Henri Faure

- Celebrating his 80th birthday on July 12, 2018
- Fundamental contributions to low-discrepancy sequences
- Mostly known for his 1982 paper "Discrépance de suites associées à un système de numération (en dimension s)", published in Acta Arithmetica
- Paper introduces what is now known as Faure sequences, originally referred to as "suite de type $P_{r,s}$"

Counting Points in Boxes with Henri Faure: From Discrepancy Bounds* to Dependence Structures**

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Outline

1. Counting tools used with HF to get discrepancy bounds
2. Dependence structure of scrambled $(0, m, s)$-nets: more counting
    1. Motivation and background
    2. Two-dimensional result
    3. The s-dimensional case

1 - Counting tools used with HF to get discrepancy bounds

- Key aspect of our work on discrepancy bounds of the form $D(N, X) \leq c_s(\log N)^s + O((\log N)^{s-1})$ for different sequences X
- Need to bound $E(J, N) = |A(J; N, X) - NV(J)|$ for any $J = [\mathbf{0}, \mathbf{z})$
- Three ingredients, used by Atanassov (2004) for Halton sequences
  1. Decompose J based on signed splittings using signed numeration systems [Faure 1981 & 1982, Atanassov 2004]
  2. Bound on the discrepancy for union of elementary intervals [Schmidt, 1977]
  3. Combinatorial arguments to bound partition obtained from splitting [Atanassov 2004, F&L 2014, 2017]
- Used this to get bounds for (t, s)-sequences (and $(t, \mathbf{e}, s)$-sequences)

#1: Signed splitting

Definition

Let be given an interval $J \subseteq I^s$, then a *signed splitting* of J is any collection of intervals $J_1, \ldots, J_n$ and respective signs $\epsilon_1, \ldots, \epsilon_n$ equal to ± 1, such that for any (finitely) additive function ν on the intervals in $I^s = [0,1)^s$, $\nu(J) = \sum_{i=1}^n \epsilon_i \nu(J_i)$.

Lemma

Let $J = \prod_{i=1}^s [0, z^{(i)}) \subseteq I^s$. Let $z_0^{(i)} = 0$, $z_{n_i+1}^{(i)} = z^{(i)}$ and let $z_j^{(i)} \in [0,1]$ be arbitrary given numbers for $1 \le j \le n_i$.
Then the intervals $\prod_{i=1}^s [\min(z_{j_i}^{(i)}, z_{j_i+1}^{(i)}), \max(z_{j_i}^{(i)}, z_{j_i+1}^{(i)}))$, with signs $\epsilon(j_1, \ldots, j_s) = \prod_{i=1}^s \operatorname{sgn}(z_{j_i+1}^{(i)} - z_{j_i}^{(i)})$, for $0 \le j_i \le n_i$, is a signed splitting of the interval J.

How discrepancy bounds require counting

$J = \prod_{i=1}^{s} [0, z^{(i)})$ where $z^{(i)} = \sum_{j=0}^{\infty} a_j^{(i)} b_i^{-j}$ and

$$|a_{j_i}^{(i)}| \leq \begin{cases} (b_i - 1)/2 & \textit{if } b_i \text{ is odd} \\ b_i/2 & b_i \text{ is even and } j_i \text{ is even} \\ (b_i - 2)/2 & b_i \text{ is even and } j_i \text{ is odd.} \end{cases}$$

Let $n_i := \lfloor \frac{\log N}{\log b_i} \rfloor$, $z_0^{(i)} = 0$, $z_{n_i+2}^{(i)} = z^{(i)}$, and $z_k^{(i)} = \sum_{j=0}^{k-1} a_j^{(i)} b_i^{-j}$ for $k = 1, \ldots, n_i + 1$. Applying Lemma 2, J is expanded in the signed splitting:

$$I(\mathbf{j}) = \prod_{i=1}^{s} [\min(z_{j_i}^{(i)}, z_{j_i+1}^{(i)}), \max(z_{j_i}^{(i)}, z_{j_i+1}^{(i)})), \qquad 0 \leq j_i \leq n_i + 1,$$

and the discrepancy function is expanded as

$$A(J; N; X) - NV(J) = \sum_{j_1=0}^{n_1+1} \cdots \sum_{j_s=0}^{n_s+1} \epsilon(\mathbf{j}) \left(A(I(\mathbf{j}); \mathcal{P}_N) - NV(I(\mathbf{j})) \right) =: \Sigma_1 + \Sigma_2,$$

where Σ_1 has the terms $\mathbf{j}$ such that $b_1^{j_1} \cdots b_s^{j_s} \leq N$ and Σ_2 has the rest.

