

Sampling to understand high dimensional functions

Part II: new material

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This course

This is a two part course.

I) **Review** of material on:

a) Functional ANOVA

b) quasi-regression

c) quasi-Monte Carlo sampling

II) **New** material on:

a) applications to missing heritability problems

b) effective dimension of some Sobolev spaces

c) new Sobol' index quantities

Part II(a): missing heritability

Based on work in progress with Or Zuk of the Broad Institute

Real world data . . . that resembles a computer experiment.

Background on SNPs

SNPs are **S**ingle **N**ucleotide **P**olymorphisms

Base pairs are A, C, G or T

At most loci, everybody gets the same

At some loci, there is a minor allele, e.g. most are A but 10% are T

SNP chips, measure 100,000s to 1,000,000s of loci

Each person has 0, 1, or 2 copies of the minor allele

Typical sample sizes

1000s of people and 100,000s of SNPs

Prototypical data

Subject	SNP ₁	SNP ₂	...	SNP _{100,000}	Height	Diabetes
1	0	0	...	1	1.7m	0
2	2	0	...	0	2.1m	1
3	1	0	...	1	1.5m	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮
1000	0	1	...	0	1.9m	1

We would like to predict based on SNPs.

Typically use p -value 10^{-8} to avoid false positives.

The few discoveries explain only a little of phenotype (eg height).

Eg: height may be $\approx 80\%$ heritable but discovered genes explain only 5–10%.

Where is the missing heritability?

Quasi-regression for heritability

Genotype is $\mathbf{x} = (x_1, \dots, x_d)$. Phenotype is y .

Assume $\|\mathbf{x}\|$ and $|y|$ bounded.

Both normalized: $\mathbb{E}(y) = \mathbb{E}(x_j) = 0$ and $\mathbb{E}(y^2) = \mathbb{E}(x_j^2) = 1$.

Model

$$y_i = \sum_{j=1}^d \beta_j x_{ij} + \varepsilon_i$$

$$\mathbb{E}(x_j \varepsilon) = 0$$

ε includes environment, environment \times genes, genes \times genes

Linear heritability is

$$\sigma_L^2 = \sum_{j=1}^d \beta_j^2$$

We assume (**unrealistically**) that x_j is independent of x_k for $j \neq k$.

Holds for most pairs j, k Will require later adjustments

Quasi-regression

$$\tilde{\beta}_j = \frac{1}{n} \sum_{i=1}^n x_{ij} y_i \quad \hat{\sigma}_L^2 = \sum_{j=1}^d \tilde{\beta}_j^2$$

Recall

$$\hat{\sigma}_{L,BC}^2 = \frac{n}{n-1} (\hat{\sigma}_L^2 - \hat{B}), \quad \text{where}$$

$$\hat{B} = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^d x_{ij}^2 y_i^2 = \frac{1}{n^2} \sum_{i=1}^n \|\mathbf{x}_i\|^2 y_i^2 = O_p\left(\frac{d}{n}\right)$$

Then

$$\mathbb{E}\left(\left(\hat{\sigma}_{L,BC}^2 - \sigma_L^2\right)^2\right) = O\left(\frac{1}{n} + \frac{d^2}{n^3}\right) \quad n \geq 2, \quad d \geq 1 \quad (1)$$

We need $n \gg d^{2/3}$ i.e. $d \gg n$ ok even if β is not sparse

∃ lower bounds for estimation of non-sparse β

Candès & Davenport (2011), Raskutti, Wainwright & Yu (2009)

Concentration of measure

$$\|\mathbf{x}_i\|^2 = \sum_{j=1}^d x_{ij}^2 \approx d$$

$$\widehat{B} = \frac{1}{n^2} \sum_{i=1}^n \|\mathbf{x}_i\|^2 y_i^2$$

$$\widetilde{B} = \frac{d}{n^2} \sum_{i=1}^n y_i^2$$

We can show

$$\mathbb{E}((\widehat{B} - \widetilde{B})^2) = O\left(\frac{d}{n^2}\right)$$

So replacing $\|\mathbf{x}_i\|^2$ by d makes a negligible change

Somewhat faster

O (2000) has an example with $d = 1,000,000$ and $n = 100,000$

Additive model

$$z_j = \frac{x_j^2 - \mathbb{E}(x_j^3)x_j - 1}{\sqrt{\mathbb{E}(x_j^4) - \mathbb{E}(x_j^3)^2 - 1}}$$

$$y_i = \sum_{j=1}^d \beta_j x_{ij} + \sum_{j=1}^d \gamma_j z_{ij} + \varepsilon_i$$

