Recursive identification of smoothing spline ANOVA models

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Introduction

We discuss different approaches to the estimation and identification of smoothing splines ANOVA models:

- The ‘classical’ approach [Wahba, 1990, Gu, 2002], as improved by Storlie et al. [ACOSSO];
- the recursive approach of Ratto et al. [2007], Young [2001] [SDR].

Introduction: ACOSSO

‘a new regularization method for simultaneous model fitting and variable selection in nonparametric regression models in the framework of smoothing spline ANOVA’.

COSSO [Lin and Zhang, 2006] penalizes the sum of component norms, instead of the squared norm employed in the traditional smoothing spline method.

Storlie et al. introduce an adaptive weight in the COSSO penalty allowing more flexibility in the estimate of important functional components (using heavier penalty to unimportant ones).

Introduction: SDR

Using the the State-Dependent Parameter Regression (SDR) approach of Young [2001], Ratto et al. [2007] have developed a non-parametric approach very similar to smoothing splines, based on *recursive filtering and smoothing estimation* [the Kalman Filter, KF, combined with Fixed Interval Smoothing ,FIS, Kalman, 1960, Young, 1999]:

- couched with optimal Maximum Likelihood estimation;

- flexibility in adapting to local discontinuities, heavy non-linearity and heteroscedastic error terms.

Goals of the paper

1. develop a formal comparison and demonstrate equivalences between the ‘classical’ tensor product cubic spline approach and the SDR approach;

2. discuss advantages and disadvantages of these approaches;

3. propose a unified approach to smoothing spline ANOVA models that combines the best of the discussed methods.

State Dependent Regressions and smoothing splines: Additive models

Denote the generic mapping as $z(\mathbf{X})$, where $\mathbf{X} \in [0,1]^p$ and p is the number of parameters.

The simplest example of smoothing spline mapping estimation of z is the additive model:

$$f(\mathbf{X}) = f_0 + \sum_{j=1}^{p} f_j(X_j) \tag{1}$$

To estimate f we can use a multivariate smoothing spline minimization problem, that is, given λ, find the minimizer $f(X_k)$ of:

$$\frac{1}{N}\sum_{k=1}^{N}(z_k - f(\mathbf{X}_k))^2 + \sum_{j=1}^{p}\lambda_j \int_0^1 [f_j''(X_j)]^2 dX_j \tag{2}$$

where a Monte Carlo sample of dimension N is assumed.

This minimization problem requires the estimation of the p hyper-parameters λ_j (also denoted as smoothing parameters): GCV, GML, etc. (see e.g. Wahba, 1990; Gu, 2002).

In the recursive approach by Ratto et al. [2007], the additive model is put into a *State-Dependent Parameter Regression* (SDR) form of Young [2001]. Consider the case of $p = 1$ and $z(X) = g(X) + e$, with $e \sim N(0, \sigma^2)$, i.e.

$$z_k = s_k + e_k,$$

where $k = 1, \ldots, N$ and s_k is the estimate of $g(X_k)$.

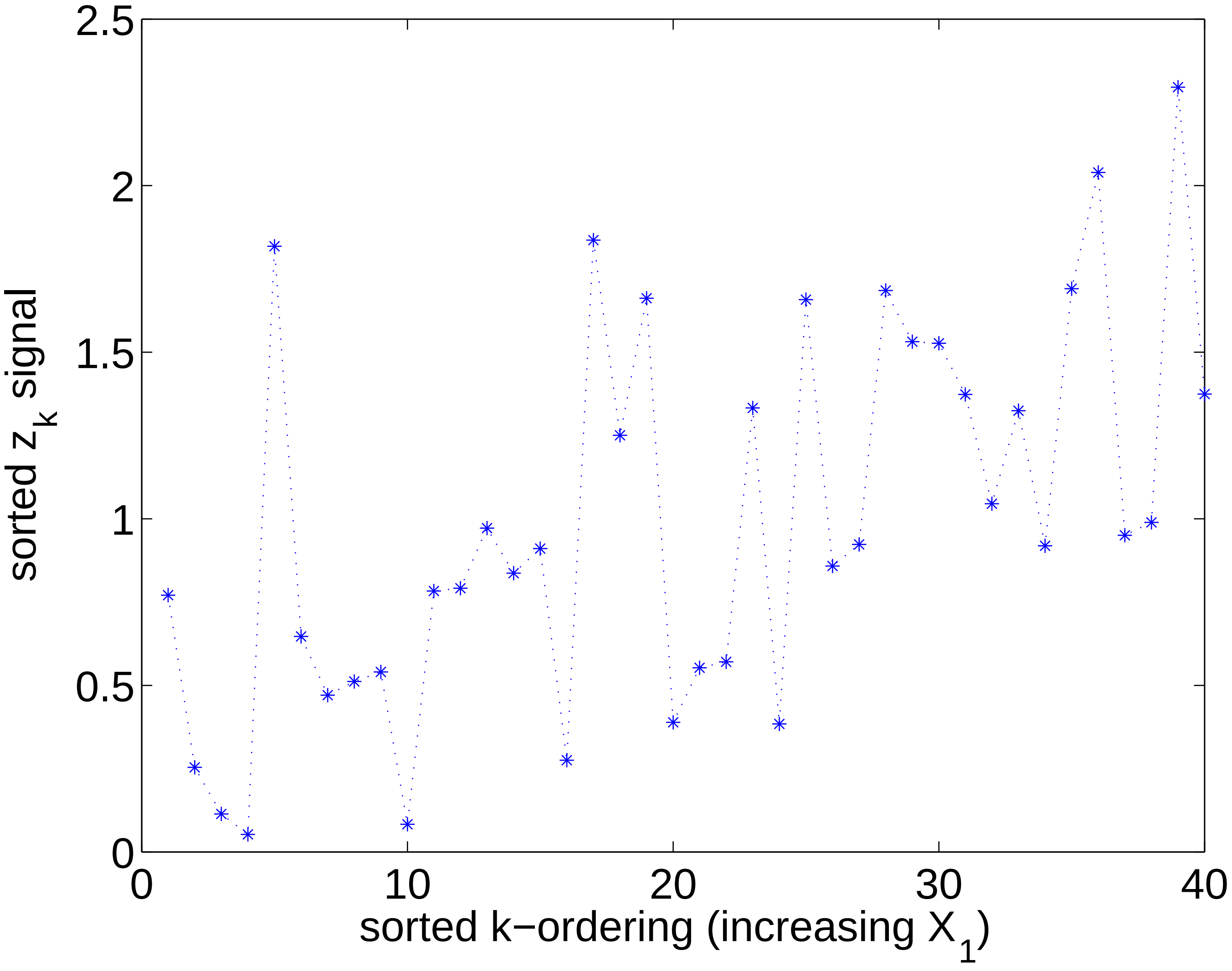
The s_k is characterized in some stochastic manner, borrowing from non-stationary time series processes and using the Generalized Random Walk (GRW) class on non-stationary random sequences [see e.g. Young and Ng, 1989, Ng and Young, 1990].

The integrated random walk (IRW) process provides the same smoothing properties of a cubic spline, in the overall State-Space (SS) formulation:

$$\begin{array}{lrcl} \text{Observation Equation:} & z_k & = & s_k + e_k \\ \text{State Equations:} & s_k & = & s_{k-1} + d_{k-1} \\ & d_k & = & d_{k-1} + \eta_k \end{array} \tag{3}$$

where d_k is the 'slope' of s_k, $\eta_k \sim N(0, \sigma_\eta^2)$ and η_k is independent of e_k.

