Markov chain quasi-Monte Carlo simulation using linear feedback shift register generators

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Introduction: Markov chain QMC

Motivation:

- We consider the problem of estimating the expectation

$$E_\pi[f(\mathbf{X})] = \int_{\mathcal{X}} f(x)\pi(dx)$$

  using Markov chain Monte Carlo (MCMC) for a probability distribution π on a state space $\mathcal{X}$ and some function $f : \mathcal{X} \to \mathbb{R}$.
- We want to improve the accuracy by replacing IID uniform random points with quasi-Monte Carlo (QMC) points.
- Traditional QMC points (e.g., Sobol', Faure, Niederreiter–Xing, ...) are not straightforwardly applicable.
- Owen–Tribble (2005) and Chen–Dick–Owen (2011) proved that MCMC remains consistent if the driving sequences are completely uniformly distributed (CUD).
- However, the definition of CUD sequences is not constructive.

Introduction: Markov chain QMC

Motivation (continued):

- To obtain point sets that approximate CUD sequences, Chen-Matsumoto-Nishimura-Owen (2012) designed short-period Tausworthe generators (i.e., linear feedback shift register generators) optimized in terms of the equidistribution property, which is a coarse measure used in pseudorandom number generation.
- Harase (2021, 2024) designed short-period Tausworthe generators in terms of the t-value, which is a central measure in the theory of (t, m, s)-nets and (t, s)-sequences.

In this talk, we outline new Tausworthe generators for Markov chain QMC and present numerical experiments using Gibbs sampling.

References:

1. S. Harase, "A table of short-period Tausworthe generators for Markov chain quasi-Monte Carlo", J. Comput. Appl. Math. 384 (2021), 113136, 12 pp.
2. S. Harase, "A search for short-period Tausworthe generators over $\mathbb{F}_b$ with application to Markov chain quasi-Monte Carlo", J. Stat. Comput. Simul. 94 (2024), no. 9, 2040–2062.

CUD sequences

Definition (CUD sequences)

A one-dimensional sequence $u_0, u_1, u_2, u_3, u_4, \ldots \in [0,1)$ is said to be completely uniformly distributed (CUD) if the overlapping s-blocks

$$(u_i, u_{i+1}, \ldots, u_{i+s-1}) \in [0,1)^s, \quad i = 0, 1, 2, \ldots,$$

are uniformly distributed for every dimension $s \geq 1$.

- Then, the non-overlapping s-blocks $(u_{is}, u_{si+1}, \ldots, u_{(i+1)s-1})$ are also uniform (Chentsov, 1967), so we can use $\{u_i\}_{i=0}^{\infty}$ in this order.
- It is desirable that the s-blocks are highly uniform (Dick–Rudolf, 2014).

Chen et al. (2012) and Harase (2021, 2024) designed "approximate" CUD sequences

$$u_0, u_1, \ldots, u_{N-2}, u_{N-1} = u_0, \ldots \quad (N-1 : \text{period length}),$$

based on short-period Tausworthe generators that run for the entire-period.

Tausworhe generators (Tausworthe, 1965)

Let $\mathbb{F}_b$ be a finite field of prime power order b.
We define Tausworthe generators over $\mathbb{F}_b$ as polynomial LCGs:

$$\begin{aligned} \boldsymbol{X}_i(x) &= \boldsymbol{q}(x)\boldsymbol{X}_{i-1}(x) \mod \boldsymbol{p}(x), \\ \boldsymbol{X}_i(x)/\boldsymbol{p}(x) &= \boldsymbol{a}_{i\sigma}x^{-1} + \boldsymbol{a}_{i\sigma+1}x^{-2} + \boldsymbol{a}_{i\sigma+2}x^{-3} + \cdots \in \mathbb{F}_b((x^{-1})). \end{aligned}$$

Here, $\boldsymbol{p}(x), \boldsymbol{q}(x) \in \mathbb{F}_b[x]$ represent a modulus and multiplier. Assume

- $\boldsymbol{p}(x)$ is a primitive polynomial with degree $\boldsymbol{m}$;
- $\boldsymbol{q}(x)$ satisfies $\gcd(\sigma, b^m - 1) = 1$, where σ is a step size such that $\boldsymbol{q}(x) = x^{\sigma} \mod \boldsymbol{p}(x)$ and $0 < \sigma < b^m - 1$.

Let $\eta : \mathbb{F}_b \to \mathbb{Z}_b = \{0, 1, \ldots, b\}$ be a bijection with $\eta(0) = 0$. Then, we transform the formal power series into the w-digit output values

$$u_i = \sum_{j=0}^{w-1} \eta(a_{i\sigma+j}) \cdot b^{-j-1} \in [0, 1) \quad (w\text{: a digit number}).$$

In this setting, the output sequence $\{u_i\}_{i=0}^{\infty}$ attains the maximal period $b^m - 1$. We assume the maximal periodicity and $w \geq m$.

Tausworhe generators (Tausworthe, 1965)

Example: $b = 3$ (base). $w = 3$ (digit number). $\eta = \mathrm{id}$.
$p(x) = x^3 + 2x^2 + x + 1 \Leftrightarrow a_i = -2a_{i-1} - a_{i-2} - a_{i-3}$.
$q(x) = x^2 + 2x (= x^5 \mod p(x))$, so the step size $\sigma = 5$.

$$00110102122210022020121112001101021222100 2 \cdots \in \mathbb{F}_3$$

$$\begin{aligned}
X_0(x)/p(x) &= 0x^{-1} + 0x^{-2} + 1x^{-3} + \cdots \mapsto u_0 = 0.001_{(3)} \\
X_1(x)/p(x) &= 1x^{-1} + 0x^{-2} + 2x^{-3} + \cdots \mapsto u_1 = 0.102_{(3)} \\
X_2(x)/p(x) &= 2x^{-1} + 2x^{-2} + 1x^{-3} + \cdots \mapsto u_2 = 0.220_{(3)} \\
&\vdots
\end{aligned}$$

Let $N := b^m$. We run Tausworthe generators for the entire period and construct the s-dimensional overlapping points
$\mathbf{u}_0 = (u_0, \ldots, u_{s-1}), \mathbf{u}_1 = (u_1, \ldots, u_s), \ldots, \mathbf{u}_{N-2} = (u_{N-2}, u_0, \ldots, u_{s-2})$. Adding the origin $\{\mathbf{0}\}$, we regard a point set

$$P_s = \{\mathbf{0}\} \cup \{\mathbf{u}_i\}_{i=0}^{N-2} \qquad (|P_s| = b^m)$$

as a QMC point set, which corresponds to a polynomial Korobov lattice.

