Normally distributed quasi-random samples combining Box–Muller and lattice rules

(work in progress)

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Motivation

$I[f]$	$\int_{[0,1]^s} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$	$\int_{\mathbb{R}^s} f(\boldsymbol{x}) \, \rho(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$

Approximated by an equal weight rule

$$Q(f; \{\boldsymbol{x}_k\}_{k=0}^{N-1}) := \frac{1}{N} \sum_{k=0}^{N-1} f(\boldsymbol{x}_k)$$

$\{\boldsymbol{x}_k\}_{k=0}^{N-1}$	uniformly distributed	distributed acc. to $\rho(\boldsymbol{x})$

Monte Carlo $\rightarrow$ quasi-Monte Carlo

good lattice rules, ...	???

Setting the scene

- Two dimensions ($s = 2$)
- Rank-1 lattice rules
- Box–Muller transform
  (cf. experiments Pillards & Cools)
- i.i.d. standard normal variates

- Work in progress . . .
  . . . Thank you Rayna!

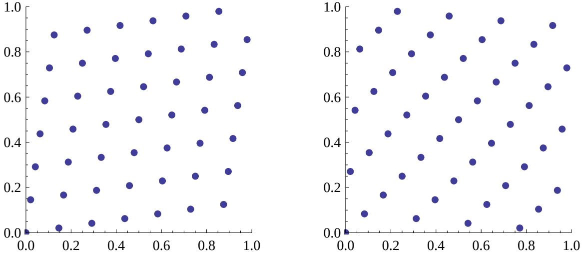
Outline

Rank-1 lattice rules

A good *rank-1 lattice rule* has uniformly distributed points

$$\boldsymbol{y}_k = \frac{k\boldsymbol{z} \bmod N}{N}, \qquad \text{for} \quad k = 0, \ldots, N-1,$$

with $\boldsymbol{z} \in \mathbb{Z}^d$ the (well chosen) *generating vector*.



$\boldsymbol{z} = [1, 7]$, $N = 48$ $\qquad$ $\boldsymbol{z} = [1, 13]$, $N = 48$

Note: the origin is always included.

The Box–Muller transform

Box & Muller (1958):

Given two uniform variates $u_1, u_2 \sim [0, 1)$ set

$$\begin{aligned} r &= \sqrt{-2\ln(1-u_1)}, \\ \theta &= 2\pi u_2. \end{aligned}$$

Then

$$\begin{aligned} x_1 &= r\cos\theta, \\ x_2 &= r\sin\theta \end{aligned}$$

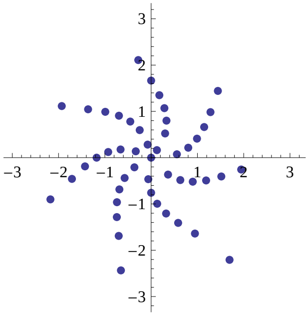
are i.i.d. standard normal variates.

Note the $1 - u_1$.

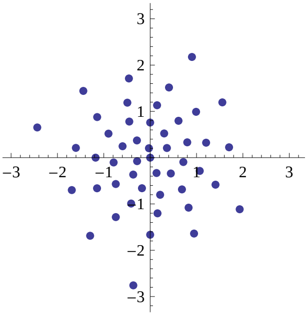
Box–Muller transformed rank-1 lattice rules

For $k = 0, \ldots, N-1$:

$$\begin{cases} r_k &= \sqrt{-2\ln(1-(kz_1/N \bmod 1))}, \\ \theta_k &= 2\pi k z_2/N, \end{cases} \qquad \begin{cases} x_{k,1} &= r_k \cos\theta_k, \\ x_{k,2} &= r_k \sin\theta_k. \end{cases}$$



$\boldsymbol{z} = [1, 7]$, $N = 48$



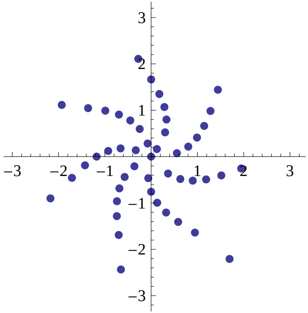
$\boldsymbol{z} = [1, 13]$, $N = 48$

$\Rightarrow$ Find a “good” generating vector $\boldsymbol{z}$!