For the recursive estimate of s_k, the MC sample has to be sorted in ascending order of X, i.e. the k and $k-1$ subscripts in (3) *denote adjacent elements under such ordering*.



2.5
2
1.5
1
0.5
0
0
10
20
30
40
sorted z_k signal
sorted k−ordering (increasing X_1)

Figure 1:

SDR procedure

1. optimize with ML (via prediction error decomposition [Schweppe, 1965]) the hyper-parameter associated with (3): NVR$= \sigma_\eta^2/\sigma^2$.

   The NVR plays the inverse role of a smoothing parameter: the smaller the NVR, the smoother the estimate of s_k.

2. Given the NVR, the FIS algorithm yields $\hat{s}_{k|N}$: the $\hat{s}_{k|N}$ from the IRW process is the equivalent of $f(X_k)$ in the cubic smoothing spline model. The recursive procedures also provide standard errors of the estimated $\hat{s}_{k|N}$.

The recursive ML optimization

In the ‘classical’ smoothing spline estimates, a ‘penalty’ is always plugged in the objective function (GCV, GML, etc.) used to optimize the λ’s, to limit the ‘degrees of freedom’ of the spline model.

In GCV we have to find λ that minimizes

$$GCV_\lambda = 1/N \cdot \frac{\sum_k (z_k - f_\lambda(X_k))^2}{(1 - df(\lambda)/N)^2}, \tag{4}$$

where $df \in [0, N]$ denotes the ‘degrees of freedom’ of the spline and where we have explicitly indicated the dependency on λ in the GCV formula.

In the recursive notation just introduced:

$$GCV_{NVR} = 1/N \cdot \frac{\sum_k (z_k - \hat{s}_{k|N})^2}{(1 - df(NVR)/N)^2}. \tag{5}$$

Without the penalty term, the optimum would always be attained at $\lambda = 0$ (or $NVR \rightarrow \infty$), i.e. perfect fit.

In SDR, however, the penalty is intrinsically plugged in by the fact that ML estimate is based on the *filtered* estimate $\hat{s}_{k|k-1} = s_{k-1} + d_{k-1}$ and not on the smoothed estimate $\hat{s}_{k|N}$, namely we find NVR that minimizes:

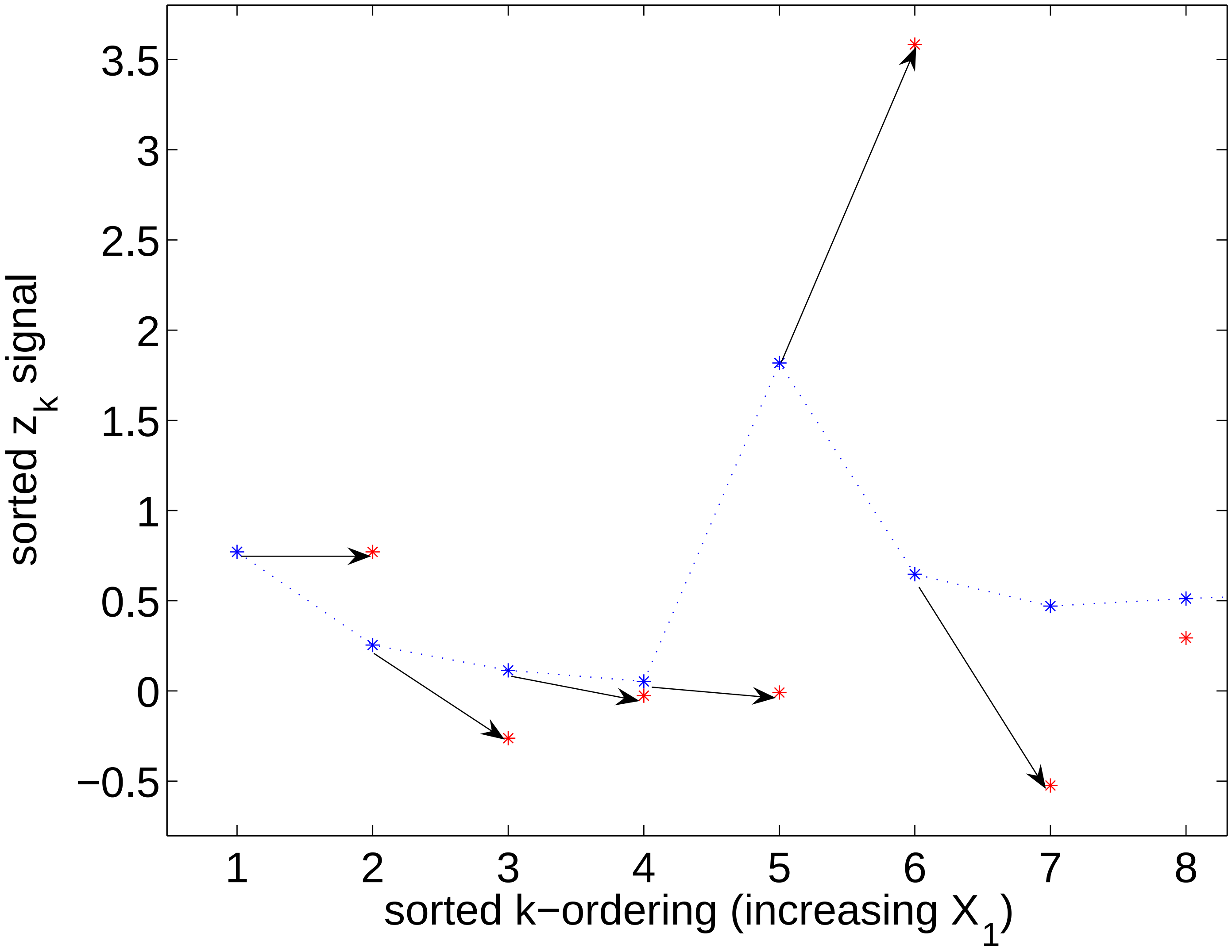
$$
\begin{aligned}
-2 \cdot \log(L) &= const + \textstyle\sum_{k=3}^{N} \log(1 + P_{k|k-1}) + (N-2) \cdot \log(\hat{\sigma^2}) \\
\hat{\sigma^2} &= \tfrac{1}{N-2} \textstyle\sum_{k=3}^{N} \tfrac{(z_k - \hat{s}_{k|k-1})^2}{(1+P_{k|k-1})}
\end{aligned}
\qquad (6)
$$

where $P_{k|k-1}$ is the one step ahead forecast error of the state $\hat{s}_{k|k-1}$ provided by the Kalman Filter.

- $\hat{s}_{k|k-1}$ is based only on the information contained in $[1, \ldots, k-1]$ while smoothed estimates use the entire information set $[1, \ldots, N]$.

- a zero variance for e_k implies $\hat{s}_{k|k-1} = s_{k-1} + d_{k-1} = z_{k-1} + d_{k-1}$, i.e. the one step ahead prediction of z_k is given by the linear extrapolation of the adjacent value z_{k-1}.

- the limit $NVR \to \infty$ $(\lambda \to 0)$ is not a 'perfect fit' situation.



2: The case of NVR→ ∞: no perfect fit for the recursive case!

Equivalence between SDR and cubic spline

To complete the equivalence between the SDR and cubic spline formulations, we need to link the NVR estimated by the ML procedure to the smoothing parameters λ.

This is easily accomplished by setting $\lambda = 1/(\mathrm{NVR} \cdot N^4)$.