Captures effects of dominant vs. recessive genes

$x_1, \dots, x_d, z_1, \dots, z_d$ are **uncorrelated**

Additive heritability

$$\sigma_A^2 = \sum_{j=1}^d \beta_j^2 + \sum_{j=1}^d \gamma_j^2$$

$$\tilde{\gamma}_j = \frac{1}{n} \sum_{i=1}^n z_{ij} y_i$$

$$\hat{\sigma}_A^2 = \sum_j (\tilde{\beta}_j^2 + \tilde{\gamma}_j^2)$$

$$\hat{\sigma}_{A,BC}^2 = \frac{n}{n-1} (\hat{\sigma}_A^2 - \hat{B}_A), \quad \text{where}$$

$$\hat{B}_A = \frac{1}{n^2} \sum_{i=1}^n (\|\mathbf{x}_i\|^2 + \|\mathbf{z}_i\|^2) y_i^2 \approx \frac{2d}{n^2} \sum_{i=1}^n y_i^2.$$

Again

$$\mathbb{E}((\hat{\sigma}_{A,BC}^2 - \sigma_A^2)^2) = O\left(\frac{1}{n} + \frac{d^2}{n^3}\right)$$

Quadratic model

$$y_i = \sum_{j=1}^d \beta_j x_{ij} + \sum_{j=1}^d \gamma_j z_{ij} + \sum_{j < k} \beta_{jk} x_{ij} x_{ik} \varepsilon_i$$

The model allows interactions.

There are $2d + d(d - 1)/2$ parameters.

$$\sigma_Q^2 = \sum_j \beta_j^2 + \sum_j \gamma_j^2 + \sum_{j < k} \beta_{jk}^2$$

For this model

Squared error $O\left(\frac{1}{n} + \frac{d^4}{n^3}\right)$ we need n of order at least $d^{4/3}$ (ouch)

It no longer works to use $\|\mathbf{x}_i\|^2 \approx d$

Could be an issue for bias adjusted quasi-regression estimation of Sobol' indices

Part II(b):

Effective dimension of some Sobolev spaces

Weighted spaces are used in QMC, starting with

Hickernell (1996) and Sloan & Woźniakowski (1998)

They downweight high order interactions and high index variables.

- 1) x_j ordinarily more important than x_{j+1}
- 2) $f_u(\mathbf{x})$ ordinarily more important than $f_v(\mathbf{x})$ for $|v| > |u|$

QMC can integrate functions in some such spaces without any curse of dimensionality

Those spaces are dominated by low order components (as follows)

Effective dimension

A function has effective dimension s in the **truncation** sense if

$$\sum_{u \subseteq \{1, 2, \dots, s\}} \sigma_u^2 \geq (1 - \varepsilon) \sigma^2$$

A function has effective dimension s in the **superposition** sense if

$$\sum_{|u| \leq s} \sigma_u^2 \geq (1 - \varepsilon) \sigma^2$$

Commonly $\varepsilon = 0.01$

QMC often succeeds on functions of low effective dimension in the superposition sense

Caflish, Morokoff & O (1997)

Weighted spaces

Pick weights $1 \geq \gamma_1 > \gamma_2 > \dots > \gamma_d > 0$. Let $\gamma_u = \prod_{j \in u} \gamma_j$.

Inner product and norm

$$\langle f, g \rangle_{W_{d,\gamma}} = \sum_{u \subseteq 1:d} \frac{1}{\gamma_u} \int \frac{\partial^{|u|} f(\mathbf{x})}{\partial \mathbf{x}_u} \frac{\partial^{|u|} \bar{g}(\mathbf{x})}{\partial \mathbf{x}_u} d\mathbf{x}$$

$$\|f\|_{W_{d,\gamma}}^2 = \langle f, f \rangle_{W_{d,\gamma}}.$$

Function class = ball

$$f \in \mathcal{B}(d, \gamma, \rho) \equiv \{f \mid \|f\|_{W_{d,\gamma}} \leq \rho\}$$

How it works

Large $|u| \implies$ small $\gamma_u \implies$ large penalty factor $1/\gamma_u$

\implies only small $\frac{\partial^{|u|} f}{\partial \mathbf{x}_u}$ are allowed

So \mathbf{x}_u not important.

