

Randomized Quasi-Monte Carlo Methods on Triangles: Extensible Lattices and Sequences

Gracia Yunruo Dong^{1,2*}, Erik Hintz³, Marius Hofert⁴,
Christiane Lemieux³

^{1*}Dept. of Statistical Sciences, University of Toronto, 700 University
Ave, Toronto, M5G1X6, Ontario, Canada.

²Dept. of Mathematics and Statistics, University of Victoria, 3800
Finnerty Road, Victoria, V8P5C2, British Columbia, Canada.

³Dept. of Statistics and Actuarial Science, University of Waterloo, 200
University Ave W, Waterloo, N2L3G1, Ontario, Canada.

⁴Dept. of Statistics and Actuarial Science, The University of Hong
Kong, Pok Fu Lam, Hong Kong.

*Corresponding author(s). E-mail(s): gracia.dong@utoronto.ca;
Contributing authors: erik.hintz@uwaterloo.ca; mhofert@hku.hk;
clemieux@uwaterloo.ca;

Abstract

Two constructions were recently proposed for constructing low-discrepancy point sets on triangles. One is based on a finite lattice, the other is a triangular van der Corput sequence. We give a continuation and improvement of these methods. We first provide an extensible lattice construction for points in the triangle that can be randomized using a simple shift. We then examine the one-dimensional projections of the deterministic triangular van der Corput sequence and quantify their sub-optimality compared to the lattice construction. Rather than using scrambling to address this issue, we show how to use the triangular van der Corput sequence to construct a stratified sampling scheme. We show how stratified sampling can be used as a more efficient implementation of nested scrambling, and that nested scrambling is a way to implement an extensible stratified sampling estimator. We also provide a test suite of functions and a numerical study for comparing the different constructions.

Keywords: quasi-Monte Carlo, triangular van der Corput sequence, lattice methods, stratified sampling

MSC Classification: 11K31 , 11K36 , 11K45 , 65D30 , 65D32

1 Introduction

Numerical integration over triangular areas is a subject that has been of interest for many decades, for example when applying finite element methods; see [Cowper \(1973\)](#) where Gaussian quadrature formulas for triangles are derived. For sampling on a two-dimensional triangle with applications in computer graphics, see [Pharr \(2019\)](#); [Basu and Owen \(2015\)](#). Rather than mapping points from the unit cube to the triangle as done in, e.g., [Heitz \(2019\)](#); [Pillards and Cools \(2005\)](#); [Fang and Wang \(1993\)](#); [Arvo \(1995\)](#), instead [Basu and Owen \(2015\)](#) have proposed two low-discrepancy constructions that construct points directly on the triangle. The first is based on a finite lattice, which attains a parallelogram discrepancy of $O(\log(n)/n)$, the best possible rate. [Brandolini et al \(2013\)](#) and work prior to this have only indicated that such a discrepancy was possible, without providing a construction. The lattice construction in [Basu and Owen \(2015\)](#) is not extensible in the sample sizes n , i.e., if n_1 points are sampled, but $n_2 > n_1$ points are needed, the entire lattice with n_2 points needs to be constructed rather than adding $n_2 - n_1$ points to the existing lattice. The second is a triangular van der Corput (vdC) sequence based on the one-dimensional vdC sequence in base 4 that places points in a two-dimensional triangle by recursively subdividing the triangle.

In this paper, we extend the work of [Basu and Owen \(2015\)](#) and explore the use of randomized quasi-Monte Carlo methods on triangles and their success in practice. Required background is reviewed in Section 2. Here, we first introduce the triangular lattice and vdC sequence of [Basu and Owen \(2015\)](#). In Section 2.5, we then show that

the vdC sequence has poor projection properties: The one-dimensional projections of
the non-randomized triangular vdC sequence contain only $2\sqrt{n} < n$ points, which can
lead to poorer integration results for functions with low effective dimension. This is
different from rank-1 lattices, which can be made fully projection regular.

We then provide an extensible lattice construction for points in the triangle that can
be randomized with a digital shift in Section 3, making this method more applicable
in practice. In Section 4, we address the issue of the poor projection properties of
the triangular vdC sequence by proposing a stratified sampling scheme using the sub-
triangles constructed in the vdC sequence as strata. We also show that, in general over
the unit interval and not only on triangles, the stratified sampling scheme has the same
distribution as the nested scrambling of the vdC sequence, while being more efficient to
implement. This connection between stratified sampling and nested scrambling allows
us to have the benefits of nested scrambling without the expensive computational
costs. This connection also allows us to show that nested scrambling provides a way
to implement an extensible stratified estimator.

Finally, although various constructions and mappings for sampling on the triangle
exist, there is little, if any, work done comparing these different methods on numerical
integration examples. This motivates the inclusion of Section 5, a numerical study
on a suite of test functions on the triangle that allow us to differentiate between the
performance of these constructions. Section 6 concludes this paper.

2 Background

In this section, we review quasi-Monte Carlo methods, some definitions and properties
of triangles, and show how one can uniformly sample within a triangle.

139 2.1 Monte Carlo and quasi-Monte Carlo methods

140

141 The *Monte Carlo* (MC) method for numerical integration uses repeated random sam-
 142 pling to obtain numerical results for integrals that either do not have a closed form
 143 or are difficult to integrate theoretically. Quantities of interest are integrals over the
 144 s -dimensional hypercube $[0, 1]^s$, which can be written as

145

146

147

148

149

150

151

152

153

154

155

156

157

158

159

160

161

162

163

164

165

166

167

168

169

170

171

172

173

174

175

176

177

178

179

180

181

182

183

184

185

186

187

188

189

190

191

192

193

194

195

196

197

198

199

200

201

202

203

204

205

$$\mu = I(f) = \int_{[0,1]^s} f(\mathbf{u}) \, d\mathbf{u},$$

where $f : [0, 1]^s \rightarrow \mathbb{R}$ is integrable. The MC estimator of $I(f)$ based on a sample of size n is

$$\hat{\mu}_{mc} = \frac{1}{n} \sum_{i=1}^n f(\mathbf{u}_i),$$

where $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ are independent and identically distributed (iid) samples from the uniform distribution over $[0, 1]^s$. From the Central Limit Theorem, the integration error is asymptotically normal with

$$\sqrt{n}(I(f) - \hat{\mu}_{mc}) \xrightarrow{D} N(0, \sigma^2),$$

where \xrightarrow{D} denotes convergence in distribution and $\sigma^2 = I(f^2) - I(f)^2$ is the variance of f , which can be estimated by the sample variance of $f(\mathbf{u}_1), \dots, f(\mathbf{u}_n)$. The MC integration error is $O_p(\frac{1}{\sqrt{n}})$, meaning that k^2 -many samples are needed to decrease the error by a factor of k . This is one of the drawbacks of the MC method, improving the accuracy of an estimate can be computationally expensive.

A way to improve the error of the estimator of our quantity of interest is to use *quasi-Monte Carlo* (QMC) methods instead of the MC method. These methods replace the randomly sampled point set of an MC estimator with a deterministic point set that is chosen to fill the unit hypercube as homogeneously as possible. Such sets are known as *low-discrepancy sequences* or low-discrepancy point sets, as the sequences cover the

area over the unit hypercube more evenly than those of a pseudo-randomly generated sequence of $\text{Uniform}[0, 1]^s$ random variables and thereby minimize the discrepancy of the point set. There are two main kinds of low-discrepancy point sets: integration lattices (Sloan and Joe, 1994) such as the Kronecker lattice of Korobov (1959), and digital nets and sequences (Dick and Pillichshammer, 2010) such as the vdC sequence of van der Corput (1935). Using QMC methods allows the error of the estimator to decrease at a faster rate than $O(\frac{1}{\sqrt{n}})$, which makes it superior for the purpose of estimation; see Owen (1997).

Quasi-random point sets can be randomized in practice to be able to estimate the variance of the *randomized Quasi-Monte Carlo* (RQMC) estimator. This randomization produces a new point set $\tilde{P}_n = \{\tilde{\mathbf{u}}_1, \dots, \tilde{\mathbf{u}}_n\}$ which satisfies that each point $\tilde{\mathbf{u}}_i \sim \text{Uniform}([0, 1]^s)$ for all i while preserving the low-discrepancy of P_n . Note that after applying the randomization function to quasi-random numbers, the generated points $\tilde{\mathbf{u}}_i$ are not independent across different i . Thus, any parts of the Monte Carlo methodology that depends on the assumption of independence will need to be adjusted when using the RQMC method.

In particular, with the MC estimator, one uses the fact that $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ are iid samples to estimate the standard error of our estimator. This cannot be done in the same way when using RQMC to estimate $I(f)$ because in that case the sample points in \tilde{P}_n are not independent. Instead, as per (Lemieux, 2009, Chapter 6.2), we create a random sample of v quasi-random estimators, which are each based on a randomized point set of size n . Let $\tilde{P}_{n,l} = \{\tilde{\mathbf{u}}_{1,l}, \dots, \tilde{\mathbf{u}}_{n,l}\}$, where $\tilde{P}_{n,1}, \dots, \tilde{P}_{n,v}$ are v independent copies of \tilde{P}_n . Define the l^{th} RQMC estimator

$$\hat{\mu}_{rqmc,l} = \frac{1}{n} \sum_{i=1}^n f(\tilde{\mathbf{u}}_{i,l}) \quad \text{for } l = 1, \dots, v,$$

231 which has expectation

232

233

234

235

236

237

238 as each $\tilde{\mathbf{u}}_{i,l} \sim \text{Uniform}([0, 1]^s)$. Thus, $\hat{\mu}_{rqmc,l}$ is an unbiased estimator of $I(f)$. The

239

240

241

242

243

244

245

246 with variance estimator

247

248

249

250

251

252

253 The empirical variance in Equation (2) can then be compared with that of the regular

254

255

256

257

258 **2.2 Point sets on the triangle**

259

260

261 In the general case, let points A, B, C lie on a hyperplane in \mathbb{R}^d , forming a non-

262

263

264

265

266

267

268

269

270

271

272

273

274

275

276

277

278

279

280

281

282

283

284

285

286

287

288

289

290

291

292

293

294

295

$$\mathbb{E}(\hat{\mu}_{rqmc,l}) = \frac{1}{n} \sum_{i=1}^n \mathbb{E}(f(\tilde{\mathbf{u}}_{i,l})) = \frac{1}{n} \sum_{i=1}^n \int_{[0,1]^s} f(\tilde{\mathbf{u}}_{i,l}) d\tilde{\mathbf{u}}_{i,l} = I(f)$$

$$\hat{\mu}_{rqmc} = \frac{1}{v} \sum_{l=1}^v \hat{\mu}_{rqmc,l}, \quad (1)$$

$$\hat{\sigma}_{rqmc}^2 = \frac{1}{v} \left(\frac{1}{v-1} \right) \sum_{l=1}^v (\hat{\mu}_{rqmc,l} - \hat{\mu}_{rqmc})^2. \quad (2)$$

$$\triangle(A, B, C) = \left\{ \lambda_1 A + \lambda_2 B + \lambda_3 C \mid \min_j \{\lambda_j\} \geq 0, \sum_{j=1}^3 \lambda_j = 1 \right\}.$$

triangle. It is thus useful to be able to map a point set constructed on one triangle to any other arbitrary triangle. Indeed, we can use an affine transformation which preserves the ratios of the lengths of parallel line segments and ratios of distances between points lying on a straight line.

Let $\Delta = \Delta(A, B, C)$ and $\Delta' = \Delta(A', B', C')$ be two arbitrary triangles. Algorithm 1 from Tymchyshyn and Khlevniuk (2019) explains how to transform a point $\mathbf{x} = (x, y) \in \Delta$ to $\mathbf{x}' = (x', y') \in \Delta'$. This transformation can be applied to every point within Δ to create a sampling scheme on Δ' . When Δ' is non-degenerate, this transformation is one-to-one. The algorithm can be extended to higher dimensions, for example, to map between simplexes.

Algorithm 1 (Transforming a point from Δ to Δ'). *Given $\Delta = \Delta(A, B, C)$, $\Delta' = \Delta(A', B', C')$, and a point $\mathbf{x} = (x, y) \in \Delta$:*

1. *Define the matrices*

$$M(\Delta) = \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ 1 & 1 & 1 \end{pmatrix} \quad \text{and} \quad M(\Delta') = \begin{pmatrix} a'_1 & b'_1 & c'_1 \\ a'_2 & b'_2 & c'_2 \\ 1 & 1 & 1 \end{pmatrix},$$

where $A = (a_1, a_2)$, $B = (b_1, b_2)$, $C = (c_1, c_2)$, $A' = (a'_1, a'_2)$, $B' = (b'_1, b'_2)$, and $C' = (c'_1, c'_2)$.

2. *Let $M(\Delta, \Delta') = M(\Delta')M(\Delta)^{-1}$ be our affine transformation matrix.*

3. *Return the point $\mathbf{x}' = (x', y')$ consisting of the first two components of the matrix-vector product*

$$(x', y', z') = M(\Delta, \Delta') \begin{pmatrix} x \\ y \\ 1 \end{pmatrix}. \quad (3)$$

We illustrate the affine transformation in Figure 1. The first four points of the scrambled triangular vdC sequence are generated on the equilateral triangle \triangle_E , and then mapped using Algorithm 1 to the right-angle triangle \triangle_R . Clearly, the ratios of distances between points are preserved, as are the low-discrepancy properties of the point set.

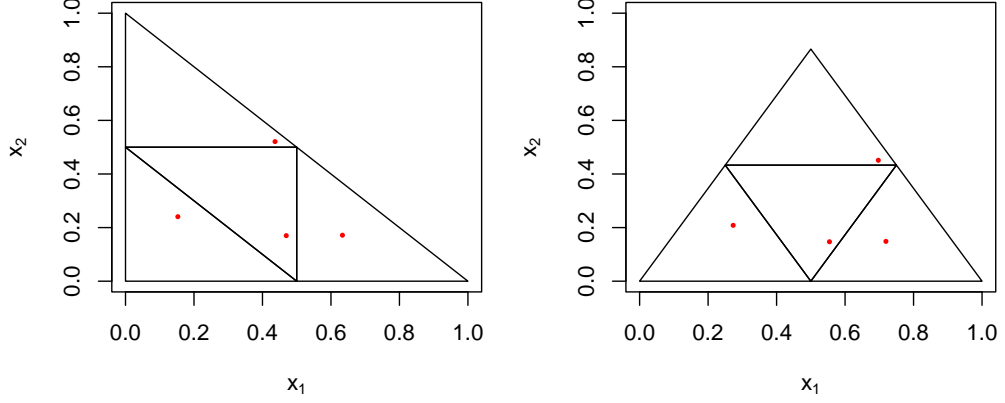


Fig. 1 Four points generated on the equilateral triangle and mapped to the right-angle triangle using Algorithm 1.