(t, m, s)-nets and t-values

In the study of QMC, the t-value is widely used as a measure of uniformity.

Definition ((t, m, s)-nets and t-values)

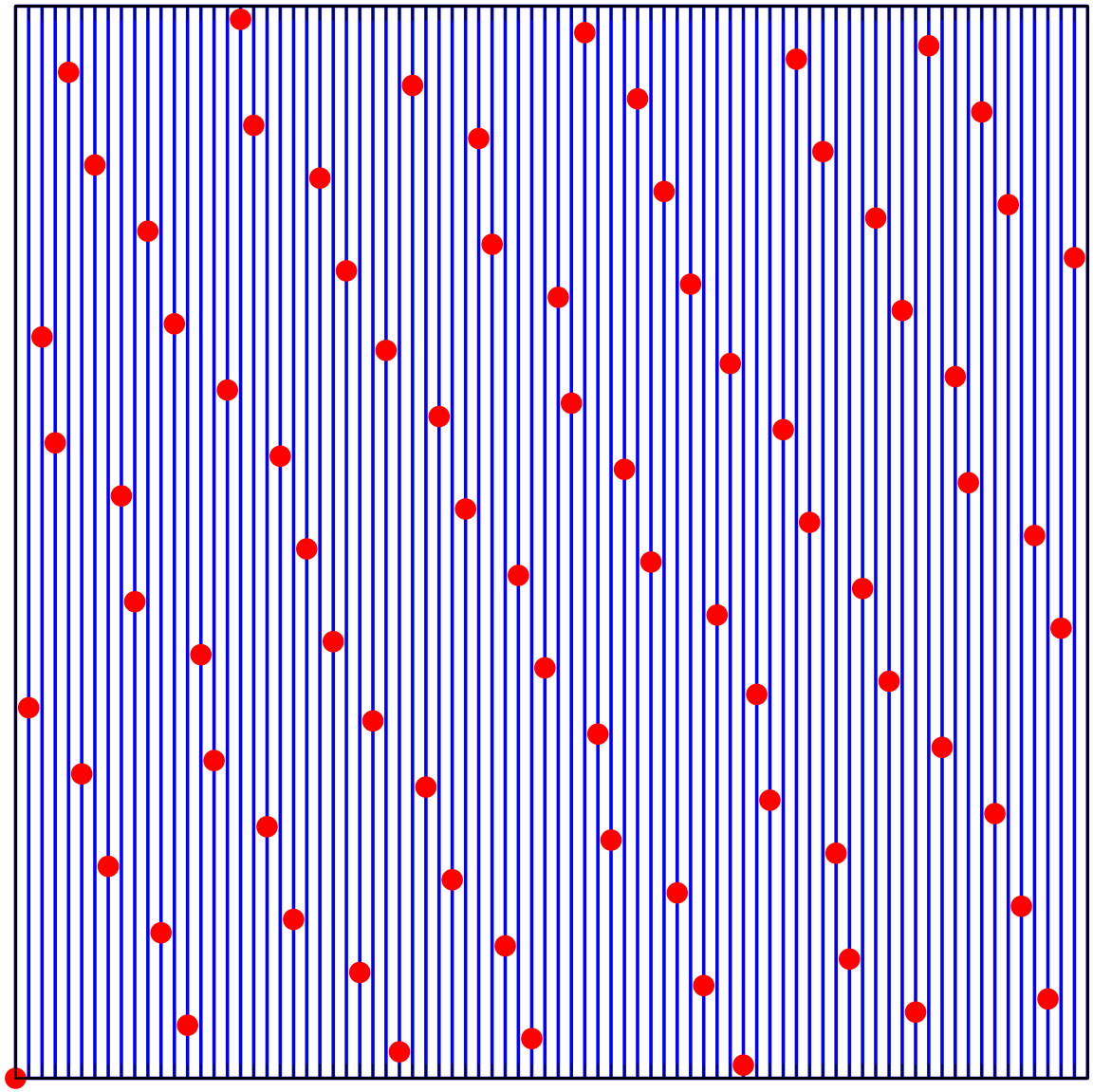
- Let $s \geq 1$ be a dimension. Let t be an integer with $0 \leq t \leq m$.
- Let E be a b-adic box $E = \prod_{j=1}^{s} \left[\frac{l_j}{b^{d_j}}, \frac{l_j+1}{b^{d_j}} \right) \subset [0,1)^s$.
- Let $P_s \subset [0,1)^s$ be a point set consisting of $N = b^m$ points.

P_s is a (t, m, s)-net in base b $\overset{\text{def}}{\iff}$ Every b-adic box E of volume b^{t-m} contains exactly b^t points of P_s.
The smallest t for which P_s is a (t, m, s)-net is called the t-value.

To construct a point set that approximates the CUD property, Harase (2021, 2024) searched a pair of polynomials $(p(x), q(x))$ whose t-values are small for each $s = 1, 2, 3, \ldots$, that is, Tausworthe generators

1. over $\mathbb{F}_2$ with t-values zero for $s = 2$ and small for $s \geq 3$; and
2. over $\mathbb{F}_4$ with t-values zero up to $s = 3$ and small for $s \geq 4$.