#2: Bound on the discrepancy for simple intervals

Lemma

Let J be an interval of the form $J = \prod_{i=1}^{s}[c_i b_i^{-d_i}, c_i' b_i^{-d_i})$ with integers c_i, c_i' satisfying $0 \leq c_i < c_i' \leq b_i^{d_i}$, and X a sequence with quality parameter t. Then for every $N \geq 1$

$$|A(J; N; X) - NV(J)| \leq b^t (c_1' - c_1) \cdots (c_s' - c_s).$$

Lemma 1 applies broadly (Halton, (t, s), $(t, \mathbf{e}, s)$)

#3: Combinatorial arguments

Original bound used by Atanassov

Lemma

Let $N \geq 1, k \geq 1$ and $b_1, \ldots, b_s$ ($b_i \geq 2$) be integers. For integers $j \geq 0, 1 \leq i \leq k$, let some numbers $c_j^{(i)} \geq 0$ be given, satisfying $c_0^{(i)} \leq 1$ and $c_j^{(i)} \leq c_i$ for $j \geq 1$, for some fixed numbers c_i ($1 \leq i \leq k$). Then

$$\sum_{\{\mathbf{j}=(j_1,\ldots,j_k)\,;\, b_1^{j_1}\cdots b_k^{j_k} \leq N\}} \prod_{i=1}^{k} c_{j_i}^{(i)} \leq \frac{1}{k!} \prod_{i=1}^{k} \left(c_i \frac{\log N}{\log b_i} + k \right). \tag{1}$$

based on argument from diophantine geometry giving for all $k \geq 1$

$$\#\{\mathbf{j} : b_1^{j_1} \ldots b_k^{j_k} \leq N\} \leq \frac{1}{k!} \prod_{i=1}^{k} \frac{\log N}{\log b_i}$$

Behavior of the discrepancy bound determined by bound on $|\Sigma_1|$:

$$|\Sigma_1| \leq \sum_{\mathbf{j}: b_1^{j_1} \cdots b_s^{j_s} \leq N} |a_{j_i}^{(i)}|$$

then use ingredients #2 (bound on $|a_{j_i}^{(i)}|$) and #3 (combinatorial argument)

- Odd base $b_i = b$: bound each $a_{j_i}^{(i)} \leq (b-1)/2$
- Even base $b_i = b$: can pair successive $a_{j_i}^{(i)}$ and bound their sum by $b-1$; gives a leading term with constant $c_s = O(\frac{b-1}{2})^s$ instead of $O(\frac{b}{2})^s$ (F&L 2012)

Combinatorial arguments (cont'd)

Variant (F&L 2014) obtained by using combinatorial property

Lemma

Given two integers $k \geq 1$ and $n \geq 0$, the number of nonnegative integers solutions of the inequality $0 \leq j_1 + \cdots + j_k \leq n$ is equal to $\binom{n+k}{k}$.

Odd base: then use

$$\sum_{\{\mathbf{j};\, b^{j_1}\cdots b^{j_k} \leq N\}} \prod_{i=1}^{k} c_{j_i}^{(i)} \leq \frac{c^k}{k!} \prod_{l=1}^{k} \left(\frac{\log N}{\log b} + l \right),$$

which gives

$$|\Sigma_1| \leq \frac{b^t}{s!} \left(\frac{b-1}{2} \right)^s \prod_{k=1}^{s} \left(\frac{\log N}{\log b} + k \right).$$

