Variance-based sensitivity analysis using harmonic analysis

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## Outline

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Bias in RBD

Numerical application

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## Rectangle rule in dimension 1



## How to generalize the design of experiments with d > 1...



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## How to generalize the design of experiments with d > 1...



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Orthogonal arrays: a very quick introduction

Consider 
$$A = OA(n, d, q, t)$$

n: number of points

d: number of factors

q: number of levels, here  $l_1 = 0$ ,  $l_2 = \frac{1}{q}, \dots, l_q = \frac{q-1}{q}$ 

i.e. 
$$A \subseteq \left\{0, \frac{1}{q}, \dots, \frac{q-1}{q}\right\}^{d}$$
 and  $|A| = n$   
t: strength,  $t \in \{0, 1, \dots, d\}$ 

#### Definition

A has strength t if each of its  $n \times t$  submatrices contains each t-uple in  $\left\{0, \frac{1}{a}, \ldots, \frac{q-1}{a}\right\}^{t}$  the same number of times.

 $\implies$  "every projection of A onto any t variables is a q-levels regular grid"

## So, what are we interested in?

Two existing methods of estimating variance-based sensitivity indices (SI)

- Fourier Amplitude Sensitivity Test (FAST): Cukier, Schaibly, Shuler, Levine... (4 papers in the 1970's), Saltelli et al. (1999)
- Random Balance Designs method (RBD): Tarantola et al. (2006)

Links to existing numerical integration theories

- lattice rules (discrete Fourier transform (DFT) on finite subgroups of the torus), mountains of papers and books beginning from the 1960's
- randomized orthogonal arrays sampling, Patterson (1954), Owen (1994)

Generalizations, improvements, error analysis...?

Tissot J.Y., Prieur C., Variance-based sensitivity analysis using harmonic analysis (*submitted*). Preprint available at http://hal.archives-ouvertes.fr/hal-00680725

## Background: harmonic ANOVA

 $X_1,\ldots,X_d$  indep. random variables f such that  $\mathbb{E}\big[f(\mathbf{X})^2\big] < +\infty$ 

• Hoeffding decomposition:

 $f(\mathbf{X}) = \sum_{\mathfrak{u} \subseteq \{1,...,d\}} f_{\mathfrak{u}}(\mathbf{X}_{\mathfrak{u}})$ 

where  $f_{\emptyset} = \mathbb{E}[f(\mathbf{X})]$  and  $\forall \mathfrak{v} \subset \mathfrak{u}, \mathbb{E}[f_{\mathfrak{u}}(\mathbf{X}_{\mathfrak{u}}) | \mathbf{X}_{\mathfrak{v}}] = 0.$ 

ANOVA decomposition:

 $Var[f(X)] = \sum_{u \subseteq \{1,...,d\}} Var[f_u(X_u)]$ 

Variance-based SI:

$$S_{u}(f, \mathbf{X}) := rac{Var[f_{u}(\mathbf{X}_{u})]}{Var[f(\mathbf{X})]}$$

If  $X_1,\ldots,X_d \sim \mathcal{U}([0,1])$ 

Hoeffding decomposition:

$$f(\mathbf{X}) = \sum_{\mathbf{k} \in \mathbb{Z}^d} c_{\mathbf{k}}(f) exp(2i\pi \mathbf{k} \cdot \mathbf{X})$$
$$= \sum_{u \subseteq \{1, \dots, d\}} \underbrace{\sum_{\mathbf{k} \in \mathbb{Z}_{u}^d} c_{\mathbf{k}}(f) exp(2i\pi \mathbf{k} \cdot \mathbf{X})}_{f_{u}(\mathbf{X}_{u})}$$

where 
$$c_{\mathbf{k}}(f) = \mathbb{E} [f(\mathbf{X})exp(-2i\pi \mathbf{k} \cdot \mathbf{X})]$$
 and  
 $\mathbb{Z}_{\mathfrak{u}}^{d} := \{\mathbf{k} \mid \forall i \in \mathfrak{u}, \ k_{i} \in \mathbb{Z}^{*} \text{ and } \forall i \notin \mathfrak{u}, \ k_{i} = 0\}$ 

$$S_{u}(f) = \frac{V_{u}(f)}{V(f)} = \frac{\sum_{\mathbf{k} \in \mathbb{Z}_{u}^{d}} |\mathbf{c}_{\mathbf{k}}(f)|^{2}}{\sum_{\mathbf{k} \in (\mathbb{Z}^{d})^{*}} |\mathbf{c}_{\mathbf{k}}(f)|^{2}}$$