Tractability over $\mathcal{B}(d, \gamma, \rho)$

Quadrature is **tractable** if the worst case error is $O(n^{-a}d^b)$

Quadrature is **strongly tractable** if the worst case error is $O(n^{-a})$, uniformly in d

(see monographs [Novak & Woźniakowski \(2008,2010\)](#))

$$\sum_{j=1}^{\infty} \gamma_j < \infty \implies \text{strong tractability, with } a = 1/2$$

$$\sum_{j=1}^{\infty} \gamma_j^{1/2} < \infty \implies \text{strong tractability, with } a = 1 - \epsilon$$

Rapid weight decay \implies no dimension effect

What sort of functions are in $\mathcal{B}(d, \gamma, \rho)$?

Strong properties \dots often come from strong assumptions

Tractability and effective dimension

When quadrature is strongly tractable,
then the functions in $\mathcal{B}(d, \gamma, \rho)$ do not have large σ_u^2 for large $|u|$.

To describe this

Find ρ^* , the smallest ρ that allows $f \in \mathcal{B}(d, \gamma, \rho)$ with $\text{Var}(f) = 1$.

Then find the largest σ_u^2 for $f \in \mathcal{B}(d, \gamma, \rho^*)$ and $|u| \geq s$.

If this $\sigma_u^2 \leq 0.01$ then $\mathcal{B}(d, \gamma, \rho)$ has effective dimension at most s

An inequality

Let f have continuous derivative $f' \in L^2[0, 1]$ with $\int_0^1 f(x) dx = 0$. Then

$$\sigma^2 = \int_0^1 f(x)^2 dx \leq \frac{1}{\pi^2} \int_0^1 |f'(x)|^2 dx.$$

Sobol' (1963) appeals to calculus of variations.

Fourier methods generalize nicely to higher dimensional analogues.

We can bound σ_u^2 by a multiple of

$$\int \left(\frac{\partial^{|u|} f(\mathbf{x})}{\partial \mathbf{x}_u} \right)^2 dx.$$

There is no reverse inequality, bounding $\int |f'|^2$ by σ^2 .

Related

Lamboni, Iooss, Popelin & Gamboa (2012)

bound Sobol' indices by integrated derivatives, for Boltzmann measures

Fourier representation

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^d} \lambda_{\mathbf{k}} e^{2\pi i \mathbf{k}^\top \mathbf{x}}$$

$$\lambda_{\mathbf{k}} = \int_{[0,1]^d} f(\mathbf{x}) e^{-2\pi i \mathbf{k}^\top \mathbf{x}} d\mathbf{x}$$

$$\text{Var}(f) = \sum_{\mathbf{k} \neq \mathbf{0}} |\lambda_{\mathbf{k}}|^2$$

After some algebra

$$\frac{\partial^{|u|} f(\mathbf{x})}{\partial \mathbf{x}_u} = \sum_{\mathbf{k} \in \mathbb{Z}^d} \lambda_{\mathbf{k}} \left((2\pi i)^{|u|} \prod_{j \in u} k_j \right) e^{2\pi i \mathbf{k}^\top \mathbf{x}}, \quad \text{and}$$

$$\|f\|_{W_{d,\gamma}}^2 = \sum_{\mathbf{k} \in \mathbb{Z}^d} |\lambda_{\mathbf{k}}|^2 \prod_{j=1}^d \left(1 + \frac{4\pi^2 k_j^2}{\gamma_j} \right)$$

Finding the dimension

$$\begin{aligned} \text{maximize} \quad & \text{Var}(f) = \sum_{\mathbf{k} \neq \mathbf{0}} |\lambda_{\mathbf{k}}|^2 \\ \text{subject to} \quad & \|f\|^2 = \sum_{\mathbf{k} \in \mathbb{Z}^d} |\lambda_{\mathbf{k}}|^2 \prod_{j=1}^d \left(1 + \frac{4\pi^2 k_j^2}{\gamma_j}\right) \leq \rho^2 \end{aligned}$$

Maximum happens when $\lambda_{\mathbf{k}} = 0$ except for $\mathbf{k} = (\pm 1, 0, 0, \dots, 0)$.