Even base: use instead Lemma 5 (from F&L 2014)

$$\sum_{\{\mathbf{j};\, b^{j_1}\cdots b^{j_k}\le N\}} \prod_{i=1}^{k} c_{j_i}^{(i)} \le \frac{1}{k!}\left(\frac{c+c'}{2}\right)^k \prod_{l=1}^{k}\left(\frac{\log N}{\log b}+2l\right),$$

with $c_{2h+1}^{(i)} \le c, c_{2h}^{(i)} \le c'$ and careful counting, which gives

$$|\Sigma_1| \le \frac{b^t}{s!}\left(\frac{b-1}{2}\right)^s \prod_{k=1}^{s}\left(\frac{\log N}{\log b}+2k\right)$$

$\rightarrow$ Same asymptotic behavior for c_s as in (F&L 2012), but actual values of c_s often smaller; compare the above with

$$\frac{b^t}{s!}\left(\frac{(b-1)\log N}{2\log b}+s\right)^s$$

Combinatorial arguments (cont'd)

Yet another way to partition the intervals $I(\mathbf{j})$ that make up Σ_1

Lemma

Assume $c_j^{(i)} \leq c_i = c$. *Then we have*

$$\sum_{\{\mathbf{j};0 \leq j_1+\cdots+j_k \leq n\}} \prod_{i=1}^{k} c_{j_i}^{(i)} \leq \sum_{m=0}^{k} c^m \binom{n}{m}\binom{k}{m} = \sum_{m=0}^{\min(k,n)} c^m \binom{n}{m}\binom{k}{m}.$$

Combinatorial arguments (cont'd)

Theorem

For any (t,s)-sequence X in an even base b and any $N \geq 1$ we have

$$D^*(N,X) \leq b^t \sum_{m=0}^{\min(s,n)} \frac{1}{m!}\binom{s}{m}\left(\frac{b-1}{2}\right)^m \prod_{l=0}^{m-1}\left(\frac{\log N}{\log b}+m-2l\right)+$$

$$b^t \sum_{k=0}^{s-1}\sum_{m=0}^{\min(k,n)} \frac{b+2}{2m!}\binom{k}{m}\left(\frac{b-1}{2}\right)^m \prod_{l=0}^{m-1}\left(\frac{\log N}{\log b}+m-2l\right),$$

Corresponding c_s from FL 2014 smaller than this for $b=2$ and $N \geq b^s$.
Amounts to show $g_s(n) \leq h_s(n)$ for $n = \log N/\log b \geq s$, where

$$g_s(n) = \frac{1}{s!}\frac{\Gamma(\frac{n}{2}+s+1)}{\Gamma(\frac{n}{2}+1)}$$

$$h_s(n) = \sum_{m=0}^{s} \frac{\binom{s}{m}}{m!}\frac{\Gamma(\frac{n+m}{2}+1)}{\Gamma(\frac{n-m}{2}+1)}.$$

2-Dependence structure of scrambled $(0, m, s)$-nets: more counting

Motivation:

- Methods such as Antithetic Variates and Latin Hypercube Sampling can be shown to never be worse than MC for functions monotone in each coordinate: what about (R)QMC?
- It is of interest to have this type of upper bounds with easily verifiable conditions on integrands.

i - Problem setup and background

- Start with randomized QMC point set $\tilde{P}_n$ where each $\mathbf{U}_i \sim U(0,1)^d$ but the $\mathbf{U}_i$'s are dependent
- Assess its dependence via distribution function

$$H(\mathbf{u},\mathbf{v};\tilde{P}_n) := \frac{2}{n(n-1)}\sum_{i=1}^{n-1}\sum_{j>i} P(\mathbf{U}_i \le \mathbf{u}, \mathbf{U}_j \le \mathbf{v}). \qquad (2)$$

- Useful to study variance of $\hat{\mu}_n = \sum_{i=1}^{n} f(\mathbf{U}_i)/n$ because

$$\mathrm{Var}(\hat{\mu}_n) = \frac{\sigma^2}{n} + \frac{n-1}{n}\sigma_{I,J}, \qquad (3)$$

where $\sigma^2 = \mathrm{Var}(f(\mathbf{U}_i))$ and

$$\sigma_{I,J} = \mathrm{Cov}(f(\mathbf{U}_I), f(\mathbf{U}_J)) = \frac{2}{n(n-1)}\sum_{i=1}^{n-1}\sum_{j>i}\mathrm{Cov}(f(\mathbf{U}_i), f(\mathbf{U}_j)).$$