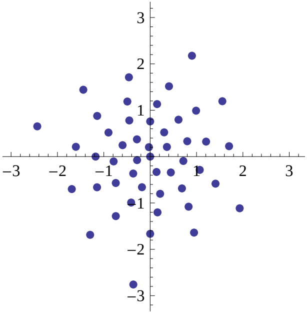
Quality criteria

- Visual
- Geometry
- Discrepancy
- Testfunctions
- Reproducing kernel

Visual quality



$\boldsymbol{z} = [1, 7], N = 48$



$\boldsymbol{z} = [1, 13], N = 48$

"Monkey-test"

→ Is our intuition right?

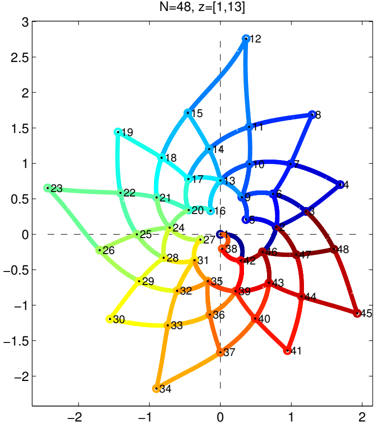
→ How to translate to objective criteria?

Geometry based quality criteria

Uniform lattice rule:

- Properties of unit cell (cf. shortest vectors)
- Less skewed is better (area vs perimeter)

Normal lattice rule unit cell?



Why discrepancy?

Koksma–Hlawka inequality for point set $P_N = \{\boldsymbol{x}_k\}_{k=0}^{N-1}$

$$|I[f] - Q_N[f]| \leqslant V(f)\, D_N\,(P_N)$$

where, using some norm $|\cdot|$

$$D_N(P_N) = |d(\{B_i\}_i, P_N)|$$

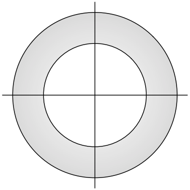
Local discrepancy: fraction of points vs. expected fraction

$$d\left(B, \{\boldsymbol{x}_k\}_{k=0}^{N-1}\right) = \frac{\#\{k, \boldsymbol{x}_k \in B\}}{N} - \int_B \rho(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}$$

$\rightarrow$ How to choose B?

r discrepancy

Unanchored:



Anchored:

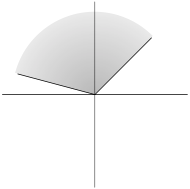
$$D_p^{\langle r \rangle}(P_N)^p := \int_0^\infty \left| \frac{\#\{P_N \cap [0,r) \times [0,2\pi)\}}{N} - \left(1 - e^{-\frac{r^2}{2}}\right) \right|^p \, dr$$

But: if $\boldsymbol{z}$ is relative prime w.r.t. N

$\rightarrow$ discrepancy independent of generating vector

θ discrepancy

Unanchored:



Anchored:

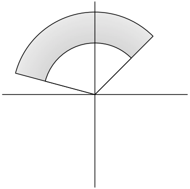
$$D_p^{\langle\theta\rangle}(P_N)^p := \int_0^{2\pi} \left| \frac{\#\{P_N \cap [0,\infty) \times [0,\theta)\}}{N} - \frac{\theta}{2\pi} \right|^p \frac{d\theta}{2\pi}$$

But: if $\boldsymbol{z}$ is relative prime w.r.t. N

$\rightarrow$ discrepancy independent of generating vector

The polar star discrepancy

Unanchored:



Anchored:

$$D_p^{\langle r,\theta\rangle}(P_N)^p := \int_0^{2\pi}\int_0^{\infty}\left|\frac{\#\{P_N \cap [0,r)\times[0,\theta)\}}{N} - \frac{\theta(1-e^{-\frac{r^2}{2}})}{2\pi}\right|^p \frac{dr\,d\theta}{2\pi}$$

For $p = \infty$, this corresponds to D_∞^* in the uniform case

Integral is undefined in the last part
$\rightarrow$ exclude interval $[r_{\max}, \infty]$ from the integration domain

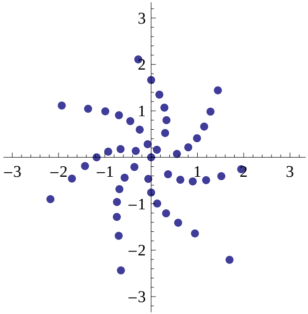
The polar star discrepancy: A formula for $p = 2$