2.3 Transforming a low-discrepancy point set from the unit square to a triangle

The end goal of creating point sets over some domain Ω is often to estimate an integral over said domain, say, $\int_{\Omega} f(\mathbf{x}) d\mathbf{x}$, where $f : \Omega \rightarrow \mathbb{R}$ is integrable. If constructing point sets on Ω directly is difficult or not possible, a natural and popular approach is to sample points from the unit hypercube $[0, 1)^d$ and to formulate this integral as

$$\mu = \int_{\Omega} f(\mathbf{x}) d\mathbf{x} = \lambda(\Omega) \int_{[0,1)^d} f(\phi(\mathbf{u})) d\mathbf{u},$$

where $\phi : [0, 1]^d \rightarrow \Omega$ for some $d \in \mathbb{N}$ is a mapping such that $\phi(\mathbf{U}) \sim \text{Uniform}(\Omega)$ for $\mathbf{U} \sim \text{Uniform}(0, 1)^d$. That is, we can estimate expectations by sampling points uniformly from the domain Ω if we can find such a mapping ϕ .

For the right-angle triangle $\Omega = \triangle$ with $0 \leq x_1 \leq x_2 \leq 1$ (which is $\Omega = \triangle((0, 0), (0, 1), (1, 1))$), Pillards and Cools (2005) give six possible transformations ϕ to map points from $\text{Uniform}[0, 1]^2$ to a uniform distribution over \triangle . Note that this right-angle triangle \triangle is not the same as \triangle_R , but as mentioned earlier, transforming points generated on one triangle to another triangle is straightforward.

1. Method *Drop*. Points are accepted if they are within \triangle and rejected otherwise. In higher dimensions, many points get lost – only 1 in every $s!$ points are kept when working in s dimensions.
2. Method *Sort*. Points rejected by the drop method are recovered by reordering the coordinates of a point in the unit square such that $x_1 \leq x_2$ to be within \triangle . This transformation is fast and continuous.
3. Method *Mirror*. We accept the points that are already in \triangle and reflect the other ones at $(1/2, 1/2)$. The resulting transformation is fast, but discontinuous.
4. Method *Origami*. Here, the sort method is recursively used within the unit square. Starting by subdividing the unit square into b^{2m} subsquares, where b and m are user-chosen integer values, with each iteration increasing the side length of the subsquare by a factor of b , until it matches the unit square. This transformation is discontinuous.
5. Method *Root*. This method is based on Fang and Wang (1993) and given by

$$\phi(u_1, u_2) = (u_1\sqrt{u_2}, \sqrt{u_2}).$$

This transformation is continuous and smooth, but the two sharp corners of the triangle are treated in different ways.

415 6. Method *Shift*. This method treats the two sharp corners of the triangle the same
416 way, in contrast with the root method. A line is drawn with slope -1 through each
417 point, and each point is then moved halfway towards the nearest axis along this
418 line. This transformation is fast, but is not generalisable to higher dimensions.
419
420

421 The “drop” method is of acceptance-rejection type in that it only keeps the points
422 in the triangle and discards the other ones. The other methods, except “root” and
423 “shift”, can be thought of as improved variants of “drop”. The method “root” is
424 originally from [Fang and Wang \(1993\)](#) and is an application of the inverse Rosen-
425 blatt transform; see [Rosenblatt \(1952\)](#). Other methods, such as introduced in [Heitz](#)
426 (2019), have been introduced for computer graphics applications, that transform points
427 from the unit square to \triangle_R with lower distortion than the “root” method, similarly
428 to the “shift” method. Although the concept of “low-distortion” is not consistently
429 defined (see [Shirley and Chiu \(1997\)](#)), such transformations aim to preserve correlation
430 between points.
431
432

433 In our numerical experiments of Section 5, we use the method “root” on the
434 bivariate Sobol’ sequence as well as on pseudo-randomly generated numbers. We
435 use this method as it is smooth, continuous, fast and can be extended to go from
436 higher-dimensional cubes to simplexes.
437
438

439 2.4 The triangular rank-2 lattice

440 In this section, we describe lattice constructions in general, and then the triangular
441 lattice of [Basu and Owen \(2015\)](#). First, we define a *lattice point set*.
442
443

$$444 P_n = \left\{ \left(\frac{i_1 z_1}{n_1} + \frac{i_2 z_2}{n_2} + \cdots + \frac{i_r z_r}{n_r} \right) \bmod 1, \ 0 \leq i_l < n_l, l = 1, \right\},$$

where the basis vectors $\mathbf{z}_1, \dots, \mathbf{z}_r \in \mathbb{R}^s$. A lattice rule is of rank t if it can be expressed in this form with $r = t$, but not $r < t$. In particular, for rank-1 lattices, we can write

$$P_n = \left\{ \left(\frac{iz_1}{n}, \frac{iz_2}{n}, \dots, \frac{iz_s}{n} \right) \bmod 1, 0 \leq i_l < n_l, l = 1, \right\},$$

based on a single generating vector $\mathbf{z} = (z_1, \dots, z_s)$. Rank-1 lattices have an advantage over higher-order lattices, as they can be made fully projection regular, i.e., each one-dimensional projection has n points. One way of constructing higher rank lattices is to employ the copy rules of [Disney and Sloan \(1992\)](#); that is, we can take a rank-1 lattice, scale it, and copy it into each of the 2^s subcubes obtained by partitioning the unit cube into two parts on each side, and obtain a rank- s lattice. Thus, rank-1 lattices are more often used. There is extensive work on choices of rank-1 lattices, both theoretical and computer searches for good lattices are available; see for example, [Dick et al \(2022\)](#); [Goda and L'Ecuyer \(2022\)](#).

[Basu and Owen \(2015\)](#) give a lattice construction for points on the triangle with optimal discrepancy: let $\alpha \in (0, 2\pi)$ be such that $\tan(\alpha)$ is a quadratic irrational number, i.e., $\tan(\alpha) = (a + b\sqrt{c})/d$ for $b, d \neq 0$ and $c > 0$ not a perfect square. The point set P_n obtained by rotating the lattice $(2n)^{-1/2}\mathbb{Z}^2$ counterclockwise by α and intersecting with \triangle satisfies $D_n^P(P_n, \triangle_R) \leq C \log n/n$. The following algorithm produces such point sets.

Algorithm 2 (Lattice construction of [Basu and Owen \(2015\)](#)). *Given the target sample size n , α such that $\tan(\alpha)$ is badly approximable in the sense of ([Basu and Owen, 2015, Definition 4.1](#)) (e.g., $\alpha = 3\pi/8$), a random vector $\mathbf{U} \sim \text{Uniform}(0, 1)^2$ (for an optional shift), an integer N , sample n points in \triangle_R as follows:*

1. Let $P = \{0, 1, \dots, N-1\}^2$ and set $\mathbf{x} \leftarrow (\mathbf{x} + \mathbf{U})/N$ for $\mathbf{x} \in P$.
2. Map $\mathbf{x} \leftarrow 2\mathbf{x} - 1 \in [-1, 1]^2$ for all $\mathbf{x} \in P$.

- 507 3. Set $\mathbf{x} \leftarrow \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix} \mathbf{x}$ for all $\mathbf{x} \in P$.
- 508
- 509
- 510 4. Set $P_n = P \cap \triangle_R$.
- 511
- 512 5. If $|P_n| \neq n$, add or remove $|P_n| - n$ points in \triangle_R to P_n .
- 513
- 514 6. Return P_n .

515 The randomization transforms the otherwise deterministic points so that $\mathbf{x} \sim$
516 $\text{Uniform}(\triangle)$ for all $\mathbf{x} \in P$, which follows readily by observing that the density of each
517 \mathbf{x} is constant if a randomization is performed. In Step 5, we can choose arbitrarily
518 which points to add or remove. We remark that the algorithm presented in (Basu
519 and Owen, 2016, p. 757) differs slightly from Algorithm 2 in that their version uses
520 $N = \lceil \sqrt{2n} \rceil + 1$ and the lattice $\{-N, \dots, N\}^2$.

527 2.5 The triangular vdC sequence

528 We now describe the triangular vdC sequence of Basu and Owen (2015), which is based
529 on the one-dimensional vdC sequence in base 4. The i^{th} point of the one-dimensional
530 vdC sequence in base b is given by $u_i = \phi_b(i - 1)$ where the radical inverse function
531 ϕ_b is defined as

$$532 \phi_b(i) = \sum_{k \geq 0} d_k b^{-k-1}, \quad i = \sum_{k \geq 0} d_k b^k \in \{0, 1, \dots\}.$$

533 With this formula, the vdC sequence places points at the left-most boundaries of each
534 of the intervals $[b^{-m}, b^{-m+1})$. Similarly, the triangular vdC sequence, based on the
535 vdC sequence in base 4, replaces the intervals with $b^m = 4^m$ congruent sub-triangles
536 and places the points in the centre of each terminal sub-triangle. Let $T = \triangle(A, B, C)$
537 denote the specific triangle which we wish to generate points on. Define the sub-triangle

of T with index d for $d \in \{0, 1, 2, 3\}$ as

$$T(d) = \begin{cases} \triangle\left(\frac{B+C}{2}, \frac{A+C}{2}, \frac{A+B}{2}\right), & d = 0, \\ \triangle\left(A, \frac{A+B}{2}, \frac{A+C}{2}\right), & d = 1, \\ \triangle\left(\frac{B+A}{2}, B, \frac{B+C}{2}\right), & d = 2, \\ \triangle\left(\frac{C+A}{2}, \frac{C+B}{2}, C\right), & d = 3. \end{cases} \quad (4)$$

For the i^{th} point in the sequence, write the base 4 representation of $i \geq 0$ as $i = \sum_{k \geq 0} d_k 4^k$. This representation has at most $K_i = \lceil \log_4(i) + 1 \rceil$ non-zero digits, which means that the expansion is finite, and we do not have to infinitely divide the triangle into sub-triangles. The original construction for the triangular vdC sequence obtains the i^{th} triangular point by mapping the integer i to the midpoint of the triangle $T(d_0, \dots, d_{K_i})$, which is recursively defined by $T(d_k, d_{k+1}) = (T(d_k))(d_{k+1})$, as detailed in Algorithm 3. For example, if we have $T = \triangle_R = \triangle((0, 0), (0, 1), (1, 0))$, then $T(2, 3) = (T(2))(3)$, where $T(2) = \triangle((0, 0.5), (0, 1), (0.5, 0.5))$. Then, $(T(2))(3) = \triangle((0.25, 0.5), (0.25, 0.75), (0.5, 0.5))$.

Algorithm 3 (Triangular vdC sequence). *Given the desired sample size n and a target triangle $\triangle(A, B, C)$, the first n points, outputted in an $n \times 2$ array \mathbf{x} , are generated as follows:*

1. For $i = 1, \dots, n$:

(a) Compute (d_0, \dots, d_{K_i}) such that $i - 1 = \sum_{k=0}^{K_i} d_k 4^k$.

(b) Initialize $T = \triangle(A, B, C)$.

(c) For $j = 0, \dots, K_i$.

Update $T = T(d_j)$ using (4).

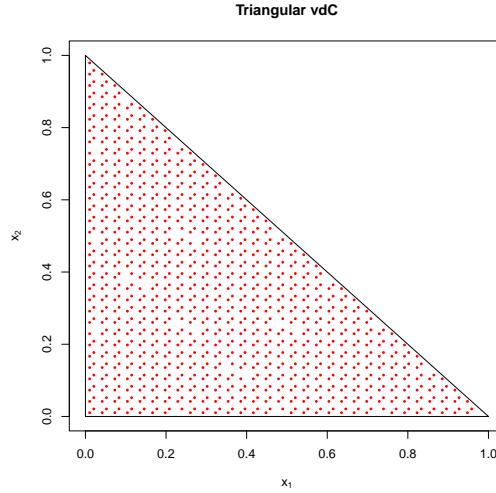
(d) Set the i^{th} coordinate $\mathbf{x}[i]$ of \mathbf{x} as $\mathbf{x}[i] = \text{mdpt}(T)$, where the midpoint function

is $\text{mdpt}(\triangle(A, B, C)) = (A + B + C)/3$ component-wise.

2. Return $\mathbf{x} = (x_1, \dots, x_n)$.

599 In other words, Algorithm 3 generates a vdC sequence in base 4, and each digit
600 of the base 4 expansion denotes which sub-triangle the point lies in. Advantages of
601 this method include that since it is based on the vdC sequence, it is extensible, bal-
602 anced, can be modified to be randomized, and it is easily implemented. However, when
603 implementing the algorithm as originally described, once the terminal sub-triangles
604 are identified, placing the sampling points at the centre of each results in points that
605 suffer from poor projection properties, as shown in Proposition 1. That is, the one-
606 dimensional projections have non-unique points, which will lead to poorer integration
607 results, especially for functions with low effective dimension where the majority of the
608 variance of the function is captured by one-dimensional projections onto these axes.

609 **Proposition 1** (Non-unique one-dimensional projections for the triangular vdC
610 sequence). *Let $T = \triangle_R$, such as in Figure 2, and denote by P_n the point set con-*
611 *sisting of the first n points produced by Algorithm 3 for $n = 4^k$ and $k > 2$. Then the*
612 *projections of P_n onto the x - and y -axis contain $2\sqrt{n} = 2^{k+1} < n$ points.*



638 **Fig. 2** The first 1000 points of the triangular vdC sequence of Basu and Owen (2015)

640
641 *Proof.* Since $n = 4^k$, each of the 4^k subtriangles contains one point, and there are 2^k
642 rows of subtriangles. In each row j , the midpoints of all upright triangles have the
643
644

same y coordinate, say y_{j1} . Similarly, the midpoints of all inverted triangles in the same row have the same y coordinate, say y_{j2} . Since there are only these two cases, the point set projects on $\{y_{ji} : j = 1, \dots, 2^k; i = 1, 2\}$, which has $2 \cdot 2^k = 2^{k+1}$ elements. The x -axis case follows similarly. \square

This behaviour where the one-dimensional projections contain non-unique points can also be observed in the equilateral triangle, as seen in Figure 6.