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## Background: harmonic estimator of the SI's

Let D be a finite subset of  $[0, 1]^d$ . Define

$$\widehat{c}_{\mathbf{k}}(f,D) := \frac{1}{|D|} \sum_{\mathbf{x} \in D} f(\mathbf{x}) exp(-2i\pi \mathbf{k} \cdot \mathbf{x})$$

 $\widehat{V}_{\mathfrak{u}}(f, \mathcal{K}_{\mathfrak{u}}, D) := \sum_{\mathbf{k} \in \mathcal{K}_{\mathfrak{u}}} |\widehat{c}_{\mathbf{k}}(f, D)|^2, \quad \mathcal{K}_{\mathfrak{u}} \text{ is a finite truncation subset of } \mathbb{Z}_{\mathfrak{u}}^d$ 

$$\widehat{V}(f,D):=\widehat{\mathrm{c}}_0(f^2,D)-\widehat{\mathrm{c}}_0(f,D)^2, \ \text{note that} \ V(f)=\mathrm{c}_0(f^2)-\mathrm{c}_0(f)^2$$

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$$\widehat{S}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, D) := rac{\widehat{V}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, D)}{\widehat{V}(f, D)}$$

 $\longrightarrow$  efficient design of experiments (DOE) *D*?

# Background: a first example (multidimensional DFT and trigonometric interpolation)



▶  $\forall \mathbf{k} \in D^*$ ,  $\widehat{c}_{\mathbf{k}}(f, D)$  is the k-th discrete complex Fourier coefficient

- $\widetilde{f}(\mathbf{x}) := \sum_{\mathbf{k}\in D^*} \widehat{c}_{\mathbf{k}}(f, D) \exp(2i\pi \mathbf{k} \cdot \mathbf{x}) \text{ is the trigo. interp. poly. (TIP) of } f$
- $\blacktriangleright \ \widehat{S}_{\mathfrak{u}}(f, D^* \cap \mathbb{Z}^d_{\mathfrak{u}}, D) = S_{\mathfrak{u}}(\widetilde{f}) \longrightarrow \text{metamodel approach}$

## Background: remark on multidimensional DFT

- generally unfeasible (curse of dimensionality)
- ▶ possible generalization: Smolyak algorithm on hyperbolic crosses (i.e. interpolation on sparse grids) ⇒ become ill-conditioned as q ↑ and d ↑, Kämmerer & Kunis (2011)





(b) hyperbolic cross(frequency domain)

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## FAST revisited

$$\widehat{S}_{\mathfrak{u}}^{\textit{FAST}}\big(f, \mathsf{K}_{\mathfrak{u}}, \mathsf{x}^{*}(\varphi, \omega)\big) = \widehat{S}_{\mathfrak{u}}\big((\mathcal{T}_{\varphi} \circ \mathcal{R}_{1})f, \mathsf{K}_{\mathfrak{u}}, \mathsf{G}(\omega)\big)$$

• 
$$\mathbf{x}^*(\varphi, \omega)$$
: DOE in classic FAST  
 $\varphi$ : random shift in  $[0, 2\pi)^d$   
 $\omega$ : "generator" of the DOE,  $\in (\mathbb{N}^*)^d$ 

• 
$$\mathcal{T}_{\varphi}$$
 and  $\mathcal{R}_1$ : linear operators on  $L^2([0,1)^d)$ 

