

# Pigeons.jl: Distributed sampling from intractable distributions

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## ABSTRACT

We introduce a software package, Pigeons.jl, that provides a way to leverage distributed computation to obtain samples from complicated probability distributions, such as multimodal posteriors arising in Bayesian inference and high-dimensional distributions in statistical mechanics. Pigeons.jl provides a simple user interface to perform such computations single-threaded, multi-threaded, and/or distributed over thousands of MPI-communicating machines. In addition, Pigeons.jl guarantees a property that we call strong parallelism invariance: the output for a given seed is identical irrespective of the number of threads and processes, which is crucial for scientific reproducibility and software validation. We describe the key features of Pigeons.jl and the approach taken to implement a distributed and randomized algorithm that satisfies strong parallelism invariance.

## Keywords

distributed computation, Bayesian inference, parallelism invariance, multi-threading, Message Passing Interface, Markov chain Monte Carlo

## 1. Introduction

In many scientific application domains, the ability to obtain samples from a probability distribution is of central interest. For instance, sampling methods have been used to discover magnetic polarization in the black hole of galaxy M87 [2] and to image the Sagittarius A\* black hole [1]. They have also been used to model the evolution of single-cell cancer genomes [23], infer plasma dynamics inside nuclear fusion reactors [14], and to identify gerrymandering in Georgia’s 2021 congressional districting plan [34]. Similarly, evaluating high-dimensional integrals or sums over complicated combinatorial spaces are related tasks that can also be solved with sampling via Markov chain Monte Carlo (MCMC) methods. However, such calculations can often be bottlenecks in the scientific process, with simulations that can last days or even weeks to finish.

Pigeons.jl<sup>1</sup> enables users to sample efficiently from challenging probability distributions and solve integration problems by imple-

menting state-of-the-art sampling algorithms [29, 27] that leverage distributed computation. Its simple user interface facilitates performing such computations single-threaded, multi-threaded, and/or distributed over MPI-communicating machines. We have stress-tested Pigeons successfully with up to 1000 machines running concurrently on a compute cluster (Sockeye) at the University of British Columbia. Further, Pigeons comes with guarantees on strong parallelism invariance wherein the output for a given seed is *identical* irrespective of the number of threads or processes. Such a level of reproducibility is rare in distributed software but of great use for the purposes of debugging in the context of sampling algorithms, which produce stochastic output. Specifically, Pigeons.jl is designed to be suitable and yield reproducible output for:

- (1) one machine running on one thread;
- (2) one machine running on several threads;
- (3) several machines running, each using one thread, and
- (4) several machines running, each using several threads.

## 1.1 Latest documentation

More in-depth documentation and additional examples can be found at: <https://pigeons.run/>.

## 1.2 Problem formulation

We describe the class of problems that can be approached using Pigeons.jl. Let  $\pi(x)$  denote a probability density<sup>2</sup> called the *target*. In many problems, e.g. in Bayesian statistics, the density  $\pi$  is typically known only up to a normalizing constant,

$$\pi(x) = \frac{\gamma(x)}{Z}, \quad Z = \int \gamma(x) dx, \quad (1)$$

where  $\gamma$  can be evaluated pointwise but  $Z$  is typically unknown. Pigeons.jl takes as input the function  $\gamma$ .

The output of Pigeons.jl can be used for two main tasks:

- (1) Approximating integrals of the form  $\int f(x)\pi(x) dx$ . For example, the choice  $f(x) = x$  computes the mean and  $f(x) = I[x \in A]$  computes the probability of  $A$  under  $\pi$ , where  $I[\cdot]$  denotes the indicator function.

<sup>1</sup>The source code for Pigeons.jl can be found at <https://github.com/Julia-Tempering/Pigeons.jl>. Pigeons.jl v0.2.0, used in the example scripts below, is compatible with Julia 1.8+.

<sup>2</sup>This density may also be a probability mass function (discrete variables). We also allow for a combination of discrete/continuous variables.

- (2) Approximating the value of the normalization constant  $Z$ . For example, in Bayesian statistics, this corresponds to the marginal likelihood, which can be used for model selection.

The Pigeons package particularly shines compared to traditional sampling approaches in the following scenarios:

- When the target density  $\pi$  is challenging due to a complex structure (e.g., high-dimensional, multi-modal, etc.).
- When the user needs not only  $\int f(x)\pi(x)dx$  but also the normalizing constant  $Z$ . Many existing tools focus on the former and struggle or fail to do the latter.
- When the target distribution  $\pi$  is defined over a non-standard space, e.g. a combinatorial object such as a phylogenetic tree.

### 1.3 What is of interest to the general Julia developer?

Ensuring code correctness at the intersection of randomized, parallel, and distributed algorithms is a challenge. To address this challenge, we designed Pigeons.jl based on a principle that we refer to as *strong parallelism invariance* (SPI). Namely, the output of Pigeons.jl is invariant to the number of machines and/or threads. Without explicitly keeping SPI in mind during software construction, the (random) output of the algorithm is only guaranteed to have the same distribution. This is a much weaker guarantee that, in particular, makes debugging difficult. However, with our notion of SPI we make debugging and software validation considerably easier. This is because the developer can first focus on the fully serial randomized algorithm, and then use it as an easy-to-compare gold-standard reference for parallel/distributed implementations. This strategy is used extensively in Pigeons.jl to ensure correctness. In contrast, testing equality in distribution, while possible (e.g., see [13]), incurs additional false negatives due to statistical error.

The general Julia developer will be interested in:

- The main causes of a violation of strong parallelism invariance that we have identified (Section 4)—some of which are specific to Julia—and how we address them in Pigeons.jl.
- The SplittableRandoms.jl<sup>3</sup> package that was developed by our team to achieve strong parallelism invariance in Pigeons.jl (Section 4.2).

## 2. Examples

In this section we present a set of minimal examples that demonstrate how to use Pigeons.jl for sampling. We also direct readers to our growing list of examples at InferHub (<https://julia-tempering.github.io/InferHub/>), which hosts a collection of posterior distributions with an emphasis on difficult (non-log-concave) problems.

We begin by installing the latest official release of Pigeons.jl:

```
using Pkg; Pkg.add("Pigeons")
```

### 2.1 Targets

To use Pigeons.jl, we must specify a target distribution, given by  $\gamma$  in Eq. (1). Numerous possible types of target distributions are supported, including custom probability densities (specified up to

a normalizing constant) written in Julia. We also allow to interface with models written in common probabilistic programming languages, including:

- Turing.jl [12] models (TuringLogPotential)
- Stan [10] models (StanLogPotential)
- Comrade.jl<sup>4</sup> models for black hole imaging (ComradeLogPotential)
- Non-Julian models with foreign-language Markov chain Monte Carlo (MCMC) code (e.g. Blang [5] code for phylogenetic inference over combinatorial spaces)

Additional targets are currently being accommodated and will be introduced to Pigeons.jl in the near future.