Example: $(0, 4, 2)$-net in base 3



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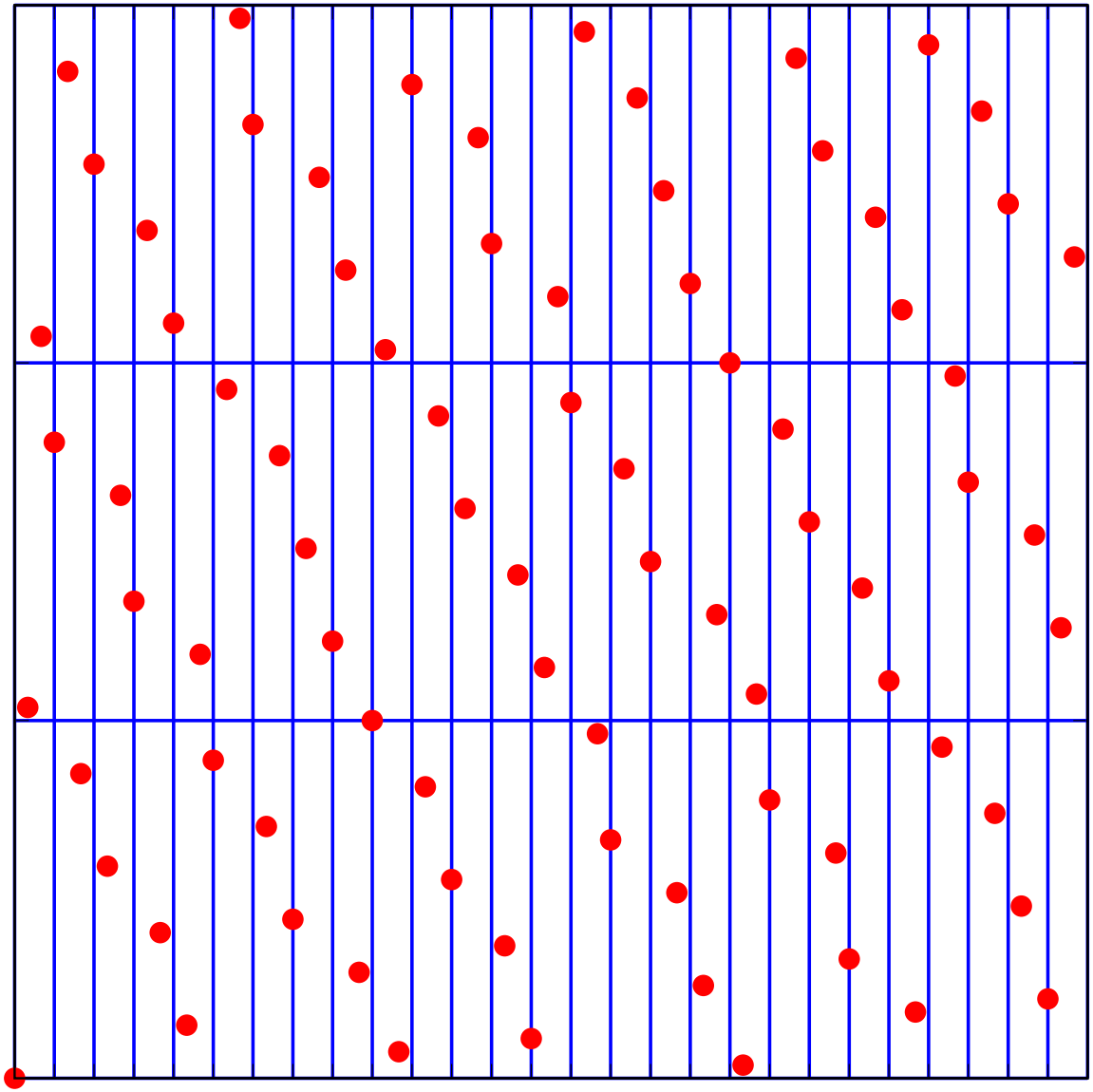

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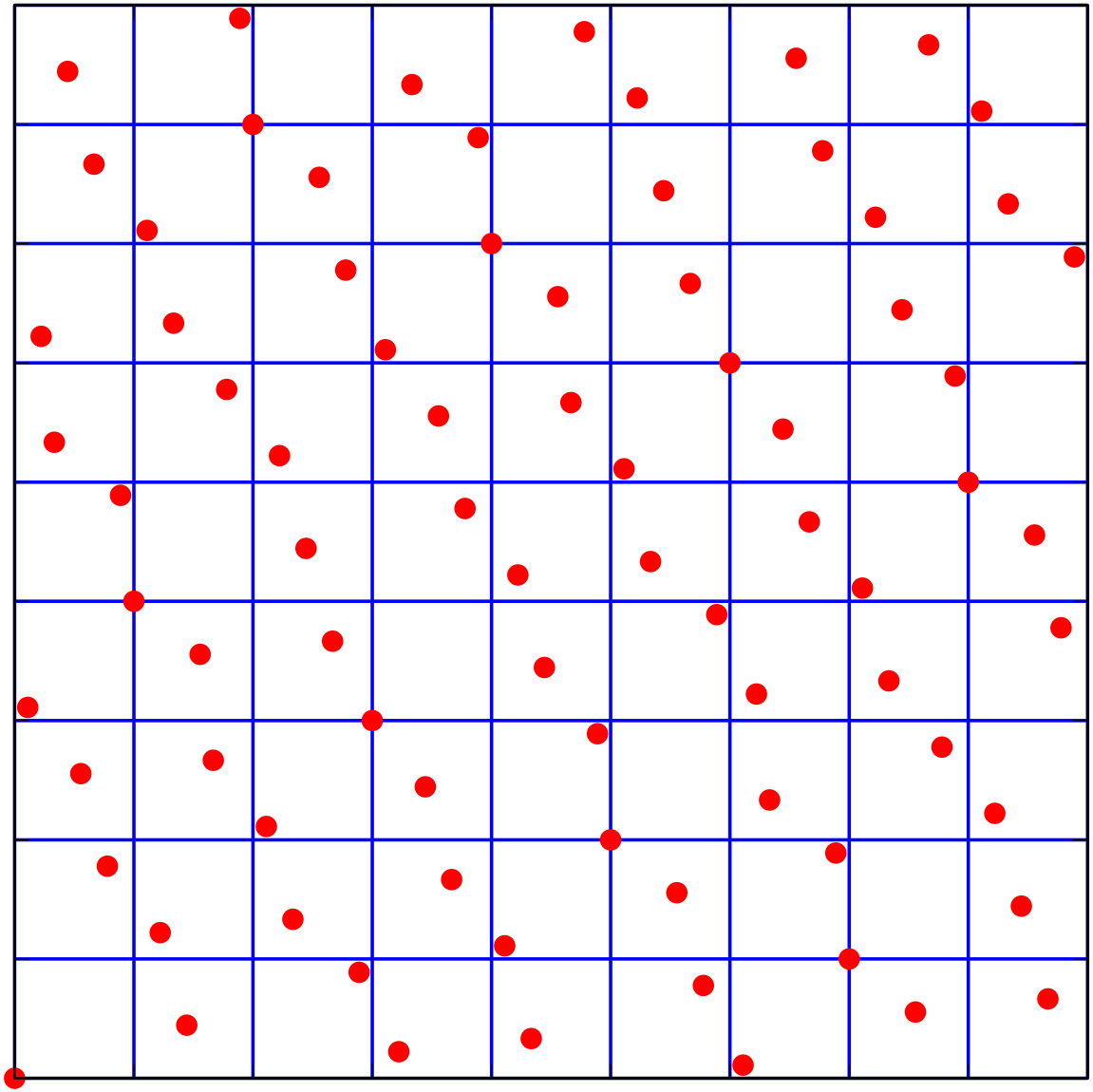

