Shapley Effects for Use as Sensitivity Measure

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Motivation

For independent variables

$$\mathbb{V}[X_1 + X_2] = \mathbb{V}[X_1] + \mathbb{V}[X_2]$$

but generally

$$\begin{aligned}\mathbb{V}[X_1 + X_2] &= \mathbb{E}[(X_1 + X_2)^2] - (\mathbb{E}[X_1 + X_2])^2 = \mathbb{E}[X_1^2] - \mathbb{E}[X_1]^2 + \mathbb{E}[X_2^2] - \mathbb{E}[X_2]^2 \\ &\quad + 2\,(\mathbb{E}[X_1 X_2] - \mathbb{E}[X_1]\,\mathbb{E}[X_2]) = \mathbb{V}[X_1] + \mathbb{V}[X_2] + 2\,\mathrm{Cov}(X_1, X_2)\end{aligned}$$

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Consequences for functional ANOVA under dependence

- Covariance terms need to be considered
- Orthogonality (strong annihilation) is lost: Hierarchical orthogonality can be used
- But this introduces dependence on the order of the factors in the model

First and last term in any ordering of the factors may receive special attention

Wanted

A concept to define main and total effects and related sensitivity indices without recurring to functional ANOVA decomposition

Back to the basics:

- Main effect S_i: Variance explained by a functional dependence on X_i

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We study a game theoretic approach:
The goal is to attribute a fair share of the variance to each input factor

Game Theory: Definitions

For d players,

- Coalition-worth value function $\mathrm{val} : 2^d \to \mathbb{R}_{\geq 0}$, 2^d: set of subsets of $[d] := \{1, \ldots, d\}$
- Coalition $\alpha \subset [d]$ lists the active players, anti-coalition $\sim \alpha = [d] \setminus \alpha$
- Marginal contribution of player i joining coalition α: $\mathrm{mar}(\alpha, i) = \mathrm{val}(\alpha \cup \{i\}) - \mathrm{val}(\alpha)$

The value function assigns a payoff to a group of players
The value function is a game if it is grounded: $\mathrm{val}(\emptyset) = 0$.

Grand total: $\mathrm{val}([d])$

Axioms for the Shapley Value

Attribute a fair share of the grand total to each player:

Theorem

The Shapley value $\Phi_i(\mathrm{val})$ *of player* i *for the payoffs* val *is uniquely characterized by the following four axioms,*

- *Pareto-efficiency:* $\sum_{i=1}^{d} \Phi_i(\mathrm{val}) = \mathrm{val}([d])$
- *Symmetry: If* $\mathrm{val}(\alpha \cup \{i\}) = \mathrm{val}(\alpha \cup \{j\})$ *for all subsets* α *containing neither* i *nor* j *then* $\Phi_i(\mathrm{val}) = \Phi_j(\mathrm{val})$
- *Linearity:* $\Phi_i(\mathrm{val}_1 + \mathrm{val}_2) = \Phi_i(\mathrm{val}_1) + \Phi_i(\mathrm{val}_2)$
- *Null-player: If for all* α, $\mathrm{val}(\alpha \cup \{i\}) = \mathrm{val}(\alpha)$ *holds then* $\Phi_i(\mathrm{val}) = 0$.

Formulas for the Shapley Value

$$\Phi_i(\mathrm{val}) = \frac{1}{d} \sum_{\alpha : i \notin \alpha} \binom{d-1}{|\alpha|}^{-1} \mathrm{mar}(\alpha, i)$$

$$\Phi_i(\mathrm{val}) = \frac{1}{d} \sum_{\alpha : i \in \alpha} \binom{d-1}{|\alpha|-1}^{-1} (\mathrm{val}(\alpha) - \mathrm{val}(\sim \alpha))$$

$$\Phi_i(\mathrm{val}) = \sum_{\alpha : i \in \alpha} \frac{\mathrm{mob}(\alpha)}{|\alpha|}$$

All three formulas satisfy the axioms which uniquely describe the Shapley value, hence define the same object.

Möbius inverses

Unique decomposition $\text{val}(\alpha) = \sum_\beta \text{mob}(\beta) u_\beta(\alpha)$
$u_\beta(\alpha) = \mathbf{1}(\beta \subset \alpha)$ (Unanimity game) codes subset inclusion
Weights: Möbius inverses / Harsanyi dividends. Implicitly defined by

$$\text{val}(\alpha) = \sum_{\beta \subset \alpha} \text{mob}(\beta).$$

This system of $2^d - 1$ linear equations can be solved by an inclusion-exclusion rule

$$\text{mob}(\alpha) = \sum_{\beta \subset \alpha} (-1)^{|\alpha|+|\beta|} \text{val}(\beta).$$

This approach is technical equivalent to the formation of higher order effects.