As a continuation of this work, [Goda et al \(2017\)](#) generalize the triangular vdC sequence by replacing the support $\{0, 1, 2, 3\}$ of the transformation in (4) by $\{(0, 0), (1, 0), (0, 1), (1, 1)\} = \mathbb{F}_2^2$, where the input strings (from \mathbb{F}_2^m for some m or \mathbb{F}_2^∞) come from a digital net. They prove that their construction gives worst case error in $\mathcal{O}((\log n)^3/n)$ for functions in $C^2(\Delta)$. Furthermore, they show that their construction includes the vdC sequence of [Basu and Owen \(2015\)](#); see ([Goda et al, 2017](#), p. 369).

3 Extensible triangular lattice constructions

We now describe our extensible triangular rank-1 and rank-2 constructions, as an extension of the triangular lattice construction. The construction in Algorithm 2 is non-extensible. In this section, we propose an extensible scheme, for which we make use of the one-dimensional vdC sequence. Recall that the i^{th} point of an extensible rank-1 lattice sequence with generating vector $\mathbf{z} \in \mathbb{Z}^d$ is defined as

$$\mathbf{u}_i = \phi_b(i)\mathbf{z} \bmod 1 \in [0, 1]^d,$$

where $\phi_b(i)$ is the i^{th} term of the vdC sequence in base b , and the modulus 1 operation is applied component-wise; see [Hickernell and Hong \(1997\)](#); [Hickernell et al \(2001\)](#).

If we want to use this idea to define a triangular Kronecker lattice sequence, then we need to introduce a more general idea extending the rank-1 case. In particular, the

691 grid that needs to be generated, given by

692

693

694

695

696

$$P = \left\{ -\frac{N}{N}, -\frac{N-1}{N}, \dots, -\frac{1}{N}, 0, \frac{1}{N}, \dots, \frac{N}{N} \right\}^2,$$

697

698

699

700

701

702

703

704

705

706

707

708

709

710

711

712

713

714

715

716

717

718

719

720

721

722

723

724

725

726

727

728

729

730

731

732

733

734

735

736

is a rank-2 lattice rather than a rank-1 lattice. We also note that the only reason why [Basu and Owen \(2015\)](#) use a grid over $[-1, 1]^2$ instead of $[0, 1]^2$ seems to be that when they rotate the points from the grid, they can just take the intersection with \triangle_R without having to perform any modulo 1 operation. However, with our proposed approach to generate an extensible grid, we will focus on generating points in $[0, 1]^2$; we can then either make use of modulo 1 operations or extend the grid to $[-1, 1]^2$.

First, we must choose the base b in which the grid will be constructed. The choice of the base b is such that whenever n is of the form b^{2k} for some $k \geq 1$, the point set P_n obtained with this method will be exactly the same as if we had proceeded with the fixed-size approach based on $N = b^k$; see [Proposition 2](#) below. We then make use of the base b decomposition of i as $i = \sum_{j \geq 0} d_j b^j$ to define the point

$$\mathbf{u}_i = (u_{i,1}, u_{i,2}) = \frac{d_0}{b}(1, 1) + \frac{d_1}{b}(0, 1) + \frac{d_2}{b^2}(1, 1) + \frac{d_3}{b^2}(0, 1) + \dots \bmod 1. \quad (5)$$

Note that the modulo 1 operation is only necessary for the second coordinate, as we have the bound

$$\frac{d_0}{b} + \frac{d_2}{b^2} + \frac{d_4}{b^3} + \dots \leq \sum_{j \geq 1} \frac{d_j}{b^k} \leq \sum_{j \geq 1} \left(\frac{1}{b}\right)^k = \frac{1}{1 - 1/b} - 1 \leq 1.$$

[Figure 3](#) shows the first 9, 50, and 81 points obtained with this method when $b = 3$.

The points \mathbf{u}_i lie in $[0, 1]^2$. Next, we rotate the points by α and can then proceed as in [Algorithm 2](#).

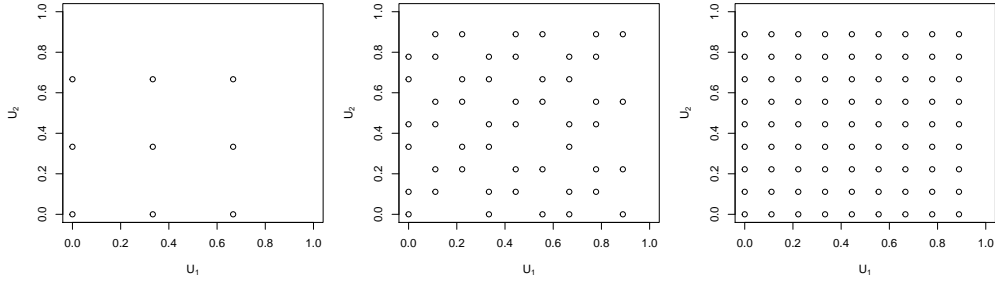


Fig. 3 First 9 (left), 50 (middle) and 81 points when using $b = 3$.

Algorithm 4 (Extensible Kronecker Lattice). *Given α, n, b , a random vector $\mathbf{U} \sim \text{Uniform}(0, 1)^2$ (for the optional shift) and a skip $s \geq 0$, sample n points in \triangle_R as follows:*

1. Set $P_n = \{\}$ and $k = 0$.
2. While $|P_n| < n$,
 - (a) Compute digits d_j such that $k + s = \sum_{j \geq 0} d_j b^j$ and compute \mathbf{u} in (5).
 - (b) Set $k \leftarrow k + 1$, $\mathbf{u} \leftarrow 2((\mathbf{u} + \mathbf{U}) \bmod 1) - 1 \in [-1, 1]^2$.
 - (c) Set $\mathbf{u} \leftarrow \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix} \mathbf{u}$.
 - (d) If $\mathbf{u} \in \triangle_R$, set $P_n = P_n \cup \{\mathbf{u}\}$.
3. Return P_n .

Proposition 2 (Equivalence of Algorithms 2 and Algorithm 4). *Let $n = b^{2k}$, $k > 0$ and $s = 0$. The sets P_n of points obtained by Algorithm 2 with $N = b^k$ and Algorithm 4 coincide.*

Proof. Assume without loss of generality that $\mathbf{U} = \mathbf{0}$. Consider the set $Q = \{\mathbf{u}_i : i = 0, \dots, n-1\}$ where the \mathbf{u}_i are as in (5). Then Q is a rank-2 lattice and can be written as $Q = \{(i/b^k, j/b^k) : 0 \leq i, j < b^k\}$. This is exactly the rectangular grid in Step 1 of Algorithm 2. Since the remaining operations (intersection and rotation) are identical in both algorithms, the result follows. \square

Algorithm 4 is based on a rank-2 lattice with generating vectors $z_1 = (1, 1)$ and $z_2 = (0, 1)$. In our numerical experiments, we also consider a rank-1 lattice with generating vector $z = (1, 182667)$; see (Cools et al, 2006, p. 26). The lattice construction allows for an easy randomization by shifting the underlying grid by a uniform vector, as originally proposed by Cranley and Patterson (1976). Figure 4 displays five independently randomized copies of the lattice points, each having a different colour.

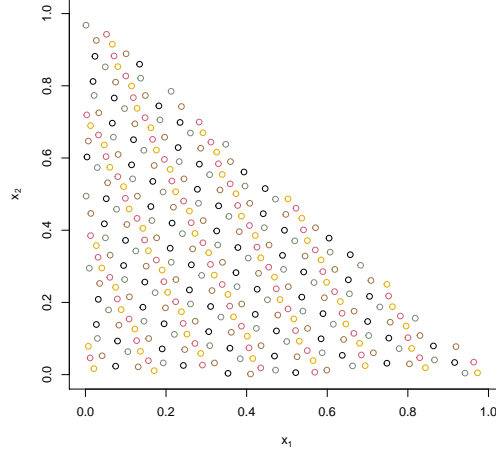


Fig. 4 Five independently randomized triangular Kronecker lattice point sets with 2^6 points each.

4 Stratified sampling based on the triangular vdC sequence

As previously mentioned, placing the sampling points at the centre of each terminal sub-triangle for the triangular vdC sequence results in points being mapped to the same coordinate on the x or y axis. Since the triangular vdC sequence is based on the one-dimensional vdC sequence over the unit interval, a natural randomization to “repair” the poor projection quality is scrambling.

In this section, we explain the equivalency between stratified sampling and the nested scrambling of Owen (1995) for any $(0, m, 1)$ -net or $(0, 1)$ -sequence. This equivalency is not limited to the vdC sequence, but will hold in general for all $(0, 1)$ -sequences, including, for example, one-dimensional projections of the Sobol' sequence.. This will allow us to then propose an efficient implementation of nested scrambling via a stratified estimator. We also show that nested scrambling is a way to implement an extensible stratified estimator. Finally, since the triangular vdC sequence is essentially a mapping from the one-dimensional vdC sequence to the two-dimensional space, it is easy to transform our proposed scrambling implementation in one dimension into a randomization method for the triangular vdC sequence.

4.1 Stratified Sampling

A simple way to reduce the variance of an estimator for the integral of a function f over the unit interval $[0, 1)$ is to stratify $[0, 1)$ into M subintervals of length p_j and allocate n_j points to the j th subinterval (with $n_1 + \dots + n_M = n$), thus resulting in the estimator

$$\hat{\mu}_{strat} = \sum_{j=1}^M p_j \frac{1}{n_j} \sum_{i=1}^{n_j} f(u_j^i),$$

where the u_j^i are iid uniforms in the j th subinterval, and independent from u_k^ℓ for $k \neq j$, $\ell = 1, \dots, n_k$. If we allocate a number of points proportional to the length of each subinterval (i.e., $n_j = np_j$ which is assumed to be an integer), then this is stratified sampling with proportional allocation. This method is guaranteed to have a lower variance than regular Monte Carlo; see (Lemieux, 2009, p. 126). Furthermore, if $n = b^m$ and we set $M = b^m$ then one point $u_j^1 = u_j$ is allocated to the j th stratum, and we get $\hat{\mu}_{strat} = \sum_{j=1}^n f(u_j)/n$ where each u_j is uniformly distributed in the j th stratum. The variance of this estimator is $\text{Var}(\hat{\mu}_{strat}) = \frac{1}{n^2} \sum_{j=1}^n \sigma_j^2$, where σ_j^2 is the variance of f within the j^{th} subinterval.

875 In the context of this section, since the number of points is not necessarily an integer
876
877 power of b , we refer to a *base b stratified sampling scheme* as a sampling scheme where
878
879 for any number of points n , if we subdivide the unit interval into subintervals with
880
881 length b^{-m} for any positive integer m , the number of points within each subinterval
882
883 is different by at most one from the number of points within any other subinterval.
884
885 That is, $|n_j - n_\ell| \leq 1$ for all $j, \ell = 1, \dots, b^m$. Stratified sampling with this property
886
887 can yield a more efficient implementation of nested scrambling, which we explain in
888
889 the next section.

890 4.2 Nested Uniform Scrambling

891
892 The nested uniform scrambling method of Owen (1995), sometimes referred to as
893
894 “Owen’s scrambling” or “nested scrambling”, scrambles a point set $P_n \subseteq [0, 1)^s$ by
895
896 applying random permutations to the digits $u_{i,j,l}$ that stem from the base b expan-
897
898 sion of $u_{i,j}$ (we write $u_{i,j} = \sum_{l=1}^{\infty} u_{i,j,l} b^{-l}$). Permutations π are randomly uniformly
899
900 distributed over all $b!$ permutations of $[0, 1, \dots, b-1]$. The permutation of each digit
901
902 depends on all the digits that came before it, and a new set of permutations is used
903
904 for each coordinate. That is, the permutation used for $u_{i,j,1}$ is π_j , the permutation
905
906 used for $u_{i,j,2}$ is $\pi_{j,u_{i,j,1}}$ (the permutation applied to the second digit $u_{i,j,2}$ depends on
907
908 the first digit $u_{i,j,1}$), the permutation used for $u_{i,j,3}$ is $\pi_{j,u_{i,j,1}u_{i,j,2}}$, and so on. That is,
909
910 to randomize the k^{th} digit of a given coordinate j , up to b^{k-1} different permutations
911
912 may be needed.

913
914 Nested scrambling is costly to implement, both in terms of time and memory. It
915
916 requires a dictionary or other lookup data structure to store all the permutations
917
918 generated, and, in addition to the time to go through all the coordinates of every
919
920 point, the lookup time for each permutation needs to be paid. However, despite being
921
922 costly to implement, nested scrambling is often used because it has the potential to
923
924 reduce the variance of the RQMC estimator in Equation (1) to $O(n^{-3} \log(n)^{s-1}) \approx$

$O(n^{-3+\epsilon})$ for sufficiently smooth functions as shown in [Owen \(1997\)](#). Use of nested scrambling is further justified by the fact that nested scrambling in base b also preserves equidistribution in base b as defined below, and satisfies the requirement of being a base b -digital scramble as defined in [Hickernell \(1996\)](#); [Hong and Hickernell \(2003\)](#); [Owen \(2003\)](#); [Wiart et al \(2021\)](#), which is also given below.

Definition 1 (Equidistribution). *We say that P_n with n of the form b^m with $m \geq 0$ for a single-base b construction, is (k_1, \dots, k_s) -equidistributed in base b if every elementary (k_1, \dots, k_s) -interval of the form*

$$I_{\mathbf{k}}(\mathbf{a}) = \prod_{\ell=1}^s \left[\frac{a_{\ell}}{b^{k_{\ell}}}, \frac{a_{\ell} + 1}{b^{k_{\ell}}} \right)$$

for $0 \leq a_{\ell} < b^{k_{\ell}}$ contains exactly $nb_1^{-k_1} \dots b_s^{-k_s}$ points from P_n , assuming \mathbf{k} is such that $n \geq b_1^{k_1} \dots b_s^{k_s}$.

