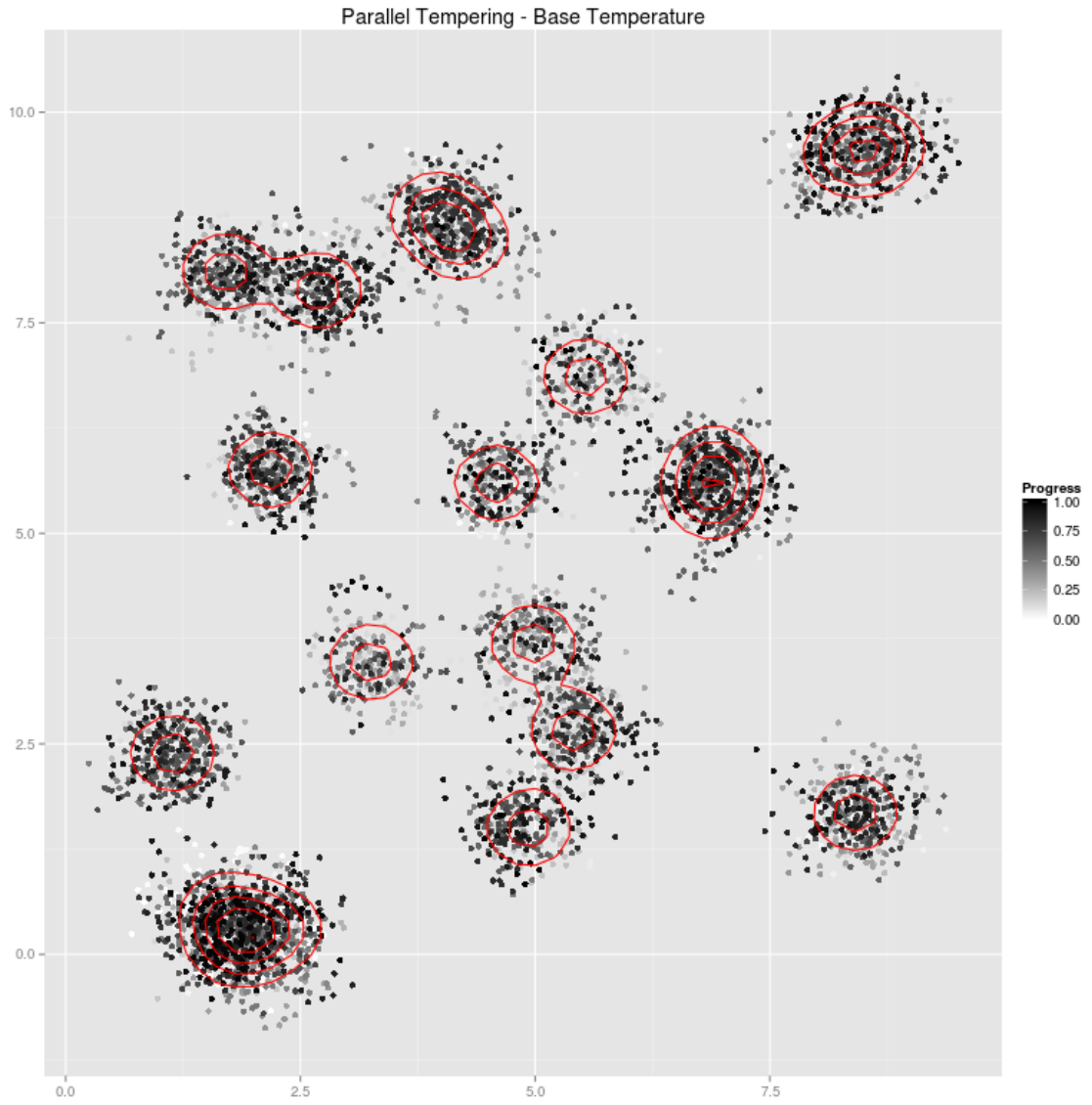


Figure 1.5: Ten Thousand Iterations of Parallel Tempering - about a quarter of which resulted in different points.

Chapter 2

Theory

In this chapter we shall expose the theoretical details of the Parallel Tempering. The following solutions are implemented in the prepared software, as described in Chapter 3.

Problem statement

Let $(\Omega, \mathfrak{F})$ be a measurable space. Ω — the State Space, a subset of a Polish space, and $\mathfrak{F}$ - countably-generated Borel subsets. Finally, denote the unit interval by $\mathcal{I} = [0, 1]$.

Problem Given a distribution $\Pi : \mathfrak{F} \mapsto \mathcal{I}$

- I absolutely continuous with respect to some measure on Ω, with a density π that we know to evaluate
- II density π known up to its proportionality factor
- III density π being multimodal

draw a sample $\{X_1, \ldots, X_N\}$ from Π so that for any function $g \in \mathbb{L}^1(\Pi)$ one can approximate well the integrals with empirical means

$$\int_\Omega g \, \mathrm{d}\, \Pi \approx \frac{1}{N} \sum_{i=1}^{N} g(X^{[i]}).$$

The rather abstract setting might seem to be an overshot, because, as the reader suspects, the most obvious and natural choice would be that of $\Omega = \mathbb{R}^N$ and $\mathfrak{F}$ the corresponding Borel sets. That, however, is not always the case — for very often one encounters some discrete spaces as well. Moreover, the abstract setting underlines the modularity of the implementation of the algorithm itself, being described in CHAPTER.

Had it been that π was not multimodal then by using the usual Metropolis-Hasting algorithm one could have easily solved the Problem. Adding condition III, however, makes the use of that algorithm problematic because of its localness — a phenomenon well visualised in CHAPTER.

The Parallel Tempering

The Parallel Tempering algorithm is based on the idea of extending our attention to the product space $(\Omega^L, \mathfrak{F}^{\otimes L}, \pi_\beta)$ equiped with a specific Markov chain[1]. The main idea is that on each copy of Ω

[1] Here $\mathfrak{F}^{\otimes L} \equiv \underbrace{\mathfrak{F} \otimes \cdots \otimes \mathfrak{F}}_{\text{L times}}$ is the usual product sigma algebra.

the corresponding chain will encounter a slightly modified version of the density of interest π. In the usual Parallel Tempering one settles for

Assumption I $\pi_\beta \propto \pi^{\beta_1} \times \cdots \times \pi^{\beta_L}$,

where $\beta = (\beta_1, \ldots, \beta_L)$ are such that $1 = \beta_1 > \cdots > \beta_L > 0$. Their inversions, $T_i = \frac{1}{\beta_i}$, called temperatures, do form therefore a growing sequence of numbers. This naming convention finds its origin in the use of the Parallel Tempering in Statistical Physics where the T_i parameters had direct interpretation.

We do stress that the normalising constants for each π^{β_l} are not assumed to be known, as we might not even know it for π itself.

A Markov Chain[2] $X \equiv \{X^{[k]}\}_{k\geq 0}$ is then constructed on Ω^L. Its construction makes explicit use of two kernels that make direct reference to π_l^β — first one, being a standard Random Walk, is responsible for the exploration of the State Space. The other, called the Swap, takes care of communication between different subchains — for X can also be thought of as being a collection of coordinate subchains

$$X^{[k]} = (X_1^{[k]}, \ldots, X_L^{[k]}).$$

Observe that the first subchain corresponds to the solution of the Problem.