•  $G(\omega)$ : cyclic group with generator  $\omega/n$ 

• 
$$\widehat{c}_{\mathbf{k}}(f, G(\omega)) = \frac{1}{n} \sum_{\mathbf{x} \in G(\omega)} f(\mathbf{x}) exp(-2i\pi \mathbf{k} \cdot \mathbf{x})$$
:  
DFT on cyclic group / rank-1 lattice rule



(a) DOE in revisited FAST

## Shift and regularization operators on $L^2([0,1]^d)$

Define  $\mathcal{R}_1$  and  $\mathcal{T}_{\varphi}$ ,  $\varphi \in [0, 2\pi)^d$ ; and also  $\mathcal{R}_p = \mathcal{R}_1 \circ \cdots \circ \mathcal{R}_1$  (p times)



## $\mathcal{R}_p$ and $\mathcal{T}_{\varphi}$ (properties)

• ANOVA decomposition is  $\mathcal{R}_p$  and  $\mathcal{T}_{\varphi}$ -invariant  $\longrightarrow S_{\mathfrak{u}}((\mathcal{T}_{\varphi} \circ \mathcal{R}_p)f) = S_{\mathfrak{u}}(f)$ 

• Riemann-Lebesgue lemma:  $|c_k(f)| \rightarrow 0$  as  $||\mathbf{k}|| \rightarrow \infty$ 

"the smoother the function, the faster the convergence"



## **RBD** revisited

$$\widehat{S}_{\{i\}}^{\mathsf{RBD}}\big(f,\mathsf{K}_{\{i\}},\mathsf{x}^{\times}(\pi,p)\big) = \widehat{S}_{\{i\}}\big((\mathcal{T}_{\widetilde{p}}\circ\mathcal{R}_p)f,\mathsf{pK}_{\{i\}},\mathsf{A}(\pi)\big)$$



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## Potential generalizations

(Operators  $\mathcal{R}_p$  and  $\mathcal{T}_{\varphi}$  are now omitted — p is set to 1 in RBD)

▶  $\widehat{S}_{\mathfrak{u}}(f, \mathcal{K}_{\mathfrak{u}}, \mathcal{G}(\boldsymbol{\omega}))$  with a group  $\mathcal{G}$  of any rank  $r \leq d$  not so easy in practice

- ►  $\widehat{S}_i(f, K_{\{i\}}, A(\pi))$  with a SI of any order:  $\widehat{S}_u(f, K_u, A(\pi))$  OK → already applied in Xu & Gertner (2011)
- $\widehat{S}_{u}(f, K_{u}, A(\pi))$  with any orthogonal array A = OA(n, d, q, t) OK

## Cubature error in FAST

Recall that 
$$\widehat{S}_{\mathfrak{u}}(f, \mathcal{K}_{\mathfrak{u}}, \mathcal{G}(\boldsymbol{\omega})) = \frac{\displaystyle\sum_{\mathbf{k}\in\mathcal{K}_{\mathfrak{u}}}\left|\widehat{c}_{\mathbf{b}}(f, \mathcal{G}(\boldsymbol{\omega}))\right|^{2}}{\widehat{c}_{\mathbf{0}}(f^{2}, \mathcal{G}(\boldsymbol{\omega})) - \widehat{c}_{\mathbf{0}}(f, \mathcal{G}(\boldsymbol{\omega}))^{2}}$$

truncation error

integration error (Poisson summation formula)

$$\widehat{\mathrm{c}}_{\mathsf{k}}ig(f, \mathcal{G}(oldsymbol{\omega})ig) - \mathrm{c}_{\mathsf{k}}(f) = \sum_{\mathsf{h}\in\mathcal{G}(oldsymbol{\omega})^{\perp}\setminus\{\mathbf{0}\}} \mathrm{c}_{\mathsf{k}+\mathsf{h}}(f)$$

where  $G(\boldsymbol{\omega})^{\perp} = \{ \mathbf{h} \in \mathbb{Z}^d \mid \mathbf{h} \cdot \boldsymbol{\omega} \equiv 0 \pmod{n} \}$  is the infinite subgroup of  $\mathbb{Z}^d$  orthogonal to G.