In what follows, we demonstrate how to use Pigeons with a Julia Turing model applied to a non-identifiable “coinflip” data set. The Bayesian model can be formulated as

$$p_1, p_2 \stackrel{\text{i.i.d.}}{\sim} U(0, 1), \quad (2)$$

$$y \mid p_1, p_2 \sim \text{Binomial}(n, p_1 p_2).$$

The random variable  $y$  is the number of heads observed on  $n$  coin flips where the probability of heads is  $p_1 p_2$ . This model is non-identifiable, meaning that it is not possible to distinguish the effects of the two different parameters  $p_1$  and  $p_2$ . As a consequence, the target distribution exhibits a complicated structure, as displayed in Fig. 1. The density of interest corresponding to this model is

$$\pi(p_1, p_2) = \gamma(p_1, p_2)/Z,$$

where

$$\gamma(p_1, p_2) = \binom{n}{y} (p_1 p_2)^y (1 - p_1 p_2)^{n-y} I[p_1, p_2 \in [0, 1]] \quad (3)$$

$$Z = \int_0^1 \int_0^1 \gamma(p_1, p_2) dp_1 dp_2. \quad (4)$$

The distribution  $\pi$  is also known as the *posterior distribution* in Bayesian statistics.

Suppose that we perform  $n = 100,000$  coin tosses and observe  $y = 50,000$  heads. We would like to obtain samples from our posterior,  $\pi$ , having collected this data. We begin by installing Turing

```
Pkg.add("Turing")
```

and then defining our Turing model and storing it in the variable `model`:

```
using Turing
@model function coinflip(n, y)
    p1 ~ Uniform(0.0, 1.0)
    p2 ~ Uniform(0.0, 1.0)
    y ~ Binomial(n, p1 * p2)
    return y
end
model = coinflip(100000, 50000)
```

From here, it is straightforward to sample from the density given by Eq. (3) up to a normalizing constant. We use non-reversible parallel

<sup>3</sup><https://github.com/Julia-Tempering/SplittableRandoms.jl>

<sup>4</sup><https://github.com/ptiede/Comrade.jl>

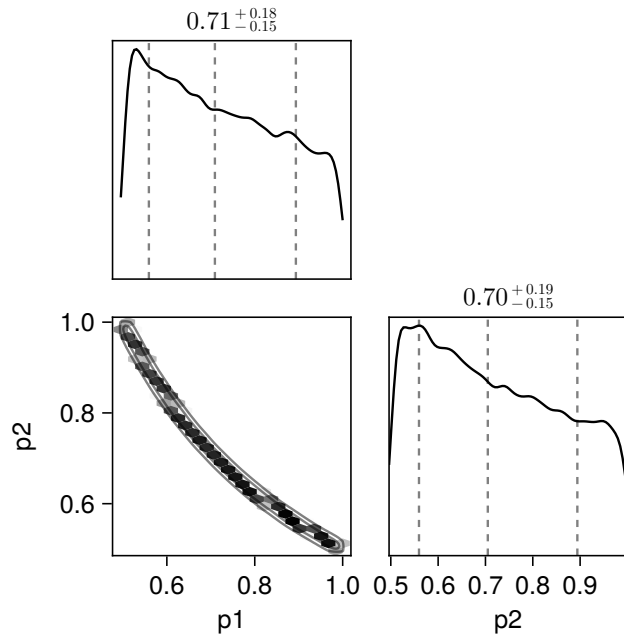


Fig. 1: Posterior distribution for the model given by Eq. (2) with  $n = 100,000$  coin flips and  $y = 50,000$  observed heads, estimated using  $2^{17}$  samples from Pigeons.jl. We present the pairwise plot for  $p_1$  and  $p_2$ , as well as the estimated densities of the marginal of the posterior for each of the two parameters. Note that because the model is non-identifiable, as we collect more data the posterior distribution concentrates around the curve  $p_1 p_2 = 0.5$ , instead of a single point, assuming that the true probability of observing heads is 0.5.

tempering [29, 30, 27, 28] (PT), Pigeons.jl’s state-of-the-art sampling algorithm, to sample from the target distribution. PT comes with several tuning parameters and [29] describe how to select these parameters effectively, which Pigeons.jl implements under the hood. We also specify that we would like to store the obtained samples in memory to be able to produce trace-plots, as well as some basic online summary statistics of the target distribution and useful diagnostic output by specifying `record = [traces, online, round_trip, Pigeons.timing_extrema, Pigeons.allocation_extrema]`. It is also possible to leave the `record` argument empty and reasonable defaults will be selected for the user. The code below runs Pigeons.jl on one machine with one thread. We use the default values for most settings, however we explain later how one can obtain improved performance by setting arguments more carefully (see Section 2.4).

```
using Pigeons
pt = pigeons(
    target = TuringLogPotential(model),
    record = [
        traces, online, round_trip,
        Pigeons.timing_extrema,
        Pigeons.allocation_extrema])
```

Note that to convert the Turing model into an appropriate Pigeons.jl target for sampling, we pass the model as an argument to `TuringLogPotential()`. Once we have stored the PT output in the variable `pt` we can access the results, as described in the fol-

lowing section. The standard output after running the above code chunk is displayed in Fig. 2 and explained in the next section. For purposes of comparison, we also run a traditional (single-chain Markov chain Monte Carlo) method.

**2.1.1 Other targets.** As mentioned previously, it is also possible to specify targets with custom probability densities, as well as Stan and Turing models. Additionally, suppose we have some code implementing vanilla MCMC, written in an arbitrary “foreign” language such as C++, Python, R, Java, etc. Surprisingly, it is very simple to bridge such code with Pigeons.jl. See <https://pigeons.run/stable/input-overview/>.

## 2.2 Outputs

Pigeons.jl provides many useful types of output, such as: plots of samples from the distribution, estimates of normalization constants, summary statistics of the target distribution, and various other diagnostics. We describe several examples of possible output below.

**2.2.1 Standard output.** An example of the standard output provided by Pigeons.jl is displayed in Fig. 2. Each row of the table in the output indicates a new tuning round in parallel tempering, with the `#scans` column indicating the number of scans/samples in that tuning round. During these tuning rounds, Pigeons.jl searches for optimal values of certain PT tuning parameters. Other outputs include:

- `restarts`: a higher number is better. Informally, PT propagates samples from an easy-to-sample distribution (the reference) to the more difficult target distribution. A tempered restart happens when a sample from the reference successfully percolates to the target. (See the subsequent sections for a more detailed description of parallel tempering.) When the reference supports i.i.d. sampling, tempered restarts can enable large jumps in the state space.
- `Λ`: the global communication barrier, as described in [29], which measures the inherent difficulty of the sampling problem. A rule of thumb to configure the number of PT chains is also given by [29], where they suggest that stable performance should be achieved when the number of chains is set to roughly  $2\Lambda$ . See Section 2.2.6 for more information.
- `time` and `alloc`: the time (in seconds) and number of allocations (in bytes) used in each round.
- `log( $Z_1/Z_0$ )`: an estimate of the logarithm of the ratio of normalization constants between the target and the reference. In many cases,  $Z_0 = 1$ .
- `min( $\alpha$ )` and `mean( $\alpha$ )`: minimum and average swap acceptance rates during the communication phase across the PT chains. See Section 3 for a description of PT communication.