The main idea behind the construction of chain X is that the subchains operating on tempered versions of π influence the subchains linked with lower temperatures by offering them their own accepted proposals. This should be highly beneficial, as more tempered chains will encounter less problems in accepting proposals from regions where the first chain would hardly ever stray.

To make this approach work at all we are still bound to make some other assumptions.

Assumption II The starting points $X^{[0]}$ are selected so that $\pi(X_l^{[0]}) > 0$ for $l \in \{1, \ldots, L\}$.

Obviously, what follows is that $\pi(X_l^{[0]})_k^\beta > 0$ as well. It is important, for otherwise, what will be demonstrated in the following sections, the algorithm would be dividing by 0 and break. Moreover, what follows from Assumption II is that the algorithm will never find itself in a point on which the density evaluates to zero.

The choice of modifying π by exponentiation, as in Assumption I, besides its simplicity[3], has considerable advantages in the analysis of the algorithm. For in the Random Walk phase of the algorithm's step suppose a proposal y is generated by the l^{th} chain from a region with less Π probability on it in comparison to the position x occupied in the last step, so that $\pi(y) < \pi(x)$. What follows,

$$\alpha_{\beta_l}(x,y) = 1 \wedge \left(\frac{\pi(y)}{\pi(x)}\right)^{\beta_l} = \left(\frac{\pi(y)}{\pi(x)}\right)^{\beta_l} > \frac{\pi(y)}{\pi(x)} = 1 \wedge \frac{\pi(y)}{\pi(x)} = \alpha_{\beta_1}(x,y),$$

which means that the probability of accepting such a proposal is larger on the more tempered chains. On the other hand, if $\pi(y) > \pi(x)$, then this probability remains the same, $\alpha_{\beta_1}(x,y) = \alpha_{\beta_k}(x,y)$. This assures that more tempered chains can make longer excursions into regions not so much Π-probable.

One cannot neglect one possibility though: if the support of π is not connected and the connected components are far away then it is highly improbable that the algorithm will give unbiased results because of poor mixing that cannot be fixed by exponentiation and some other technique should be

[2]For the algorithm step numbering we shall henceforth use the square brackets notation.

[3]For in general one could settle for some other kind of homotopic deformation.

used. We stress this point because in computer simulations one might tumble upon this problem because of the finite arithmetic — the rounding of numbers to zero.

As pointed out before, the update mechanism of the Parallel Tempering consists of two stages. Assume that the algorithm has reached n^{th} step, $X^{[n-1]}$. Following notation used in Miasojedow, Moulines and Vihola (2013a), we introduce two kernels that act subsequently on $X^{[n-1]}$

$$X^{[n-1]} \overset{M_{\Sigma,\beta}}{\to} \widetilde{X}^{[n-1]} \overset{\mathcal{S}_\beta}{\to} X^{[n]}.$$

We shall refer to $\mathcal{S}_\beta$ and $M_{\Sigma,\beta}$ as to the swap kernel and the random-walk kernel respectively[4]. These will be now presented in greater detail.

The Random Walk Kernel

Take a point in the State Space, $x = (x_1, \ldots, x_{\mathrm{L}}) \in \Omega^L$. To assign probabilities to the proposal of the next step, given x, we consider events $A_i \in \mathfrak{F}$. We shall assume that

Assumption III Random Walk proposal generation occurs independently on all subchains

$$M_{\Sigma,\beta}(x, A_1 \times \cdots \times A_L) = \prod_{l=1}^{L} M_{\Sigma_l,\beta_l}(x_l, A_l).$$

The $M_{\Sigma_l,\beta_l}(x_l, A_l)$ corresponds to standard Metropolis kernel, as in Geyer (2012). To be more precise

$$M_{\Sigma_l,\beta_l}(x_l, A_l) \equiv \int_A \alpha_{\beta_l}(x_l, y_l) q_{\Sigma_l}(y_l - x_l) \mathrm{d}y_l + \mathbb{I}(x_l, A) r(x_l) \tag{2.1}$$

where

$$r(x_l) = \int [1 - \alpha_{\beta_l}(x_l, y_l)] q_{\Sigma_l}(y_l - x_l) \mathrm{d}y_l$$

is the probability of not accepting the proposal and the subprobability density of accepting the update [5] is

$$\alpha_{\beta_l}(x_l, y_l) \equiv 1 \wedge \frac{\pi^{\beta_l}(y_l)}{\pi^{\beta_l}(x_l)}. \tag{2.2}$$

To understand why M_{Σ_l,β_l} is given by Eq. 2.1 we note that the role of the kernel is to assign probability to the next step of the algorithm given that the previous one assumed value x[6]. The Metropolis-Hastings algorithm goes as follows[7]:

Algorithm 2.0.1 (Metropolis-Hastings).
Require: *$X^{[0]}$ such that $\pi(X^{[0]}) \neq 0$*
  procedure Metro*($X^{[0]}$, N)*
    for $n \in \{0, \ldots, N-1\}$ ***do***
      Draw proposal $Y \sim q(X^{[n]}, y)\mathrm{d}\, y$
      Draw $U \sim \mathcal{U}(0,1)$
      if $U \leq \alpha(X^{[n]}, Y)$ ***then***

[4] M as Metropolis.
[5] Also known as the Hastings ratio.
[6] So we abstract here from how the actual value x was obtained, being mysteriously revailed to us by Nature, under the guise of random number generator. In fact kernels and their duals play principal role in the Bayesian statistics.
[7] We omit the inverse temperatures for time being.

$X^{[n+1]} \leftarrow Y$
else
$X^{[n+1]} \leftarrow X^{[n]}$
end if
end for
end procedure

Therefore, one should assign probability to event $\{X^{[n+1]} \in A\}$ for all $A \in \mathfrak{F}$. But this is done, as

$$\int_A \alpha(x,y)q(x,y)\mathrm{d}\,y = \int_A \mathcal{P}\Big(U \leq \alpha(x,y)\Big)q(x,y)\mathrm{d}\,y =$$
$$= \int_A \mathcal{P}\Big(U \leq \alpha(x,Y)|Y=y\Big)q(x,y)\mathrm{d}\,y = \mathcal{P}\Big(U \leq \alpha(x,Y), Y \in A\Big) =$$
$$= \mathcal{P}\Big(X^{[n+1]} \neq X^{[n]}, X^{[n+1]} \in A\Big)$$

where we assume Y to be drawn out of the proposal distribution and U to be independent of it. Setting $A = \Omega$ one notices that[8]

$$\mathcal{P}\Big(X^{[n+1]} = X^{[n]}\Big) = \int [1-\alpha(x,y)]q(x,y)\mathrm{d}\,y = r(x)$$

— precisely as claimed.

In the above equations the proposal distribution being used, following notation from Geyer (2012), is $q(x_l, y_l) = q_{\Sigma_l}(y_l - x_l)$, where q_{Σ_l} is the density of $\mathcal{N}(0, \Sigma_l)$.

The simple form of Eq. 2.2 stems from proposal distribution symmetry,

$$q(x_l, y_l) = q(y_l, x_l).$$

The choice of α is motivated by assuring the self-adjointness of the $M_{\Sigma,\beta}$ operator, which in turn implies that distribution Π is preserved, so that

$$\Pi M_{\Sigma,\beta} = \Pi. \tag{2.3}$$

As indicated by Miasojedow *et al.* (2013b), the implementation of $M_{\Sigma,\beta}$ consists of separate simulation of M_{Σ_l,β_l} for each of the coordinate chains, $X_l^{[n-1]}$.