Definitions for the s-dimensional case

- A vector $\mathbf{X}$ of rv's is Negative Upper Orthant Dependent (NUOD) if

$$P(X_1 \geq x_1, \ldots, X_d \geq x_d) \leq \prod_{l=1}^{d} P(X_l \geq x_l).$$

- A vector $\mathbf{X}$ of rv's is Negative Lower Orthant Dependent (NLOD) if

$$P(X_1 \leq x_1, \ldots, X_d \leq x_d) \leq \prod_{l=1}^{d} P(X_l \leq x_l).$$

- NLOD Sampling scheme:

$$H(\mathbf{u}, \mathbf{v}; \tilde{P}_n) := \frac{2}{n(n-1)} \sum_{i=1}^{n-1} \sum_{j>i} P(\mathbf{U}_i \leq \mathbf{u}, \mathbf{U}_j \leq \mathbf{v}) \leq \prod_{l=1}^{s} u_l v_l$$

- Can define NUOD sampling scheme similarly

ii-Two-dimensional result (L (2017))

- Can prove that a scrambled $(0, m, 2)$-net is an NUOD sampling scheme and get

Result: Let f be a function defined over $[0,1]^2$ that is monotone in each coordinate. Let $\hat{\mu}_n$ be the estimator for $I(f)$ based on a scrambled $(0, m, 2)$-net in base b, and let $\hat{\mu}_{mc,n}$ be the MC estimator for $I(f)$ based on $n = b^m$ points. Then

$$\mathrm{Var}(\hat{\mu}_n) \leq \mathrm{Var}(\hat{\mu}_{mc,n}).$$

iii-s-dimensional case

- Can prove that a scrambled $(0, m, s)$-net is an NUOD/NLOD sampling scheme.
- Use explicit representation of pdf $\psi_m^s(\mathbf{x}, \mathbf{y})$ of pair of distinct points to write

$$H(\mathbf{u}, \mathbf{v}; \tilde{P}_n) = \frac{2}{n(n-1)} \sum_{i=1}^{n-1} \sum_{j>i} P(\mathbf{U}_i \le \mathbf{u}, \mathbf{U}_j \le \mathbf{v}) = \int_{\mathbf{0}}^{(\mathbf{u},\mathbf{v})} \psi_m^s(\mathbf{x}, \mathbf{y}) d\lambda$$

and then show

$$\int_{\mathbf{0}}^{(\mathbf{u},\mathbf{v})} \psi_m^s(\mathbf{x}, \mathbf{y}) d\lambda \le \int_{\mathbf{0}}^{(\mathbf{u},\mathbf{v})} d\lambda \qquad \text{for any } \mathbf{u}, \mathbf{v}$$

- Implies variance of net-based estimator no larger than MC for any quasi-monotone function

Partitioning the space

Definition

For $x, y \in [0,1]$, let $\gamma_b(x,y)$ be the exact number of initial digits shared by x and y in their base b expansion, i.e. the smallest number i such that

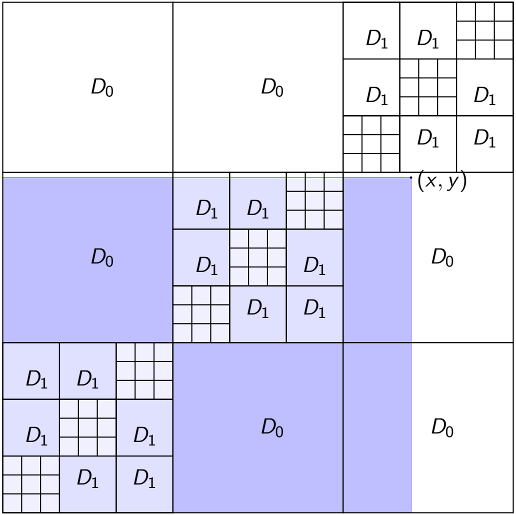
$$\lfloor b^i x \rfloor = \lfloor b^i y \rfloor \quad \text{but} \quad \lfloor b^{i+1} x \rfloor \neq \lfloor b^{i+1} y \rfloor.$$

For $\mathbf{x}, \mathbf{y} \in [0,1]^s$, let $\gamma_b^s(\mathbf{x},\mathbf{y}) = \sum_{j=1}^s \gamma_b(x_j, y_j)$.