We get $\|f\|^2 = \text{Var}(f)(1 + 4\pi^2/\gamma_1)$, so $\rho^{*,2} = 1 + 4\pi^2/\gamma_1$.

$$\sigma_u^2 = \sum_{\mathbf{k}_u \in (\mathbb{Z} - \{0\})^{|u|}} |\lambda_{\mathbf{k}_u : \mathbf{0}_{-u}}|^2$$

$$\text{Similarly} \quad \max_{f \in \mathcal{B}(d, \gamma, \rho^*)} \sigma_u^2 = \frac{1 + 4\pi^2/\gamma_1}{\prod_{j \in u} (1 + 4\pi^2/\gamma_j)}$$

If $|u|$ is large and γ_j decay rapidly \dots then σ_u^2 must be small

Effective dimensions

$$\text{For } \gamma_j = j^{-1.01}$$

Just barely strongly tractable

Truncation dimension is 97

Superposition dimension is 2

$$\text{For } \gamma_j = j^{-2}$$

Almost $O(n^{-1+\epsilon})$ uniformly in d

Truncation dimension is 10

Superposition dimension is 1

These use $\varepsilon = 0.01$

At $\varepsilon = 0.0001$ superposition dimensions rise to 3 and 2

Part II(c): new Sobol' indices

Recall

$$\underline{\tau}_u^2 = \sum_{v \subseteq u} \sigma_v^2$$

$$\overline{\tau}_u^2 = \sum_{v \cap u \neq \emptyset} \sigma_v^2$$

$$\underline{\tau}_u^2 = \iint f(\mathbf{x}) (f(\mathbf{x}_u : \mathbf{z}_{-u}) - f(\mathbf{z})) \, d\mathbf{x} \, d\mathbf{z}$$

What other quantities can we get?

In principal we can get any σ_u^2 from

$$\sigma_u^2 = \sum_{v \subseteq u} (-1)^{|u-v|} \tau_v^2$$

we prefer

- 1) unbiased estimates
- 2) low variance
- 3) averages of squared differences to differences of squares
- 4) to avoid $O(2^d)$ integrals, or even $O(d^2)$ integrals

The set of possibilities

$$\sum_{u \subseteq \mathcal{D}} \sum_{v \subseteq \mathcal{D}} \lambda_{u,v} \iint f(\mathbf{x}_u : \mathbf{z}_{-u}) f(\mathbf{x}_v : \mathbf{z}_{-v}) d\mathbf{x} d\mathbf{z}$$

where

$$\mathbf{y} = \mathbf{x}_u : \mathbf{z}_{-u} \implies y_j = \begin{cases} x_j, & j \in u \\ z_j, & j \notin u \end{cases}$$

and

$$\lambda_{u,v} \in \mathbb{R}$$

A 2^{2d} dimensional space of Sobol' quantities (overparameterized)

We only want $\sum_u \delta_u \sigma_u^2$ for $\delta \in \mathbb{R}^{2^d}$

Special subsets

1) Squares

$$\iint \left(\sum_u \lambda_u f(\mathbf{x}_u : \mathbf{z}_{-u}) \right)^2 d\mathbf{x} d\mathbf{z} \quad \text{Nonnegative}$$

2) Bilinear

$$\iint \left(\sum_u \lambda_u f(\mathbf{x}_u : \mathbf{z}_{-u}) \right) \left(\sum_u \gamma_u f(\mathbf{x}_u : \mathbf{z}_{-u}) \right) d\mathbf{x} d\mathbf{z} \quad \text{Fast}$$

3) All for one

$$\iint \left(\sum_u \lambda_u f(\mathbf{x}_u : \mathbf{z}_{-u}) \right) f(\mathbf{z}) d\mathbf{x} d\mathbf{z} \quad \text{Simple}$$

4) Contrast

$$\sum_u \sum_v \lambda_{u,v} = 0 \quad \text{Free of } f_{\emptyset}^2$$

The basis

$$\iint f(\mathbf{x}_u:\mathbf{z}_{-u})f(\mathbf{x}_v:\mathbf{z}_{-v}) d\mathbf{x} d\mathbf{z} = f_{\emptyset}^2 + \mathcal{I}_{\text{NXOR}(u,v)}^2$$