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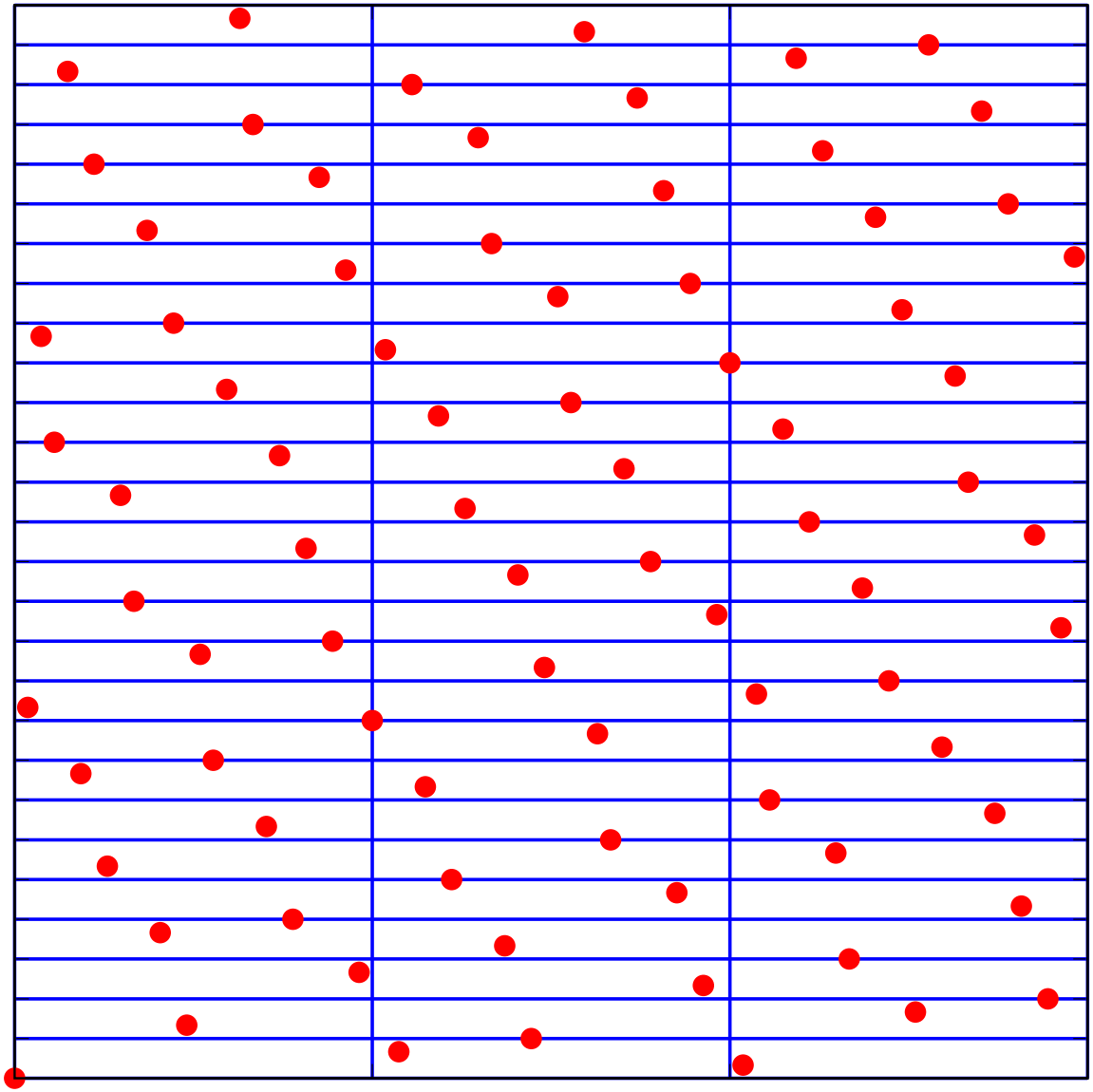
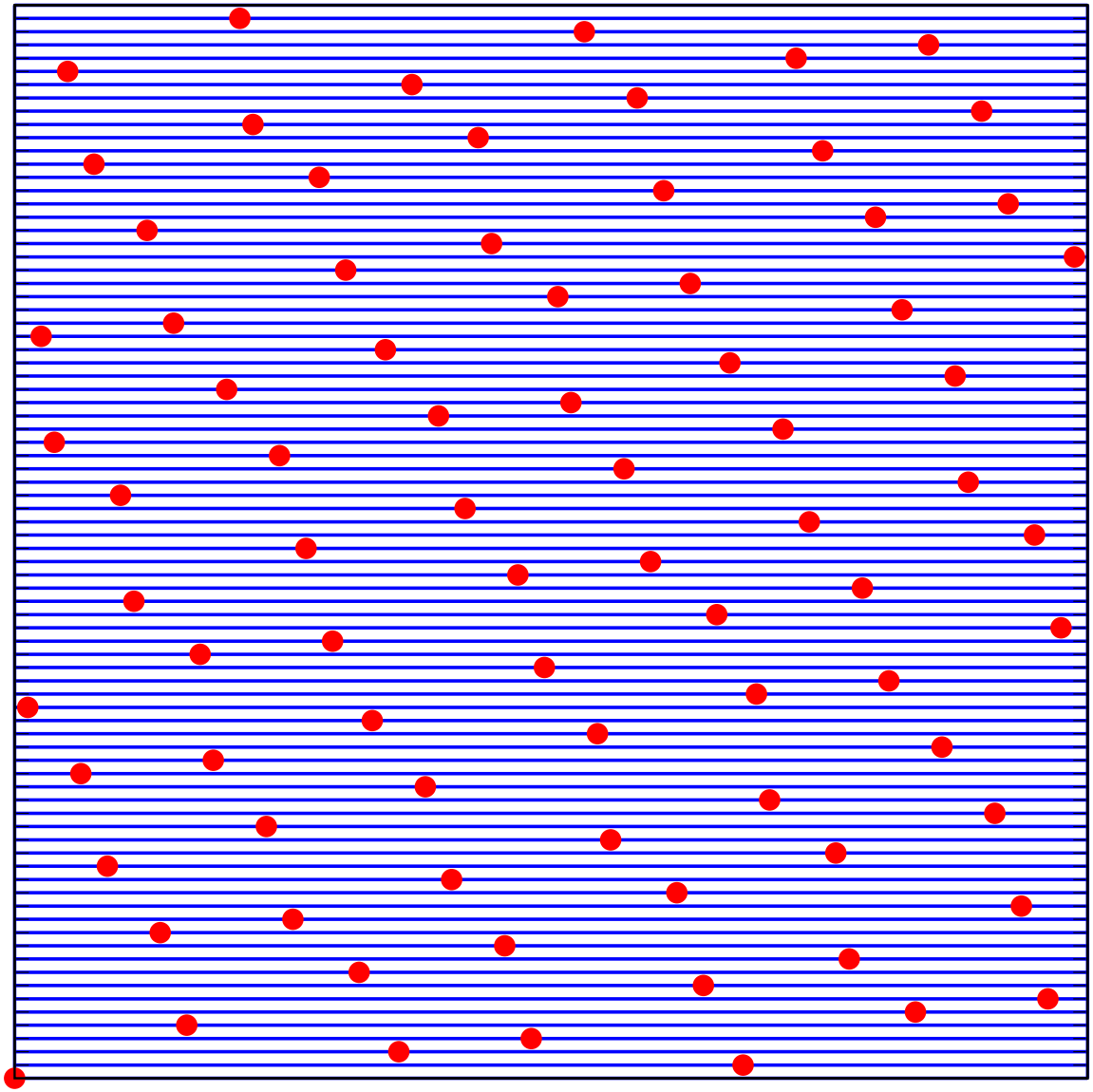