The swap kernels

Now we address the question of how to interlace the independent chains generated with kernel $M_{\Sigma,\beta}$. We want to swap the generated states so that chains with higher temperature influence the regions of lower temperatures. Being more precise, the swapping gives some possibility to the chains with lower temperatures to find themeselves in states that would otherwise be very unlikely to happen, the path leading to them being very unlikely to occur - these paths are rendered more probable for the chains with higher temperature. The swaps are made at random so that the probability of swaps takes into account some properties of π evaluated on the last points from all the chains.

Before passing to detailed description of different ways the swaps might be made, which we call Strategies, let us first describe the properties of the swap kernel $\mathcal{S}_\beta$ common to all Strategies. In all cases, we rely on the following assumption

[8] Under the sensible assumption that the proposal distribution does not have any atom in x — this is usually automatically assumed by considering a distribution that is absolutely continous w.r. to Lebesgue measure.

ASSUMPTION IV At one step of the algorithm, there will be only one possible swap between a chosen at random pair of coordinates.

The restriction here is not so much in the number of swaps per step. What seems to be more relevant is rather the constraint to a particular subset of the group of all permutations — for one could certainly envisage that any random permutation could take place. However, it simplifies the interpretation of STRATEGIES that are to be described.

Let us denote the swap operator by S_{ij}, so that

$$S_{ij}x = (x_1, \dots, x_{i-1}, x_j, x_{i+1}, \dots, x_{j-1}, x_i, x_{j+1}, \dots, x_L).$$

We require $\mathcal{S}_\beta(x, \circ)$ to be a measure concentrated on the set of all possible pairs of swaps between coordinates of $x = (x_1, \dots, x_L)$, i.e. on the set $\mathfrak{S}_x \equiv \{S_{ij}x : i < j\}$. We note that the proposal measure for the swap kernel $\mathcal{Q}$ is of the following form

$$\mathcal{Q}(x, A) \equiv \sum_{i<j} p_{ij}(x) \mathbb{I}_A(S_{ij}x)$$

Then, the swap kernel would be of the following form, for any $x \in \Omega^L$ and A

$$\mathcal{S}_\beta(x, A) = \int_A \alpha_{\text{swap}}(x, y)\mathcal{Q}(x, \mathrm{d}\, y) + r(x)\mathcal{I}(x, A)$$

where $r(x) = 1 - \int\limits_{\Omega^L} \alpha_{\text{swap}}(x, y)\mathcal{Q}(x, \mathrm{d}\, y)$. Plugging $\mathcal{Q}$ permits us to write

$$\begin{aligned}\int_A \alpha_{\text{swap}}(x, y)\mathcal{Q}(x, \mathrm{d}\, y) &= \sum_{i<j} p_{ij}(x) \int \alpha_{\text{swap}}(x, y)\mathbb{I}_A(y)\delta_{S_{ij}x}(\mathrm{d}\, y) \\ &= \sum_{i<j} p_{ij}(x)\alpha_{\text{swap}}(x, S_{ij}x)\mathbb{I}_A(S_{ij}x),\end{aligned}$$

so that finally

$$\mathcal{S}_\beta(x, A) = \sum_{i<j} p_{ij}(x)\alpha_{\text{swap}}(x, S_{ij}x)\mathbb{I}_A(S_{ij}x) + \Big(1 - \sum_{i<j} p_{ij}(x)\alpha_{\text{swap}}(x, S_{ij}x)\Big)\mathcal{I}(x, A),$$

where

$$\alpha_{\text{swap}}(x, y) = \frac{\pi_\beta(\mathrm{d}\, y)\mathcal{Q}(y, \mathrm{d}\, x)}{\pi_\beta(\mathrm{d}\, x)\mathcal{Q}(x, \mathrm{d}\, y)} \wedge 1$$

is the Radon-Nikodym derivative of two measures. It's calculated with respect to measure $\mu(\mathrm{d}\, x, \mathrm{d}\, y) \equiv \pi(\mathrm{d}\, x)\mathcal{Q}(x, \mathrm{d}\, y)$. The measure that is being differentiated is μ composed with the exchange coordinates operation, $R(x, y) = (y, x)$[9]. So finally $\alpha_{\text{swap}} \equiv \frac{\mathrm{d}\,\mu \circ R^{-1}}{\mathrm{d}\,\mu}$.

Observe that thanks to the proposal's support finiteness we actually get

$$\alpha_{\text{swap}}(x, y) = \frac{\pi_\beta(y)\mathcal{Q}(y, x)}{\pi_\beta(x)\mathcal{Q}(x, y)} \wedge 1.$$

Now, since $y \in \mathfrak{S}_x$, the tagetted π_β is a tensor of measures, $Q(x, S_{ij}x) = p_{ij}(x)$, and $Q(S_{ij}x, x) = p_{ij}(S_{ij}x)$ [10], we get finally

[9] Which is obviously measurable in the appropriate sense.

[10] Here we pass from measure notation to probability function notation, $\mathcal{Q}(x, \{S_{ij}x\}) = \mathcal{Q}(x, S_{ij}x)$. We can do it because $\mathcal{Q}$ is purely atomic given x.

$$\alpha_{\text{swap}}(x, S_{ij}x) = \Big[\Big(\frac{\pi(x_j)}{\pi(x_i)}\Big)^{\beta_i-\beta_j}\frac{p_{ij}(S_{ij}x)}{p_{ij}(x)}\Big] \wedge 1$$

In our computer simulations several swapping strategies have been tested. For instance,

STRATEGY I $p_{ij}(x) \propto \frac{\pi(x_j)}{\pi(x_i)} \wedge \frac{\pi(x_i)}{\pi(x_j)} = \exp\Big(-\big|\log(\pi(x_j)) - \log(\pi(x_i))\big|\Big)$.

In this particular the proportionality is in fact equality, because the above expression is transposition symmetric and this considerably simplifies the statistical sum analysis. In general, we want $p_{ij}(x) \propto h(x_i, x_j)$ for some function h. Thus,

$$\frac{p_{kl}(S_{kl}x)}{p_{kl}(x)} = \frac{\frac{h(x_l,x_k)}{A(\tilde{x}_{kl})+f(x_k)+g(x_l)+h(x_l,x_k)}}{\frac{h(x_k,x_l)}{A(\tilde{x}_{kl})+f(x_l)+g(x_k)+h(x_k,x_l)}} = \underbrace{\frac{h(x_l,x_k)}{h(x_k,x_l)}}_{\text{'direct effect'}} \times \underbrace{\frac{A(\tilde{x}_{kl})+f(x_l)+g(x_k)+h(x_k,x_l)}{A(\tilde{x}_{kl})+f(x_k)+g(x_l)+h(x_l,x_k)}}_{\text{'distribution effect'}},$$

where $\tilde{x}_{kl}$ is x without its k^{th} and l^{th} coordinates, $f(x_l) = \sum_{i<l, i\neq k} h(x_i, x_l)$, and $g(x_k) = \sum_{j>k, i\neq l} h(x_k, x_j)$. As we see it is fairly straightforward to compare the above expression to 1 if the 'distribution effect' equals 1, and difficult had it been the other case. To assure this happens, one can settle for a function h that is transposition invariant, $h(x, y) = h(y, x)$. This is certainly the case of STRATEGY I. In this strategy therefore we are promoting exactly swaps between coordinates whose proposals have relatively the same π density values, i.e. $\pi(x_j) \approx \pi(x_i)$.