In the general additive case (1), the recursive procedure just described needs to be applied, in turn, for each term $f_j(X_{j,k}) = \hat{s}_{j,k|N}$, requiring a different sorting strategy for each $\hat{s}_{j,k|N}$.

Hence the 'backfitting' procedure, as described in Young [2000, 2001], is exploited.

Finally, the estimated NVR$_j$'s can be converted into λ_j values and the additive model put into the standard cubic spline form.

State Dependent Regressions and smoothing splines: ANOVA models with interaction functions

The additive model concept (1) can be generalized to include 2-way (and higher) interaction functions via the functional ANOVA decomposition. For example, we can let

$$f(\mathbf{X}) = f_0 + \sum_{j=1}^{p} f_j(X_j) + \sum_{j<i}^{p} f_{j,i}(X_j, X_i) \tag{7}$$

In the ANOVA smoothing spline context, corresponding optimization problems with interaction functions and their solutions can be obtained conveniently with the reproducing kernel Hilbert space (RKHS) approach (see Wahba 1990). In the SDR context, an interaction function is formalized as the product of two states

$$f_{1,2}(X_1, X_2) = s_1 \cdot s_2,$$

each of them characterized by an IRW stochastic process.

Hence the estimation of a single interaction term $z(\mathbf{X}_k) = f(X_{1,k}, X_{2,k}) + e_k$ is formalized as:

$$\begin{array}{lrcl} \text{Observation Equation:} & z_k & = & s^I_{1,k} \cdot s^I_{2,k} + e_k \\ \text{State Equations: } (j = 1, 2) & s^I_{j,k} & = & s^I_{j,k-1} + d^I_{j,k-1} \\ & d^I_{j,k} & = & d^I_{j,k-1} + \eta^I_{j,k} \end{array} \tag{8}$$

where $I = 1, 2$ is a multi-index denoting the interaction term under estimation and $\eta^I_{j,k} \sim N(0, \sigma^2_{\eta^I_j})$. The two terms $s^I_{j,k}$ are estimated iteratively by running the recursive procedure in turn.

- take an initial estimate of $s^{I}_{1,k}$ and $s^{I}_{2,k}$ by regressing z with the product of simple linear or quadratic polynomials $p_1(X_1) \cdot p_2(X_2)$ and set $s^{I,0}_{j,k} = p_j(X_{j,k})$;

- iterate $i = 1, 2$:
  - fix $s^{I,i-1}_{2,k}$ and estimate NVR^{I}_{1} and $s^{I,i}_{1,k}$ using the recursive procedure;
  - fix $s^{I,i}_{1,k}$ and estimate NVR^{I}_{2} and $s^{I,i}_{2,k}$ using the recursive procedure;

- the product $s^{I,2}_{1,k} \cdot s^{I,2}_{2,k}$ obtained after the second iteration provides the recursive SDR estimate of the interaction function.

Unfortunately, in the case of interaction functions we cannot derive an explicit and full equivalence between SDR and cubic splines of the type mentioned for first order ANOVA terms. Therefore, in order to be able to exploit the estimation results in the context of a smoothing spline ANOVA model, we take a different approach, similarly to the ACOSSO case.

Very short summary of ACOSSO

Assume that $f \in \mathcal{F}$, where $\mathcal{F}$ is a RKHS. $\mathcal{F}$ can be written as an orthogonal decomposition $\mathcal{F} = \{1\} \oplus \{\bigoplus_{j=1}^{q} \mathcal{F}_j\}$, where each $\mathcal{F}_j$ is itself a RKHS and $j = 1, \ldots, q$ spans over ANOVA terms of various order. We re-formulate (2) for the general case with interactions as the function f that minimizes:

$$\frac{1}{N}\sum_{k=1}^{N}(z_k - f(\mathbf{X}_k))^2 + \lambda_0 \sum_{j=1}^{q}\frac{1}{\theta_j}\|P^j f\|_{\mathcal{F}}^2 \tag{9}$$

where the q-dimensional vector of θ_j smoothing parameters needs to be optimized somehow.

The COSSO [Lin and Zhang, 2006] penalizes the sum of norms, which allows to identify the informative predictor terms f_j with an estimate of f that minimizes

$$\frac{1}{N}\sum_{k=1}^{N}(z_k - f(\mathbf{X}_k))^2 + \lambda\sum_{j=1}^{q}\|P^j f\|_{\mathcal{F}} \tag{10}$$

using a single smoothing parameter λ. COSSO improves considerably the problem (9) with $\theta_j = 1$ and is much more computationally efficient than the full problem (9) with optimized θ_j's.

In the adaptive COSSO (ACOSSO) of Storlie et al., $f \in \mathcal{F}$ minimizes

$$\frac{1}{N}\sum_{k=1}^{N}(z_k - f(\mathbf{X}_k))^2 + \lambda \sum_{j=1}^{q} w_j \|P^j f\|_{\mathcal{F}} \tag{11}$$

where $0 < w_j \leq \infty$ are weights that depend on an initial estimate of $\tilde{f}$, either using (9) with $\theta_j = 1$ or the COSSO estimate (10). The adaptive weights are obtained as $w_j = \|P^j \tilde{f}\|_{L_2}^{-\gamma}$, with $\gamma = 2$ typically and the L_2 norm $\|P^j \tilde{f}\|_{L_2} = (\int (P^j \tilde{f}(\mathbf{X}))^2 d\mathbf{X})^{1/2}$.

Combining SDR and ACOSSO for interaction functions

Obvious way: the SDR estimates of additive and interaction function terms can be taken as the initial $\tilde{f}$ used to compute the weights in the ACOSSO.

However, the SDR identification and estimation provides a more detailed information about f_j terms that is worth exploiting.

We define $\mathcal{K}_{\langle j \rangle}$ the reproducing kernel of an additive term $\mathcal{F}_j$ of the ANOVA decomposition of the space $\mathcal{F}$.

In the cubic spline case, this is constructed as the sum of two terms

$$\mathcal{K}_{\langle j \rangle} = \mathcal{K}_{01\langle j \rangle} \oplus \mathcal{K}_{1\langle j \rangle}$$

where $\mathcal{K}_{01\langle j \rangle}$ is the r.k. of the parametric (linear) part and $\mathcal{K}_{1\langle j \rangle}$ is the r.k. of the purely non-parametric part.

The second order interaction terms are constructed as the tensor product of the first order terms, for a total of four elements, i.e.

$$\begin{aligned}
\mathcal{K}_{\langle i,j\rangle} &= (\mathcal{K}_{01\langle i\rangle} \oplus \mathcal{K}_{1\langle i\rangle}) \otimes (\mathcal{K}_{01\langle j\rangle} \oplus \mathcal{K}_{1\langle j\rangle}) \\
&= (\mathcal{K}_{01\langle i\rangle} \otimes \mathcal{K}_{01\langle j\rangle}) \oplus (\mathcal{K}_{01\langle i\rangle} \otimes \mathcal{K}_{1\langle j\rangle}) \\
&\quad \oplus (\mathcal{K}_{1\langle i\rangle} \otimes \mathcal{K}_{01\langle j\rangle}) \oplus (\mathcal{K}_{1\langle i\rangle} \otimes \mathcal{K}_{1\langle j\rangle})
\end{aligned} \tag{12}$$

In general, one should attribute a specific coefficient $\theta_{\langle\cdot\rangle}$ to each single element of the r.k. of $\mathcal{F}_j$ [see e.g. Gu, 2002, Chapter 3], i.e. two θ's for each main effect, four θ's for each two-way interaction, and so on.