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 $\rightarrow$  main issue: "constructing  $G(\omega)$  which minimizes the error in some sense"

## Classic approach: error minimization=avoiding interferences

- ▶ interference between **k** and **h**  $\iff \widehat{c}_{k}(f, G(\omega)) = \widehat{c}_{h}(f, G(\omega))$
- criterion to avoid the interference between k and h:

 $\mathcal{P}(\mathbf{k},\mathbf{h},\boldsymbol{\omega})$  :  $(\mathbf{k}-\mathbf{h})\cdot\boldsymbol{\omega}\not\equiv 0 \pmod{n}$ 

Proposition 1

Let  $K = \cup_{\mathfrak{u} \neq \emptyset} K_{\mathfrak{u}}$   $(K_{\mathfrak{u}} \subseteq \mathbb{Z}_{\mathfrak{u}}^d)$  and  $G(\omega)$  of order n such that

 $\forall \mathbf{k}, \mathbf{h} \in K, \ \mathbf{k} \neq \mathbf{h}, \ \mathcal{P}(\mathbf{k}, \mathbf{h}, \boldsymbol{\omega}) \ is \ true.$ 

If n = |K| then

 $\widetilde{f}_{\kappa}(\mathbf{x}) = \sum_{\mathbf{k}\in\kappa} \widehat{c}_{\mathbf{k}}(f, G(\omega)) \exp(2i\pi \mathbf{k} \cdot \mathbf{x})$  is the t.i.p. of f at the nodes  $\mathbf{g} \in G(\omega)$ and  $\widehat{S}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, G(\omega)) = S_{\mathfrak{u}}(\widetilde{f}_{\kappa}) \longrightarrow$  metamodel approach

**Remarks**: (1)  $|K| < n \implies$  metamodel approach but weaker conclusion (2) computational complexity  $O(n^d)$  (basic exhaustive algorithm)

New approach: error minimization=achieving the (optimal) rate of convergence in a space of smooth functions

Weighted Korobov space  $\mathcal{H}_{\alpha,\gamma,d}$ ,  $\alpha > 1$ ,  $\gamma = (\gamma_{\mathfrak{u}}) \geq 0$  (RKHS)

• 
$$f \in \mathcal{H}_{\alpha,\gamma,d} \Longrightarrow |c_{\mathbf{k}}(f)| \le \frac{\gamma_{\mathfrak{u}_{\mathbf{k}}}||f||_{\mathcal{H}_{\alpha,\gamma,d}}}{\prod_{i \in \mathfrak{u}_{\mathbf{k}}}|k_{i}|^{\alpha/2}}, \ (\mathfrak{u}_{\mathbf{k}} = \{i \mid k_{i} \neq 0\})$$

Constructing  $\omega$  in rank-1 lattice rules

$$\blacktriangleright B^{opt}_{\alpha,\gamma,d}(n) = \min_{\omega \mid o(G(\omega)) = n} \sup_{||f||_{\mathcal{H}_{\alpha,\gamma,d}} \leq 1} |\widehat{c}_0(f, G(\omega)) - c_0(f)|$$

▶ objective: constructing  $\omega$  such that  $G(\omega)$  achieves a nearly optimal rate of convergence  $B_{\alpha,\gamma,d}(n) \ge B_{\alpha,\gamma,d}^{opt}(n)$ 

Korobov-type construction O(dn<sup>2</sup>) (Korobov, 1960)
 component-by-component construction O(d<sup>2</sup>n<sup>2</sup>) (Sloan & Reztsov, 2002)
 fast CBC construction O(dn log(n)) (using FFT) (Nuyens & Cools, 2004)
 fast CBC construction for embedded lattice rules O(dn log(n)<sup>2</sup>) (Cools et al., 2006)

## New approach (cont.)

#### **Proposition 2**

Let  $f \in \mathcal{H}_{\alpha,\gamma,d}$  and  $B_{\alpha,\gamma,d}(n)$  defined as previously. There exists  $G(\omega)$  of order n such that:

• if 
$$f^2 \in \mathcal{H}_{\alpha',\gamma',d}$$
,  $|\widehat{V}(f,G(\omega)) - V(f)| = O(B_{\alpha,\gamma,d}(n)) + O(B_{\alpha',\gamma',d}(n))$   
and  $\beta = \beta(n)$  such that

where  $\mathcal{Z}_{d,\beta} = \{ \mathbf{k} \mid \prod_{i=1}^{d} \max(1, |k_i|) \leq \beta \}$ : Zaremba cross (=hyperbolic cross)



## Bias in RBD

Recall that

$$\widehat{S}_{\mathfrak{u}}(f, \mathcal{K}_{\mathfrak{u}}, \mathcal{A}(\pi)) = \frac{\widehat{V}_{\mathfrak{u}}(f, \mathcal{K}_{\mathfrak{u}}, \mathcal{A}(\pi))}{\widehat{V}(f, \mathcal{A}(\pi))} = \frac{\sum_{\mathsf{k} \in \mathcal{K}_{\mathfrak{u}}} \left|\widehat{c}_{\mathsf{k}}(f, \mathcal{A}(\pi))\right|^{2}}{\widehat{c}_{\mathsf{0}}(f^{2}, \mathcal{A}(\pi)) - \widehat{c}_{\mathsf{0}}(f, \mathcal{A}(\pi))^{2}}$$

Let A be an OA(n, d, q, t) and  $\mu$  the normalized counting measure on  $(\mathfrak{S}_n)^d$ 

• we are interested in 
$$\mathbb{E}_{\mu}\Big[\widehat{V}(f, A(\pi))\Big]$$
 and  $\mathbb{E}_{\mu}\Big[\widehat{V}_{\mathfrak{u}}(f, \mathcal{K}_{\mathfrak{u}}, A(\pi))\Big]$ 

► let 
$$f \in \mathcal{H}_{\alpha} = \mathcal{H}_{\alpha,1}$$
 (unweighted Korobov space), we have  
$$\mathbb{E}_{\mu}\Big[ |\widehat{c}_{\mathsf{k}}(f, A(\pi))|^2 \Big] = |c_{\mathsf{k}}(f)|^2 + Var_{\mu}\Big[\widehat{c}_{\mathsf{k}}(f, A(\pi))\Big] + O(q^{-\alpha/2})$$

## Bias in RBD (cont.)

Theorem 1 ([Owen, 1994] revisited as a duality relation) Denote  $D = \{0, \frac{1}{q}, \dots, \frac{q-1}{q}\}^d$ , we have

$$Var_{\mu}\left[\widehat{c}_{0}(f,A(\pi))\right] = \frac{1}{n^{2}}\sum_{|\mathfrak{u}|>t}\left(\sum_{r=0}^{|\mathfrak{u}|}B(\mathfrak{u},r)(1-q)^{r-|\mathfrak{u}|}\right)\left(\sum_{\mathbf{k}\in\mathbb{Z}_{\mathfrak{u}}^{d}\cap(-\frac{q}{2},\frac{q}{2})^{d}}\left|\widehat{c}_{\mathbf{k}}(f,D)\right|^{2}\right)$$

where

$$B(\mathfrak{u},r) = \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbf{1}_{|\{l \in \mathfrak{u}, A_{il} = A_{jl}\}|=r}$$

consists of the number of pairs of rows  $(A_i, A_j)$  that match on exactly r of the axes in u.

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**Remark**: note that t = 0 and n = 1 leads to Parseval's identity.