Example: $(0, 4, 2)$-net in base 3



Search algorithm

We briefly introduce the search algorithm (Harase, 2021 and 2024).

Theorem (Niederreiter, 1992) and (Tezuka–Fushimi, 1993)

Let $p(x)$ and $q(x) \in \mathbb{F}_b[x]$ be a modulus and multiplier of Tausworthe generators. Then, the 2-dimensional point set P_2 attains the t-value zero (in base b) if and only if the partial quotients in the continued fraction of $q(x)/p(x)$ are all of degree 1.

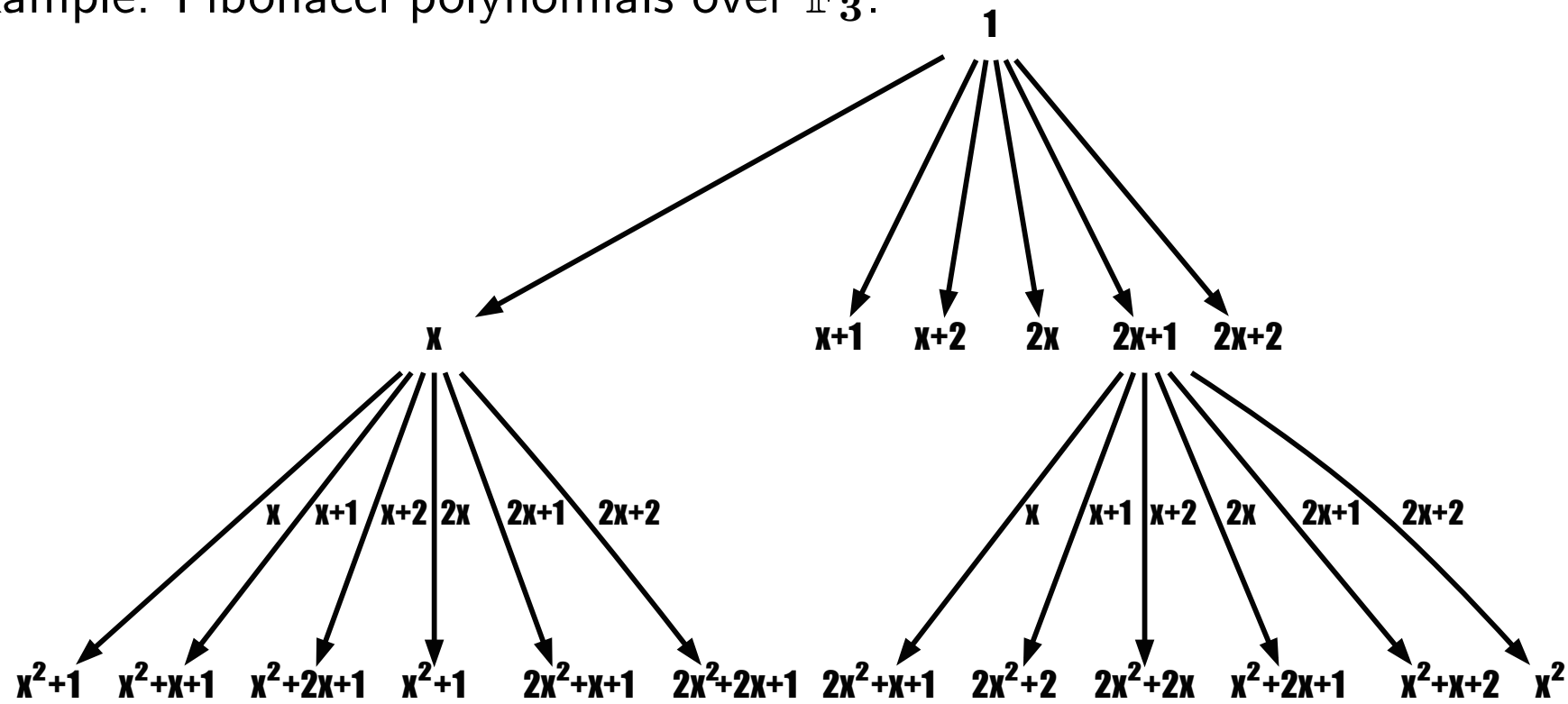
To obtain such pairs $(p(x), q(x))$, we consider a polynomial analogue of Fibonacci numbers over $\mathbb{F}_b$ (cf., Tezuka and Fushimi (1993)):

$$
\begin{aligned}
&F_k(x) = A_k(x)F_{k-1}(x) + F_{k-2}(x), \quad k = 1, 2, \ldots, m, \\
&F_{-1}(x) = 0, F_0(x) = 1, \\
&A_k(x) = \beta x + \gamma, \quad \beta \in \mathbb{F}_b^* \text{ and } \gamma \in \mathbb{F}_b.
\end{aligned}
$$

Then, the partial quotients in the continued fraction of $F_{m-1}(x)/F_m(x)$ are all of degree 1, i.e., $F_{m-1}(x)/F_m(x) = [0; A_m, A_{m-1}, \cdots, A_1]$.

Fibonacci polynomials over $\mathbb{F}_b$ and tree structures

Example: Fibonacci polynomials over $\mathbb{F}_3$.



$$F_k(x) = A_k(x)F_{k-1}(x) + F_{k-2}(x), \quad k = 1, 2, \ldots, m$$
$$F_{-1}(x) = 0, F_0(x) = 1$$
$$A_k(x) = \beta x + \gamma, \quad \beta \in \mathbb{F}_b^* \text{ and } \gamma \in \mathbb{F}_b.$$

From all the pairs $(F_m(x), F_{m-1}(x))$, we choose a suitable pair $(p(x), q(x))$ with t-values zero for $s = 2$ and small for $s \geq 3$.

Comparison of the t-values: our new vs existing results

A search for Tausworthe generators over $\mathbb{F}_2$ (Harase, 2021):

$m = 16$

dim. s	2	3	4	5	6	7	8	9	10	11	12	13	14	15
New	0	3	4	7	7	8	10	10	10	11	11	11	11	11
Existing	3	4	5	8	8	8	8	8	10	10	10	10	10	10

(Existing: Tausworthe generators developed by Chen et al. (2012).)

A search for Tausworthe generators over $\mathbb{F}_4$ (Harase, 2024):

$m \backslash s$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
5	0	0	0	1	1	2	2	2	2	2	2	2	2	2	2
6	0	0	0	1	2	2	2	2	3	3	3	3	3	3	3
7	0	0	0	1	2	2	2	3	3	3	3	3	3	4	4
8	0	0	0	1	2	4	4	4	4	4	4	4	4	4	4
9	0	0	0	1	3	3	3	3	3	4	4	4	4	4	4
10	0	0	0	2	2	3	3	3	4	4	4	5	5	6	6

Numerical example: 3-dimensional Gaussian Gibbs

We provide numerical examples to confirm the performance of Markov chain QMC.

We consider the three-dimensional Gaussian (normal) distribution $\mathcal{N}(\mu, \Sigma)$, where

$$\mu = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \Sigma = \begin{pmatrix} 1 & 0.3 & -0.2 \\ 0.3 & 1 & 0.5 \\ -0.2 & 0.5 & 1 \end{pmatrix}.$$