**2.2.2 Plots.** It is straightforward to obtain plots of samples from the target distribution, such as trace-plots, pairwise plots, and density plots of the marginals.

To obtain posterior densities and trace-plots, we first make sure that we have the third-party `MCMCChains.jl`<sup>5</sup>, `StatsPlots.jl`<sup>6</sup>, and `PlotlyJS.jl`<sup>7</sup> packages installed via

```
Pkg.add("MCMCChains", "StatsPlots", "PlotlyJS")
```

<sup>5</sup><https://github.com/TuringLang/MCMCChains.jl>

<sup>6</sup><https://github.com/JuliaPlots/StatsPlots.jl>

<sup>7</sup><https://github.com/JuliaPlots/PlotlyJS.jl>

#scans	restarts	$\Lambda$	time(s)	allc(B)	$\log(Z_1/Z_0)$	$\min(\alpha)$	$\text{mean}(\alpha)$
2	0	1.04	0.383	3.48 e+07	-4.24 e+03	0	0.885
4	0	4.06	0.00287	1.79 e+06	-16.3	4.63 e-06	0.549
8	0	3.49	0.00622	3.55 e+06	-12.1	0.215	0.612
16	0	2.68	0.0161	7.46 e+06	-10.2	0.518	0.703
32	0	4.29	0.0353	1.37 e+07	-11.8	0.222	0.524
64	3	3.17	0.0699	2.86 e+07	-11.5	0.529	0.648
128	8	3.56	0.139	5.53 e+07	-11.5	0.523	0.605
256	12	3.38	0.241	1.1 e+08	-11.6	0.526	0.625
512	37	3.48	0.473	2.22 e+08	-12	0.527	0.614
1.02 e+03	77	3.55	0.895	4.46 e+08	-11.8	0.571	0.605

Fig. 2: Standard output provided by Pigeons.jl. Rows indicate tuning rounds of the PT algorithm with an exponentially increasing number of PT iterations (#scans). Columns indicate various useful diagnostics, such as the amount of memory allocations per round (in bytes), time (in seconds), and estimates of the log of the normalization constants. The output is described in greater detail in Section 2.2.6 and has been modified to exclude columns that are not described in the paper.

With the `pt` output object from before for our non-identifiable coin-flip model, we can run the following:

```
using MCMCChains, StatsPlots, PlotlyJS
plotlyjs()
samples = Chains(
    sample_array(pt), variable_names(pt))
my_plot = StatsPlots.plot(samples)
display(my_plot)
```

The output of the above code chunk is an interactive plot that can be zoomed in or out and exported as an HTML webpage. A modified static version of the output for the first parameter,  $p_1$ , is displayed in the top panel of Fig. 3, along with a comparison to the output from a single-chain algorithm in the bottom panel of the same figure.

To obtain pair plots, we add the `PairPlots.jl`<sup>8</sup> and `CairoMakie.jl`<sup>9</sup> packages:

```
Pkg.add("PairPlots", "CairoMakie")
```

and then run

```
using PairPlots, CairoMakie
my_plot = PairPlots.pairplot(samples)
display(my_plot)
```

The output of the above code chunk with an increased number of samples is displayed in Fig. 1.<sup>10</sup>

**2.2.3 Estimate of normalization constant.** The (typically unknown) constant  $Z$  in Eq. (1) is referred to as the *normalization constant*. In many applications, it is useful to approximate this constant. For example, in Bayesian statistics, this corresponds to the marginal likelihood and can be used for model selection.

As a side-product of PT, we automatically obtain an approximation to the natural logarithm of the normalization constant. This is done

automatically using the stepping stone estimator [33]. The estimate can be accessed using

```
stepping_stone(pt)
```

In the case of the normalization constant given by Eq. (4) for  $n = 100,000$  and  $y = 50,000$ , we can exactly obtain its value as  $\log(Z) \approx -11.8794$ . Note that this is very close to the output provided in Fig. 2.

**2.2.4 Online statistics.** Pigeons has facilities to support cases requiring large memory. For instance, we allow for the computation of online statistics, as well as off-memory sample storage. Having specified the use of the `online` recorder in our call to `pigeons()`, we can output some basic summary statistics of the marginals of our target distribution. For instance, it is straightforward to estimate the mean and variance of each of the marginals of the target with

```
using Statistics
mean(pt); var(pt)
```

Other constant-memory statistic accumulators are made available in the `OnlineStats.jl` [11] package. To add additional constant-memory statistic accumulators, we can register them via `Pigeons.register_online_type()`, as described in our online documentation. For instance, we can also compute constant-memory estimates of extrema of our distribution.

**2.2.5 Off-memory processing.** When either the dimensionality of the model or the number of samples is large, the obtained samples may not fit in memory. In some cases it may be necessary to store samples to disk if our statistics of interest cannot be calculated online and with constant-memory (see Section 2.2.4). We show here how to save samples to disk when Pigeons.jl is run on a single machine. A similar interface can be used over MPI.

First, we make sure that we set `checkpoint = true`, which saves a snapshot at the end of each round in the directory `results/all/<unique directory>` and is symlinked to `results/latest`. Second, we make sure that we use the disk recorder by setting `record = [disk]`, along with possibly any other desired recorders. Accessing the samples from disk can

<sup>8</sup><https://github.com/seffal/PairPlots.jl>

<sup>9</sup><https://github.com/JuliaPlots/CairoMakie.jl>

<sup>10</sup>The code chunk above requires Julia 1.9.

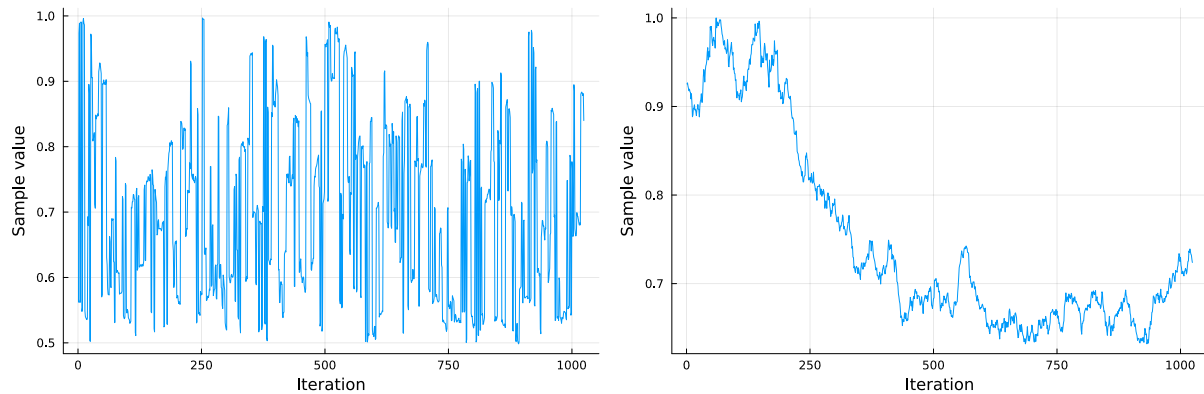


Fig. 3: Trace-plots for the first parameter,  $p_1$ , in the non-identifiable coinflip Turing model. **Left:** Samples from Pigeons.jl using PT with 10 chains. Note that the trace-plot indicates fast mixing/exploration across the state space. **Right:** Single-chain Markov chain Monte Carlo. Note that the trace-plot explores the state space much more slowly when we do not use PT.

then be achieved in a simple way using the Pigeons.jl function `process_sample()`.