In fact, each $\mathcal{F}_j$ would be optimally fitted by opportunely choosing weights in the sum of $\mathcal{K}_{\langle \cdot, \cdot \rangle}$ elements.

The SDR estimate $\hat{s}_j^I$ of the interaction (8) can be easily decomposed into the sum of a linear ($\hat{s}_{01\langle j \rangle}^I$) and non-parametric term ($\hat{s}_{1\langle j \rangle}^I$) providing:

$$\hat{s}_i^I \cdot \hat{s}_j^I = \hat{s}_{01\langle i \rangle}^I \hat{s}_{01\langle j \rangle}^I + \hat{s}_{01\langle i \rangle}^I \hat{s}_{1\langle j \rangle}^I + \hat{s}_{1\langle i \rangle}^I \hat{s}_{01\langle j \rangle}^I + \hat{s}_{1\langle i \rangle}^I \hat{s}_{1\langle j \rangle}^I, \quad (13)$$

that is a proxy of the four elements of the r.k. of the second order tensor product cubic spline.

the optimal use of the SDR identification and estimation in the ACOSSO framework is to apply specific weights to each element of the r.k. $\mathcal{K}_{\langle \cdot, \cdot \rangle}$, using the L_2 norms of each of the four elements in (13).

Examples

Storlie et al. [2008] performed an extensive analysis and comparison of meta-modelling approaches for the estimation of total sensitivity indices. Main conclusions:

- simple models like quadratic regressions and additive smoothing splines can work very well specially for small sample sizes;
- for larger sample sizes, more flexible approaches (MARS, ACOSSO, MLE GP in particular) can provide better estimation;
- GP does not outperform smoothing methods in estimating sensitivity indices.

The present paper does not modify substantially these results on sensitivity indices estimation; we concentrate here on the forecast performance (out-of-sample R^2).

We compared the combined SDR-ACOSSO approach with ACOSSO and DACE on several examples:

- we checked the behavior of SDR in identifying single 2-way interaction functions;
- we performed full emulation exercises, considering multivariate analytic functions

Note: we used Gaussian correlation function in DACE. Preliminary cross-checks with generalized exponential correlation function indicate a much better behavior (not shown here): DACE results presented here may be too 'pessimistic' and the comparison unfair.

Examples: single surface fitting

Consider surfaces $z(X_1, X_2) = g(X_1, X_2) + e$, with $e \sim N(0, \sigma)$, with signal to noise ratios $SNR = V(z)/V(e)$: very large ($SNR > 10$), middle ($SNR \sim 3$), very small ($SNR \sim 0.1$).

Compared SDR, standard GCV estimation and DACE using a training MC sample $\mathbf{X}$ of 256 elements and tested the out-of sample performance of each method in predicting the 'noise-free' signal $g(X_1, X_2)$ using a new validation sample $\mathbf{X}^*$ of dimension 256. We repeated this exercise on 100 random replicas for each function and each SNR. We considered 9 types of surfaces of increasing order of complexity (i.e. 27 different surface identification, each replicated 100 times).