Using γ^s we partition the unit hypercube $[0,1]^s \times [0,1]^s$ as

$$[0,1]^s \times [0,1]^s = \bigcup_{i=0}^{\infty} D_i^s, \text{ where } D_i^s = \{(\mathbf{x},\mathbf{y}) \in [0,1]^{2s} : \sum_{j=1}^s \gamma_b(x_j, y_j) = i\}.$$

The D_i's: will be used to partition box $[0, x] \times [0, y]$



Pdf of pair of distinct points from scrambled net

Counting points in boxes again...

Definition

Let P_n be a digital $(0, m, s)$-net in base b. We define

$$M(m, s) = \#\{P_n \cap [b^{-1}, 1]^s\}.$$

Lemma

$$M(m, s) = \sum_{k=0}^{s} (-1)^k \binom{s}{k} \max\{b^{m-k}, 1\}$$

for all $m \in \mathbb{Z}$ *and* $s \geq 1$*. Moreover* $M(m, s) = (b-1)^s b^{m-s}$ *when* $m \geq s$*.*

Proposition

Let $\psi_m^s(\mathbf{x},\mathbf{y})$ *be the joint pdf of two distinct points* $(\mathbf{U}_I,\mathbf{U}_J)$ *randomly chosen from a scrambled* $(0,m,s)$*-net in base* b*. Then*

$$\psi_m^s(\mathbf{x},\mathbf{y}) = \frac{b^m}{b^m-1}\frac{b^s}{(b-1)^s}\frac{M(m-i,s)}{b^{m-i}}$$

when $(\mathbf{x},\mathbf{y}) \in D_i^s$*, i.e.* $\sum_{j=1}^s \gamma_b(x_j,y_j) = i$*. Moreover*

1. *if* $(\mathbf{x},\mathbf{y}) \in D_i^s$ *and* $i \le m-s$*, then* $\psi_m^s(\mathbf{x},\mathbf{y}) = \frac{b^m}{b^m-1}$*, and*
2. *if* $(\mathbf{x},\mathbf{y}) \in D_i^s$ *and* $i \ge m$*, then* $\psi_m^s(\mathbf{x},\mathbf{y}) = 0$*.*

Sketch of NLOD proof

Let $\psi : [0,1]^s \times [0,1]^s \to \mathbb{R}$ be a bounded function taking the constant value ζ_i on D_i^s for all $i \in \mathbb{N}$. Our goal is to understand when

$$G(x,y) := \int_{R(\mathbf{x},\mathbf{y})} \psi d\lambda \leq \mathbf{xy} \qquad \text{for all } \mathbf{x},\mathbf{y} \in [0,1]^s,$$

where $R(\mathbf{x},\mathbf{y}) = [\mathbf{0},\mathbf{x}] \times [\mathbf{0},\mathbf{y}]$.

For each $m \in \mathbb{Z}$ and $s \geq 1$ we define

$$\zeta_m^s = \left(\frac{b^s}{(b-1)^s}\frac{M(m-i,s)}{b^{m-i}}\right)_{i=0}^{\infty} \text{ and } \mu_m = \begin{cases} \frac{b^m}{b^m-1} & \text{if } m \geq 1, \\ 0 & \text{otherwise.} \end{cases}$$

Note that with this notation the value vector of our pdf ψ_m^s is $\mu_m \zeta_m^s$.

Proposition

Suppose $\psi : [0,1]^s \times [0,1]^s \to \mathbb{R}$ *is a function that takes the constant value* ζ_i *on* D_i^s *for each* $i \geq 0$ *and is integrable over* $R(\mathbf{1},\mathbf{1})$*. Then*

$$\int_{R(\mathbf{x},\mathbf{y})} \psi d\lambda \leq \mathbf{xy} \cdot \sup_{k \in \mathbb{N}} \langle S^k \xi^s, \zeta \rangle$$