Not exclusive or

$j \in u$	$j \in v$	XOR(u, v)	NXOR(u, v)
0	0	0	1
0	1	1	0
1	0	1	0
1	1	0	1

$$j \in \text{NXOR}(u, v) \iff j \in u \cap v \text{ or } j \in u^c \cap v^c$$

Proof

$$\begin{aligned}
& \iint f(\mathbf{x}_u : \mathbf{z}_{-u}) f(\mathbf{x}_v : \mathbf{z}_{-v}) \, d\mathbf{x} \, d\mathbf{z} \\
&= \sum_{w \subseteq \mathcal{D}} \sum_{w' \subseteq \mathcal{D}} \iint f_w(\mathbf{x}_u : \mathbf{z}_{-u}) f_{w'}(\mathbf{x}_v : \mathbf{z}_{-v}) \, d\mathbf{x} \, d\mathbf{z} \\
&= \sum_{w \subseteq \mathcal{D}} \iint f_w(\mathbf{x}_u : \mathbf{z}_{-u}) f_w(\mathbf{x}_v : \mathbf{z}_{-v}) \, d\mathbf{x} \, d\mathbf{z} \\
&= \sum_w 1_{w \subseteq (u \cap v) \cup (u^c \cap v^c)} \int f_w(\mathbf{x})^2 \, d\mathbf{x} \\
&= \sum_{w \subseteq \text{NXOR}(u, v)} \int f_w(\mathbf{x})^2 \, d\mathbf{x} \\
&= f_{\emptyset}^2 + \tau_{\text{NXOR}(u, v)}^2.
\end{aligned}$$

All for one

$$\begin{aligned}
 & \sum_v \lambda_v \iint f(\mathbf{x}) f(\mathbf{x}_v : \mathbf{z}_{-v}) \, d\mathbf{x} \, d\mathbf{z} \\
 &= \sum_v \lambda_v \left(f_{\emptyset}^2 + \tau_{\text{NXOR}(\mathcal{D}, v)}^2 \right) \\
 &= f_{\emptyset}^2 \sum_v \lambda_v + \sum_v \lambda_v \tau_v^2
 \end{aligned}$$

Combinations with $\sum_{v \subseteq \mathcal{D}} \lambda_v = 0$ are free of f_{\emptyset}^2

For τ_u^2 take

$$\lambda_v = \begin{cases} (-1)^{|u-v|} & u \subseteq v \\ 0 & \text{else.} \end{cases}$$

(Lots of alternation)

Mean squares

If $\sum_v \lambda_v = 0$ then the following is a nonnegative estimate of a linear combination of σ_u^2

$$\begin{aligned} & \iint \left(\sum_v \lambda_v f(\mathbf{x}_v : \mathbf{z}_{-v}) \right)^2 d\mathbf{x} d\mathbf{z} \\ &= \sum_v \sum_w \lambda_v \lambda_w \iint f(\mathbf{x}_v : \mathbf{z}_{-v}) f(\mathbf{x}_w : \mathbf{z}_{-w}) d\mathbf{x} d\mathbf{z} \\ &= \sum_v \sum_w \lambda_v \lambda_w \tau_{\text{NXOR}(w,v)}^2 \end{aligned}$$

Combinations with $\sum_{v \subseteq \mathcal{D}} \lambda_v = 0$ are free of f_{\emptyset}^2

Q: What can we get as a square?

A: $\bar{\tau}_u^2$ and Υ_u^2 (but what else?)

Cannot get $\underline{\tau}_u^2$ as a square

$$\iint \left(\lambda_0 f(\mathbf{z}) + \lambda_1 f(\mathbf{x}_u : \mathbf{z}_{-u}) + \lambda_d f(\mathbf{x}) \right)^2 d\mathbf{x} d\mathbf{z}$$

with $\lambda_0 = A, \lambda_d = B, \lambda_1 = -A - B, \text{ WLOG } f_\emptyset = 0$

XOR	\emptyset	u	\mathcal{D}		NXOR	\emptyset	u	\mathcal{D}
\emptyset	\emptyset	u	\mathcal{D}	\rightarrow	\emptyset	\mathcal{D}	$-u$	\emptyset
u	u	\emptyset	$-u$		u	$-u$	\mathcal{D}	u
\mathcal{D}	\mathcal{D}	$-u$	\emptyset		\mathcal{D}	\emptyset	u	\mathcal{D}

τ_{NXOR}^2	\emptyset	u	\mathcal{D}					
\emptyset	σ^2	$\underline{\tau}_{-u}^2$	0	\rightarrow				
u	$\underline{\tau}_{-u}^2$	σ^2	$\underline{\tau}_u^2$					
\mathcal{D}	0	$\underline{\tau}_u^2$	σ^2					

$$\rightarrow \begin{aligned} & \sigma^2(A^2 + B^2 + (A + B)^2) \\ & - \underline{\tau}_u^2 B(A + B) - \underline{\tau}_{-u}^2 A(A + B) \end{aligned}$$