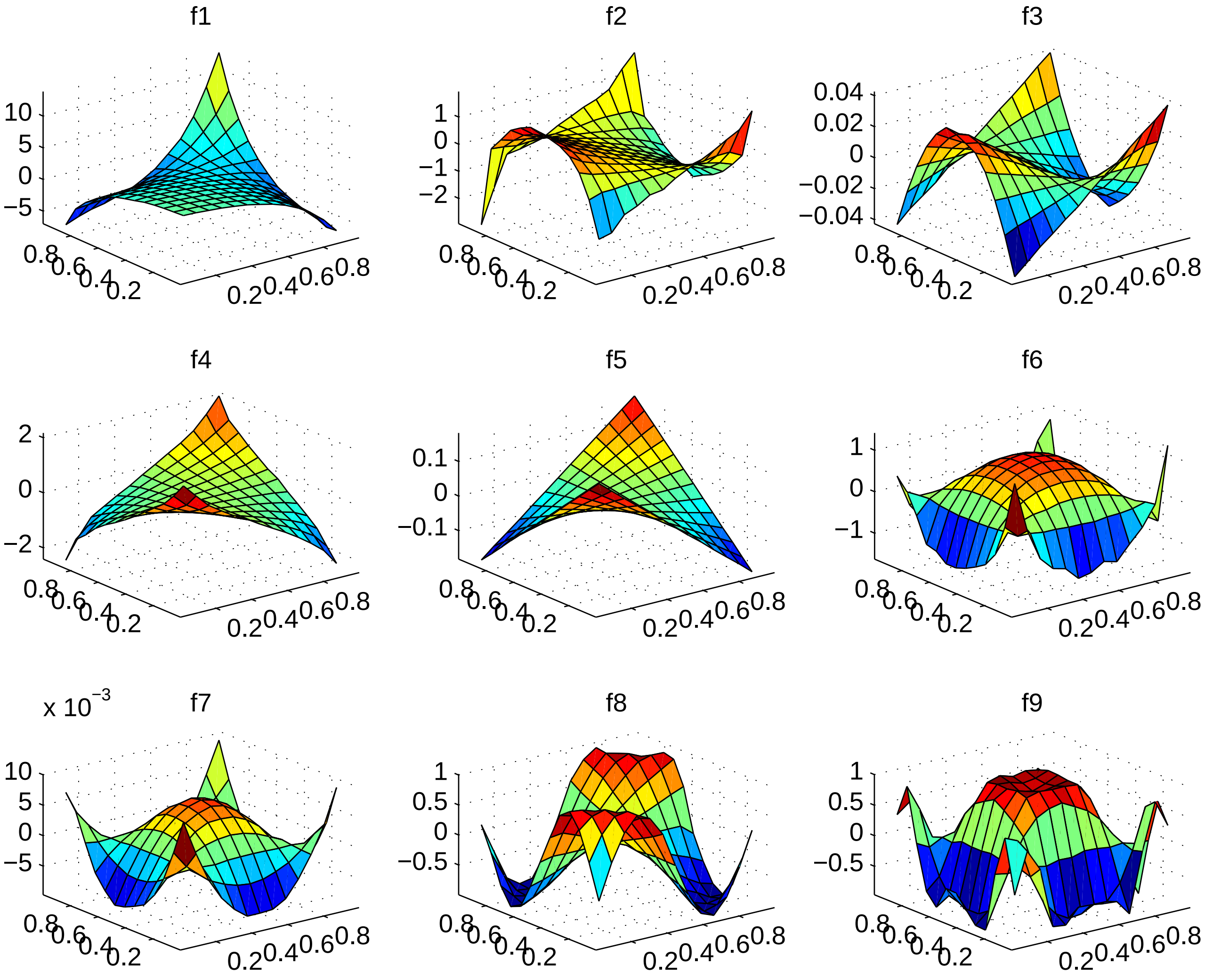


Figure 3: Shape of the surfaces considered

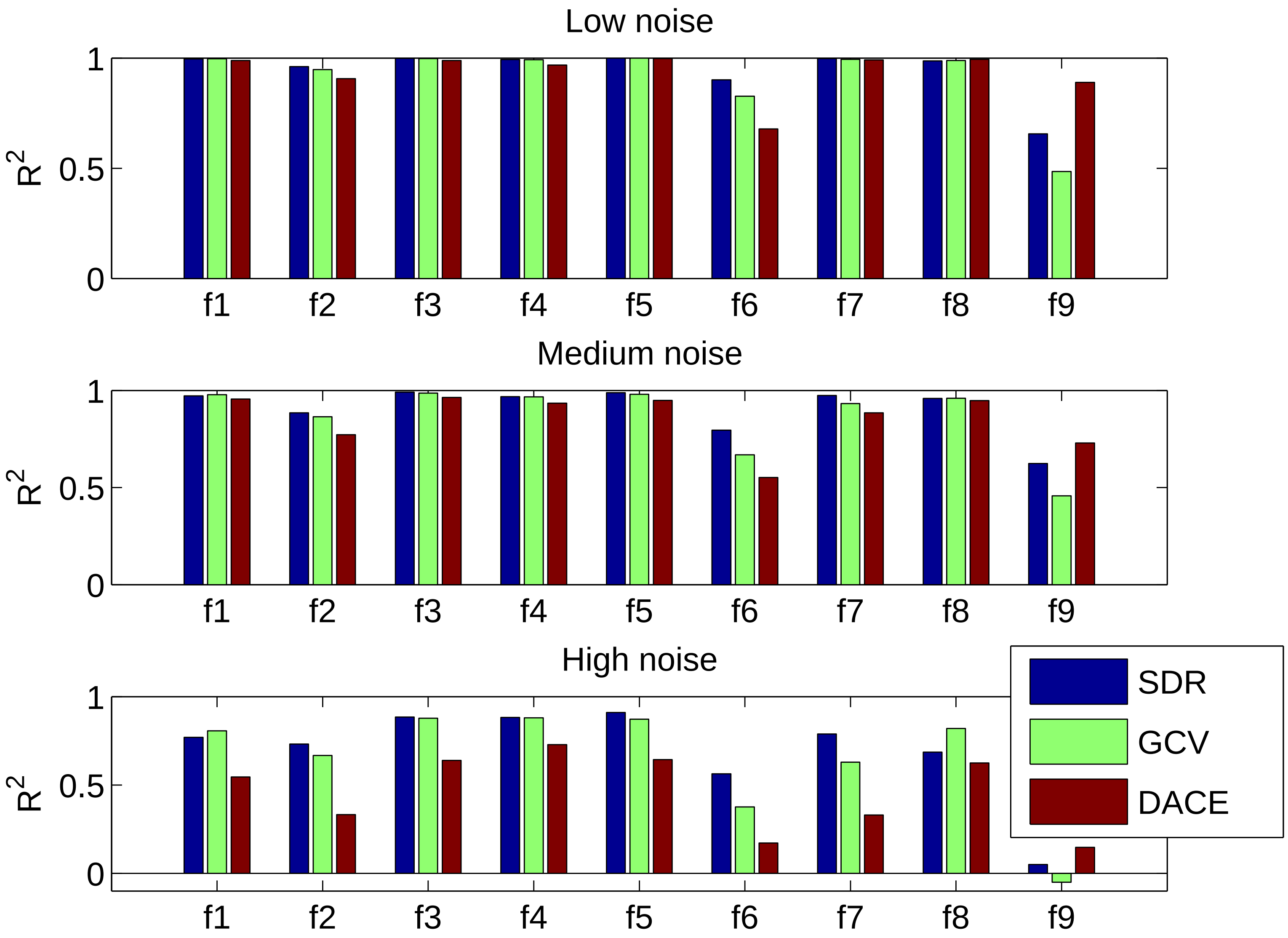


Figure 4: Out of sample R^2

Only for one out of the nine surfaces, DACE outperformed SDR or GCV estimation. In the other cases, SDR and GCV gave similar results, when the four terms in (13) have similar weights, while SDR was extremely efficient in better identifying surfaces characterized by different weights. These results suggested that SDR identification step can provide significant added value in smoothing spline ANOVA modelling.

Examples: full emulation

We considered the analytic Sobol' g-function [Saltelli et al., 2000] with different dimension p and degree of interaction (denoted as 'simple' and 'nasty' in Table 1).

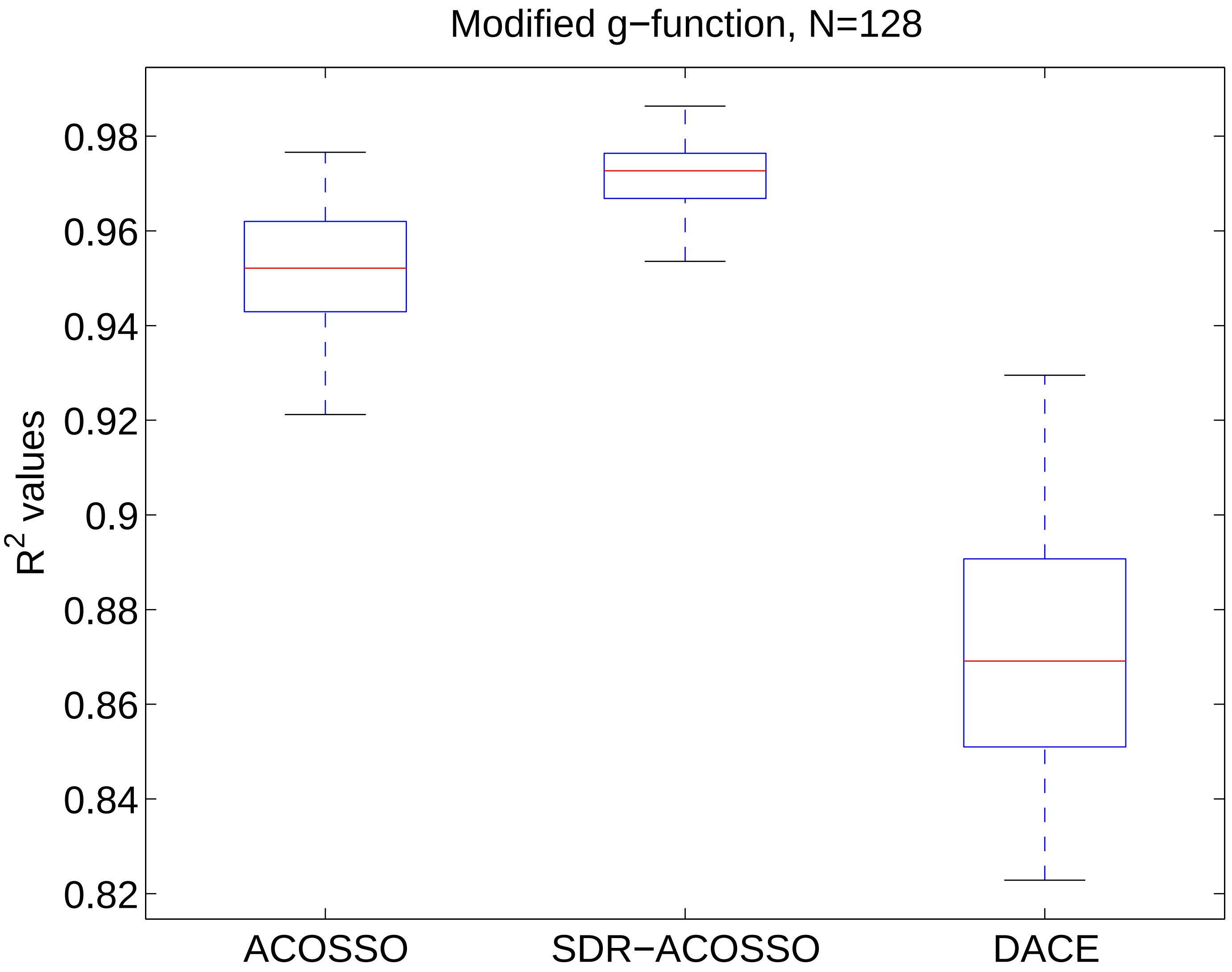
We also analyzed a modified version of the Sobol' g-function, and two test functions used in Storlie et al..

