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OPTIMAL DESIGNS FOR NONPARAMETRIC ESTIMATION OF ZEROS OF REGRESSION FUNCTIONS

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ABSTRACT. We investigate nonparametric estimators of zeros of a regression function and its derivatives and we derive the distribution of design points minimizing the expected width of a confidence interval and the expected variance of the proposed estimator.

The main goal of this contribution is to derive the optimal distribution of design points for a nonparametric regression estimator of the so-called *zero of a regression function*, i.e., the location in which the unknown regression function intersects the horizontal axis.

A survey of literature concerning optimal design for nonparametric regression models may be found in [20]. The immediately following discussion [7] suggests that there seem to exist two different general approaches. One approach uses the classical optimal design theory in order to find a finite set of support points with associated weights minimizing, e.g., the sum of variances of the nonparametric regression estimator in some pre-defined points [5], [12]. The other approach uses calculus of variations in order to find designs minimizing *Asymptotic Integrated Mean Squared Error* (AIMSE) of the nonparametric regression estimator [3], [4], [10]. Similar ideas underlie also the derivation of minimax and maximin designs, i.e., designs minimizing the maximum of AIMSE or designs maximizing the minimum power of a test over a class of alternatives [1], [2]; cf. also [21].

In contrast to the previously proposed optimal designs [1]–[5], [10], [12], we aim to find the design minimizing the variability of the *empirical zero*, i.e., the location at which the nonparametric regression estimator intersects the horizontal axis, instead of minimizing the variability of the nonparametric regression estimator itself. Similarly as in [10], the optimal design is obtained by applying standard calculus of variations. The main advantage of our approach is that prior

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information may be used very naturally. In Section 2, we obtain similar designs as [10] but the interpretation of our result seems to be more straightforward.

A similar approach to optimal design has been previously used in [8] for nonparametric estimator of the location of maximum with constant bandwidth. In this paper, we concentrate on the empirical zero of an arbitrary derivative of the regression function and we derive the optimal distribution of design points also for local (adaptive) bandwidths.

Introduction. We consider a fixed-design nonparametric regression model, i.e.,

$$Y_i = m(x_i) + \varepsilon_i \qquad \text{for} \quad i = 1, \dots, n, \tag{1}$$

where Y_i's are observations of a response variable, $0 \leq x_1 < \cdots < x_n \leq 1$ are fixed values of the explanatory variable defined by a probability density function $f_X(.)$ (i.e., $\int_{x_{i-1}}^{x_i} f_X(u)\,du \doteq 1/n$), and ε_i's are iid centered random errors. In Sections 1 and 2, we will consider also heteroscedastic random errors.

We are mainly interested in estimation of the *zero* of $m(.)$, i.e., the x-coordinate of the point in which the unknown regression function $m(.)$ intersects the horizontal axis. The zero is sometimes also called a *root* of the equation $m(.) = 0$. We also investigate estimators of zeros of derivatives of $m(.)$. The symbol ξ_ν denotes the zero of $m^{(\nu)}(.)$, the νth derivative of $m(.)$.

In Section 1, we start by investigating the asymptotic distribution of the empirical zero, i.e., the value at which the nonparametric regression estimator $\hat{m}^{(\nu)}(.)$ meets the horizontal axis. In Section 2, we obtain the distribution of design points minimizing some measures of variability of the empirical zero. Finally, a short simulation study is contained in Section 3.

Gasser-Müller estimator. Assuming that we observe n pairs of observations (Y_i, x_i), $i = 1, \dots, n$, from the nonparametric regression model (1), the Gasser-Müller (GM) estimator [6] of $m^{(\nu)}(.)$ is defined as

$$\hat{m}_{n,b_n,\nu}(x) = \frac{1}{b_n^{\nu+1}} \sum_{i=1}^{n} \int_{s_{i-1}}^{s_i} K_\nu\left(\frac{x-u}{b_n}\right) du Y_i, \tag{2}$$

where $s_{i-1} = \frac{1}{2}(x_i + x_{i-1})$, b_n is the bandwidth, and $K_\nu(.)$ is a kernel function of order (ν, k) [6], i.e., the support of the Lipschitz continuous function $K_\nu(.)$ is the interval $\langle -1, 1\rangle$ and

$$\int_{-1}^{1} K_\nu(x) x^j\,dx = \begin{cases} (-1)^\nu \nu! & \text{for } j = \nu, \\ 0, & 0 \leq j < k,\ j \neq \nu, \\ (-1)^k k! B_{k,k} & \text{for } j = k. \end{cases} \tag{3}$$

In the following, we fix the parameters ν and k and a kernel function $K_\nu(.)$ of order (ν, k).