STRATEGY II $p_{ij}(x) \propto \frac{\pi(x_j)}{\pi(x_i)} \wedge 1 = \exp\Big(-\big[\log(\pi(x_j)) - \log(\pi(x_j))\big]\Big) \wedge 1$.

This strategy breaks the symmetry of the previous one rendering the evaluation of the effect on the α_{swap} challenging, if not impossible. The main idea behind this strategy was to

The subsequent strategies are again functions of the fist strategy.

STRATEGY III $p_{ij}(x) \propto \Big(\frac{\pi(x_j)}{\pi(x_i)} \wedge \frac{\pi(x_i)}{\pi(x_j)}\Big)^{|\beta_i-\beta_j|} = \exp\Big(-|\beta_i - \beta_j| \times \big|\log(\pi(x_j)) - \log(\pi(x_i))\big|\Big)$.

This strategy permits us to soften a bit the requirement that $\pi(x_j) \approx \pi(x_i)$. This effect is strengthened for coordinates that are similarly tempered, i.e. where $\beta_i - \beta_j \approx 0$. Swaps between adjacent chains will be therefore more probable.

One can also use a strategy that incorporates some distance measure between points, ρ being any quasi-metric. STRATEGY IV is a good example of such procedure - the more distant the points, the less probable it is for them to get swapped.

STRATEGY IV $p_{ij}(x) \propto \Big(\frac{\pi(x_j)}{\pi(x_i)} \wedge \frac{\pi(x_i)}{\pi(x_j)}\Big)^{\frac{|\beta_i-\beta_j|}{1+\rho(x_i,x_j)}} = \exp\Big(-\frac{|\beta_i-\beta_j|\times|\log(\pi(x_j))-\log(\pi(x_i))|}{1+\rho(x_i,x_j)}\Big)$.

Finally, for purposes of comparisons with Baragatti *et al.* (2013), we include also strategies that are STATE SPACE independent, i.e. the probability of swaps does not depend on the evaluations of the density π in the sample points. Such naïve strategies include

STRATEGY V $p_{ij} = \frac{2}{\text{L(L}-1)}$

and

STRATEGY VI $p_{ij} = \frac{1}{\text{L}-1}\mathbb{I}_{\{|i-j|=1\}}$

amounting to choosing uniformly among all possible swaps and all neighbouring-in-temperature swap respectively.

Chapter 3

Implementation

In this chapter we will present the implementation of the Parallel Tempering algorithm, as described in Chapter 2.

The analysis of the algorithm in all its complexity called for the development of a more structurised template for carrying out numerical computations. The Parallel Tempering algorithm, being an extension to the Metropolis-Hastings algorithm, does naturally share many similarities its structure. Both algorithms can have very abstract formulations and can be carried out theoretically on any countably- generated measurable space. Practical considerations would never go that far. However, one cannot, in principle, discard the use of Stochastic Simulations in solving many real-life modelling problems such as, for instance, the Bayesian model selection, or Ising-type modelling of crystallic structures. The mulitude of potential applications calls for a reasonably flexible implemention of the Parallel Tempering algorithm. To overcome these problems, the object-oriented paradigm was used in this work, so that the State Space and the Algorithm were two separate entities.

Having realised the need for modularity, it seemed natural to take the whole idea one step further and develop a general template for Metropolis-Hastings-like simulations, going way beyond the idea of a task-specific computer programme. For there are other potential developments of the Metropolis-Hastings algorithm that are being used, all baring strong similarities in stuctures of these algorithms. Our template's goal was therefore to provide basic building blocks used for simulations, leaving the practitioners concentrate on the analysis. The template is codenamed stochasticSimulations and that shall be the **R** package name when shipped.

R offers several implemented meta-structures that enable basic object oriented programming techniques. Among these there are the **S3** classes, **S4** classes, and the most recent Reference Classes. The implementation the template, was carried out using Reference Classes. This choice was dictated by several reasons. First, only **S4** classes and Reference Classes offer the possibility of basic type verification[1]. This assured that no serious errors were introduced in the implementation phase and that users cannot provide absurd input for the algorithm. Moreover, Reference Classes are claimed to be the only implementation of objects in **R** that use passing arguments by reference, and a priori could saved some time in the calculations on unnecessary object copying[2]. Finally, Reference Classes are considered to be highly compatible with **C++** precompiled programmes being called from **R**. This is a clear advantage, as the future shipments of stochasticSimulations are planned to be implemented in **C++**, so that users can simulate faster that the whole programme was more memory efficient.

[1] Still far from the **C++** standards though.

[2] No serious differences in execution time were actually spoted when comparing both the functionally programmed prototype with the object-oriented final version, however.

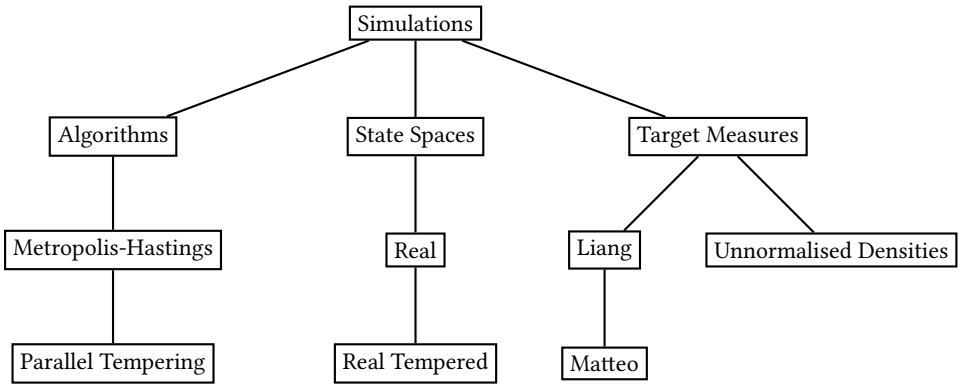


Figure 3.1: Current operational entity-relations diagram.

3.1. Division into objects

To assure real modularity of our template, more divisions were proposed than only the one mentioned at the beginning of this chapter. The overall structure is represented in Figure 3.1.

We already mentioned the separation of the Algorithm from the State Space. It is useful to think of the Algorithm as of a decision-maker. Its role is restricted to making decisions on acceptance or rejections of the proposals generated by the State Space and then on giving orders to the State Space to perform subsequent actions. The information on which the Algorithm bases its decisions depends on the points from the State Space only indirectly, via the evaluations of densities[3] at the proposal points. For in phase of the Random Walk the decision is based on the evaluation of

$$\alpha_\beta(x_l, y_l) = 1 \wedge \frac{\pi^{\beta_l}(y_l)}{\pi^{\beta_l}(x_l)} = R\Big(\pi(y_l), \pi(x_l)\Big),$$

and in the Random Swap phase — upon evaluation of one of the strategies, and additionally, in case of Strategy IV, of the quasi metric

$$p_{ij}(x) = S\Big(\pi(x_i), \pi(x_j), \underbrace{\rho(x_i, x_j)}_{\text{Random Swap only}}\Big)$$

A third candidate for an entity thus appears - namely an object whose methods would serve to measure some characteristic of the State Space sample points for the use in the decision-making of the Algorithm. We called this entity the Target Measure.