We considered a training sample of dimension 256 (or 128) to estimate the emulators and used a new validation sample of the same dimension to check the out of sample performance. We repeated the analysis 100 times for each function and each method (using LHS).

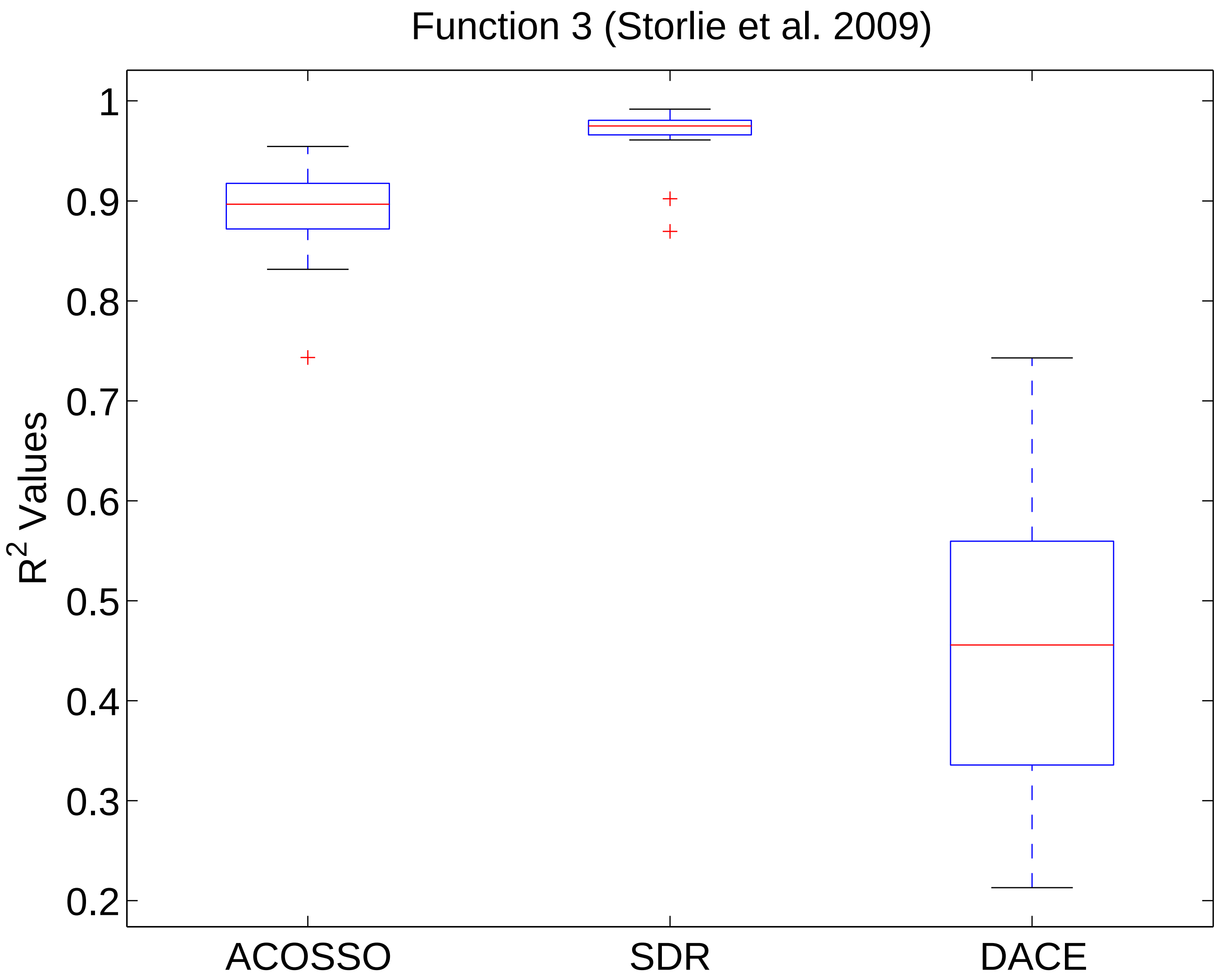
We also performed analyzes at increasing sample size, from 128 to 1024, using Sobol' quasi-Monte Carlo sequences.

$method$	$p = 4$ 'simple'	$p = 4$ 'nasty'	$p = 8$ 'simple'	$p = 10$ 'nasty'
SDR-ACOSSO	0.9994	0.8633	0.9928	0.1922
ACOSSO	0.9986	0.7910	0.9163	0.1963
DACE	0.9932	0.8174	0.9715	-0.0247

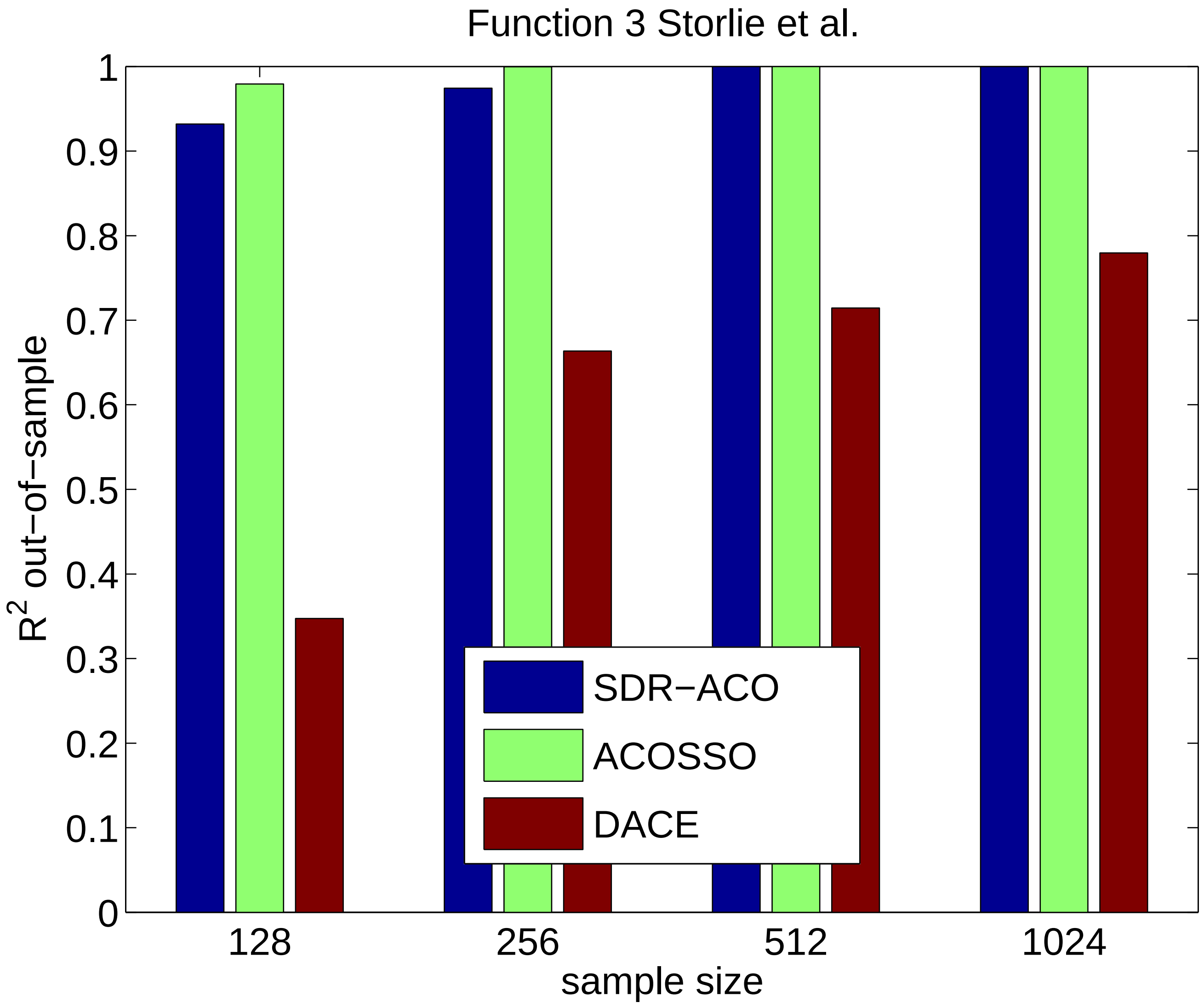
Table 1: SDR-ACOSSO, ACOSSO and DACE: average R^2 (out of sample) computed on 100 replicas for different types of the Sobol' g-function.