## Bias in RBD (cont.)

#### **Proposition 3**

Let A = OA(n, d, q, t) free of the coincidence defect (= no two rows of A agree in any t + 1 columns). If there exists  $\alpha > 2t + 1$  such that  $f \in \mathcal{H}_{\alpha}$  then (1) if  $f^2 \in \mathcal{H}_{\alpha}$ , then  $\mathbb{E}_{\mu} \Big[ \widehat{V}(f, A(\pi)) \Big] = V(f) - \frac{1}{n} \sum_{|\mathfrak{u}| > t} V_{\mathfrak{u}}(f) + o(n^{-1})$ (2)  $\mathbb{E}_{\mu} \Big[ \widehat{V}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, A(\pi)) \Big] = V_{\mathfrak{u}}(f) + \frac{B}{n} + \varepsilon_{trunc}(f, K_{\mathfrak{u}}) + o(n^{-1})$ where  $B \leq |K_{\mathfrak{u}}| (V(f) + c_0(f)^2)$ 

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In practice,

- no bias correction needed for  $\widehat{V}(f, A(\pi))$
- $\frac{B}{n}$  could be greater than  $V_{u}(f)$

## Bias correction in RBD

(1) A = OA(n, d, q, 1)

$$\begin{split} \widehat{V}_{i}^{c}(f, K_{\{i\}}, A(\pi)) &= \frac{n}{n - |K_{\{i\}}|} \widehat{V}_{i}(f, K_{\{i\}}, A(\pi)) - \frac{|K_{\{i\}}|}{n - |K_{\{i\}}|} \widehat{V}(f, A(\pi)) \\ \widehat{V}_{ij}^{c}(f, K_{\{i,j\}}, A(\pi)) &= \frac{n}{n + 1} \widehat{V}_{ij}(f, K_{\{i,j\}}, A(\pi)) \\ &- \frac{|K_{\{i,j\}}|}{n + 1} (\widehat{V}(f, A(\pi)) + \widehat{c}_{0}(f, A(\pi))) \end{split}$$

(2) A = OA(n, d, q, 2)

$$\begin{aligned} \widehat{V}_{i}^{e}(f, K_{\{i\}}, A(\pi)) &= \widehat{V}_{i}(f, K_{\{i\}}, A(\pi)) \\ \widehat{V}_{ij}^{e}(f, K_{\{i,j\}}, A(\pi)) &= \frac{n}{n - |K_{\{i,j\}}|} \widehat{V}_{ij}(f, K_{\{i,j\}}, A(\pi)) \\ &- \frac{|K_{\{i,j\}}|}{n - |K_{\{i,j\}}|} (\widehat{V}(f, A(\pi)) - \widehat{V}_{i} - \widehat{V}_{j}) \end{aligned}$$

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Analytical test case: Sobol's g-function



## Analytical test case (cont.)

First test case: RBD + bias correction

• 
$$d = 6$$
,  $\mathbf{a} = (0, 0, 1, 1, 9, 9)$ 

- n = 1681

   (a) A = OA(1681, 6, 1681, 1)
   (b) A = OA(1681, 6, 41, 2) (Bush's construction)
- truncation sets based on a Zaremba cross ( $\beta = 12$ )
- boxplots of 200 independent replicates

Second test case: FAST (new approach)

•  $d = 30, a = (0, 0.5, 1, 1.5, 2, \dots, 14.5)$ 

► embedded lattice rule  $G(\omega) = (G(\omega, n))_{n=2^{10}..2^{19}}$  $n_{\max} = 2^{19} \approx 5.10^5$  $j < k \Longrightarrow G(\omega, 2^j) \subset G(\omega, 2^k)$ 

• truncation sets based on a Zaremba cross  $(\beta(n) = 0.8n^{1/4})$ 

## RBD - first-order sensitivity indices



For each index, from the left to the right: strength 2, strength 1 and strength 1 with bias correction.

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## RBD – second-order sensitivity indices



For each index, from the left to the right: strength 2, strength 2 with bias correction, strength 1 and strength 1 with bias correction.

## FAST - first-order sensitivity indices



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## FAST – first-order sensitivity indices (log/log)



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## FAST - second-order sensitivity indices



## FAST – second-order sensitivity indices (log/log)



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## Summary

We revisited FAST and RBD in light of

- DFT on cyclic groups/lattice rules
- randomized ortogonal array sampling

FAST: we proposed a new approach based on lattice rules

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RBD: we generalized RBD to any orthogonal array we proposed a bias correction method

## That's all folks!

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