Assumption. The following assumptions are used in Section 1 in order to derive the asymptotic distribution of the nonparametric estimator of ξ_ν, i.e., the zero of $m^{(\nu)}(.)$, the νth derivative of the unknown regression function $m(.)$

(A1) The function $m^{(k)}(.)$ is Lipschitz continuous.

(A2) The Lipschitz continuous kernel function $K_\nu(.)$ with support $\langle -1, 1\rangle$ is of order (ν, k), where $\nu \geq 0$, $k > \nu + 1$ and the difference $k - \nu$ is even.

(A3) The bandwidth $b_n \to 0$, $nb_n^2 \to \infty$, $nb_n^{2\nu+1} \to \infty$ as $n \to \infty$.

(A4) The density of design points, $f_X(x) > \delta_f > 0$, is Lipschitz (γ_f)-continuous with $0 < \gamma_f \leq 1$, i.e., $|f_X(u) - f_X(v)| \leq L_f |u - v|^{\gamma_f}$ for all u and $v \in \langle 0, 1\rangle$ and for some $L_f > 0$.

(A5) The random errors ε_i are iid and $E|\varepsilon_i|^r < \infty$ for some $r > 2$. Denoting $\varepsilon_i = \varepsilon_n(x_i)$, where $\varepsilon_n(x)$ is defined for all $x \in \langle 0, 1\rangle$, we assume that $E\varepsilon_n(x) = 0$ and $\mathrm{Var}\{\varepsilon_n(x)\} = \sigma^2(x)$, where the function $\sigma^2(.)$ is Lipschitz continuous and there exist $0 < \delta_\sigma$ and $D_\sigma < +\infty$ such that $\delta_\sigma < \sigma^2(x) < D_\sigma$ for all $x \in \langle 0, 1\rangle$.

Assuming independent and identically distributed (iid) random errors, the rate of uniform strong consistency and asymptotic normality of GM estimator is derived in [6], [9], [11]. The uniform strong consistency and asymptotic normality of nonparametric regression estimators under various mixing assumptions is investigated in [16], [18].

For simplicity, we discuss only iid random errors although the asymptotic results in Sections 1 and 2 are valid also for strongly mixing random errors: the asymptotic normality of GM estimator may be established by using a Central Limit Theorem for nonstationary weakly dependent triangular arrays of random variables [14] and the uniform strong consistency rate, needed for establishing the asymptotic normality of empirical zero, may be derived by applying a Hoeffding type exponential inequality for strongly mixing sequences [17] and by proceeding similarly as in [9], [11].

Assuming iid random errors, the asymptotic distribution of empirical zero is described in the following Section 1.

1. Asymptotic distribution of empirical zero

The symbol $\hat{\xi}_{n,b_n,\nu}$ denotes the *empirical zero* of $m_{n,b_n,\nu}(.)$, i.e., a solution of the equation $\hat{m}_{n,b_n,\nu}(\hat{\xi}_{n,b_n,\nu}) = 0$. The empirical zero is a natural estimator of the zero ξ_ν.

In order to establish the asymptotic distribution of $\hat{\xi}_{n,b_n,\nu}$, we use an additional assumption concerning the geometry of the function $m(.)$ close to ξ_ν:

(A6) The zero ξ_ν is unique. There exist a, b, $c > 0$, and $\tau \geq 1$ such that $0 < a < \xi_\nu < b < 1$, $m^{(\nu)}(.)$ is strictly monotonous on $\langle a, b \rangle$ and $|m^{(\nu)}(t)| \geq c|t - \xi_\nu|^\tau$ for $t \in \langle a, b \rangle$.