Definition 2 $((t, m, s)$ -nets). *We say that a point set P_n in base b has a quality parameter t if P_n is (k_1, \dots, k_s) -equidistributed for all s -dimensional vectors of non-negative integers $\mathbf{k} = (k_1, \dots, k_s)$ such that $k_1 + \dots + k_s \leq m - t$. We then refer to P_n as a (t, m, s) -net in base b .*

Definition 3 $((t, s)$ -sequences). *We say a sequence is a (t, s) -sequence in base b if for every integer $m \geq 0$, every point set of the form $\mathbf{u}_j, \dots, \mathbf{u}_{j+b^m-1}$, where j is of the form $j = vb^m + 1$ for some $v \geq 0$, is a (t, m, s) -net.*

Definition 4 (Base b -digital scramble). *A randomization \mathcal{S} is a base b -digital scrambling if the following two properties hold: Let $U_{i,\ell} = \sum_{r=1}^{\infty} U_{i,\ell,r} b^{-r}$, that is, $U_{i,\ell,r}$ represents the r^{th} digit in the base b expansion of the ℓ^{th} coordinate of the i^{th} point \mathbf{u}_i in the scrambled point set \tilde{P}_n . Then we must have:*

1. Each $\mathbf{u}_i \sim \text{Uniform}([0, 1]^s)$;

967 2. For two distinct points $\mathbf{u}_i = \mathcal{S}(\mathbf{v}_i), \mathbf{u}_j = \mathcal{S}(\mathbf{v}_j)$ and for each coordinate $\ell = 1, \dots, s$,
 968
 969 if the two deterministic points $V_{i,\ell}, V_{j,\ell}$ have the same first r digits in base b and
 970 differ on the $(r+1)^{\text{th}}$ digit, then:
 971
 972 (a) the scrambled points $(U_{i,\ell}, U_{j,\ell})$ also have the same first r digits in base b ;
 973
 974 (b) the pair $(U_{i,\ell,r+1}, U_{j,\ell,r+1})$ is uniformly distributed over $\{(k_1, k_2), 0 \leq k_1 \neq k_2 <$
 975 $b\}$;
 976
 977 (c) the pairs $(U_{i,\ell,v}, U_{j,\ell,v})$ for $v > r+1$ are mutually independent and uniformly
 978 distributed over $\{(k_1, k_2), 0 \leq k_1, k_2 < b\}$.
 979
 980
 981

982 4.3 Nested Scrambling as Stratified Sampling

983
 984 We now show that we can implement a nested scrambled vdC sequence via a base b
 985 stratified sampling scheme on the unit interval, as the two methods produce point sets
 986 with the same joint distribution. First, we show that the scrambled vdC sequence in
 987 base b is a $(0, 1)$ -sequence in base b . Since scrambling in the constructing base does not
 988 change the t parameter, it is sufficient to show that the deterministic vdC sequence is
 989 a $(0, 1)$ -sequence.
 990
 991

992 **Lemma 1** (A consecutive subset of the vdC sequence is a $(0, m, 1)$ -net). *Any point set*
 993 *P_n that is made up of $n = b^m$ consecutive points from the vdC sequence constructed*
 994 *in base b is a $(0, m, 1)$ -net in base b .*
 995
 996

997 *Proof.* If we consider the first m digits in the base b expansion of each point $u_i \in P_n$,
 1000 there is exactly one point with each of the unique b^m combinations of digits; see (Dong
 1001 and Lemieux, 2022, Section 5). That is, there is exactly one point in each of the m -
 1002 elementary intervals and thus, by definition, a $(0, m, 1)$ -net in base b , and thus P_n is
 1003 m -equidistributed in base b . □
 1004
 1005

1006 **Lemma 2** (A consecutive subset of a vdC sequence has the same properties as the
 1007 initial portion of a $(0, 1)$ -sequence). *Any point set P_n that is made up of n consecutive*
 1008
 1009
 1010
 1011
 1012

points from a vdC sequence in base b has the same equidistribution properties as the first n points of a $(0, 1)$ -sequence in base b .

Proof. The result follows by observing that every point set P_k made up of $k = b^m$ consecutive points from the vdC sequence in base b is a $(0, m, 1)$ -net in base b (by Lemma 1). \square

Lemma 3 (Equivalence of the scrambled vdC sequence and stratified sampling for $n = b^m$). *Let $\hat{\mu}_{scr,n} = \frac{1}{n} \sum_{i=1}^n f(\tilde{u}_i)$ where $\tilde{u}_i, i = 1 \dots n$, are the first n points of a scrambled vdC sequence in base b . If $n = b^m$ for some positive integer m , then $\hat{\mu}_{scr,n}$ corresponds to the estimator that uses stratified sampling with proportional allocation.*

Proof. Since the first b^m points of the scrambled vdC sequence in base b is a $(0, m, 1)$ -net in base b (by Lemma 1), its equidistribution properties mean that there is exactly one point in each of the b^m subintervals, and the scrambling as defined in Definition 4 has the point placed independently and uniformly within each of the b^m subintervals. This is exactly stratified sampling with proportional allocation. \square

However, in general, n is not a power of b . In this case, we argue that the equidistribution properties of the $(0, 1)$ -sequence are such that the scrambled vdC estimator (by Lemma 2) places a number of points in the intervals $[jb^{-l}, (j+1)b^{-l})$ that are different by at most one from each other for $l \leq m$ for $m = \lfloor \log_b n \rfloor$.

To explain how to implement this estimator using our base b stratified sampling algorithm, we introduce the following notation. Write $n = \lambda b^m + r$, with the quotient $\lambda = \lfloor n/b^m \rfloor$ and remainder r satisfying $0 \leq r < b^m$. Further, break down r as $r = kb + j$, where $0 \leq j < b$. We also define M to be the smallest integer power of b greater than or equal to n . That is, $M = b^q$, where $q = \lceil \log_b n \rceil$.

In Proposition 3 we will prove that we can implement $\hat{\mu}_{scr,n}$ for any sample size n as a base b stratified sampling estimator over strata of the form $[jb^{-l}, (j+1)b^{-l})$ for $l = 1, \dots, m$. This is done by using the vector $[N_1, \dots, N_M]$, where N_j is the number

of points in $[jb^{-q}, (j+1)b^{-q})$ (either 0 or 1). That is, N_j counts the number of points in the smallest meaningful stratum: strata of size b^{-q} or smaller can have at most 1 point, thus there is no reason to subdivide further.

The scrambled vdC estimator satisfies the following properties:

1. $N_j \in \{0, 1\}$, $j = 1, \dots, M$, $\sum_{j=1}^M N_j = n$, and
2. The N_j 's have the same marginal distribution.

To define the scrambled estimator, we simply need to generate the vector of N_j 's with the properties listed above. Rather than obtaining these N_j via scrambling, we propose a more efficient procedure for sampling a vector of N_j 's given a base b and a number of points n in Algorithm 5 (the latter samples N_1, \dots, N_M for computing $\hat{\mu}_{scr, n}$).

Constant	Definition
n	Number of points to generate (input)
b	Base (input)
q	$q = \lceil \log_b n \rceil$
m	$m = \lfloor \log_b n \rfloor$
M	$M = b^q$
λ	$\lfloor n/b^m \rfloor$
r	$r = n - \lambda b^m$
k	$k = \lfloor \log_b r \rfloor$
j	$j = r - kb$

Table 1 Constants used in Algorithm 5.

Algorithm 5 (Sampling N_1, \dots, N_M for computing $\hat{\mu}_{scr, n}$). *Given input $n \in \mathbb{N}$ and*

$b \geq 2$, sample N_1, \dots, N_M as follows:

1. *Initialize n and b . Calculate the constants $q, m, M, \lambda, r, k, j$ as summarized in Table 1.*
2. *If $M = n$, return $N_j = 1$ for $j = 1, \dots, M$.*
3. *If $m = 0$, then $n = \lambda$, and $M = b$. Randomly choose λ of the b N_j 's to be 1 and $b - \lambda$ of the N_j 's to be 0, and return N_j for $j = 1, \dots, M$.*

4. If $m > 0$, we recursively generate the N_j 's in each of the b sub-intervals of the form $[jb, (j+1)b)$, $j = 0, \dots, b-1$ as follows:
- (a) Generate a vector of n_i 's of length b that sums to n with $b-r$ entries of λb^{m-1} and r entries of $\lambda b^{m-1} + 1$:
- (i) Randomly choose a subset \mathcal{I} of indices j from $\{1, \dots, b\}$.
- (ii) If $i \in \mathcal{I}$, then $n_i = \lambda b^{m-1} + k + 1$.
- (iii) Otherwise, $n_i = \lambda b^{m-1} + k$.
- (b) For each $i = 1, \dots, b$, we generate $N_{(i-1)b^{m+1}}, \dots, N_{ib^m}$ by restarting at Step 1 with the same base b but with $n = n_i$, and $q = m$. At this step, we have b recursive calls to the function.
5. Return N_1, \dots, N_M .

Note that in Step 4b, when we return to Step 1, if n_i is a power of b , q is not guaranteed to be equal to $\lceil \log_b n \rceil$, as it can also take on the value $\lceil \log_b n \rceil + 1$. For example, this case may arise when sampling $n = 10$ points in base 3. We would need to allocate these 10 points into 27 strata, so we will need to put 3 points into 9 strata. So even though $3 = 3^1$, we would want $q = 2$ as $9 = 3^2$: q is counting how many times we need to subdivide the unit interval.

After acquiring the N_j 's using Algorithm 5, we must generate the point set. This process is straightforward. To generate the point set based on the N_j , for every $j = 1 \dots M$, if $N_j = 1$, generate a point uniformly in the interval $[jb^{-q}, (j+1)b^{-q})$. If $N_j = 0$, do not generate a point in the interval.

Proposition 3 (Equivalence of stratified sampling and the one-dimensional vdC sequence). *The point set created using Algorithm 5 to define the N_j 's is such that pairs of distinct points have the same joint distribution as those coming from a scrambled vdC point set and thus the corresponding estimators have the same first two moments.*

Proof. We must derive the joint pdf of pairs of randomly chosen distinct points from the point set created using Algorithm 5, and show that it is the same as the joint pdf

1151 of pairs of randomly chosen distinct points from a one-dimensional scrambled vdC
1152 point set. To do so, we need the following definitions taken from [Wuart et al \(2021\)](#);
1153 [Dong and Lemieux \(2022\)](#):
1154

1155 **Definition 5** ($\gamma_b(x, y)$). For $x, y \in [0, 1)$, let $\gamma_b(x, y) \geq 0$ be the exact number of initial
1156 digits shared by x and y in their base b expansion, i.e. the smallest number $i \geq 0$ such
1157 that $\lfloor b^i x \rfloor = \lfloor b^i y \rfloor$ but $\lfloor b^{i+1} x \rfloor \neq \lfloor b^{i+1} y \rfloor$. If $x = y$ then we let $\gamma_b(x, y) = \infty$.
1158
1159

1160 **Definition 6** (Counting numbers $N_b(i; P_n)$ and $M_b(k; P_n)$). Let $P_n = \{U_1, \dots, U_n\}$
1161 be a point set in $[0, 1)$ and $b, i, k \in \mathbb{N}, b \geq 2$. Then,
1162

- 1163 1. $N_b(i; P_n)$ is the number of ordered pairs of distinct points (U_l, U_j) in P_n such that
1164 $\gamma_b(U_l, U_j) = i$,
1165
- 1166 2. $M_b(k; P_n)$ is the number of ordered pairs of distinct points (U_l, U_j) in P_n such that
1167 $\gamma_b(U_l, U_j) \geq k$, and
1168
- 1169 3. $N_b(k; P_n, U_l) = \sum_{e \in \{0, 1\}} (-1)^{|e|} M_b(k + e; P_n, U_l)$.
1170
1171

1172 (Proof, continued.) The joint pdf of a one-dimensional scrambled vdC is
1173
1174

$$\psi(x, y) = \begin{cases} \frac{N_b(i; P_n)}{n(n-1)} \frac{b^{1+i}}{(b-1)}, & \text{if } i < \infty, \\ 0, & \text{if } i = \infty, \end{cases}$$

1175 where P_n refers to the first n points of the deterministic vdC sequence.
1176

1177 We now show that the scrambled vdC point set and the point set constructed
1178 using the proposed base b stratified sampling method from Algorithm 5 yield the same
1179 $M_b(k; P_n)$ as defined in Definition 6. This means that $N_b(i; P_n)$ and thus the joint pdf
1180 $\psi(x, y)$ for all pairs of points (x, y) are then the same for both methods.
1181
1182

Since the base b vdC sequence is equivalent to a one-dimensional Halton sequence,
we know from [Dong and Lemieux \(2022\)](#) that in this case $M_b(k; P_n)$ is given by:

$$_{vdC}M_b(k; P_n) = \left\lfloor \frac{n-1}{b^k} \right\rfloor \left(2n - \left\lfloor \frac{n-1}{b^k} \right\rfloor b^k - b^k \right). \quad (6)$$

For any k , we can write $n = qb^k + r$, where $q = \lfloor \frac{n}{b^k} \rfloor$ and $0 \leq r < b^k$. By construction of the base b stratified sampling estimator, we divide the unit interval into b^k segments and any pairs of points in the same segment will share at least k initial common digits. There are $b^k - r$ of these segments with q points, and r segments with $q + 1$ points. Thus, the number of ordered pairs of points that are in the same segment is $(b^k - r)q(q - 1) + r(q + 1)q$. Substituting $r = n - qb^k$, we have $_{SS}M_b(k; P_n) = 2nq - q^2b^k - qb^k$ for the point set created via base b stratified sampling. Now, we substitute $q = \lfloor \frac{n}{b^k} \rfloor$ and simplify to get

$$_{SS}M_b(k; P_n) = 2n \left\lfloor \frac{n}{b^k} \right\rfloor - \left\lfloor \frac{n}{b^k} \right\rfloor^2 b^k - \left\lfloor \frac{n}{b^k} \right\rfloor b^k = \left\lfloor \frac{n}{b^k} \right\rfloor \left(2n - \left\lfloor \frac{n}{b^k} \right\rfloor b^k - b^k \right).$$

This is very similar to (6), except with $\lfloor \frac{n-1}{b^k} \rfloor$ rather than $\lfloor \frac{n}{b^k} \rfloor$. We show that $_{SS}M_b(k; P_n) = _{vdC}M_b(k; P_n)$ by considering the following two cases:

1. $\lfloor \frac{n}{b^k} \rfloor = \lfloor \frac{n-1}{b^k} \rfloor$. This case occurs when $r \neq 0$. If this is the case, then we conclude $_{SS}M_b(k; P_n) = \lfloor \frac{n-1}{b^k} \rfloor (2n - \lfloor \frac{n-1}{b^k} \rfloor b^k - b^k) = _{vdC}M_b(k; P_n)$ and we are done.
2. $\lfloor \frac{n}{b^k} \rfloor \neq \lfloor \frac{n-1}{b^k} \rfloor$. In this case, $r = 0$ and $\lfloor \frac{n}{b^k} \rfloor = \frac{n}{b^k} = q$, as well as $\lfloor \frac{n-1}{b^k} \rfloor = \frac{n}{b^k} - 1 = q - 1$. Then, we can write $_{SS}M_b(k; P_n)$ as

$$_{SS}M_b(k; P_n) = \frac{n}{b^k} \left(2n - \frac{n}{b^k} b^k - b^k \right) = \frac{n}{b^k} (2n - n - b^k) = \frac{n^2}{b^k} - n.$$

1243 Similarly, we can write ${}_{vdC}M_b(k; P_n)$ as:

1244

1245

1246

1247

1248

1249

1250

1251

1252 Thus, ${}_{SS}M_b(k; P_n) = {}_{vdC}M_b(k; P_n)$, as needed.

1253

1254 Hence, we find that ${}_{SS}M_b(k; P_n) = {}_{vdC}M_b(k; P_n)$ and thus that ${}_{SS}N_b(k; P_n) =$

1255

1256 ${}_{vdC}N_b(k; P_n)$ for all k . This implies that ${}_{SS}\psi(x, y) = {}_{vdC}\psi(x, y)$ for all $(x, y) \in [0, 1)^2$.