**2.2.6 PT diagnostics.** We describe how to produce some key parallel tempering diagnostics from [29].

The global communication barrier, denoted  $\Lambda$  in Pigeons.jl output, can be used to approximately inform the appropriate number of chains. Based on [29], stable PT performance should be achieved when the number of chains is set to roughly  $2\Lambda$ . This can be achieved by modifying the `n_chains` argument in the call to `pigeons()`. The global communication barrier is shown at each round and can also be accessed with

```
Pigeons.global_barrier(pt)
```

The number of restarts per round can be accessed with

```
n_tempered_restarts(pt)
```

These quantities are also displayed in Fig. 2. Many other useful PT diagnostic statistics and plots can be obtained, as described in our full documentation.

## 2.3 Parallel and distributed PT

One of the main benefits of Pigeons.jl is that it allows users to easily parallelize and/or distribute their PT sampling efforts. We explain how to run MPI locally on one machine and also how to use MPI when a cluster is available.

**2.3.1 Running MPI locally.** To run MPI locally on one machine using four MPI processes and one thread per process, use

```
pigeons(
  target = TuringLogPotential(model),
  on = ChildProcess(
    n_local_mpi_processes = 4,
    n_threads = 1))
```

**2.3.2 Running MPI on a cluster.** Often, MPI is available via a cluster scheduling system. To run MPI over several machines:

- (1) In the cluster login node, follow the Pigeons.jl installation instructions in our online documentation.
- (2) Start Julia in the login node, and perform a one-time setup by calling `Pigeons.setup_mpi()`.
- (3) In the Julia REPL running in the login node, run:<sup>11</sup>

```
pigeons(
  target = TuringLogPotential(model),
  n_chains = 1_000,
  on = MPI(n_mpi_processes = 1_000,
    n_threads = 1))
```

The code above will start a distributed PT algorithm with 1,000 chains on 1,000 MPI processes each using one thread. Note that for the above code chunks involving `ChildProcess()` and `MPI()` to work, it may be necessary to specify dependencies in their function calls. See <https://pigeons.run/stable/mpi/> for details.

## 2.4 Additional options

In the preceding example we only specified the target distribution and let Pigeons.jl decide on default values for most other settings of the inference engine. There are various settings we can change, including: the random seed (`seed`), the number of PT chains (`n_chains`), the number of PT tuning rounds/samples (`n_rounds`), and a variational reference distribution family (`variational`), among other settings. For instance, we can run

```
pigeons(
  target = TuringLogPotential(model),
  n_rounds = 10,
  n_chains = 10,
  variational = GaussianReference(),
  seed = 2
)
```

<sup>11</sup>In version 0.4.0 of Pigeons, the function `MPI` has been renamed `MPIProcesses` to avoid a clash with the library `MPI.jl`.



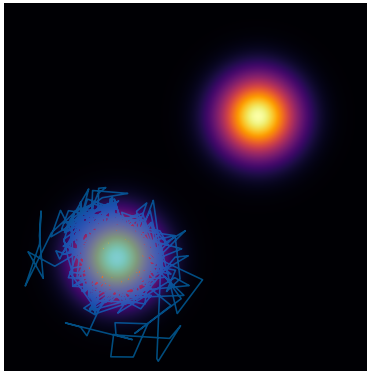


Fig. 4: A simple bimodal distribution from which traditional MCMC methods may struggle to obtain samples. Blue lines display output from 1,000 iterations of a Metropolis-Hastings random walk MCMC algorithm. The sampler in this figure is visibly trapped in one of the two modes.

which runs PT with the same Turing model target as before and explicitly states that we should use 10 PT tuning rounds with 10 chains (described below). In the above code chunk we also specify that we would like to use a Gaussian variational reference distribution. That is, the reference distribution is chosen from a multivariate Gaussian family that lies as close as possible to the target distribution in order to improve the efficiency of PT. We refer readers to [27] for more details. When only continuous parameters are of interest, we encourage users to consider using `variational = GaussianReference()` and setting `n_chains_variational = 10`, for example, as the number of restarts may substantially increase with these settings.

### 3. Parallel tempering

Pigeons.jl provides an implementation of distributed parallel tempering (PT) described in [29], which we outline in Algorithm 1. This section gives both a brief overview of PT and some details of its distributed implementation.

In this section we assume a basic understanding of Markov chain Monte Carlo (MCMC) methods. For readers unfamiliar with MCMC, it is important to know that it is a method to obtain approximate samples from a distribution. However, with traditional MCMC methods, the samples may be heavily correlated instead of independent and may fail to sufficiently explore the full space of the distribution (see Fig. 4); PT is a method that aims to address these issues. For a more in-depth review of PT, we refer readers to [27].

#### 3.1 Overview of PT

Suppose that we would like to estimate integrals involving  $\pi$ , such as  $\int f(x)\pi(x)dx$ . These integrals may be multivariate and even include combinations of continuous and discrete variables (where sums replace integrals in the discrete case). One method is to obtain samples from  $\pi$  to approximate such integrals. Often, the distribution  $\pi$  can be challenging for traditional MCMC methods—such as Metropolis-Hastings, slice sampling, and Hamiltonian Monte Carlo—because of its structure. For example, in a bimodal example such as the one illustrated in Figure 4, traditional methods might remain in one of the two modes for an extremely long period of time.

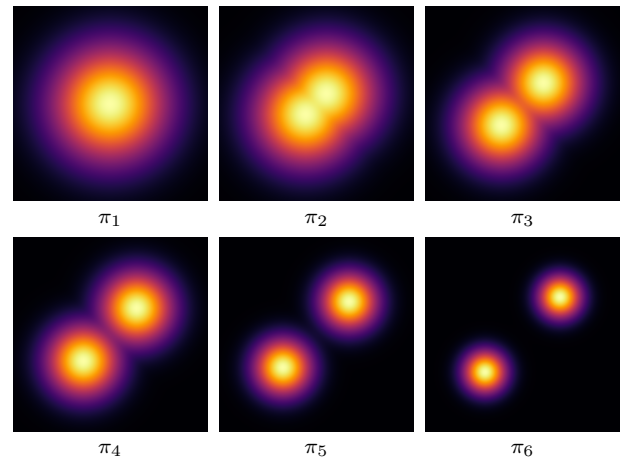


Fig. 5: Heatmaps of six distributions lying on an annealing path from a unimodal reference distribution  $\pi_1$ , from which it is straightforward to obtain samples, and ending at  $\pi_N$ , which is in this case the bimodal distribution from Figure 4. (Note that in this case the colours between the heatmaps are not directly comparable because the densities of intermediate distributions are not normalized.)