The very idea behind the Target Measure entity is that it should serve as a container for user-defined probability function or a density together with every additional data-structure required for its evaluation. Moreover, in case the user was interested in testing the Parallel Tempering algorithm's potential against some analytically tractable toy-example, or in case this example was easy to simulate using a simpler or potentially more efficient technique than MCMC, the Target Measure entity would be the place to store any additional method of carrying out calculations regarding this particular distribution. For example, in our simulations (confront Chapter simulationsAndResults) we could additionally provide efficient methods for quantile simulations and evaluates of the real distribuant. Implementations of these functions were collected as methods of the appropriately named instatiation of the Target Measure structure.

[3] In the discrete case – probability functions

The reason for separating the Target Measure from the State Space is again dictated by the modularity requirement. Totally different models can be modelled on the same State Space, the only difference being the way the probability is assigned. It is therefore natural to define an entity whose task will be to serve as a warehouse for sample points, together with efficient methods or reading them, and in the end – presenting the results to the user. These things, to some extent, can be done for any probability measure defined by the user.

The Object Oriented paradigm gives the programmer also the tool of Inheritance. Its role is to assure no code getting copied when several programmes share the same structure and differ only at some minor implementation details. In our implementation we have noticed that the Parallel Tempering algorithm, being an extension to the Metropolis-Hastings, differs only in the appearance of the swap stage and its methods, the Random Walk stage being almost the same[4]. The Parallel Tempering algorithm inherits from the Metropolis-Hastings methods that are used for generating Random Walk proposals and updating the stored density evaluations. The Metropolis-Hastings in its turn inherits fields from the Algorithm entity — a virtual class, whose role is to store variables that can be used in any algorithm whatsoever, e.g. containing information on the user-supplied maximal number of iterations, or binary information on whether the calculations are done in the burn-in period, this being important for efficient storing of simulated points, or whether the simulation has been already carried out which is important for proper visualisation of the results.

Some of the entities must contain pointers to other entities in order to be able to call methods of other entities when needed[5]. Because of certain Reference Classes limitations[6], the Algorithm has a pointer on the State Space, which in its turn has a pointer on the Target Measure. Under different circumstances, different realisations of objects will appear as the Algorithm, the State Space, and the Target Measure. For instantance, if the user wanted to carry out standard Metropolis-Hastings calculations on the three-dimensional euclidean space and check how it copes with the density function he provided, then the programme would have to first initialise the Unnormalised Density being the instantiation of the Target Measure entity. Then, initialise the Real space, as an instatiation of the State Space, and create a pointer on the Unnormalised Density. Finally, it would have to initialise the Metropolis-Hastings being the operational Algorithm, and set the pointer on the previously initialised Real space. To automate this chain of initialisations, a controller entity was established under the name of Simulation. The Simulation greets the user, checks whether he is not interested in one of the preprogrammed examples of how different algorithms behave (compare to Chapter simulationsAndResults), and then instantiates all different entities using the user-provided informations.

For reasons of user-friendliness, additional functions were written, whose names follow a simple convention. The name of the algorithm can be composed of up to two substings: the first substring being the name of the algorithm used, and the second - the name of some standard State Space. The functions serve as wrappers for more general Reference Class constructor of the Simulation object. Continuing on the above-mentioned example, the user would simply had to call[7]

```
Example <- metropolisReal(
  n = 1000,
  spaceDim = 2,
  targetDensity = userDefinedDensity
)
```

[4]The difference being that it is called for several chains instead of one.

[5]Remember the Algorithm being compared to a decision maker.

[6]As pointed out before, Reference Classes are relatively new, and, as such, poorly documented. With trial and error it has been checked, that this particular choice of entity-nesting simply works.

[7]The convention is known under the name of camelCase.

to initialise the simulation of the Metropolis-Hastings algorithm on the Real state space, with userDefinedDensity being an R-implemented unnormalised density function[8]. If he was to use the Parallel Tempering algorithm approach, the initialisation code would be

```
Example <- paralleltemperingRealtempered(
  n = 1000,
  spaceDim = 2,
  targetDensity = userDefinedDensity
)
```

The presented object structure is far from final. Hopefully it will evolve in time, trying to match the needs of various users. We plan to the separate the swap distributions from the Parallel Tempering entity, giving the user the possibility to check swapping strategies tailored to his needs. Moreover, the existance of the Real Tempered entity stems from purely technical reasons of proper visualisation. The optimal solution would be to create a special controller class for visualisation that would take into account differences in the information presentation of results created through the use of different algorithms and provide some basic solutions.

To guarantee user-friendliness, the most common State Space— the multidimensional Euclidean space — has been provided, so that the user can carry out computations specifying only the required minimum - the density function of the measure of interest. With future releases of the software, more standard State Spaces are scheduled for implemention as well, giving the practitioners experience the potentials and drawbacks of Metropolis-Hastings-like stochastic simulations.

3.2. Functions and Methods

A detailed enumeration of headers of the implemented methods together with brief description can be found in Appendix A.

3.3. Two-dimensional Колмогоров-Смирнов distance

In order to check how different strategies approximate the toy-example distribution described in the next chapter, one had to settle for some kind of criterion. Recall that the general Problem is to approximate an integral

$$\int_{\Omega} g \, \mathrm{d}\, \Pi \approx \frac{1}{\mathrm{N}} \sum_{i=1}^{\mathrm{N}} g(X^{[i]}).$$

One of the principal results in the Ergodic Theory is that one should observe weak convergence of empirical measures to the Target Measure Π on almost all trajectories. The sample measures are simply taken to be

$$\Pi_{\mathrm{N}}(A) \equiv \frac{1}{\mathrm{N}} \sum_{i=1}^{\mathrm{N}} \mathbb{I}_A(X^{[i]}),$$

for $A \in \mathfrak{F}$. The weak convergence means that for any function $f : \Omega \mapsto \mathbb{R}$ bounded and continous and a fixed $\omega \in \Omega$ one observes

[8] In future versions C++ calls will be usable.

$$\Pi_{\mathrm{N}} f(\omega) \equiv \frac{1}{\mathrm{N}} \sum_{i=1}^{\mathrm{N}} \mathbb{I}_A\Big(X^{[i]}(\omega)\Big) f\Big(X^{[i]}(\omega)\Big) \xrightarrow{\mathrm{N}\to\infty} \int_\Omega f(x)\Pi(\mathrm{d}\, x),$$

and we denote it by $\Pi_{\mathrm{N}} \rightharpoonup \Pi$. The above-mentioned result is simply

$$\mathcal{P}\Big(\Pi_{\mathrm{N}} \rightharpoonup \Pi\Big) = 1.$$

If so, it is obvious that if the theorem holds, then on almost all trajectories one would also observe

$$\mathcal{P}\left(\sup_{x\in\mathbb{R}^{\mathrm{K}}} \Big|F(x) - \hat{F}_{\mathrm{N}}(x)\Big| \to 0\right) = 1,$$

where $\hat{F}_{\mathrm{N}}$ is the Empirical Cumulative Distribution Function — **ECDF**. If so, then if the values of the trajectory-based **ECDF** were far away from the true distribuant, the approximation would be of poor quality. Therefore, if one is to compare different algorithms in their task to solve the Problem, as we do when applying different Swap Strategies, then a natural measure for such comparison is exactly the evaluation of the Колмогоров-Смирнов distance

$$d_{KS}\Big(F, \hat{F}_{\mathrm{N}}(\omega)\Big) \equiv \sup_{x\in\mathbb{R}^{\mathrm{K}}} \Big|F(x) - \hat{F}_{\mathrm{N}}(x)(\omega)\Big|.$$

But since it is trajectory-dependent, then a better way would be to carry out several hundreds of simulations and check for the differences in the mean values of the Колмогоров-Смирнов distance and its variance and use these quantities as proxies for our test. This is of course a heuristics, for the reasoning to be precise one would have to consider if the process has the huge bulk of its probability centered around the mean function.