1257

1258 Thus, the estimator implemented using the base b stratified sampling has the same

1259

1259 first two moments as the scrambled vdC estimator. \square

1260

1261 Since n is not necessarily an integer power of b , our estimator does not inherit

1262

1263 properties of stratified sampling with proportional allocation. However, its connection

1264

1265 to nested scrambling implies we can apply results about the variance of scrambled

1266

1266 estimators for $(0, 1)$ -sequences as found, e.g., in [Gerber \(2015\)](#). That is, even though

1267

1268 the variance is not guaranteed to be no higher than for Monte Carlo for any function

1269

1269 (as a purely stratified sampling estimator based on proportional allocation would),

1270

1271 the superior asymptotic bounds for the variance of a scrambled estimator apply. Also,

1272

1273 since we know the scrambled vdC estimator produces an unbiased estimator (see [Dong](#)

1274

1274 and [Lemieux \(2022\)](#)) this means Algorithm 5 also produces an unbiased estimator.

1275

1276

1277

1277 4.4 Comparative efficiency analysis for fixed n

1278

1279

1280 Using the above connection between scrambling and base b stratified sampling, for

1281

1281 fixed n we can implement scrambling by sampling the N_j 's as in Algorithm 5 and

1282

1283 once those intervals where a point will be placed have been identified, we simply place

1284

1285 a point uniformly in that interval. This approach is computationally more efficient

1286

1286 than proceeding via recursive permutations, as is required when implementing nested

1287

1288 scrambling.

The recursive Algorithm 5 for base b stratified sampling has $\lceil \log_b(n) \rceil$ layers, and each call to the function has b sub-calls. Thus, in total, there are $b + b^2 + \dots + b^{\lceil \log_b(n) \rceil} = O(n)$ operations. For nested scrambling of the vdC sequence, we need to scramble the first $\lfloor \log_b(n-1) \rfloor + 1$ digits for each of the n points. This means that the number of operations needed is $O(n \log(n))$. In addition, permutations have to be stored in a lookup dictionary. There are b combinations of 1 digit, b^2 combinations of 2 digits, and so on. Thus, the amount of storage needed for nested scrambling is $b + 2b^2 + \dots + (\lfloor \log_b(n-1) \rfloor + 1)b^{\lfloor \log_b(n-1) \rfloor + 1} = O(n \log(n))$. Another advantage of the base b stratified sampling algorithm is that it does not require any additional storage for a lookup dictionary, as the nested scrambling algorithm does.

Figure 5 shows the runtime needed to generate $n = 2000, 4000, \dots, 200\,000$ points from the scrambled base 4 vdC sequence needed to construct point sets on the triangle. Our base b stratified sampling implementation is compared with nested scrambling and shown to be more computationally efficient. Furthermore, an increase in runtime occurs only at integer powers of 4. We also report, in the legend, a growth rate of the runtime α , such that the runtime is proportional to n^α . This is estimated by the regression coefficient α of $\log(\text{runtime}) = \alpha \log(n) + c$. α is estimated to be 1.07 for stratified sampling and 1.21 for nested scrambling, showing that, indeed, stratified sampling has close to linear time complexity while nested scrambling has a higher time complexity.

4.5 From the one-dimensional vdC sequence to the triangular vdC sequence

It is now straightforward to use the ideas presented thus far for the one-dimensional vdC sequence to construct a scheme to sample n points on an arbitrary triangle. The M “strata” are now the sub-triangles, and we can use Algorithm 5 to sample the number of points in each sub-triangle, say N_1, \dots, N_M . Then, sample N_j (either 0 or

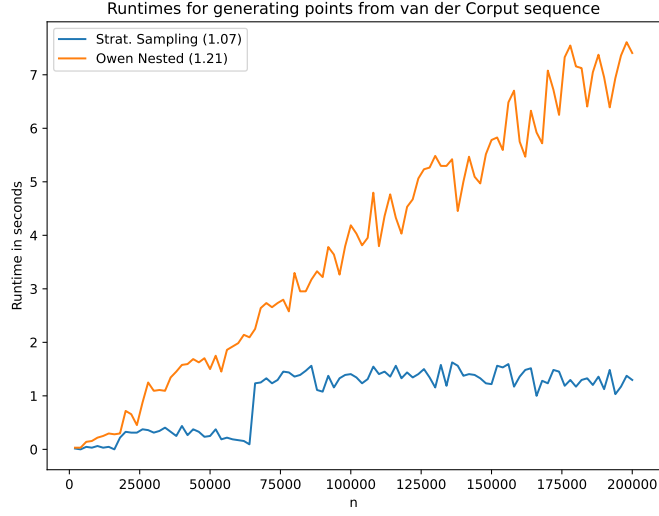


Fig. 5 Runtime comparison for generating a scrambled vdC sequence in base 4 using Owen’s Scrambling vs Stratified Sampling. Estimated growth rate for the runtimes are in parentheses in the legends.

1) points uniformly in each sub-triangle for $j = 1, \dots, M$, for example, using one of the methods described in Section 2.3. This estimator can also be extended using the method described in Appendix A.

An algorithm similar to Algorithm 3 can be used to sample in the triangle – the steps are described in Algorithm 6. Again, the sampling scheme subdivides the triangle into a finer and finer partition of triangles until each sub-triangle gets at most one point. The differences are that we now fill the sub-triangles in a non-deterministic order (that still satisfies the equidistribution properties), and as well, the points within each sub-triangle are uniformly placed rather than put in the centre.

Algorithm 6 (Mapping the stratified sampling estimator to the triangle). *Given input $n \geq 1$ and target triangle $\triangle(A, B, C)$, generate the first n points, outputted in an $n \times 2$ array \mathbf{x} , as follows:*

1. Generate a vector of indexes I_1, \dots, I_n using Algorithm 5 with base $b = 4$. Each of the indexes $0 \leq I_i \leq 4^{\lceil \log_4 n \rceil} - 1$, so we know that the base 4 representation

<i>is finite for each index. The representation has at most $K_i = \lceil \log_4(i) + 1 \rceil$ digits,</i>	1381
<i>which means that the expansion is finite, and we do not have to infinitely divide</i>	1382
<i>the triangle into sub-triangles.</i>	1383
2. For $i = 1, \dots, n$:	1384
(a) Compute (d_0, \dots, d_{K_i}) such that $I_i = \sum_{k=0}^{K_i} d_k 4^k$;	1385
(b) Initialize $T = \triangle(A, B, C)$;	1386
(c) For $j = 0, \dots, K_i$,	1387
Update $T = T(d_j)$ using (4);	1388
(d) Set the i^{th} point $\mathbf{x}[i]$ to be a random uniformly sampled point within T . In our	1389
implementation, we use the “root” method as described in Section 2.3;	1390
3. Return \mathbf{x} .	1391
This avoids the poor projection properties of the original triangular vdC sequence	1392
as seen in Figure 6, and it provides a way to randomize the point set to allow for error	1393
estimation.	1394
We note that this method of mapping points from the one-dimensional vdC	1395
sequence to the two-dimensional triangle can be done in other bases – for any base b	1396
such that b is a perfect square, we can map a scrambled vdC sequence in base b to the	1397
triangle, which is simply divided into b sub-triangles of equal size. The enumeration	1398
of the sub-triangles does not matter – after scrambling, (or, equivalently, stratified	1399
sampling), the points are uniformly distributed between the sub-triangles.	1400
Proposition 4 (Unbiasedness of $\hat{\mu}_{scr,n}$). <i>The estimator $\hat{\mu}_{scr,n}$ is unbiased.</i>	1401
<i>Proof.</i> The statement is equivalent to showing that each point is marginally uniformly	1402
distributed over the triangle. Without loss of generality, the marginal pdf f for the	1403
	1404
	1405
	1406
	1407
	1408
	1409
	1410
	1411
	1412
	1413
	1414
	1415
	1416
	1417
	1418
	1419
	1420
	1421
	1422
	1423
	1424
	1425
	1426

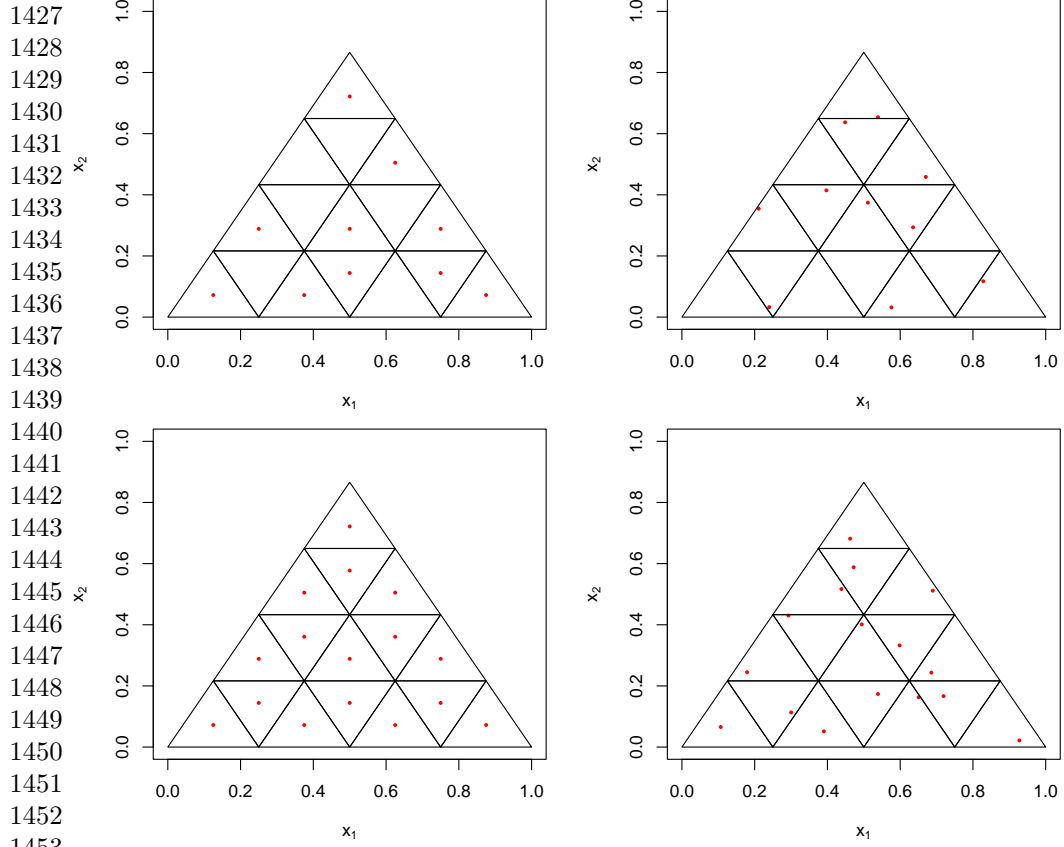


Fig. 6 Examples of the triangular vdc points generated on \triangle_E , with $n = 10$ (top) and $n = 16$ (bottom). The images on the left have each point at the centre of the terminal sub-triangle, while the images on the right have the points scrambled. For the $n = 10$ case, the sub-triangles with points are selected via stratified sampling.

point $\mathbf{u} = (u_1, u_2)$ uniformly distributed over \triangle_E is:

$$f(\mathbf{u}) = \begin{cases} \frac{2}{\sin(\pi/3)}, & \text{if } 0 \leq u_1 \leq 1/2 \text{ and } u_2 \leq u_1 \tan(\pi/3) \\ & \text{or } 1/2 \leq u_1 \leq 1 \text{ and } (1 - u_1) \tan(\pi/3), \\ 0, & \text{otherwise.} \end{cases}$$

For the stratified sampling estimator with given $n \geq 1$, we subdivide the triangle into 4^q sub-triangles each with area $\frac{2}{\sin(\pi/3)4^q}$. Since each sub-triangle is chosen with equal probability (as the N_j share the same marginal distribution), and we uniformly

sample within each of the n sub-triangles, the value of the pdf f within the sub-triangle is equal to the reciprocal of its area, $\frac{\sin(\pi/3)4^q}{2}$. Then, a point sampled using the stratified sampling algorithm has marginal pdf $g(\mathbf{u})$ given by

$$g(\mathbf{u}) = \begin{cases} \frac{\sin(\pi/3)4^q}{2 \times \# \text{ sub-triangles}}, & \text{if } \mathbf{u} = (u_1, u_2) \in \triangle_E, \\ 0, & \text{otherwise,} \end{cases}$$

$$= \begin{cases} \frac{2}{\sin(\pi/3)}, & \text{if } \mathbf{u} = (u_1, u_2) \in \triangle_E, \\ 0, & \text{otherwise.} \end{cases}$$

Thus, since $g(\mathbf{u}) = f(\mathbf{u})$, the stratified sampling algorithm samples uniformly over the triangle and thus the resulting estimator is unbiased. \square

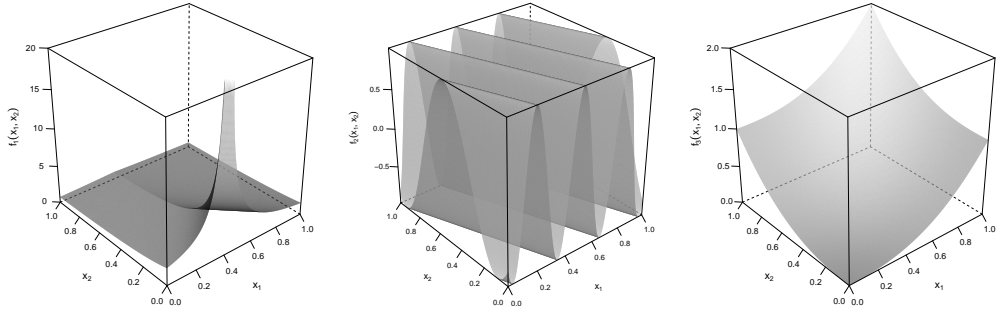
5 Numerical experiments

Now that we have described our proposed lattice and randomized triangular vdC constructions for a point set on the triangle, we compare their performance on numerical integration problems with existing constructions. There are very few, if any, numerical experiments on the triangle that compare RQMC integration variances, so we hope that these experiments give insight towards the performance of the various methods.