τ_u^2 as a square

We get

$$\begin{aligned} & \iint \left(Af(\mathbf{z}) - (A+B)f(\mathbf{x}_u:\mathbf{z}_{-u}) + B\lambda_d f(\mathbf{z}) \right)^2 d\mathbf{x} d\mathbf{z} \\ &= \sigma^2(A^2 + B^2 + (A+B)^2) - \tau_u^2 B(A+B) - \tau_{-u}^2 A(A+B) \end{aligned}$$

To eliminate σ^2 and τ_{-u}^2 we need $A = B = 0$.

Substitution $\tau_{-u}^2 = \sigma^2 - \bar{\tau}_u^2$ does not help.

Introducing more terms inside the square means more terms that need to cancel (e.g. τ_v^2 for $v \neq u$)

Weighted sums of squares

$$\sum_{r=1}^R \alpha_r \iint \left(\sum_{u \subseteq \mathcal{D}} \lambda_{r,u} f(\mathbf{x}_u : \mathbf{z}_{-u}) \right)^2 d\mathbf{x} d\mathbf{z}$$

The coefficient of $\sigma_{\mathcal{D}}^2$ is:

$$\sum_{r=1}^R \alpha_r \sum_{u \subseteq \mathcal{D}} \lambda_{r,u}^2$$

We cannot make this 0 without $\alpha_r < 0$ (or trivially $\lambda_{r,u} = 0$ or all $\alpha_r = 0$)

So . . . no unbiased nonnegative estimate of τ_u^2 . (checkmate)

Bilinear, with $O(d)$ evaluations

Suppose $\lambda_u = 0$ for $|u| \notin \{0, 1, d-1, d\}$. Same for $\gamma_v = 0$.

Then the rule

$$\sum_u \sum_v \lambda_u \gamma_v \iint f(\mathbf{x}_u : \mathbf{z}_{-u}) f(\mathbf{x}_v : \mathbf{z}_{-v}) d\mathbf{x} d\mathbf{z}$$

takes $O(d)$ computation \dots not $O(d^2)$.

For $j \neq k$, let j represent $\{j\}$ and $-j$ represent $-\{j\}$ etc.

$O(d)$ pairs, with $k \neq j$

$$\begin{array}{c} \text{XOR} \\ \emptyset \\ j \\ -j \\ \mathcal{D} \end{array} \begin{array}{c} \emptyset \\ j \\ k \\ -j \\ -k \\ \mathcal{D} \end{array} \left[\begin{array}{cccccc} \emptyset & j & k & -j & -k & \mathcal{D} \\ j & \emptyset & \{j, k\} & \mathcal{D} & -\{j, k\} & -j \\ -j & \mathcal{D} & -\{j, k\} & \emptyset & \{j, k\} & j \\ \mathcal{D} & -j & -k & j & k & \emptyset \end{array} \right]$$

$$\begin{array}{c} \text{NXOR} \\ \emptyset \\ j \\ -j \\ \mathcal{D} \end{array} \begin{array}{c} \emptyset \\ j \\ k \\ -j \\ -k \\ \mathcal{D} \end{array} \left[\begin{array}{cccccc} \mathcal{D} & -j & -k & j & k & \emptyset \\ -j & \mathcal{D} & -\{j, k\} & \emptyset & \{j, k\} & j \\ j & \emptyset & \{j, k\} & \mathcal{D} & -\{j, k\} & -j \\ \emptyset & j & k & -j & -k & \mathcal{D} \end{array} \right]$$

$\tau_{\text{NXOR}}^2(u, v)$

Assuming $f_\emptyset = 0$ (WLOG if $\sum_u \lambda_u = 0$)

$$\tau_{\text{NXOR}}^2 \begin{matrix} & \emptyset & j & k & -j & -k & \mathcal{D} \\ \begin{matrix} \emptyset \\ j \\ -j \\ \mathcal{D} \end{matrix} & \left[\begin{array}{cccccc} \sigma^2 & \tau_{-j}^2 & \tau_{-k}^2 & \tau_j^2 & \tau_k^2 & 0 \\ \tau_{-j}^2 & \sigma^2 & \tau_{\{j,k\}}^2 & 0 & \tau_{\{j,k\}}^2 & \tau_j^2 \\ \tau_j^2 & 0 & \tau_{\{j,k\}}^2 & \sigma^2 & \tau_{\{j,k\}}^2 & \tau_{-j}^2 \\ 0 & \tau_j^2 & \tau_k^2 & \tau_{-j}^2 & \tau_{-k}^2 & \sigma^2 \end{array} \right] \end{matrix}$$