To resolve this issue, PT constructs a sequence of  $N$  distributions,  $\pi_1, \pi_2, \dots, \pi_N$ , where  $\pi_N$  is usually equal to  $\pi$ . The distributions are chosen so that it is easy to obtain samples from  $\pi_1$  with the sampling difficulty increasing as one approaches  $\pi_N$ . An example of such a sequence of distributions, referred to as an *annealing path*, is shown in Figure 5.

We now turn to explain how this path of distributions can be used to enhance sampling from the target distribution,  $\pi$ . PT operates by first obtaining samples from each distribution on the path in parallel (referred to as an *exploration phase*). Then, samples between adjacent distributions are swapped (referred to as a *communication phase*). The communication phase in PT is crucial: it allows for the discovery of new regions of the space of the target distribution such as the top-right mode of the distribution presented in Figure 4.

#### 3.2 Local exploration and communication

A central data structure in Pigeons is the `Replica`, a Julia struct that we will often refer to in the remainder of this section. A single `Replica` stores a `state` variable and a `chain` integer, among other entries. At the beginning of PT,  $N$  `Replica`s are created, one for each distribution on the annealing path, and the chain entries in the  $N$  replicas are initialized at  $1, 2, \dots, N$ , respectively. For a given `Replica`, if the chain number is  $i$  and the state is  $x$ , then this means that the sample corresponding to the  $i$ -th distribution in the sequence  $\pi_1, \dots, \pi_N$  is currently at location  $x$ .

In the local exploration phase, each `Replica`'s state is modified using an MCMC move targeting  $\pi_i$ , where  $i$  is given by `Replica.chain`. The MCMC move can either modify `Replica.state` in-place, or modify the `Replica.state` field. This operation is indicated by the `local_exploration` function in Algorithm 1.

In the communication phase, PT proposes swaps between pairs of replicas. In principle, there are two equivalent ways to do a swap. In the first implementation, the `Replica`s could exchange their `state` fields. Alternatively, they could exchange their `chain` fields. Because we provide distributed implementations, we use the latter as

it ensures that the amount of data that needs to be exchanged between two machines during a swap can be made very small (two floating point numbers), resulting in an exchange of  $O(N)$  messages of size  $O(1)$ . Note that this cost does not vary with the dimensionality of the state space, in contrast to the first implementation that would transmit  $O(N)$  messages of size  $O(d)$ , where  $d$  is the dimension of the state space, incurring a potentially very high communication cost for large values of  $d$ .

### 3.3 Distributed implementation

A distributed implementation of PT is shown in Algorithm 1 and we describe the details of the implementation below. For pedagogy, we first present the algorithm in the special case where the number of machines available is equal to the number of Replicas and distributions,  $N$ . However, Pigeons also allows for the more general case where the number of machines is not necessarily equal to  $N$ . We outline how Pigeons achieves this in Section 3.3.3.

**3.3.1 Distributed mapping from chains to machines.** Recall that our theoretical  $O(1)$  message size for communication between two machines is achieved by exchanging chain indices between Replicas instead of their states. However, in order to achieve this low cost, a specialized distributed data structure is needed to maintain a mapping from chain indices to machine identifiers. To motivate it, we start with an illustrative example. Suppose we have  $N = 4$  distributions, chains, replicas, and machines, and that machine 1 is exploring chain 2 while machine 4 is exploring chain 3. At one point, the Replica at chain 2 (machine 1) might need to exchange chain indices with the Replica that has chain index 3 (machine 4). However, a priori it is not clear how machine 1 should know that it should communicate with machine 4 because it has no knowledge about the chain indices on the other machines.

To resolve this issue, we introduce a special data structure called a `PermutedDistributedArray`. In the case where the number of replicas is equal to the number of available machines, the construction is quite simple and effectively results in each machine storing one additional integer. Considering the same example above, the solution to the problem is to have machine 1 (chain 2 wanting to communicate with chain 3) communicate with machine 3. Machine 3 stores in its `dist_array` variable of type `PermutedDistributedArray` the value 4, which is the machine number that stores chain 3. By updating these `PermutedDistributedArray` variables at each communication step, we can ensure that each machine  $j$  is aware of which machine number currently stores chain  $j$ . Therefore, the machines act as keys in a dictionary for the communication permutations. An illustration of communication between four machines is provided in Fig. 6. We note that with a `PermutedDistributedArray` we make special assumptions on how we access and write to the array elements. Several MPI processes cooperate, with each machine storing data for a slice of this distributed array, and at each time step an index of the array is manipulated by exactly one machine. Thanks to this, we do not need to resort to global MPI synchronization steps.

**3.3.2 MPI implementation details.** We use the `MPLjl` [8] package to support communication between machines. In Algorithm 1, the function `swap_stat()` extracts the sufficient statistic required by each partner of a swap. The swap sufficient statistic contains two elements: (1) a uniformly distributed random number, and (2) the log of the ratio  $\pi_c(x_t)/\pi_{c'}(x_t)$ , up to a normalization constant which may depend on  $c$  and  $c'$  but not  $x_t$ . The function

**Algorithm 1** Distributed PT on machine  $j$  (one replica per machine)

---

**Require:** Initial state  $x_0$ , sequence of distributions  $\{\pi_i\}_{i=1}^N$ , number of iterations  $T$ , machine number  $j$

```

1: chain  $\leftarrow j$  ▷ current chain number
2: dist_array[j]  $\leftarrow j$  ▷ chain  $j$  is on machine  $j$ 
3: for  $t$  in  $1, 2, \dots, T$  do
4:    $x_t \leftarrow \text{local\_exploration}(\pi_{\text{chain}}, x_{t-1})$ 
5:    $c_t \leftarrow \text{chain}$ 
6:   if is_even( $t$ ) = is_even(chain) then
7:     direction  $\leftarrow +1$ 
8:   else
9:     direction  $\leftarrow -1$ 
10:  end if
11:  partner  $\leftarrow \text{chain} + \text{direction}$ 
12:  if partner = 0 then
13:    partner  $\leftarrow 1$  ▷ Encode boundaries as self-interaction
14:  else if partner =  $N + 1$  then
15:    partner  $\leftarrow N$ 
16:  end if
17:  my_stat  $\leftarrow \text{swap\_stat}(x_t, \text{chain}, \text{partner})$ 
18:  to_machine  $\leftarrow \text{permuted\_get}(\text{dist\_array}, \text{partner})$ 
19:  partner_stat  $\leftarrow \text{transmit}(\text{my\_stat}, \text{to\_machine})$ 
20:  if swap_accepted(my_stat, partner_stat) then
21:    chain  $\leftarrow \text{partner\_chain}$ 
22:  end if
23:  permuted_set!(dist_array, chain,  $j$ )
24: end for
25: return  $\{(x_t, c_t)\}_{t=1}^T$ 

```

---

`transmit()` is used to exchange these statistics between the two partners of a proposed swap. In order to make an accept-reject decision, the two machines use the same uniform sample (using an arbitrary, fixed convention, namely the shared sufficient statistic's uniform from the lowest interacting chain index) to make a common swap decision (where the acceptance ratio is the sum of the two exchanged log ratios, (2)).