To test the performance of the different triangular constructions, we consider the following 2-dimensional test functions over the right-angle triangle \triangle_R with corners at $(0, 0)$, $(0, 1)$, $(1, 0)$:

1. $f_1(x, y) = (|x - \beta| + y)^d + (|y - \beta| + x)^d / 2$ This function has two singularities, so we anticipate this function to be harder to integrate than the others. This function is based on $f(x, y) = (|x - \beta| + y)^d$ from [Pillards and Cools \(2005\)](#). The integral evaluates to $\frac{1}{(d+1)(d+2)} ((d+1/2)(1-\beta)^{d+2} + (\beta+1)^{d+2}/2 - \beta^{d+2})$ over \triangle_R .

1519 2. $f_2(x, y) = \cos(2\pi\beta + \alpha_1x + \alpha_2y)$, from [Pillards and Cools \(2005\)](#). This is a smooth
1520 oscillatory function. The integral evaluates to $\frac{1}{\alpha_2}(\frac{1}{\alpha_1 - \alpha_2}(\cos(2\pi\beta + \alpha_2) - \cos(2\pi\beta +$
1521 $\alpha_1)) + \frac{1}{\alpha_1}(\cos(2\pi\beta + \alpha_1) - \cos(2\pi\beta)))$ over \triangle_R .
1522
1523 3. $f_3(x, y) = x^{\alpha_3} + y^{\alpha_3}$. Since this is the sum of univariate functions, it will help us
1524 determine if poor one-dimensional projections affect the integration power of the
1525 point set. The integral evaluates to $\frac{2}{(\alpha_3+1)(\alpha_3+2)}$ over \triangle_R .
1526
1527 We use $\beta = 0.4, d = -0.9, \alpha_1 = e^3, \alpha_2 = e^2, \alpha_3 = 2.5$ and estimate $\mu_j = \int_{\triangle_R} f_j(\mathbf{x}) d\mathbf{x}$,
1528 whose theoretical values are known for $j = 1, 2, 3$. Figure 7 displays f_k for $k = 1, 2, 3$
1529 with these parameter settings. Although the figures show the functions over the unit
1530 square, we integrate over the right-angle triangle \triangle_R only.



1536 **Fig. 7** Test functions f_1 (left), f_2 (middle) and f_3 (right) used in the numerical study.

1537
1538 We also estimate the value at time 0 of a European basket call option with maturity
1539 $T = 1$ based on two underlying assets that follow a lognormal distribution each.
1540 Formally, the value of the option is

$$C_0 = E \left[\max \left(0, e^{-rT} \left(\frac{1}{2} \sum_{j=1}^2 S_j(T) - K \right) \right) \right],$$

1541 where $S_j(T)$ is the price of the asset j at maturity $T = 1$. The lognormal model means
1542 we can write $S_j(T) = S_j(0)e^{(r-\sigma^2/2)T+\sigma\sqrt{T}Z}$, where $Z \sim N(0, 1)$ is a standard normal
1543 random variable.
1544

For our applications, we use the following parameters: the strike price K is either 45, 50, or 55 (to account for out-of-the-money, at-the-money, and in-the-money); the asset price at time 0 is $S_0 = 50$; the risk-free rate $r = 0.05$; the volatility $\sigma = 0.3$, and the maturity $T = 1$ year.

We consider two types of dependence structures between the two lognormal assets in the basket. Each dependence structure is the copula implied by the uniform distribution on a triangle. We start with the following two triangles: $\triangle((0,0), (0,1)(1,0))$ and $\triangle((1,1), (0,1)(1,0))$. For each triangle, we generate point sets on that triangle and transform them to marginally standard uniform distributions with their marginal CDFs, $F(x_i) = 1 - (1 - x_i)^2$ for $i = 1, 2$ for $\triangle((0,0), (0,1), (1,0))$ and $F(x_i) = 1 - x_i^2$ for $i = 1, 2$ for $\triangle((1,1), (0,1), (1,0))$ to obtain samples from the corresponding copula. Figure 8 shows such copula samples, where the underlying triangles were generated using the rSobol' + root method as detailed in the following section. The

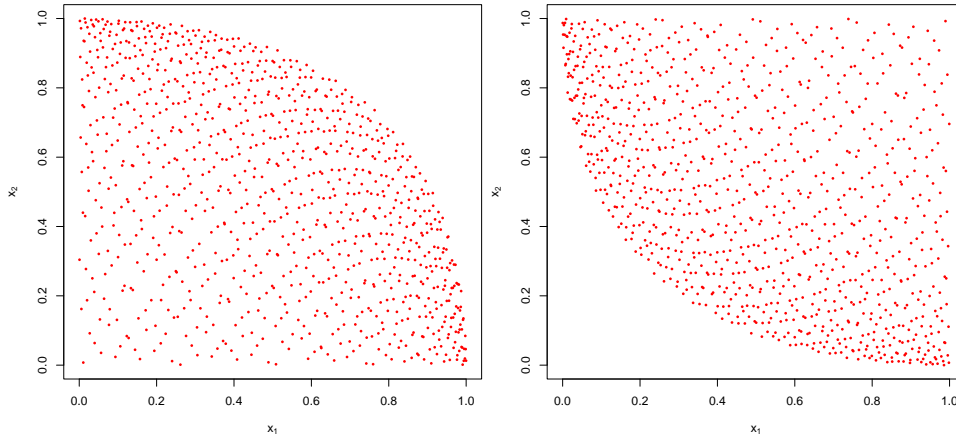


Fig. 8 Samples from the copulas based on $\triangle((0,0), (0,1)(1,0))$ (left) and $\triangle((1,1), (0,1)(1,0))$ (right) used in the basket option pricing example.

triangle-implied-copulas are used to model scenarios in which the asset prices are not simultaneously high (first triangle) or not simultaneously low (second triangle).

We compare the following randomized methods to estimate μ_j .

1611 1. PRNG + root: This is equivalent to the MC method; we generate pseudo-random
1612 points in the unit square and then apply the “root” method from Pillards and Cools
1613 (2005).
1614
1615 1616 2. rSobol’ + root: Here, the Sobol sequence randomized with a digital shift is
1617 generated, and then the “root” method from Pillards and Cools (2005) is applied.
1618
1619 1620 3. rLattice1: This refers to using Algorithm 4 with the rank-1 lattice of Cools et al
1621 (2006) and $\alpha = 3\pi/8$, randomized with a shift.
1622
1623 1624 4. rLattice2: This refers to the rank-2 lattice of Basu and Owen (2015), randomized
1625 with a shift. This method is not extensible, so a new point set must be generated
1626 every time n is changed.
1627
1628 1629 5. rvdC: This refers to our randomized triangular vdC sequence based on stratified
1630 sampling.
1631
1632 If necessary, Algorithm 1 is then used to transform the points to the desired triangle.
1633 The first $n = 1000$ points from these constructions are shown in Figure 9.
1634
1635 For each method and each sample size $n \in 2^4, 2^5, \dots, 2^{17}$, $v = 25$ randomizations
1636 were used. The estimates are obtained as the sample average of the realizations, while
1637 the variance is estimated as the sample variance of the v independent draws. Figure 10
1638 displays the results for the two-dimensional test functions. We also report the conver-
1639 gence speed (as measured by the regression coefficient α of $\log(\widehat{\text{Var}}) = \alpha \log(n) + c$
1640 displayed in the legend). We can see from the results that the bivariate Sobol’ sequence
1641 mapped to the triangle using the “root” method is typically the best performing
1642 method on these test functions. It does particularly well on function f_2 , which can
1643 be explained by the parameters chosen for this function, in conjunction with how the
1644 root transformation is applied to map to the triangle \triangle_R . Indeed, since we use the
1645 mapping $(1 - \sqrt{u_1}, \sqrt{u_1}u_2)$, it means the corresponding function on $[0, 1]^2$ is smoother
1646 than f_2 , i.e., it oscillates with a lower frequency. This is unlike what is happening
1647 for function f_3 , where the methods sampling directly on the triangle deal with a sum
1648
1649
1650
1651
1652
1653
1654
1655
1656

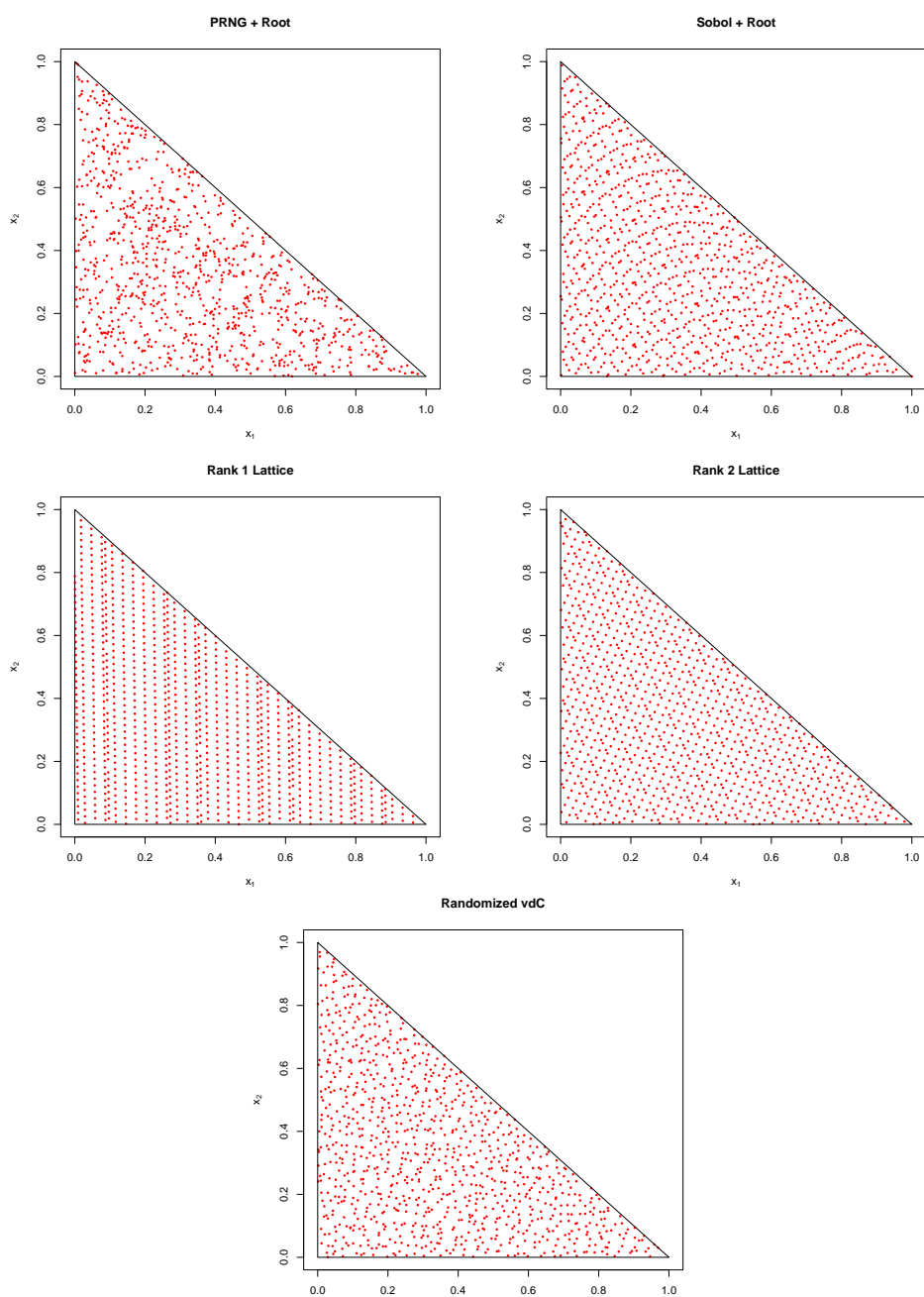


Fig. 9 First $n = 1000$ points of the point sets used in our experiments.

1703 of univariate functions, while the corresponding function on $[0, 1)^2$ based on the root
1704 transformation is truly two-dimensional.

1706 Our stratified sampling method is approximately equal in performance to the
1707 lattice-based methods, except for f_3 where it does better and is in fact essentially
1708 as good as the Sobol' + root method. The variance reduction of stratified sampling
1709 is more pronounced for functions where the within-strata variance is small and the
1710 between-strata variance is larger. Nested scrambling also has been shown to have sig-
1711 nificant variance reductions for smooth functions. Thus, it is unsurprising that for the
1712 function f_3 , the stratified sampling scheme has the best performance out of the three
1713 test functions, as it is the smoothest function with the most between-strata variance.

1719 Figures 11 and 12 display the results for the basket option pricing problem. Again,
1720 we also report the convergence speed in the legend. For all strike prices, the results
1721 are based on the same $v = 25$ randomized point sets. As was the case for the two-
1722 dimensional test functions, we can see from the results that the bivariate Sobol'
1723 sequence mapped to the triangle using the "root" method is typically the best per-
1724 forming method on these test functions. Our stratified sampling-based estimator tends
1725 to outperform the lattice-based methods. These results suggest that point sets directly
1726 constructed to have a low discrepancy in the integration space of interest may be
1727 outperformed by point sets obtained by applying a well-chosen transformation to a
1728 low-discrepancy point set constructed over the unit cube. Gaining a better under-
1729 standing of when and why this happens is something that we plan to investigate in
1730 the near future.