$$\sum_j \tau_j^2 = \sum_j \sigma_j^2 \quad \sum_j \sum_{k \neq j} \tau_{\{j,k\}}^2 = d(d-1)\sigma^2 - \sum_u (2(d-1) - |u|)|u|\sigma_u^2$$

$$\sum_j \tau_{-j}^2 = d\sigma^2 - \sum_u |u|\sigma_u^2 \quad \sum_j \sum_{k \neq j} \tau_{\{j,k\}}^2 = \sum_{u:|u|=2} \sigma_u^2 + 2 \sum_j \sigma_j^2$$

Using $O(d)$ terms

We can estimate

$$\sum_u \sigma_u^2 1_{|u|=1}$$

$$\sum_u \sigma_u^2 1_{|u|=2} \quad !$$

$$\sum_u |u| \sigma_u^2$$

$$\sum_u |u|^2 \sigma_u^2$$

Another $O(d)$ quantity

Largest element in u :

$$\lceil u \rceil = \begin{cases} \max\{j \mid j \in u\}, & u \neq \emptyset \\ 0, & u = \emptyset. \end{cases}$$

Then

$$\begin{aligned} \sum_{j=1}^{d-1} \bar{\tau}_{\{1,2,\dots,j\}^c}^2 &= \sum_u \sigma_u^2 \sum_{j=1}^{d-1} 1_{u \cap \{1,\dots,j\}^c \neq \emptyset} \\ &= \sum_u \sigma_u^2 \sum_{j=1}^{d-1} 1_{u \cap \{j+1,\dots,d\} \neq \emptyset} \\ &= \sum_u \sigma_u^2 (\lceil u \rceil - 1). \end{aligned}$$

A mean dimension in the truncation sense.

Easier to compute than effective dimension.

Optimal estimates

Sobol's estimates have been improved (!!) recently:

Kucherenko, Feil, Shah, Mauntz (2011), and

Janon, Klein, Lagnoux, Nodet & Prieur (2012) (Grenoble)

$$\text{Let } \eta^2 = \sum_u \delta_u \sigma_u^2.$$

We would like

$$\mathbb{E}(\hat{\eta}^2) = \eta^2 \quad \text{and,} \quad \text{Var}(\hat{\eta}^2) = \text{minimum.}$$

Using variance components theory

Unfortunately $\text{Var}(\hat{\eta}^2)$ depends on 4'th moments

Fortunately There is a theory of **MIN**imum **Q**uadratic **N**orm **UN**biased **E**stimates (MINQUE)*

Unfortunately They do not appear to be available for crossed random effects

Fortunately We can choose where to sample and our estimator.

* C. R. Rao (1970s)

Speculation

For all for one $\sum_u \lambda_u \tau_u^2$

$$\text{minimize } \sum_u \lambda_u^2$$

$$\text{subject to } \sum_u \lambda_u \tau_u^2 = \sum_u \delta_u \sigma_u^2$$

$$\text{and } \sum_u \lambda_u = 0.$$

This ignores # of function evaluations. So instead

$$\text{minimize } \left(\sum_u \lambda_u^2 \right) \times \left(\sum_u 1_{\lambda \neq 0} \right) = \|\lambda\|_2^2 \times \|\lambda\|_0$$

Merci, la deuxieme fois

- GDR Coordinators: Clémentine Prieur, Bertrand Iooss, Fabien Mangeant
- Scientific and organizing committee
- Françoise Poggi
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MCQMC 2014

Please come to Leuven for MCQMC 2014.

Sensitivity for extremes

Gary Tang asked about sensitivity measures that are more attuned to extreme values of $f(\boldsymbol{x})$.

Some joint work with Josef Dick:

- 1) Transform $f(\boldsymbol{x})$ (don't like)
- 2) Analysis of skewness $\int f(\boldsymbol{x})^3 d\boldsymbol{x}$ (don't like either)
- 3) Analysis of fourth moment $\int f(\boldsymbol{x})^4 d\boldsymbol{x}$ (don't like either)
- 4) Estimate $\int f_u(\boldsymbol{x})^4 d\boldsymbol{x}$ (like much more, still testing!)