Main and total effects for games

Let us therefore introduce (unnormalized) main and total effects based on the coalition-worth value function,

- Main effects $S_i = \mathrm{val}(\{i\}) = \mathrm{mar}(\emptyset, i) = \mathrm{mob}(\{i\})$
- Total effects $T_i = \sum_{\alpha:i\in\alpha} \mathrm{mob}(\alpha)$

Note that always

$$
\begin{aligned}
T_i &= \sum_{\alpha:i\in\alpha} \mathrm{mob}(\alpha) = \sum_{\alpha} \mathrm{mob}(\alpha) - \sum_{\alpha:i\notin\alpha} \mathrm{mob}(\alpha) \\
&= \mathrm{val}([d]) - \sum_{\alpha\subset\sim i} \mathrm{mob}(\alpha) = \mathrm{val}([d]) - \mathrm{val}(\sim i)
\end{aligned}
$$

Shapley Effects

Grand total: Output variance
Players: Input factors

Consider the value function $\text{val}(\alpha) = \mathbb{V}[\mathbb{E}[Y|X_\alpha]]$:
If $\alpha = \emptyset$ then we have to compute the variance of a constant value, i.e. val is a game
If $\alpha = [d]$ and $y = f(x_1, \ldots, x_d)$ is a square integrable deterministic function then $\text{val}([d]) = \mathbb{V}[\mathbb{E}[Y|X_{[d]}]] = \mathbb{V}[Y]$, i.e. the grand total is the output variance

How to compute the Shapley effects

Sobol' method, pick-and-freeze with conditionally independent sampling

```
for i=1:d; w0=1; for j=1:i-1; w0=w0*(d-i+j)/j; end; w(i)=w0; end % weights
[ua,ub]=createsample(d,n,randomsource); za=norminv(ua); zb=norminv(ub);
C=chol(S); na=za*C; nb=zb*C; xa=trafo(normcdf(na)); xb=trafo(normcdf(nb));
ya=model(xa);yb=model(xb); Vy=(yb-ya)'*(yb-ya)/n/2; Shap=ones(1,d)*Vy;
for i=1:2^(d-1)-1 % loop only over half of the indices
 g=logical(bitget(i,1:d)); sz=sum(g); D=chol([S(g,g),S(g,¬g);S(¬g,g),S(¬g,¬g)]);
 D11=D(sz+1:end,sz+1:end); D22=D(1:sz,1:sz);D21=D(1:sz,sz+1:end);
 ni=na;ni(:,¬g)=zb(:,¬g)*D11+na(:,g)*(D22\D21); xi=trafo(normcdf(ni));
 yi=model(xi); sz=k-sz; E=chol([S(¬g,¬g),S(¬g,g);S(g,¬g),S(g,g)]);
 E11=E(sz+1:end,sz+1:end); E22=E(1:sz,1:sz); E21=E(1:sz,sz+1:end); nj=na;
 nj(:,g)=zb(:,g)*E11+na(:,¬g)*(E22\E21);  xj=trafo(normcdf(nj));
 yj=model(xj); sz=k-sz; bal=(yj-yi)'*(yj+yi-2*ya)/(2*n); % bal =val(g)-val(¬g)
 Shap(g)=Shap(g)+bal/w(sz); Shap(¬g)=Shap(¬g)-bal/w(d-sz);
end, Shap=Shap/d;
```

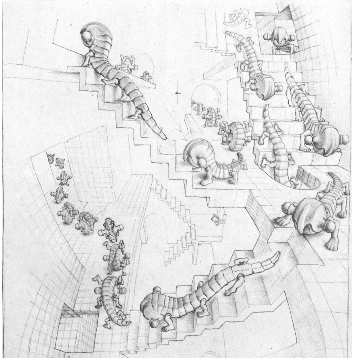
Code Discussion

- `d` input dimension, `n` basic sample block size, `model` vectorized simulator, `trafo` marginal transformation from $[0,1]^d$, `createsample` create two basic sample blocks (not shown)
- Implemented are Gaussian Copula dependence structures
- Via Cholesky decompositions of reordered covariance matrices
- Using the second Shapley formula with a balanced value function
- Computationally costly: Visits half of all subsets, pick-and-freeze design for each of them, symmetric design

Goda "Crawling Centipede" approach

With a winding stairs approach one can compute val(α) for $\alpha = \{1, 2, \ldots, i\}$ (consecutive indices).