1741 6 Conclusion

1743 In this paper, we provided an extensible rank-1 lattice construction for points in the
1744 triangle that can be randomized with a shift. We also examined the projection qualities
1745 of the triangular vdC sequence, and we improved upon the triangular vdC sequence
1746

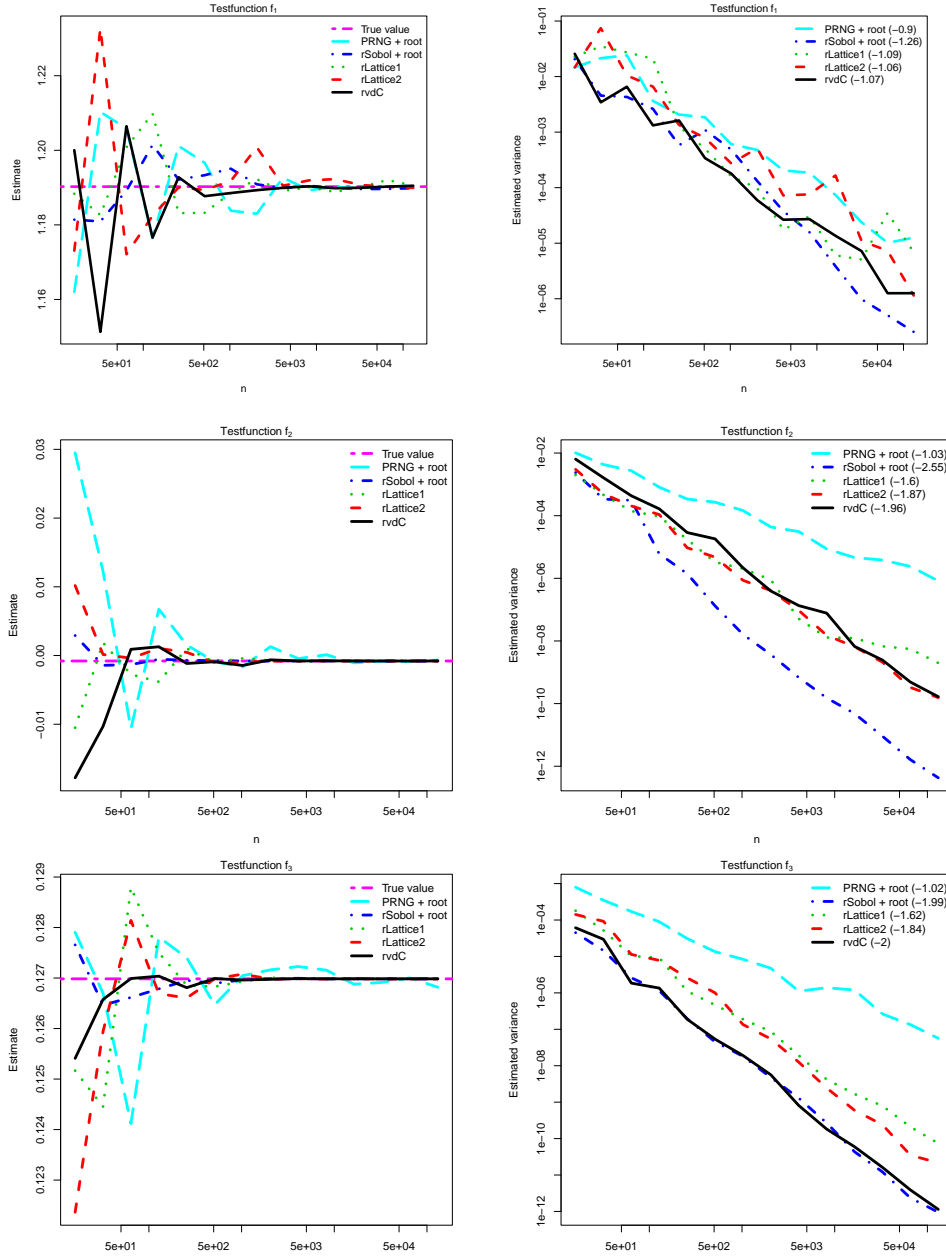


Fig. 10 Estimates (left) and estimated variances (right) when integrating f_1^n (top), f_2 (middle) or f_3 (right). For each n , $v = 25$ randomizations were used. Regression coefficients for the estimated variance are in parentheses in the legends.

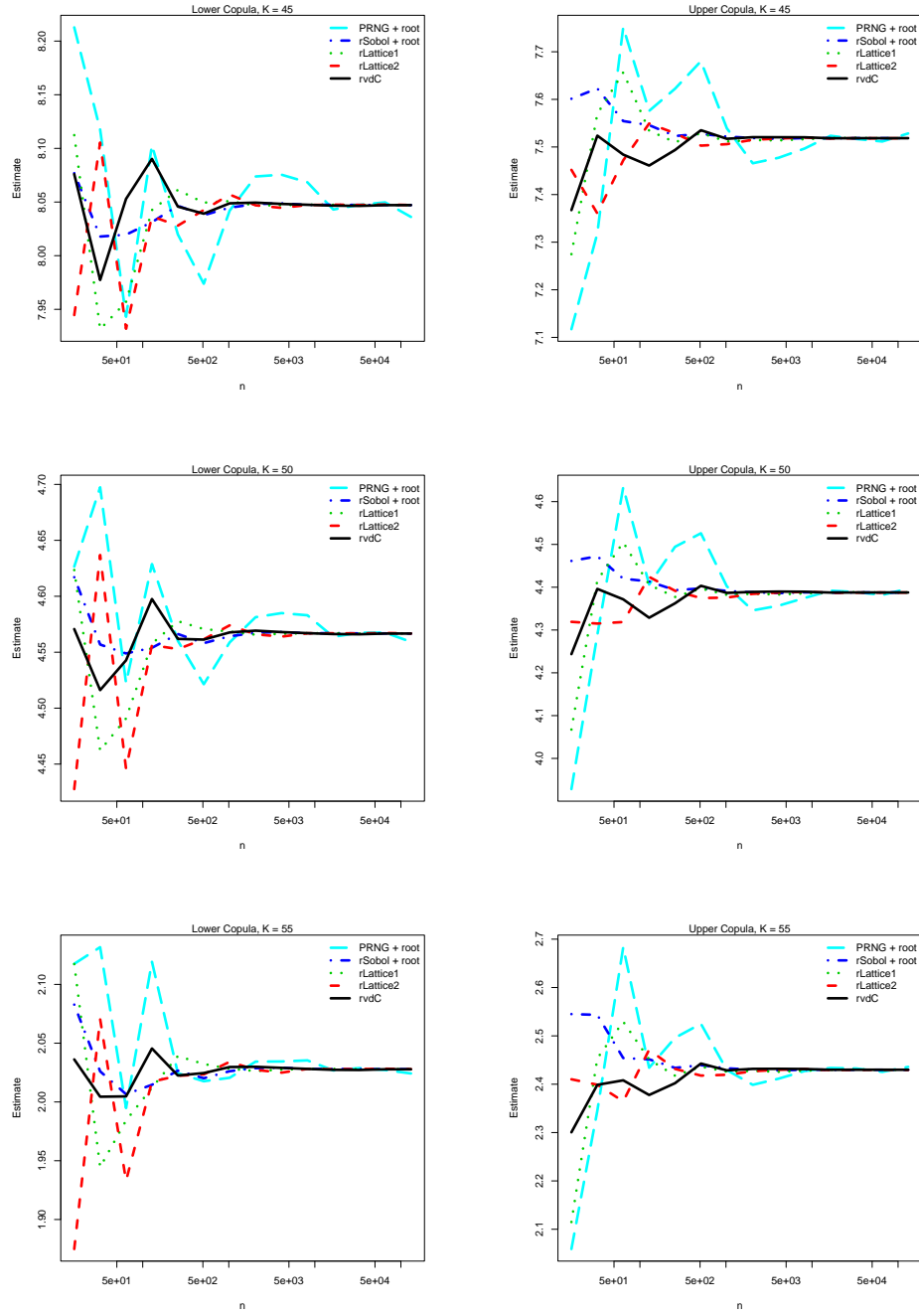


Fig. 11 Estimates when integrating the basket option pricing problem. For each n , $v = 25$ randomizations were used.

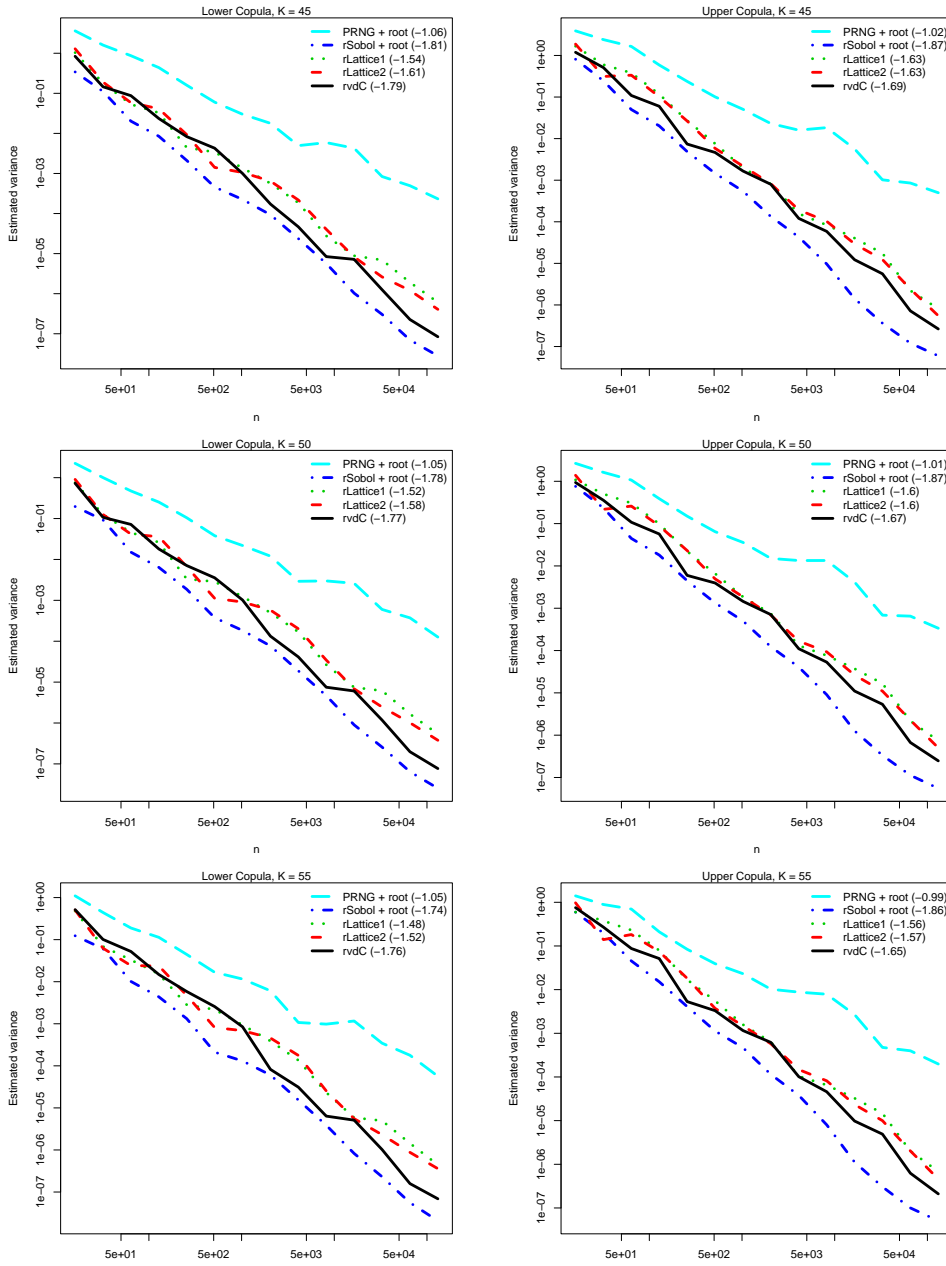


Fig. 12 Estimated variances when integrating the basket option pricing problem. For each n , $v = 25$ randomizations were used. Regression coefficients are in parentheses in the legends.

1887 of [Basu and Owen \(2015\)](#) by proposing a sampling scheme that uses their idea of
1888
1889 recursively subdividing the triangle, but with superior one-dimensional projections.
1890 We also showed that the scrambled sequence can be efficiently implemented using
1891
1892 stratified sampling, giving the benefits of the reduced variance without the additional
1893
1894 computational costs. This connection between stratified sampling and scrambling also
1895 gives an extensible stratified estimator. We give a test suite of functions and include
1896
1897 a numerical study to compare the different sampling constructions over a triangular
1898
1899 region.

1900 Future work in this area includes extending similar stratified sampling schemes
1901
1902 onto other surfaces, such as surfaces of spheres and simplexes. We would also like to
1903
1904 explore constructions and applications that require sampling on multiple triangles,
1905
1906 such as surfaces constructed with a mesh of triangles.

1907 1908 **Declarations**

1909 1910 1911 **Funding**

1912
1913 This work was supported by the Natural Science and Engineering Research Council
1914
1915 of Canada (NSERC) via grant 238959 to CL and the Canadian Statistical Sciences
1916
1917 Institute (CANSSI) via the CANSSI Distinguished Postdoctoral Fellowship program
1918
1919 to GD.

1920 1921 **Conflicts of interest/Competing interests**

1922
1923 The authors have no conflicts of interest to declare that are relevant to the content of
1924
1925 this article.

1926
1927
1928
1929
1930
1931
1932

Availability of data and material

No datasets were analysed during the current study. R implementation of the algorithms described within this article and R code for the numerical experiments are available upon request.

Authors' contributions

Gracia Dong and Erik Hintz wrote the main manuscript text and code required for the numerical experiments. Erik Hintz developed the methodology in Section 3. Gracia Dong developed the methodology in Section 4. Christiane Lemieux and Marius Hofert supervised the project. All authors reviewed the manuscript.