For $\boldsymbol{z} \in \mathbb{Z}_N^2$, with z_1 relatively prime to N,
$R = r_{\max}(P_N(\boldsymbol{z})) = \sqrt{2 \ln N}$ and $c = N/(N-1)$, we have

$$
\begin{aligned}
(D_2^{\langle r,\theta\rangle}(P_N))^2 = \frac{1}{3}\left(\frac{\sqrt{\pi}}{2}\operatorname{erf}(R) - \sqrt{2\pi}\operatorname{erf}\left(\frac{R}{\sqrt{2}}\right) + R\right) c \\
- \frac{2}{N}\sum_{k=0}^{N-1}\frac{1-y_{k,2}^2}{2}\left(R - r_k + \sqrt{\frac{\pi}{2}}\left(\operatorname{erf}\left(\frac{r_k}{\sqrt{2}}\right) - \operatorname{erf}\left(\frac{R}{\sqrt{2}}\right)\right)\right) c \\
+ \frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{\ell=0}^{N-1}(1-\max(y_{k,2}, y_{\ell,2}))\,(R - \max(r_k, r_\ell))\, c.
\end{aligned}
$$

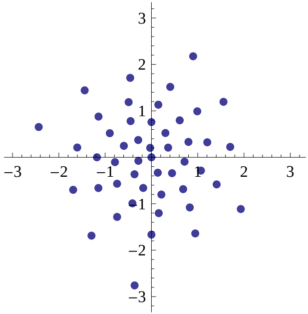
Similar to Warnock's formula for $T^\star$

The polar star discrepancy: results



$\boldsymbol{z} = [1, 7]$, $N = 48$

$D_2^{\langle r,\theta \rangle}(P_N) = 0.052361$



$\boldsymbol{z} = [1, 13]$, $N = 48$

$D_2^{\langle r,\theta \rangle}(P_N) = 0.033277$

→ Complies with the “monkey-test” for this example

Quality based on testfunctions

Similar to TESTPACK (Genz 1987):

- 11 function families for $\mathbb{R}^s$ (Hill-Robinson 2003)
- Analytical solutions known
- Typical difficulties (peak, oscillating, decaying, ...)
- Random translation parameters
  determine only location of difficulty
  $\rightarrow$ average case error

$\rightarrow$ Results allow to discriminate $\boldsymbol{z}$'s
$\rightarrow$ Does not always corresponds to the “monkey-test”

Reproducing kernel approach

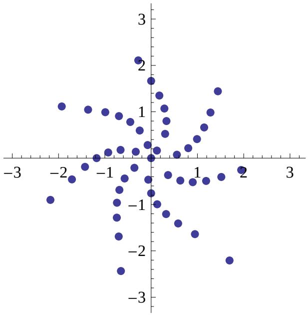
First attempt: kernel from Kuo-Woźniakowski 2010

$$K_\gamma(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(-\gamma^2 \|\boldsymbol{x} - \boldsymbol{y}\|_2^2\right)$$

This leads to a worst case error

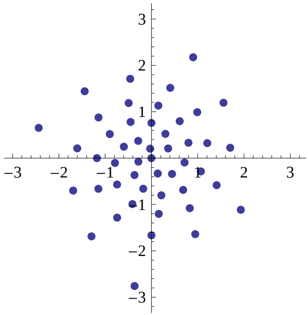
$$\begin{aligned} e_\gamma^2(P_N) \quad &:= \quad \frac{1}{4\gamma^2 + 1} \\ &+ \quad \frac{1}{(2\gamma^2 + 1)\, N} \sum_{k=0}^{N-1} \exp\left(-\frac{\gamma^2}{2\gamma^2 + 1} \|\boldsymbol{x}_k\|_2^2\right) \\ &+ \quad \frac{1}{N^2} \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} \exp\left(-\gamma^2 \|\boldsymbol{x}_k - \boldsymbol{x}_l\|_2^2\right) \end{aligned}$$

Reproducing kernel approach results



$\boldsymbol{z} = [1, 7], N = 48$

$e^2_{\gamma=0.5}(P_N) = 1.518109$



$\boldsymbol{z} = [1, 13], N = 48$

$e^2_{\gamma=0.5}(P_N) = 1.518036$

→ Results very close to each other, but

→ Complies with the “monkey-test” for this example

Closing remarks

Conclusions:

- Good generating vectors are not always transferable
- Different quality criteria can be defined

Current work

- Explore other discrepancy measures
- Experiment with different kernels
- Generalise
  - Correlated normal variates
  - Higher dimensions ($s > 2$)