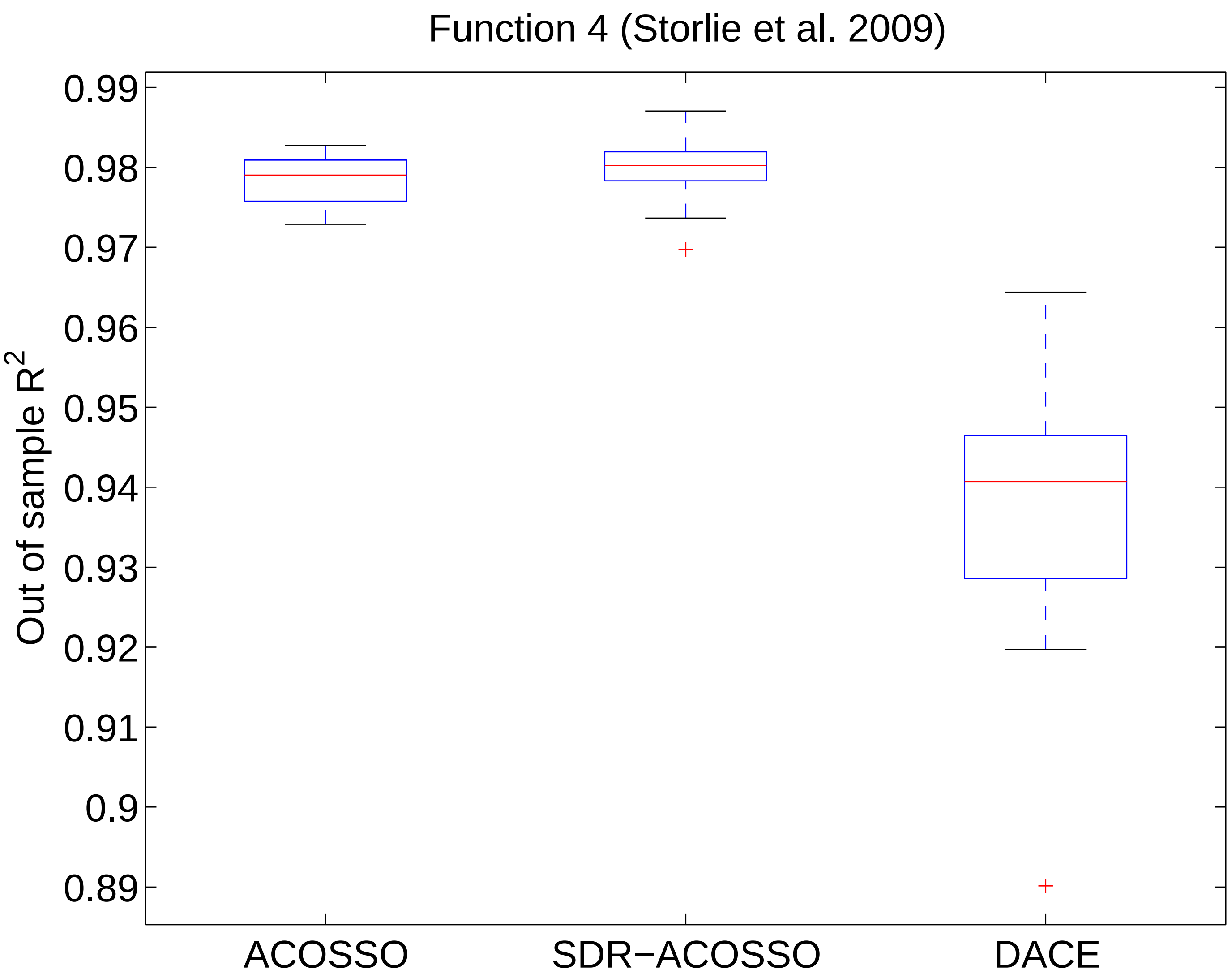
5: Out of sample R^2 for the modified g-function. N=128.



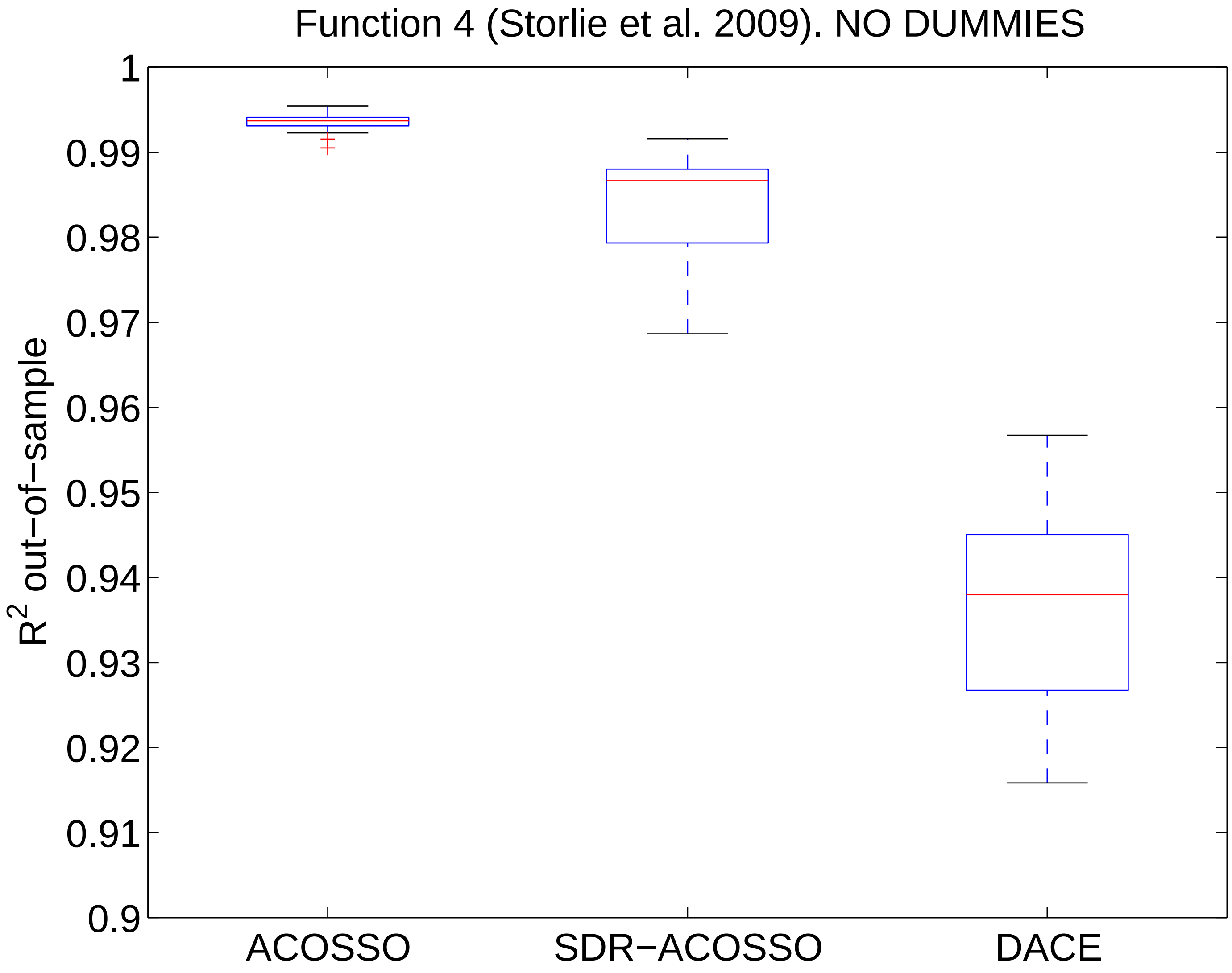
: Out of sample R^2 for the additive Example 3 in Storlie et al. N=128.