In Algorithm 1 we also introduce the functions `permuted_get()` and `permuted_set!()`, which operate on a `PermutedDistributedArray` as described in Section 3.3.1. Given the current machine's `dist_array` and the partner chain with which it should communicate, `permuted_get()` returns the machine number that holds the partner chain. Given the current machine's `dist_array`, chain number, and machine number  $j$ , `permuted_set!()` updates the `PermutedDistributedArray` variables with the updated permutation.

**3.3.3 Load balancing.** So far we have assumed, for pedagogy, that the number of machines  $M$  is equal to the number of chains  $N$ . This restriction is not present in Pigeons, so we now describe how the code base generalizes Algorithm 1. First, the  $N$  replicas are shared between the  $M$  machines so that each machine contains either  $\lceil N/M \rceil$  or  $\lfloor N/M \rfloor$  replicas. Each machine's replicas are called the local replicas. The allocation of replicas to machine is fixed over the whole execution of the algorithm and maintained using the `LoadBalance` struct. Second, the code performing local exploration is enclosed in a loop over the local replicas, and if the option “`multithreaded = true`” is used in the `pigeons(...)` call, the exploration loop is performed in a `@threads` for loop. Finally, the functions used in the communication, `permuted_get`, `permuted_set!`, `transmit`, etc., are vectorized to accommodate

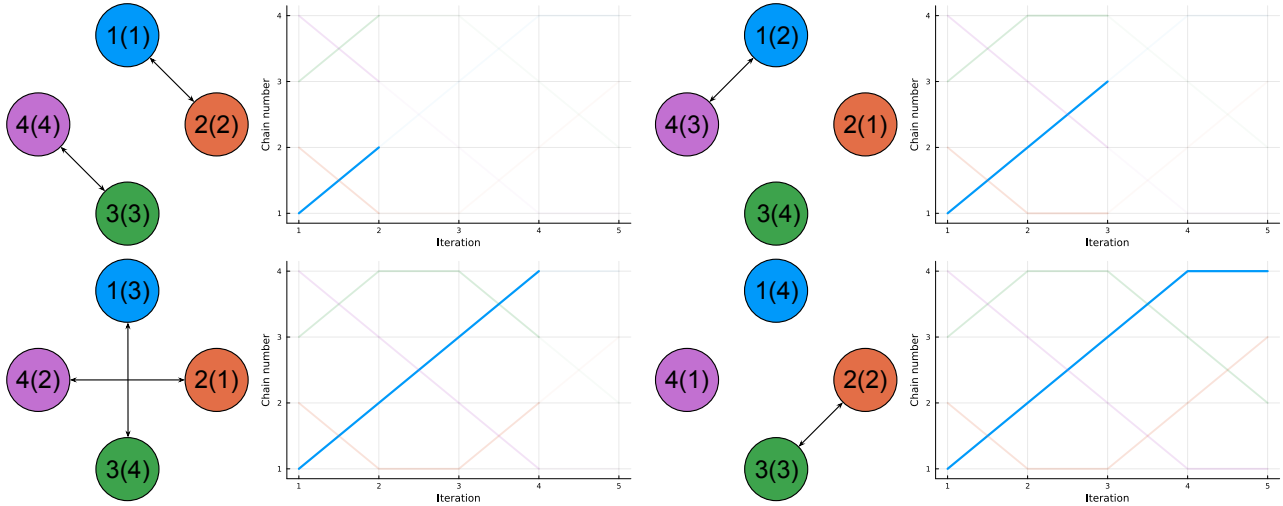


Fig. 6: A summary of communication between four machines with  $N = 4$  PT chains. Circles represent machines with the machine number in the center of the circle. Different colours are also used for different machines. Numbers in parentheses represent the chain that is currently being explored by that machine. Arrows indicate communication occurring between machines to exchange chain indices. To keep track of which chains are stored on which machine, we introduce the `dist_array` of type `PermutedDistributedArray`, described in Section 3.3.1, which is of length  $N$ . The  $j$ -th element of `dist_array` at a given time step indicates which machine number is storing chain index  $j$ . The bolded curve in the figures to the right indicate the trajectory of the first Replica over the course of each of the communication steps. **Top left:** the PT replicas are initialized and the first communication step is proposed. At this time step, `dist_array` = [1, 2, 3, 4]. **Top right:** after the first successful communication step, we now have `dist_array` = [2, 1, 4, 3]. **Bottom left:** The second communication step is completed and `dist_array` = [2, 4, 1, 3]. **Bottom right:** The third communication step is completed and `dist_array` = [4, 2, 3, 1].

that chain and partner are no longer integers but rather sets of integers. In particular, the permuted distributed array is designed so that each machine is responsible for tracking machine allocations for  $\lceil N/M \rceil$  or  $\lfloor N/M \rfloor$  chains instead of a single one.

### 3.4 Weak scaling of PT

We study the weak scaling properties of Pigeons' implementation of PT. In this setup, we consider a varying problem size proportional to the number of processes used. The number of chains is our definition of the problem size; this is in line with previous heuristics that establish that the problem difficulty is generally proportional to the optimal number of chains in PT [29]. In particular, we consider a multivariate normal target distribution and vary the dimension  $d \in \{2^1, 2^2, \dots, 2^{12}\}$  for the distributed setup and  $d \in \{2^1, 2^2, \dots, 2^{10}\}$  for the parallel (shared memory) setup. The number of chains is set to  $\lceil \sqrt{d} \rceil$  according to PT tuning suggestions [29] and for the distributed and parallel settings we set the number of processes or threads equal to the number of chains. Within each chain we use the autoMALA sampler [4], which is a gradient-based sampler with automatic step size selection in the Metropolis-adjusted Langevin algorithm. Ten different seeds are used in order to obtain approximate 95% confidence intervals of the speedup.

The weak scaling results for both the distributed memory parallelism (DMP) and shared memory parallelism (SMP) settings are presented in Fig. 7. We see that we obtain an approximately linear speedup as we increase the number of processes.

### 3.5 Relevance of DMP versus SMP

We emphasize again that Pigeons supports both shared memory parallelism (SMP) and distributed memory parallelism (DMP). However, in certain cases, it might be useful to run parallel tem-

pering with many chains or to run several instances of parallel tempering at once. In such cases, the DMP setup is the most natural if the requested number of chains is very large. Another notable example of the benefit of DMP is for the multi-GPU use case. For instance, in some situations the likelihood evaluation of a single chain may require its own GPU (e.g., if one is running a Fast Fourier Transform on a GPU). Additionally, DMP can be useful when the user's code is not thread safe. In such cases, concurrency can still be achieved via DMP. Our implementation in Pigeons ensures that the communication cost in the DMP setup is minimal. In most cases, the communication cost is negligible compared to other computations performed on each process.

## 4. Strong parallelism invariance

In this section we describe potential violations of strong parallelism invariance (SPI) that can occur in a distributed setting. We also explain how we avoid these issues by using special distributed reduction schemes and splittable random number generators. Insights provided in this section can be applied to general distributed software beyond Julia.