References

- Arvo J (1995) Stratified sampling of spherical triangles. In: Proceedings of the 22nd annual conference on Computer graphics and interactive techniques, pp 437–438, <https://doi.org/10.1145/218380.218500>
- Basu K, Owen A (2015) Low discrepancy constructions in the triangle. SIAM Journal on Numerical Analysis 53(2):743–761. <https://doi.org/10.1137/140960463>
- Basu K, Owen A (2016) Transformations and Hardy–Krause variation. SIAM Journal on Numerical Analysis 54(3):1946–1966. <https://doi.org/10.1137/15M1052184>
- Brandolini L, Colzani L, Gigante G, et al (2013) A Koksma–Hlawka inequality for simplices. In: Trends in harmonic analysis. Springer, p 33–46, https://doi.org/10.1007/978-88-470-2853-1_3
- Cools R, Kuo F, Nuyens D (2006) Constructing embedded lattice rules for multivariate integration. SIAM Journal on Scientific Computing 28(6):2162–2188. <https://doi.org/10.1137/06065074X>

1979 van der Corput J (1935) Verteilungsfunktionen i & ii. In: Nederl. Akad. Wetensch.
 1980
 1981 Proc., pp 1058–1066
 1982
 1983 Cowper G (1973) Gaussian quadrature formulas for triangles. International Journal
 1984
 1985 for Numerical Methods in Engineering 7(3):405–408. [https://doi.org/10.1002/nme.](https://doi.org/10.1002/nme.1620070316)
 1986 [1620070316](https://doi.org/10.1002/nme.1620070316)
 1987
 1988
 1989 Cranley R, Patterson TNL (1976) Randomization of number theoretic methods for
 1990
 1991 multiple integration. SIAM Journal on Numerical Analysis 13(6):904–914. [https:](https://doi.org/10.1137/0713071)
 1992 [//doi.org/10.1137/0713071](https://doi.org/10.1137/0713071)
 1993
 1994
 1995 Dick J, Pillichshammer F (2010) Digital nets and sequences: discrepancy theory and
 1996
 1997 quasi-Monte Carlo integration. Cambridge University Press, [https://doi.org/10.](https://doi.org/10.1017/CBO9780511761188)
 1998 [1017/CBO9780511761188](https://doi.org/10.1017/CBO9780511761188)
 1999
 2000
 2001 Dick J, Goda T, Suzuki K (2022) Component-by-component construction of ran-
 2002
 2003 domized rank-1 lattice rules achieving almost the optimal randomized error rate.
 2004 Mathematics of Computation 91(338):2771–2801. [https://doi.org/10.1090/mcom/](https://doi.org/10.1090/mcom/3769)
 2005 [3769](https://doi.org/10.1090/mcom/3769)
 2006
 2007
 2008 Disney S, Sloan IH (1992) Lattice integration rules of maximal rank formed by copying
 2009
 2010 rank 1 rules. SIAM journal on numerical analysis 29(2):566–577. [https://doi.org/](https://doi.org/10.1137/0729036)
 2011 [10.1137/0729036](https://doi.org/10.1137/0729036)
 2012
 2013
 2014 Dong GY, Lemieux C (2022) Dependence properties of scrambled halton sequences.
 2015
 2016 Mathematics and Computers in Simulation [https://doi.org/10.1016/j.matcom.2022.](https://doi.org/10.1016/j.matcom.2022.04.016)
 2017 [04.016](https://doi.org/10.1016/j.matcom.2022.04.016)
 2018
 2019
 2020 Fang K, Wang Y (1993) Number-theoretic methods in statistics, vol 51. CRC Press
 2021
 2022
 2023
 2024

Gerber M (2015) On integration methods based on scrambled nets of arbitrary size. Journal of Complexity 31(6):798–816. <https://doi.org/10.1016/j.jco.2015.06.001>

Goda T, L’Ecuyer P (2022) Construction-free median quasi-monte carlo rules for function spaces with unspecified smoothness and general weights. SIAM Journal on Scientific Computing 44(4):A2765–A2788. <https://doi.org/10.1137/22m1473625>

Goda T, Suzuki K, Yoshiki T (2017) Quasi-Monte Carlo integration for twice differentiable functions over a triangle. Journal of Mathematical Analysis and Applications 454(1):361–384. <https://doi.org/10.1016/j.jmaa.2017.04.051>

Heitz E (2019) A low-distortion map between triangle and square. HAL preprint

Hickernell FJ (1996) The mean square discrepancy of randomized nets. ACM Transactions on Modeling and Computer Simulation (TOMACS) 6(4):274–296. <https://doi.org/10.1145/240896.240909>

Hickernell FJ, Hong HS (1997) Computing multivariate normal probabilities using rank-1 lattice sequences. In: Golub GH, Lui SH, Luk FT, et al (eds) Proceedings of the Workshop on Scientific Computing (Hong Kong). Springer-Verlag, Singapore, p 209–215

Hickernell FJ, Hong HS, L’Ecuyer P, et al (2001) Extensible lattice sequences for quasi-Monte Carlo quadrature. SIAM Journal on Scientific Computing 22:1117–1138. <https://doi.org/10.1137/s1064827599356638>

Hong HS, Hickernell FJ (2003) Algorithm 823: Implementing scrambled digital sequences. ACM Transactions on Mathematical Software (TOMS) 29(2):95–109. <https://doi.org/10.1145/779359.779360>

2071 Korobov A (1959) The approximate computation of multiple integrals. In: Dokl. Akad.
 2072 Nauk SSSR, pp 1207–1210
 2073
 2074
 2075 Lemieux C (2009) Monte Carlo and Quasi-Monte Carlo Sampling. Springer Series
 2076 in Statistics, Springer New York, <https://doi.org/10.1007/978-0-387-78165-5>, URL
 2077 <https://books.google.ca/books?id=wj5OyydZ5bkC>
 2078
 2079
 2080
 2081 Owen AB (1995) Randomly permuted (t, m, s) -nets and (t, s) -sequences. In: Monte
 2082 Carlo and quasi-Monte Carlo methods in scientific computing. Springer, p 299–317,
 2083 https://doi.org/10.1007/978-1-4612-2552-2_19
 2084
 2085
 2086
 2087 Owen AB (1997) Scrambled net variance for integrals of smooth functions. The Annals
 2088 of Statistics 25(4):1541–1562. <https://doi.org/10.1214/aos/1031594731>
 2089
 2090
 2091 Owen AB (2003) Variance and discrepancy with alternative scramblings. ACM Trans-
 2092 actions of Modeling and Computer Simulation 13(4). [https://doi.org/10.1145/](https://doi.org/10.1145/945511.945518)
 2093 [945511.945518](https://doi.org/10.1145/945511.945518)
 2094
 2095
 2096
 2097 Pharr M (2019) Adventures in sampling points on triangles. URL [https://pharr.org/](https://pharr.org/matt/blog/2019/02/27/triangle-sampling-1)
 2098 [matt/blog/2019/02/27/triangle-sampling-1](https://pharr.org/matt/blog/2019/02/27/triangle-sampling-1), accessed: 2022-06-14
 2099
 2100
 2101 Pillards T, Cools R (2005) Transforming low-discrepancy sequences from a cube to
 2102 a simplex. Journal of computational and applied mathematics 174(1):29–42. [https:](https://doi.org/10.1016/j.cam.2004.03.019)
 2103 [//doi.org/10.1016/j.cam.2004.03.019](https://doi.org/10.1016/j.cam.2004.03.019)
 2104
 2105
 2106
 2107 Rosenblatt M (1952) Remarks on a multivariate transformation. The Annals of
 2108 Mathematical Statistics 23(3):470–472. <https://doi.org/10.1214/aoms/1177729394>
 2109
 2110
 2111 Shirley P, Chiu K (1997) A low distortion map between disk and square. Journal of
 2112 graphics tools 2(3):45–52
 2113
 2114
 2115
 2116

Sloan IH, Joe S (1994) Lattice methods for multiple integration. Oxford University Press	2117 2118 2119 2120
Tymchyshyn V, Khlevniuk A (2019) Beginner's guide to mapping simplexes affinely. ResearchGate preprint https://doi.org/10.13140/RG.2.2.13787.41762	2121 2122 2123 2124
Wiat J, Lemieux C, Dong GY (2021) On the dependence structure and quality of scrambled (t, m, s) -nets. Monte Carlo Methods and Applications https://doi.org/10.1515/mcma-2020-2079	2125 2126 2127 2128 2129 2130
Appendix A Extending a stratified estimator	2131 2132 2133
The approach described in Section 4, where we used the connection between stratified sampling and nested scrambling to give a faster implementation of nested scrambling, works well when n is fixed. Now, we use the connection between base b stratified sampling and nested scrambling to show how to extend a stratified estimator. Typically, stratified sampling is applied for fixed n and if a larger point set is needed, a new one is generated from scratch instead of only generating the additional points. Here, we argue that the nested permutations used for scrambling can be thought of as a way to allow for a stratified estimator to be extended easily, i.e., for points to be added without having to restart with a completely new stratified estimator. This works by recursively choosing a stratum at each level that has the least number of points, as explained in Algorithm 7. For simplicity, we deal directly with the stratum sample sizes N_1, \dots, N_M as generated by Algorithm 5 instead of the point set P_n , since after generating the strata sample sizes, it is simply a matter of placing a point uniformly within each stratum j with corresponding $N_j = 1$. This algorithm essentially works by recursively subdividing the interval into b subintervals, and randomly choosing one with the least points to add the next point into.	2134 2135 2136 2137 2138 2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2149 2150 2151 2152 2153 2154 2155 2156 2157 2158 2159 2160 2161 2162

2163 If we are working directly with the point set and not the strata, then we must
 2164 modify Algorithm 7 by changing Step 2a so that we first determine which b^q strata
 2165 are equivalent to 1, and set the rest to 0. Then in the following step, when putting 2
 2166 points within the same interval of size b^{-q} , since one of the N_j would already be set
 2167 to 1 based on the point that is already there, we only select the second subinterval
 2168 of size b^{-q+1} without replacement. Likewise, before Step 3a, we must first populate
 2169 N_1, \dots, N_M based on the existing point set.
 2170
 2171 **Algorithm 7** (Extending a stratified estimator). *Given N_1, \dots, N_M and a base b , we*
 2172 *sample one additional point as follows.*
 2173
 2174 1. Set $n = \sum_{j=1}^M N_j$.
 2175
 2176 2. If $n = M$, then we have to increase the number of strata from $M = b^q$ to $M = b^{q+1}$.
 2177
 2178 (a) Initialize $N_1, \dots, N_{b^{q+1}} = 0$.
 2179
 2180 (b) Randomly select an interval of size b^{-q} to contain two points. Subdivide this
 2181 interval into b intervals, and randomly select two of these subintervals to have
 2182 a point, i.e., $N_j = 1$.
 2183
 2184 (c) Subdivide the other intervals of size b^{-q} into b intervals, and randomly select
 2185 one of these intervals to have a point, i.e., $N_i = 1$.
 2186
 2187 (d) Return $N_1, \dots, N_{b^{q+1}}$.
 2188
 2189 3. If $n \neq M$, we do not need to increase the number of strata. We work with N_1, \dots, N_M .
 2190
 2191 (a) Divide the unit interval into b subintervals such that each of these subintervals
 2192 is represented by M/b strata.
 2193
 2194 (b) Let $L_j = \sum_{i=1}^{M/b} N_{(M/b)(j-1)+i}$ for $j = 1, \dots, b$.
 2195
 2196 (c) The L_j will differ by at most one. Randomly pick a j from the L_j that have the
 2197 minimum number of points.
 2198
 2199 (d) If $L_j = 0$, randomly choose one of the M/b strata to place a point in.
 2200
 2201 (e) If $L_j > 0$, repeat this algorithm from Step 2 on the j^{th} subinterval.
 2202
 2203 (f) Return N_1, \dots, N_M .
 2204
 2205
 2206
 2207
 2208

We now illustrate Algorithm 7 with an example showing how to extend a scrambled estimator from $n = 7$ to $n = 10$ when working in base 3. Let P_7 be the original point set with 7 points. Denote by Q_l the number of points in $[(l-1)/3, l/3)$ for $l = 1, 2, 3$ within P_7 . That is, $Q_1 = N_1 + N_2 + N_3$, $Q_2 = N_4 + N_5 + N_6$, and $Q_3 = N_7 + N_8 + N_9$. That is, Q_l and N_j both enumerate strata, just of different sizes. Given that $7 = 2 \times 3 + 1$, when constructing the estimator for $n = 7$ we would have had to sample N_1, \dots, N_9 such that one of Q_1, Q_2, Q_3 is equal to 3 and the other two are equal to 2. Say we have $Q_1 = Q_2 = 2, Q_3 = 3$. Then $N_7 = N_8 = N_9 = 1$ and we also need to choose two indices in each of $\{1, 2, 3\}$ and $\{4, 5, 6\}$ whose corresponding N_j will be set to 1. Say we choose 1, 3, 4, 5.

If we then want to add 3 points to go to $n = 10 = 1 \times 9 + 1$, it means we are now working with a stratified estimator over strata of size $1/27$ instead of $1/9$. In this case, we have that Q_ℓ now represents the total number of points in each interval of size $1/9$, and only one of them will be equal to 2 with the other 8 being equal to 1.

Rather than jumping directly to $n = 10$, let us explain how each point is added.

1. ($n = 8$) Choose which of the two intervals of size $1/9$ with no point will have a point uniformly sampled in it.
2. ($n = 9$) Sample a point uniformly in the last interval of size $1/9$ that has no point.
3. ($n = 10$) Choose one of the 9 intervals of size $1/9$ which will have a second point placed in it (i.e., for which Q_1, \dots, Q_9 will be equal to 2, as they are currently all equal to 1); determine in which of the intervals of size $1/27$ the point lies that is already placed in this interval of size $1/9$; randomly choose one of the two empty intervals of size $1/27$ to place the second point and then place a point uniformly in it.

Since intervals are always chosen without replacement within the group of b intervals of size b^{-q} we are currently working with, it is clear that if we initially generate

2255 a random permutation of $[1, \dots, b]$, we are simply deciding beforehand in which order
2256
2257 points will be added within this group of sub-intervals.

2258
2259
2260
2261
2262
2263
2264
2265
2266
2267
2268
2269
2270
2271
2272
2273
2274
2275
2276
2277
2278
2279
2280
2281
2282
2283
2284
2285
2286
2287
2288
2289
2290
2291
2292
2293
2294
2295
2296
2297
2298
2299
2300