The principal problem with the KS test is that it is computationally expensive and somewhat unpopular to carry out in the multidimensional set-up. Because of the lack of appropriate **R**-package, the whole procedure had to be reconsidered and implemented.

Suppose we are given a simulation with $\tilde{\mathrm{N}}$ iterations after the burn-in period. It often happens that the algorithm stays for more than one iteration in certain sample points[9]. We count the occurences of that points and then normalise them dividing them by $\tilde{\mathrm{N}}$ and call the result *a charge*. Thus, we are given a matrix with sample coordinates and their charges. If the target measure π is absolutely continous with respect to the Lebesgue measure, then the points generated by accepted proposals should all differ on both of their coordinates, the measure of any submanifold of $\mathbb{R}^{\mathrm{K}}$ being zero. If that is not the case, then we simply face the problem of computer's finite arithmetics and could solve it by a longer binary representation of the real numbers. In practice that is an extremely unlikely event and we will neglect it. Therefore we will from now on focus on points with distinct coordinates and refer to the number of thereof by N. The world *sample* will also be applied only to the uppermentioned points.

The computations of the **KS** distance might be computationally expensive, requiring, in pesimistic case, evaluation of the true Cumulative Distribution Function F in approximately $\frac{\mathrm{N}^{\mathrm{K}}}{\mathrm{K}!}$ points[10]. To see that, let us focus in all of this section on the bivariate case[11].

[9] In fact we can easily control the point sejour-time due to the random walk by manipulating the proposal step's distribution parameters. In case of the kernel generated by the conditional normal distribution, it suffices to diminish the entries of the covariance matrix.

[10] The exact number being equal to number of points on the intersection of a $\mathrm{K}+1$ dimensional simplex with the coordinates summing to N, and the $\mathbb{Z}^{\mathrm{K}+1}$ lattice.

[11] ...the generalisation to higher dimension being straighforward.

Figure 3.2: Sample points and level sets of an examplary **ECDF**.

Observe, that the level sets of any **ECDF** are uniquely determined by the sample points (as A, B, C and D in Figure 3.2) and points generated from them by taking the vectorised maximum

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \vee \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} a_1 \vee b_1 \\ a_2 \vee b_2 \end{bmatrix},$$

such as E in Figure 3.2.

One of the easiest way of establishing the values on the level sets of $\hat{F}_{\mathrm{N}}$ is by considering a square, $(\mathrm{N}+2) \times (\mathrm{N}+2)$ matrix B, as in Figure 3.3. The entries of B correspond to values of $\hat{F}_{\mathrm{N}}$ on certain rectangles. Take the set of all x-coordinates of sample-points, Φ_x, and the set of all y-coordinates of sample-points, Φ_y. Add to them the coordinates of two dummy points: (x_0, y_0) and $(x_{\mathrm{N}+1}, y_{\mathrm{N}+1})$ We enumerate points of these sets in the ascending order,

$$\Phi_x = \{x_0 < x_1 < \cdots < x_{\mathrm{N}} < x_{\mathrm{N}+1}\}$$

and

$$\Phi_y = \{y_0 < y_1 < \cdots < y_{\mathrm{N}} < y_{\mathrm{N}+1}\}.$$

Then, the $\hat{F}_{\mathrm{N}}$ function is constant on rectangles

$$R_{ij} = [x_i, x_{i+1}) \times [y_j, y_{j+1}),$$

where $i, j \in \{0, 1, \ldots, \mathrm{N}+1\}$. It is easy to realise now, that the number of level sets depends on the number of sample points and points generated by them using the vectorised maximum, $\hat{\mathrm{N}} = \#\{z : \exists x, y \in \mathrm{Sample} x, y \neq z \text{ and } z = x \vee y\}$. This number is easily seen to be the greatest if all sample points could be arranged so that their x-coordinates strictly increase and y-coordinates strictly decrease.

To actually derive the **KS** distance we must assume that we can evaluate not only the true **CDF** F, but also its two marginals[12]. Similarly to its univariate counterpart, the **KS** distance can be calculated on only a finite number of points. Consider any rectangle. $\hat{F}_{\mathrm{N}}$ is constant on it. So the **KS** distance depends solely on the evaluations of F on that set. But F is a distribuant - a function monotone in all its arguments, and so the maximum distance from $\hat{F}_{\mathrm{N}}$ can be attained only on the

[12]Limits of all the possible subsets of coordinates in infinity.

Figure 3.3: Relation between B matrix and **ECDF** level sets.

vertices of the rectangle. On the border rectangles ($R_{i,\mathrm{N}+1}$ and $R_{\mathrm{N}+1,j}$) the evaluation simplifies to vertices adjacent to R_{ij} rectangles and it is there, where we have to evaluate the marginals instead of F. $\hat{F}_{\mathrm{N}}$ is equal to zero on rectangles on the southern and western extremities. Thus we put $B_{i0} = B_{0j} = 0$.

The rest of the algorithm is based on the dynamic programming approach introduced by Ni and Vingron (2012) for comparing lists of changes in gene expression under different scoring regimes. The overall algorithm proceeds as follows:

Algorithm 3.3.1 (2D-ECDF).

1: $KS := 0$
2: $\mathrm{J} = \mathrm{N} + 1$
3: *Read* α
4: *Prepare* Φ_x *and* Φ_y.
5: ***while*** $i \in \{1, \ldots, \mathrm{N}+1\}$ ***do***
6: ***while*** $j \in \{1, \ldots, \mathrm{J}\}$ ***do***
7: $B_{ij} \leftarrow \begin{cases} B_{i-1,j-1} + \textit{charge}, & R_{ij}\textit{'s upper-left vertex contains a sample-point} \\ B_{i,j-1} + B_{i-1,j} - B_{i-1,j-1}, & \textit{otherwise.} \end{cases}$
8: ***if*** $i, j < \mathrm{N}+1$ *and* $B_{ij} > B_{i,j-1} \vee B_{i-1,j}$ ***then***
9: $F_{ij} \leftarrow F(x_i, y_j)$
10: ***else if*** $j = \mathrm{N}+1$ ***then***
11: $F_{ij} \leftarrow F(x_i, \infty)$
12: ***else if*** $i = \mathrm{N}+1$ ***then***
13: $F_{ij} \leftarrow F(\infty, y_j)$
14: ***end if***
15: ***for*** $a \in \{i-1, i\}$ *and* $b \in \{j-1, j\}$ ***do***
16: $A \leftarrow |F_{ij} - B_{ab}|$
17: ***if*** $A > KS$ ***then***

```
18:                 KS ← A
19:             end if
20:             if F_ij ∧ B_ij > 1 − KS − α then
21:                 J ← j − 1
22:             end if
23:         end for
24:         j ← j + 1
25:     end while
26:     i ← i + 1
27: end while
```

Important changes with respect to Ni and Vingron (2012) can be seen in line 16 and the introduction of two extra variables J and α in lines 6, 21, and 20. The introduction of J stems from the observation, that if both F and $\hat{F}_{\mathrm{N}}$ are already in the interval $(1 - KS, 1]$, then any further evaluations of KS to the East and North from the grid point under study could not result in a bigger difference then the one already observed. Parameter α enlarges that band further to $(1-KS-\alpha, 1]$, so that the true **KS** distance will not be larger than by α from the value already established. We have also noted that it is not important to evaluate the real distribuant at every point of the matrix B. Rather than that, we note that because F is a distribuant, evaluations are required on South-Eastern edges of the level sets, such as points A, B, C, D, and E on Figure 3.3. That is the reason behind code in line 9. Other changes seem to be of minor importance and result from discretisation of the *a priori* continous problem.