We have identified two factors that can cause violations of our previously-defined SPI that standard Julia libraries do not automatically take care of:

- (1) **Non-associativity of floating point operations:** When several workers perform distributed reduction of floating point values, the output of this reduction will be slightly different depending on the order taken during reduction. When these reductions are then fed into further random operations, this implies that two randomized algorithms with the same seed but using a different number of workers will eventually arbitrarily diverge.



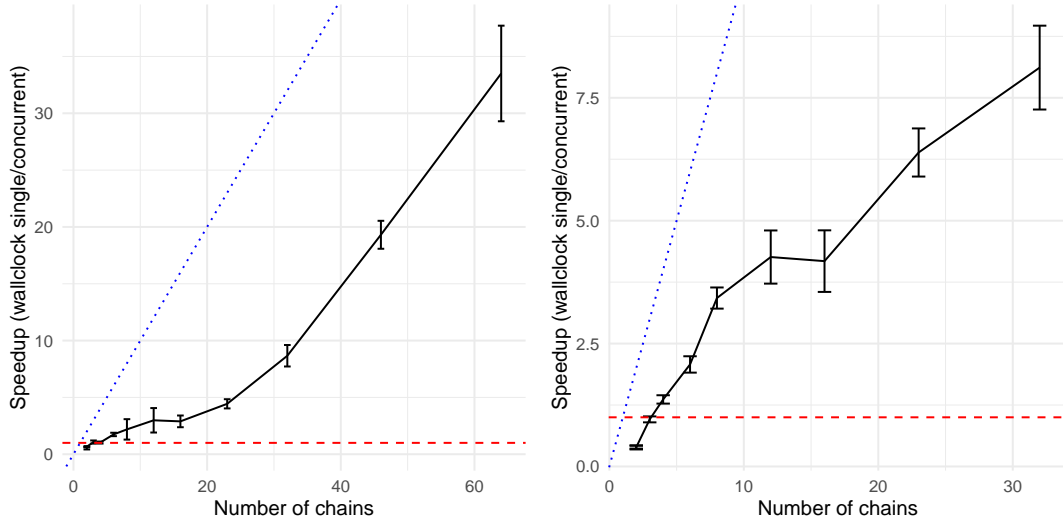


Fig. 7: Weak scaling results for PT in both the distributed (MPI, **left**) and parallel (Julia threads, **right**) settings with approximate 95% confidence intervals for the speedup relative to single-thread execution. The blue dotted line represents a hypothetical speedup equal to the number of processes/threads. The red dashed line indicates a speedup of one for reference.

- (2) **Global, thread-local, and task-local random number generators:** These are the dominant approaches to parallel random number generators in current languages, and an appropriate understanding of these RNGs is necessary. In particular, in Julia it is important to understand the behaviour of the `@threads` macro.

Our focus in the remainder of this section is to describe how our implementation solves the two above issues.

#### 4.1 Distributed reduction and floating point non-associativity

After each round of PT, the machines need to exchange information such as the average swap acceptance probabilities, statistics to adapt a variational reference and adjust annealing parameters, and so on. For instance, suppose our `state` is univariate and real-valued and that each `Replica` keeps track of the number of times the target chain  $N$  is visited as well as the mean of the univariate `states` from the target chain. To obtain the final estimate of the mean of the target distribution, we would like to pool the mean estimates from each of the `Replicas`, weighted by the number of times that each `Replica` visited the target chain. This process involves summing floating-point values that are located on each of the `Replicas`/machines and is an example of a reduction scheme.

To illustrate why distributed reduction with floating point values can violate strong parallelism invariance if not properly implemented, we consider the following toy example. Suppose we have 8 machines storing the floating point numbers  $\{1x, 2x, \dots, 8x\}$ , as illustrated in Fig. 8, where we use  $x = 10e^1 \approx 27.1828$  in the following examples. In this case, if our reduction procedure is to sum the floating point numbers, we know that our final answer should be approximately  $36x$ . However, depending on the exact order in which floating point addition is carried out, the answers might not all be the same and exactly equal to  $36x$ . For instance, in Fig. 8 we see that the order of operations for eight machines would be given

by

$$((1x + 2x) + (3x + 4x)) + ((5x + 6x) + (7x + 8x)) \approx 978.5814582452562.$$

In contrast, with two machines, one possible order of operations might be

$$(((1x + 2x) + 3x) + 4x) + (((5x + 6x) + 7x) + 8x) \approx 978.5814582452563.$$

A possible reduction tree for two machines is illustrated in Fig. 9.

To avoid the issue of non-associativity of floating point arithmetic, we ensure that the order in which operations are performed is exactly the same, irrespective of the number of processes/machines and threads. This is achieved by making sure that every value to be added—if addition is our reduction operation—is a leaf node in a reduction tree that is invariant to the number of machines available to perform the computation. For instance, if  $N$  values are to be reduced, then the reduction tree would have  $N$  leaf nodes. If  $M$  machines are available, these machines are then assigned in such a way that the order of operations is as if there were  $N$  machines available. To do so, it may be necessary for a machine to “communicate with itself”, imitating the behaviour that would be present if there were  $N$  machines available. Fig. 10 and Fig. 11 illustrate the reduction procedure for eight and two machines, respectively.

#### 4.2 Splittable random streams

Another building block towards achieving SPI is a *splittable random stream* [18, 7]. Julia uses *task-local* random number generators, a notion that is related to (but does not necessarily imply) strong parallelism invariance. A *task* is a unit of work on a machine. A task-local RNG would then mean that a separate RNG is used for each unit of work, hopefully implying strong parallelism invariance if the number of tasks is assumed to be constant. Unfortunately, this is not the case when a separate task is created for each thread of execution in Julia. We note that the `@threads` macro in

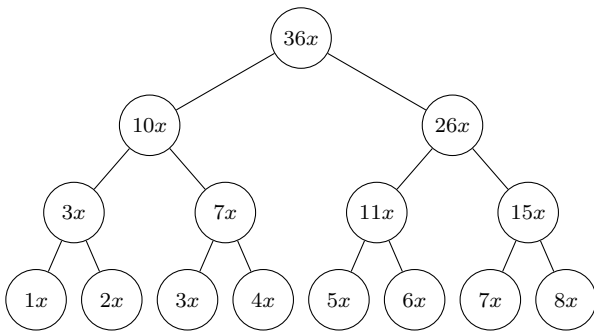


Fig. 8: Adding eight floating point numbers  $\{1x, 2x, \dots, 8x\}$  across eight machines. Additions in each row of the tree can be performed in parallel. The final result is stored in the root node of the tree and can be represented by the expression  $((1x + 2x) + (3x + 4x)) + ((5x + 6x) + (7x + 8x))$ , indicating the order of operations.