$\xi^s = (\mathrm{Vol}(D_i^s))_{i=0}^{\infty}$, *and* $\zeta = (\zeta_i)_{i=0}^{\infty}$*. In particular*

$$\int_{R(\mathbf{x},\mathbf{y})} \psi d\lambda \leq \mathbf{xy}$$

for all $\mathbf{x}, \mathbf{y} \in [0,1]^s$ *if and only if* $\langle S^k \xi^s, \zeta \rangle \leq 1$ *for all* $k \in \mathbb{N}$*.*

Here S is the shift operator: $S(\eta_0, \eta_1, \ldots) = (0, \eta_0, \eta_1, \ldots)$

Theorem

A scrambled $(0, m, s)$-net in base b is a NLOD sampling scheme and a NUOD sampling scheme.

Proof.

By previous proposition, need to show that $\langle S^k \xi^s, \mu_m \zeta_m^s \rangle \le 1$ for all $k \in \mathbb{N}$. When $k < m$ we have

$$\langle S^k \xi^s, \mu_m \zeta_m^s \rangle = \langle \xi^s, \mu_m (S^*)^k \zeta_m^s \rangle \le \langle \xi^s, \mu_{m-k} \zeta_{m-k}^s \rangle = \int_{[0,1]^{2s}} \psi_{m-k}^s d\lambda = 1$$

because $\mu_m \le \mu_{m-k}$. Otherwise $k \ge m$ and we have

$$\langle S^k \xi^s, \mu_m \zeta_m^s \rangle = \langle \xi^s, \mu_m \zeta_{m-k}^s \rangle = \langle \xi^s, 0 \rangle = 0.$$

□

Key result used: $bV_i \ge V_{i-1}$ where $V_i = D_i \cap \{[0, x] \times [0, y]\}$

Implication for variance estimation (in progress)

With an explicit integral representation for

$$\mathrm{Cov}(f(\mathbf{U}_I), f(\mathbf{U}_J)) = \int\int f(\mathbf{x})f(\mathbf{y})\psi(\mathbf{x},\mathbf{y})d\lambda$$

we can estimate this covariance term as an integral over $[0,1]^{2s}$, using two copies of a scrambled $(0,m,s)$-net
and then

$$\hat{\mathrm{Var}}(\hat{\mu}_n) = \frac{\hat{\sigma}^2}{n} + \frac{n-1}{n}\hat{\sigma}_{I,J},$$

Some References

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Generalized Hoeffding's Lemma

- Multivariate integration by parts (Mardia and Thompson 1972):

- Let μ_F be a finite signed measure over $[0,1]^s$. Assume that f is integrable with respect to μ_F over $[0,1)^s$ and that it admits the representation

$$f(\mathbf{u}) = \int_{\mathbf{v} \leq \mathbf{u}} g(\mathbf{v}) d\eta_f(\mathbf{v}), \tag{4}$$

for every $\mathbf{u} \in [0,1)^s$, where η_f is a finite signed Borel measure over $[0,1]^s$, and g is a Borel-measurable integrable function with respect to $\mu_F \times \eta$. Then we have

$$\int_{[0,1)^s} f(\mathbf{u}) d\mu_F(\mathbf{u}) = \int_{[0,1)^s} g(\mathbf{u}) \mu_F([\mathbf{u}, \mathbf{1}]) d\eta_f(\mathbf{u}).$$

Generalization of Hoeffding's lemma

Lemma

Let $\mathbf{U}$ *and* $\mathbf{V}$ *be random vectors over* $[0,1]^d$ *with joint survival function* $T(\mathbf{u},\mathbf{v})$ *and marginal survival functions* $R(\mathbf{u})$ *and* $S(\mathbf{v})$*, respectively. Let* f *be a function defined over* $[0,1]^s$ *satisfying the representation* (4) *with function* g *and measure* η_f*. Then*

$$\mathrm{Cov}(f(\mathbf{U}), f(\mathbf{V})) = \int_{[0,1]^{2d}} (T(\mathbf{u},\mathbf{v}) - R(\mathbf{u})S(\mathbf{v}))g(\mathbf{u})g(\mathbf{v})d\eta_f(\mathbf{u})d\eta_f(\mathbf{v}),$$

assuming f *satisfies all integrability conditions required for this covariance term to be well defined.*