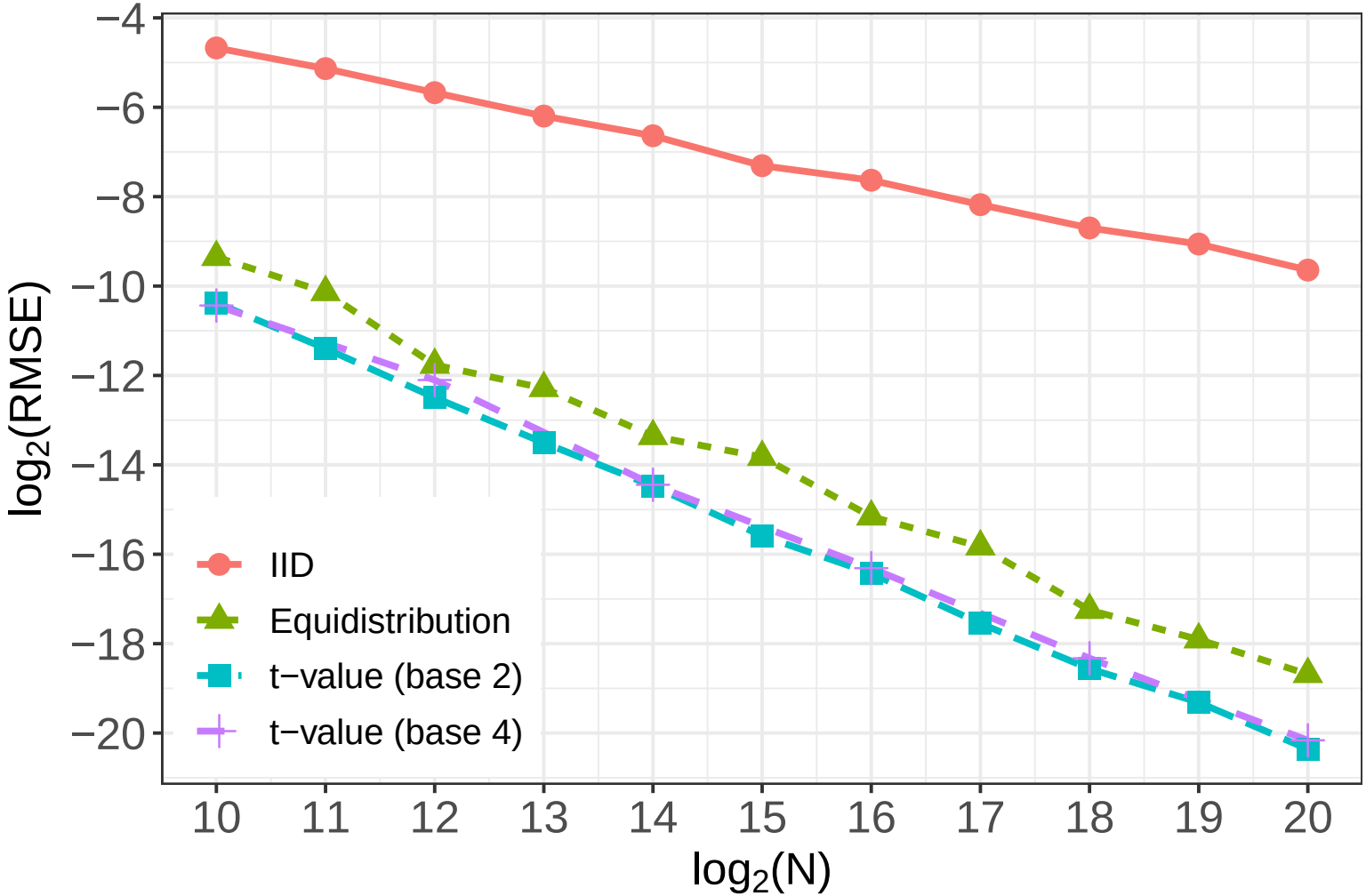
Then, a Gibbs sampling scheme can be implemented as the iteration of the calculation of one-dimensional normal distribution as follows:

$$X_k \mid \mathbf{X}_{-k} \sim \mathcal{N}(\mu_k + \Sigma_{k,-k}\Sigma_{-k,-k}^{-1}(\mathbf{X}_{-k} - \mu_{-k}), \Sigma_{k,k} - \Sigma_{k,-k}\Sigma_{-k,-k}^{-1}\Sigma_{-k,k})$$

for $k = 1, 2, 3$.

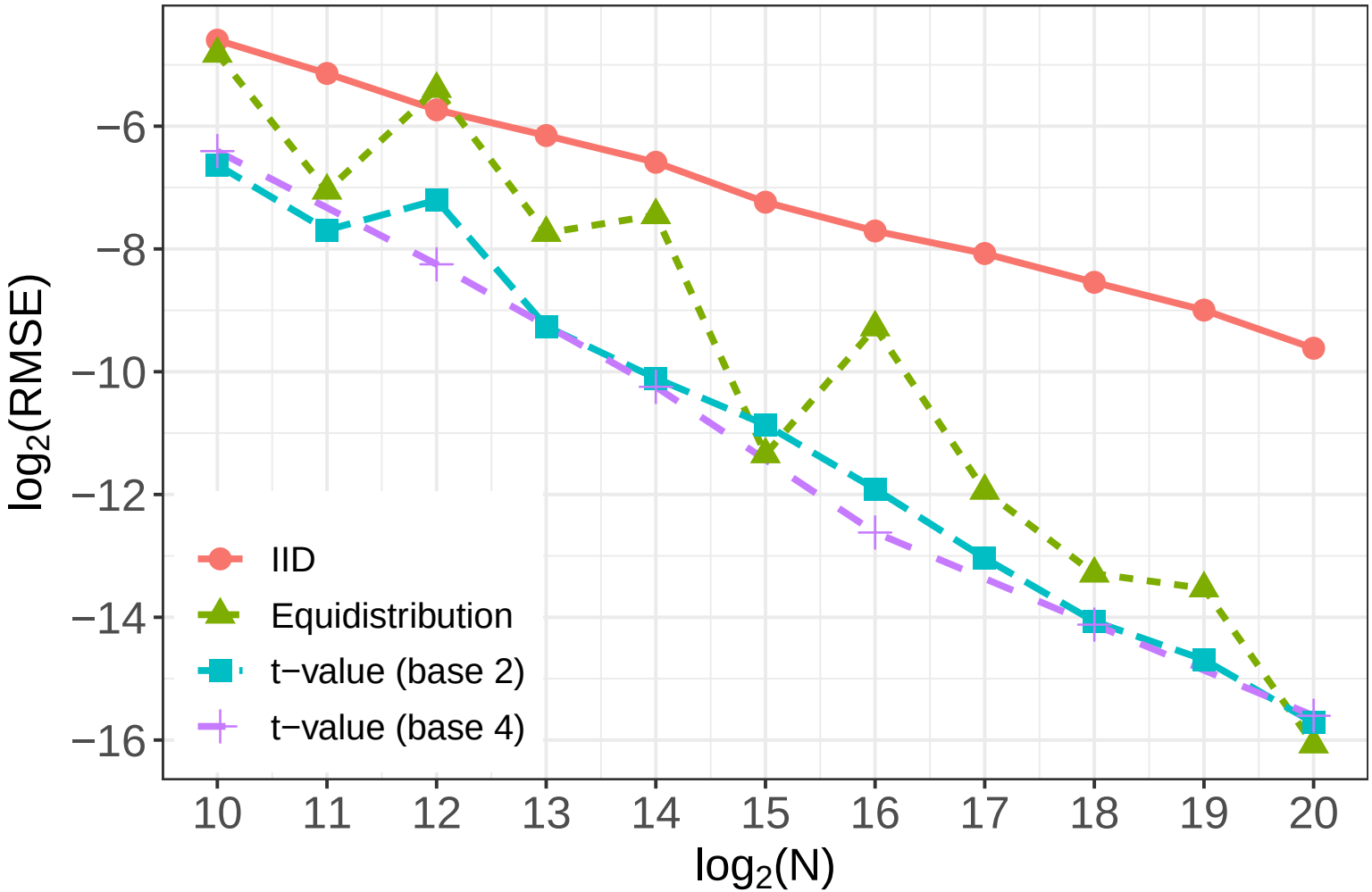
Numerical example: 3-dimensional Gaussian Gibbs