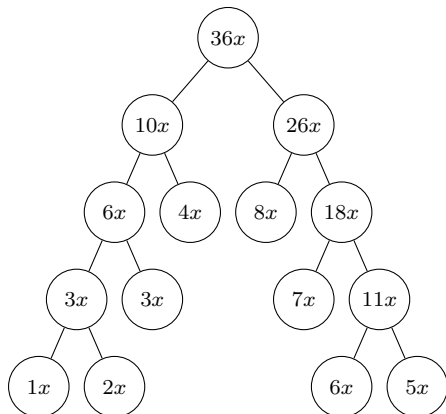


Fig. 9: One possible way of adding eight floating point numbers  $\{1x, 2x, \dots, 8x\}$  across two machines. The final result is stored in the root node of the tree and can be represented by the expression  $((1x + 2x) + 3x) + 4x + (((5x + 6x) + 7x) + 8x)$ . Note that the order of operations in this expression is different from the one presented in Fig. 8.

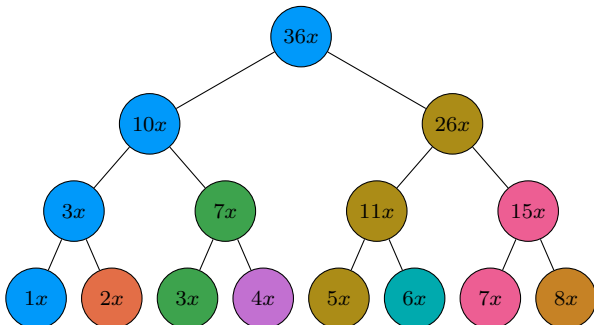


Fig. 10: Addition of eight floating point numbers across eight machines with a guarantee on SPI. Each machine is represented by a different colour. The final result can be represented by the expression  $((1x + 2x) + (3x + 4x)) + ((5x + 6x) + (7x + 8x))$ .

Julia creates `nthreads()` tasks and thus `nthreads()` pseudorandom number generators. This can break strong parallelism invariance as the output may depend on the number of threads.

To motivate splittable random streams, consider the following toy example that violates our notion of SPI:

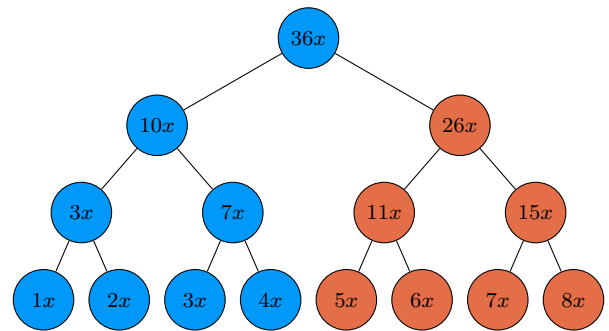


Fig. 11: Addition of eight floating point numbers across two machines with a guarantee on SPI. Each machine is represented by a different colour. The final result can be represented by the expression  $((1x + 2x) + (3x + 4x)) + ((5x + 6x) + (7x + 8x))$ , which is the same as that given by eight machines in Fig. 10.

```
using Random
import Base.Threads.@threads

println("Num. of threads: $(Threads.nthreads())")

const n_iters = 10000
result = zeros(n_iters)
Random.seed!(1)
@threads for i in 1:n_iters
    result[i] = rand()
end
println("Result: $(last(result))")
```

With eight threads, this outputs:

```
Num. of threads: 8
Result: 0.25679999169092793
```

Julia guarantees that if we rerun this code, as long as we are using eight threads, we will always get the same result, irrespective of the multi-threading scheduling decisions implied by the `@threads`-loop. Internally, Julia works with task-local RNGs and the `@threads` macro spawns `nthreads()` number of task-local RNGs. For this reason, with a different number of threads, the result is different:

```
Num. of threads: 1
Result: 0.8785201210435906
```

In this simple example above, the difference in output is perhaps not too concerning, but for our parallel tempering use case, the distributed version of the algorithm is significantly more complex and difficult to debug compared to the single-threaded one. We therefore take task-local random number generation one step further and achieve SPI, which guarantees that the output is not only reproducible with respect to repetitions for a fixed number of threads, but also for different numbers of threads or processes.

A first step to achieve this is to associate one random number generator to each `Replica`. To do so, we use our `SplittableRandoms.jl` package, which is a Julia implementation of Java `SplittableRandoms`. Our package offers an implementation of `SplitMix64` [26], which allows us to turn one seed into an arbitrary collection of pseudo-independent RNGs. A quick example of how to use the

SplittableRandoms.jl library is given below. By splitting a master RNG using the `split()` function, we can achieve SPI even with the use of the `@threads` macro.

```
using Random
using SplittableRandoms: SplittableRandom, split
import Base.Threads.@threads

println("Num. of threads: $(Threads.nthreads())")

const n_iters = 10000
const master_rng = SplittableRandom(1)
result = zeros(n_iters)
rngs = [split(master_rng) for _ in 1:n_iters]
Random.seed!(1)
@threads for i in 1:n_iters
    result[i] = rand(rngs[i])
end
println("Result: $(last(result))")
```

With one and eight threads, the code above outputs

```
Num. of threads: 1
Result: 0.4394633333251359
```

```
Num. of threads: 8
Result: 0.4394633333251359
```

## 5. Related work

Automated software packages for Bayesian inference have revolutionized Bayesian data analysis in the past two decades, and are now a core part of a typical applied statistics workflow. For example, packages such as BUGS [20, 21, 22], JAGS [15], Stan [10], PyMC3 [24], and Turing.jl [12] have been widely used in many scientific applications.

These software packages often provide two key user-facing components: (1) a probabilistic programming language (PPL), which allows users to specify Bayesian statistical models in code with a familiar, mathematics-like syntax; and (2) an inference engine, which is responsible for performing computational Bayesian inference once the model and data have been specified. Pigeons.jl focuses on the development of a new inference engine that employs distributed, high-performance computing.

Inference engines available in existing software packages are varied in their capabilities and limitations. For instance, the widely-used Stan inference engine is only capable of handling real-valued (i.e., continuous) parameters. Other tools, such as JAGS, are capable of handling discrete-valued parameters but are limited in their capability to handle custom data-types (e.g. phylogenetic trees). Of those that have the capability to model arbitrary data types, none have an automatically distributed implementation to our knowledge. Turing.jl [12] offers another popular inference engine and PPL, however Pigeons.jl allows one to interface with several different PPLs as well as to easily perform distributed computation.

There is also a vast literature on distributed and parallel Bayesian inference algorithms [3, 6, 9, 16, 17, 19, 25, 31, 32, 35]. These methods unfortunately do not lead to widely usable software packages because they either introduce unknown amounts of approxi-

mation error, involve significant communication cost, or reduce the generality of Bayesian inference.

## 6. Conclusion

Pigeons.jl is a Julia package that enables users with no experience in distributed computing to efficiently approximate posterior distributions and solve challenging Lebesgue integration problems over a distributed computing environment. The core algorithm behind Pigeons.jl is distributed, non-reversible parallel tempering [29, 27]. Pigeons.jl can be used in a multi-threaded context, as well as distributed over up to thousands of MPI-communicating machines. Further, Pigeons.jl is designed so that for a given seed, the output is *identical* regardless of the number of threads or processes used.

## 7. Acknowledgements

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