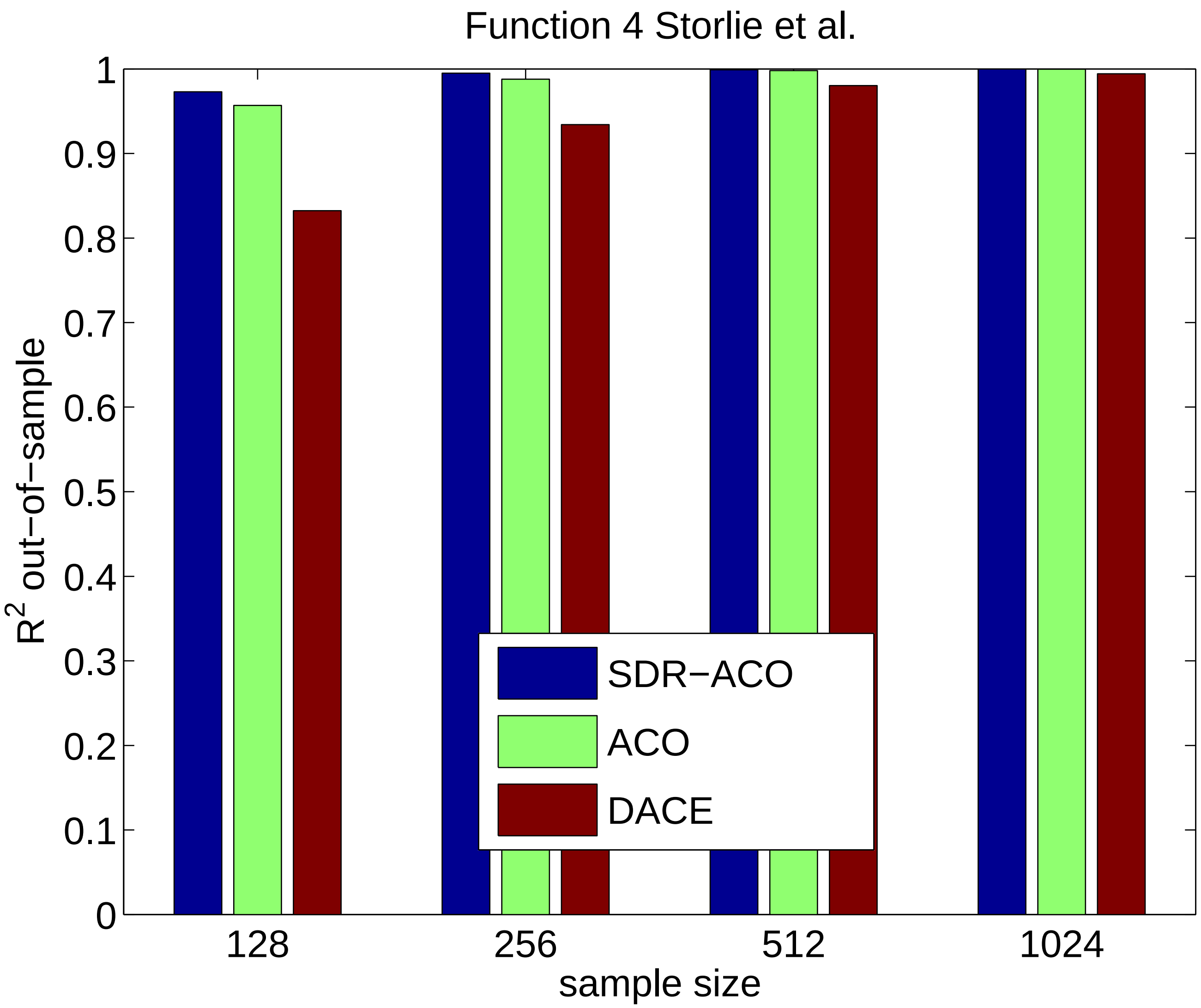
: Out of sample R^2 for the additive Example 3 in Storlie et al. Quasi-MC.



: Out of sample R^2 for the non-additive Example 4 in Storlie et al. N=256.



: Out of sample R^2 for the non-additive Example 4 in Storlie et al. N=256.



10: Out of sample R^2 for the non-additive Example 4 in Storlie et al.. Quasi-MC.

Conclusions: out-of-sample performance

- SDR is extremely rapid, efficient and accurate in identifying *additive models*: recursive algorithms avoid the inversion of large matrices needed in the other methods (ACOSSO, DACE).

- In ANOVA models with interactions, ACOSSO confirms its good performances (efficiency and relatively low computational cost). SDR-ACOSSO improves ACOSSO in many cases, although at the price of a significantly higher computational cost.

- for additive models the advantage of SDR is in both low computational cost and of accuracy,

- when interactions are included the greater accuracy of SDR-ACOSSO has a cost. SDR-ACOSSO and ACOSSO also compare very favorably with respect to DACE in many cases, even if there are cases where DACE outperforms SDR-ACOSSO in out-of-sample prediction.

- Further comparisons using generalized exponential correlation function in DACE are in progress: first results indicate a better performance of DACE w.r.t. present results; still ACOSSO / SDR-ACOSSO appear competitive.

Conclusions: computational burden

- SDR (for additive models) and ACOSSO (for models with interactions) are advisable choices for a *rapid and reliable* emulation exercise (when simpler QREG methods fail).

- Should ACOSSO be unable to explain a large part of the mapping, SDR-ACOSSO or DACE should be taken into consideration.

- DACE is not necessarily the best choice when the model is supposed to be very complex and with significant interactions: the interpolation constraint may imply spurious identification of interaction terms involving unimportant X's;

- SDR-ACOSSO can provide detailed information about the form of each additive and interaction term of a truncated the ANOVA decomposition, often allowing very good out-of-sample predictions.

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