We estimate $E[X_1]$ with true value 0 by taking the sample mean.
We calculate RMSEs using 300 digital shifts.



Numerical example: 3-dimensional Gaussian Gibbs

We estimate $E[X_1X_2X_3]$ with true value 0 by taking the sample mean.
We calculate RMSEs using 300 digital shifts.



Numerical example: Bayesian linear regression

We use the Boston housing data.
Harrison and Rubinfeld (1978) built a linear regression model given by

$$\begin{aligned}\log(\mathrm{MEDV}) = {} & \beta_0 + \beta_1 \mathrm{CRIM} + \beta_2 \mathrm{ZN} + \beta_3 \mathrm{INDUS} + \beta_4 \mathrm{CHAS} + \beta_5 \mathrm{NOX}^2 \\ & + \beta_6 \mathrm{RM}^2 + \beta_7 \mathrm{AGE} + \beta_8 \log(\mathrm{DIS}) + \beta_9 \log(\mathrm{RAD}) + \beta_{10} \mathrm{TAX} \\ & + \beta_{11} \mathrm{PTRATIO} + \beta_{12} \mathrm{B} + \beta_{13} \log(\mathrm{LSTAT}) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \tau^2),\end{aligned}$$

where

- The housing price MEDV is a response variable;
- The constant term, CRIM, . . . , LSTAT are 14 explanatory variables.

We now consider Bayesian inference (e.g., see Hoff (2009)).

- Assume that $\beta = (\beta_0 \ldots, \beta_{13})$ and τ^2 are independent and follow the normal and inverse-gamma prior distributions.
- We calculate the posterior mean estimates $E[\beta]$ and $E[\tau^2]$ by running the Gibbs sampler for $N = 2^{16}$ iterations after a burn-in period.

Numerical example: Bayesian linear regression

The following table shows a summary of sample variances of posterior mean estimates $E[\beta_i]$ and $E[\tau^2]$ using 300 digital shifts.

$N = 2^{16}$					
Parameter	β_0	β_1	β_2	β_3	β_4
IID	3.07e-07	2.74e-11	4.13e-12	8.43e-11	1.64e-08
Equidistribution	9.28e-12	6.59e-16	1.07e-16	2.37e-15	4.71e-13
t-value (base 2)	1.40e-12	9.12e-17	1.82e-17	3.55e-16	1.71e-13
t-value (base 4)	1.73e-12	9.86e-17	1.71e-17	4.20e-16	7.31e-14
Parameter	β_5	β_6	β_7	β_8	β_9
IID	1.72e-07	2.22e-11	4.26e-12	1.54e-08	5.87e-09
Equidistribution	4.73e-12	6.69e-16	1.14e-16	4.70e-13	1.67e-13
t-value (base 2)	7.11e-13	7.65e-17	8.86e-18	4.47e-14	1.42e-14
t-value (base 4)	9.01e-13	1.24e-16	1.63e-17	7.71e-14	3.20e-14
Parameter	β_{10}	β_{11}	β_{12}	β_{13}	τ^2
IID	2.25e-13	3.48e-10	1.89e-13	1.09e-08	7.35e-11
Equidistribution	6.91e-18	1.08e-14	4.52e-18	2.34e-13	2.36e-15
t-value (base 2)	1.18e-18	1.36e-15	6.42e-19	3.02e-14	9.24e-16
t-value (base 4)	1.36e-18	2.28e-15	1.20e-18	4.68e-14	1.00e-15

Conclusion

Summary:

- For Markov chain QMC, we conducted a search of short-period Tausworthe generators in terms of the t-value, that is, Tausworthe generators
  1. over $\mathbb{F}_2$ with t-values zero for $s = 2$ and small for $s \geq 3$; and
  2. over $\mathbb{F}_4$ with t-values zero up to $s = 3$ and small for $s \geq 4$.
- In the parameter search, we used Fibonacci polynomials over $\mathbb{F}_b$.
- We reported numerical examples using Gibbs sampling in which our new Tausworthe generators perform comparable to or even better than the existing Tausworthe generators (Chen et al., 2012).

References:

1. S. Harase, "A table of short-period Tausworthe generators for Markov chain quasi-Monte Carlo", J. Comput. Appl. Math. 384 (2021), 113136, 12 pp.
2. S. Harase, "A search for short-period Tausworthe generators over $\mathbb{F}_b$ with application to Markov chain quasi-Monte Carlo", J. Stat. Comput. Simul. 94 (2024), no. 9, 2040–2062.

The code in C is available at `https://github.com/sharase`.