Goda's approach: Randomize the index were the innovation enters



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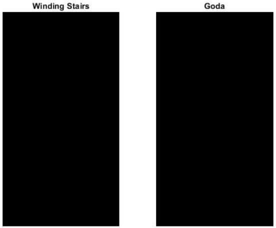

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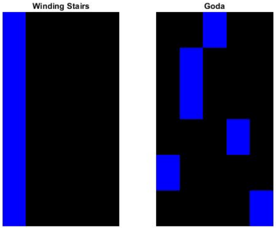

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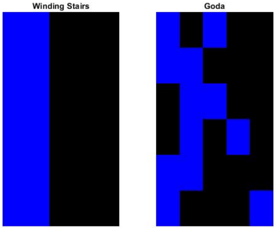

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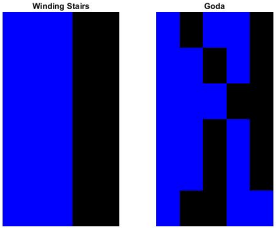

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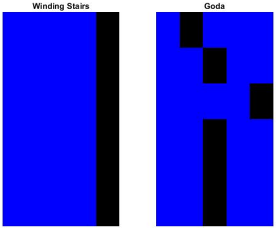

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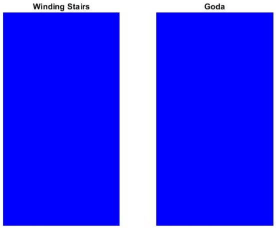

Shapley effects, Goda's method

```
x = rand(n,d);  y = rand(n,d); % MC sample
[¬, pm] = sort(rand(n,d),2);  % random permutation
z = x; fz1 = func(trafo(z)); fx = fz1; % save fx as reference point
phi1 = zeros(1,d); phi2 = zeros(1,d);
for j=1:d
   % activate indices from permutation matrix
   ind = bsxfun(@eq,pm(:,j),1:d); % compare column with row
   z(ind) = y(ind); % copy over next pick'freeze dimension (per run)
   fz2 = func(trafo(z));
   fmarg = ((fx-fz1/2-fz2/2).*(fz1-fz2))';  % update
   phi1 = phi1 + fmarg*ind/n;
   fz1 = fz2;
end
```

Code Discussion

- `d` input dimension, `n` basic sample block size, `func` vectorized simulator, `trafo` marginal transformation from $[0,1]^d$
- Only input independence (1D innovation injection)
- Reference point is the $f(x)$ output, but may also consider differences to $f(y)$
- Original version offers error estimate
- Computationally cheap: $(d+1)\cdot n$ vs. $(2^d-1)\cdot n$

Analytical Example: Gauss Linear

Input: Multivariate normal distribution with covariance Σ

Simulation model: $Y = \beta^0 + \beta^T X$, $X \in \mathbb{R}^d$

All conditional distributions are Gaussian, all conditional expectations are linear

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Theorem

Under Gauss linear, unnormalized main, total and Shapley effects are given by

$$S_j = \beta^T \left(\frac{\Sigma_{[d],j}\Sigma_{j,[d]}}{\Sigma_{j,j}} \right) \beta = \beta^T \left(\frac{\Sigma_{[d],j}\Sigma_{[d],j}^T}{\Sigma_{j,j}} \right) \beta$$

$$T_j = \beta_j^2 \frac{\det(\Sigma)}{\det(\Sigma_{-j,-j})}$$

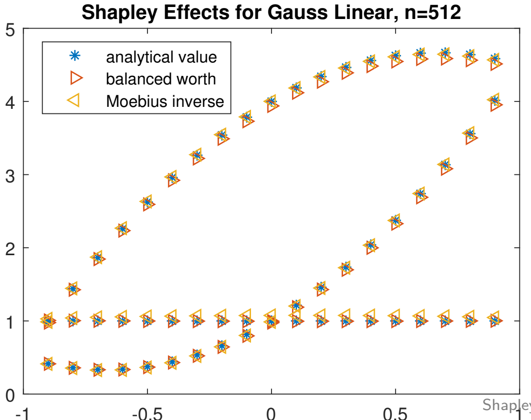
$$\Phi_j = \frac{1}{d} \sum_{j \in u} \binom{d-1}{|u|-1}^{-1} \beta^T \left(\Sigma_{[d],u}\Sigma_{u,u}^{-1}\Sigma_{u,[d]} - \Sigma_{[d],-u}\Sigma_{-u,-u}^{-1}\Sigma_{-u,[d]} \right) \beta$$

Output variance is $\mathbb{V}[Y] = \beta^T \Sigma \beta$.

Feed the Code

Input: $X \sim \mathcal{N}(0, \Sigma)$ with $\Sigma = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \varrho\sigma \\ 0 & \varrho\sigma & \sigma^2 \end{pmatrix}$, $\sigma = 2$, ϱ is varied within $[-1, 1]$

Model $Y = f(X_1, X_2, X_3) = X_1 + X_2 + X_3$



Thank You!

Questions, Comments

mailto:elmar.plischke@tu-clausthal.de

Preprints, Scripts, Stuff

https://artefakte.rz-housing.tu-clausthal.de/epl/

GitLab Repository

https:
//gitlab.gwdg.de/elmar.plischke/global-sensitivity-analysis-collection