Our impelementation of the **KS** distance calculator might not the optimal one. As pointed out by Bentley (1980) the problem of calculating values of an **ECDF** only in the sample points could be solved in $\mathcal{O}(\mathrm{N}\log(\mathrm{N}))$ iterations. The existence of an algorithm requiring only $\mathcal{O}(\hat{\mathrm{N}}\log(\hat{\mathrm{N}}))$ operations, interesting in its own sake and probably rather straightforward, will be object of further research.

Chapter 4

Simulations and Results

Recall that Liang-Wang example of a multimodial function:

$$f(x) = \sum_{i=1}^{20} \frac{\omega_i}{\sigma_i \sqrt{2\pi}} \exp\Big(- \frac{(x-\mu_i)^{\mathrm{t}}(x-\mu_i)}{2\sigma_i^2}\Big),$$

where $\sigma_1 = \cdots = \sigma_{20} = 0.1$, $\omega_1 = \cdots = \omega_{20} = 0.05$ and the means μ_i are enlisted in Chapter 1.

Another example is inspired by paper by Baragatti *et al.* (2012). The goal is to test different swapping strategies in finding also less accentuated modes of probability. For that reason, the following mixture of normal distributions was considered

$$f(x) = \frac{1}{10}\frac{1}{2\pi\sigma_1^2} \exp\Big(- \frac{||x-\mu_1||^2}{2\sigma_1^2}\Big) + \frac{9}{10}\frac{1}{2\pi\sigma_2^2} \exp\Big(- \frac{||x-\mu_2||^2}{2\sigma_2^2}\Big),$$

where $\sigma_1 = 0.7$ and $\sigma_2 = 0.05$ and the means are

μ_1	μ_2
2	8
2	8

Summary

Appendices

Appendix A

Description of implemented methods within objects

Algorithm

R code	Description
`initialize = function( iterationsNo = NULL, burnIn = 2000L, ... )`	This method initialises the Algorithm object. The default setting of the iterations number to NULL is technical and bypasses an error in the Reference Classes implementation: the Reference Classes objects have their constructors that are again Reference Classes objects. Calling the constructor automatically calls generation of the underlying object. This cannot be constructed properly without user-provided inputs. An easy solution is to include in that objects an if statement that checks whether what happens is not the above-mentioned case and construct an empty structure if that is so. A typical burn-in is set to 2000 steps.

`show = function(...)`
`anteSimulationShow = function(...)`
`postSimulationShow = function(...)`
	These bulk methods divide are responsible for the exploration of the inputs and outputs of the algorithm in the terminal.

R code	Description
`getDataForVisualisation = function(...)`	Orders the state space to manipulate the data so that plotting procedures of the **ggplot2** package could handle them
`makeStepOfTheAlgorithm = function(iteration, ...)`	Calls procedures responsible for execution of a single algorithm step: in case of the Metropolis-Hastings algorithm it executes the Random Walk. In case of the Parallel Tempering algorithmit undertakes both the Random Walk and the Random Swap.
`turnOnBurnIn = function(...)` `turnOffBurnIn = function(...)`	These methods pass the information to the State Space on whether it should avoid remembering sample points because of the burn-in period, or not.
`simulate = function(...)`	Starts the simulation process.

Metropolis-Hastings

R code	Description
`insertChainNames = function(...)`	Stores the names of different chains.

R code	Description
`prepareSimulation = function(...)`	Initialises values needed before the simulation.
`acceptanceRejection = function(...)`	Tabularises different chains statistics on rejection and acceptance in the Random Walk phase.
`randomWalk = function(...)`	Performs the random walk step: it asks the state-space to generate the logs of unnormalised probabilities evaluated in the proposed points and then performs the usual rejection part. All this could be done parallely if it was needed - this feature will be shipped with version 2.0.
`randomWalkRejection = function(...)`	Here the Hastings quotients get compared with randomly generated values from the unit interval. All values are taken in logs for numerical stability.
`getLogAlpha = function(...)`	Substracts logarithms of evaluations of the unnormalised densities in the proposal points from their last step counterparts.
`triggerUpdate- -AfterRandomWalk = function(...)`	This procedure updates the State Space after an operation consisting of accepting any new proposal in the random-walk phase of the algorithm. Updates are also needed in the probabilities of the last states stored in a field in the parallel-tempering object.
`updateAfterRandomWalk = function(...)`	This procedure updates the information gathered by the Algorithm: it updates the correct logarithms of the unnormalised densities and notes which chains did move in the Random Walk.

ParallelTemperings

R code	Description
`insertStrategyNo = function( strategyNo )`	Checks whether user inserted correct swapping strategy number.
`getNeighbours = function(...)`	Generates the indices of the neighbouring chains in the lexicographic ordering.
`insertTranspositions = function(...)`	Prepares the dictionary between lexicographic ordering and pair ordering of possible swaps; evaluates the maximal number of potential swaps and inititiates a matrix that stores information on the transitions that occured throughout the simulation.
`plotHistory = function(...)`	Prepares a plot of the swaps distribution that occured during the simulation.
`writeSwaps = function( directoryToWrite, ... )`	Prepares a **.csv** file containing the swap history.
`swapHistory = function(...)`	Tabularizes the information on swap history. First row enumerates how many swaps of a given type were proposed. The second one enumerates how many of these were actually accepted.

R code	Description
`swap = function( iteration )`	Performs the swap phase of a given step of the algorithm.
`swapProposalGeneration = function(...)`	Generates the proposal for the Swap. The function differentiates between state-dependent and state-independent swaps. It stores the information about the swap for later analysis. It also marks which chains did exchange their last sample points.
`swapRejectionAndUpdate = function( iteration, ... )`	Performs the rejection in the swap step and the resulting update. Basing on the information of which interchanges did occur, it reavaluates the values of the unnormalised probabilities of swaps. It calculate Hastings quotients for the Swap phase and performs rejection. After the rejection it updates the swap history and the values of the above-mentioned probabilities. Finally, it orders the State Space to reshuffle the sample points and store them.
`updateSwapUProbs = function( transpositions--ForUpdate, ... )`	Updates values of unnormalised probabilities of swap.
`findTranspositions--ForUpdate = function(...)`	Finds numbers of transpositions in the lexical ordering whose probabilities must be updated after the random walk phase.

R code	Description
`updateSwapUProbs = function( transpositions–ForUpdate )`	Updates values of unnormalised probabilities of swap.
`generateTranspositions = function( chainNumbers )`	Creates a matrix that enlists all possible transpositions of supplied indices of the temperature vector.
`translateLexicTo–Transpositions = function( lexics )`	Translates transpositions ennumbered lexicographically into pairs of corresponding numbers.
`translateTranspositions–ToLexic = function( transpositions )`	Lexicographically orderes given pairs of transpositions.
`swapStrategy = function( transposition )`	Calculates the unnormalised probabilities of swaps, based on the preinserted strategy number.

StateSpaces

R code	Description
`insertInitialStates = function( initialStates = matrix( ncol=0, nrow=0), spaceDim = 0L, chainsNo = 0L, ... )`	Checks whether the user inserted correct initial states. If their dimension is different then the dimension supplied by the user, or they were not enough of them, i.e. less than the number of chains, or if initial states were not supplied, it generates new ones uniformly from a hypersquare $[0, 10]^{\text{Problem Dimenstion}}$.
`turnOnBurnIn = function(...)` `turnOffBurnIn = function(...)`	These methods pass the information to the State Space on whether it should avoid remembering sample points because of the burn-in period, or not.
`proposeLogsOfUMeasures = function(...)`	Calls the Target Measure to evaluate the logarithms of unnormalalised density or probability function.
`randomWalkProposal = function(...)`	Generates the proposal in the Random Walk phase and returns the results to the Algorithm.
`updateStatesAfter-RandomWalk = function(...)` `updateStatesAfterSwap = function(...)`	Realises the call from the Algorithm to update the required parameters.

R code	Description
`calculateBetweenSteps = function(...)`	General wrapper for updates to be executed between the Random Walk phase and the Random Swap phase.

Real (State Space)

R code	Description
`insertInitialStates = function( initialStates = matrix( ncol=0, nrow=0), spaceDim = 0L, chainsNo = 0L, ... )`	Checks whether the user inserted correct initial states. If their dimension is different then the dimension supplied by the user, or they were not enough of them, i.e. less than the number of chains, or if initial states were not supplied, it generates new ones uniformly from a hypersquare $[0, 10]^{\text{Problem Dimenstion}}$.
`createDataStorage = function(...)`	Creates an appropriately big matrix for the storage of sample points.
`insertProposal- -Covariances = function( proposalCovariances = matrix( ncol=0, nrow=0 ), ... )`	Checks whether the user provided correct proposal covariances. The user can provide one matrix if he wants the covariances to be the same for all chains. If that is not the case, the user is obliged to provide a list of matrices that contains as many matrices as there are temperature levels. If the user provides wrong data, unit variances are to be chosen. If the user provides an object whose type is neither matrix, nor list, then the algorithm stops.

R code	Description
`checkCovariance = function(covarianceMatrix, ...)`	Returns true of the given object is a matrix and its dimensions match the dimension of the State Space provided by the user beforehand.

Real Tempered (State Space)

R code	Description
`insertTemperatures = function(temperatures, ...)`	Checks whether the user inserted correct temperature values and stores them.
`getIteration = function(iteration = 1L, type = 'initial states', ...)`	For a given iteration extracts results of a given step type, to choose among 'initial states', 'random walk', and 'swap'.
`prepareDataForPlot = function(...)`	Reshuffles the entire history of states so that the entire result conforms to the data frame templates of **ggplot2**
`plotAllTemperatures = function(...)`	Performs a plot of all simulated chains with an overlayed map of the real density from the Liang example.

R code	Description
`plotBasics = function( algorithmName, ... )`	Performs a plot of the base level temperature chain of main interest with an overlayed map of the real density from the Liang example.
`measureQuasiDistance = function( iState, jState, ... )`	Measures the quasi distance between states needed for.

Target Measure

R code	Description
`measure = function(...)`	Evaluates the density or the probability function at a given point.
`establishTrueValues = function(...)`	Evaluates the values of the provided density on a grid $[-2, 12]^2$ with the mesh set at 0.1. These are to be plotted so that the user may compare the results of the simulation with how it really looks.

Target Unnormalised Densities

R code	Description
`initialize = function( targetDensity = function(){}, ... )`	Stores the unnormalised density function provided by the user.

Target Liang Densities and Matteo Densities

R code	Description
`initialize = function( iterationsNo = NULL, quantile- -SimulationsNo=, mixturesNo =, mixturesWeight = , mixturesMeans = , sigma = , weightConstant = , algorithmName = 'Liang', ... )`	Initialises the reference example of the Liang density described in detail in chapter ....
`plotDistribuant = function(...)`	Plots the distibuant of Liang density based on the grid points from $[-2, 12]^2$ with the mesh set at 0.1.
`distribuant = function( x, ... )`	Calculates the true value of Liang's measure distribuant at point x. It serves as a reference value when evaluating the Колмогоров-Смирнов distance.

R code	Description
`marginalDistribuant = function( proposedState, coordinateNo, ... )`	Calculates the true value of Liang's measure marginal distribuants at point x. One can insert the coodinate number, i.e. 1 or 2, which does not assume the infinite value. It serves as a reference value when evaluating the Колмогоров-Смирнов distance.
`getSquareGrid = function( minimum, maximum, mesh, ... )`	Prepares the matrix with values from $[-2, 12]^2$ with the mesh set at 0.1.
`getQuantiles = function( simulationsNo, ... )`	Simulates the values of Liang Measure's quantiles using Monte Carlo simulation scheme.
`simulateQuantiles = function( simulationsNo, ... )`	Writes down the results of the quantile simulation for further calculations. This function is handy when trying to evaluate visually the correctness of different simulation strategies.
`measureDistance−−FromMeans = function( point, ... )`	Calculates the distance of a given point from all of the means in the mixture of the 20 gaussian densities.

R code	Description

`classify = function(`
`  point,`
`  ...`
`)`
	Start the classification procedures. Their aim is to prescribe the sample points to particular densities that are components of the Liang mixture of measures. The aim of this procedure is to check whether the presence of the sample points in the approximity of modes approximates well their probability input to the whole distribution, which is set to $1/20^{\text{th}}$.

`classifyByLength =`
`  function(`
`  point,`
`  ...`
`  )`
	Performs the classification of sample points to the modes using the distance-from-mean criterion.

`classifyByChiSquare =`
`  function(`
`  point,`
`  ...`
`  )`
	Performs the classification of sample points to the modes using the minimal-chi-square criterion.

`getFirstAndSecondMoments =` `  function(...)`	Calculates all first and second true moments of the Liang distribution.

R CODE	DESCRIPTION

```
initialize  =
  function(
    space = ,
    algo = ,
    target = ,
    example = ,
    iterationsNo = ,
    burnIn = ,
    chainsNo = ,
    spaceDim = ,
    initialStates = ,
    targetDensity = ,
    temperatures = ,
    strategyNo = ,
    quasiMetric = ,
    covariances = ,
    detailedOutput = ,
    save = ,
    trialNo = ,
    evaluateKS = ,
    integratedFunction=,
    rememberStates = ,
    evaluateSojourn = ,
    ...
)
```

Initialises the simulation - prepares the appropriate TARGET MEASURE, links it to appropriate STATE SPACE, chooses the right ALGORITHM.

```
checkTemperatures =
  function(
    temperatures,
    ...
  )
```

Checks whether the user provided correct temperatures.

```
setIterationsNo =
  function(
    iterationsNo,
    ...
  )
```

Checks whether the user provided correct maximal number of iterations that the algorithm is to execute and stores it.

R code	Description
`write = function(...)`	Creates the file where the results of the simulations will get stored, in the `./data` catalogue, under a naming including the number of iterations, number of simulations, and the number of used strategy, in case the user has chosen the Parallel Tempering algorithm. Also, it calls the particular saving procedure of different objects.
`furnishResults = function(...)`	Prepares a vector containing the statistics on a particular run of the simulation. Among them: the strategy number, the rejections of the Random Walk, the rejections of the Random Swap, the Колмогоров-Смирнов statistic, the sojourn estimates, and the integral estimates.
`simulate = function(...)`	Performs the simulation.

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