Proposition 1. *Assume that assumptions (A1)–(A6) hold,* $nb_n^{2\nu+3}/\log n \to \infty$*, the kernel* $K_\nu(.)$ *is differentiable,* $K_\nu(-1) = K_\nu(1) = 0$*, the derivative* $K'_\nu(.)$ *is Lipschitz continuous, the regression function* $m(.)$ *is* $(k+1)$*-times continuously differentiable, and* $m^{(\nu+1)}(\xi_\nu) \neq 0$*. If* $n^{1/2} b_n^{k+1/2} \to d \geq 0$*, then*

$$\left(nb_n^{2\nu+1}\right)^{1/2} \left(\hat{\xi}_{n,b_n,\nu} - \xi_\nu\right) \xrightarrow{\mathcal{D}} N\!\left(-\frac{dB_{k,k} m^{(k)}(\xi_\nu)}{m^{(\nu+1)}(\xi_\nu)}, \frac{\sigma^2(\xi_\nu)}{f_X(\xi_\nu)} \frac{V}{\{m^{(\nu+1)}(\xi_\nu)\}^2} \right). \tag{4}$$

P r o o f. The proof is a modification of the proof of Theorem 3.1 in [11]. $\square$

1.1. Constant bandwidth

Looking at the mean and the variance of the asymptotic distribution of the empirical zero given in Proposition 1 and replacing d^2 by nb_n^{2k+1}, it is easy to express the *Mean Squared Error* (MSE)

$$\begin{aligned} \mathrm{MSE}(\hat{\xi}_{n,b_n,\nu}) = {} & b_n^{2k-2\nu} \left(\frac{B_{k,k} m^{(k)}(\xi_\nu)}{m^{(\nu+1)}(\xi_\nu)} \right)^2 \\ & + \frac{1}{nb_n^{2\nu+1}} \frac{\sigma^2(\xi_\nu)}{f_X(\xi_\nu)} \frac{V}{\{m^{(\nu+1)}(\xi_\nu)\}^2}. \end{aligned}$$

Assuming that the bias term is not equal to zero, i.e., assuming that the kth derivative of the regression function $m^{(k)}(\xi_\nu) \neq 0$, we may calculate the bandwidth that minimizes the MSE

$$\begin{aligned} b_{0,n} &= n^{-1/(2k+1)} \left[\frac{2\nu+1}{2k-2\nu} \frac{\sigma^2(\xi_\nu) V}{f_X(\xi_\nu) \{B_{k,k} m^{(k)}(\xi_\nu)\}^2} \right]^{1/(2k+1)} \\ &= O\!\left(n^{-1/(2k+1)}\right). \end{aligned} \tag{5}$$

1.2. Local bandwidth

The precision of measurements sometimes depends on location and, in some situations, we may assume that $\sigma^2(x_i) = \sigma^2 w(x_i)$, where $w(.) > 0$ is a known function and $\sigma^2 > 0$ is an unknown constant. Apart of the variance function $w(.)$, the bandwidth may depend also on the known density of design points. From (5), we obtain that the asymptotically optimal *local bandwidth* satisfies

$$b_{0,n,f,w}(x) \propto \left(\frac{w(x)}{nf_X(x)} \right)^{1/(2k+1)}. \tag{6}$$

For homoscedastic random errors, the local bandwidth is defined by (6) with $w(.) \equiv 1$.

2. Optimal designs

In the nonparametric regression setup, the problem of finding the optimal distribution of design points has been previously addressed in [10] from the point of view of the *Integrated Mean Squared Error* (IMSE) of the GM kernel regression estimator $\hat{m}(x)$. Choosing a probability measure H with a positive and continuous density $h(.)$ on $\langle 0,1\rangle$ and considering

$$\text{IMSE} = E\int\big\{\hat{m}(x)-m(x)\big\}^2 dH(x) \approx \frac{1}{nb_n}\int K^2(s)\,ds\int\frac{h(x)}{f_X(x)}\,dx,$$

the *Asymptotic IMSE* (AIMSE) optimal density of design points, with constant bandwidth and homoscedastic random errors, is

$$f_X^*(x) = h(x)^{1/2}\Big/\int h(u)^{1/2}\,du \propto h(x)^{1/2}, \tag{7}$$

see [10] for more details.

Unfortunately, the probability measure H lacks any clear interpretation and, therefore, the AIMSE optimal design is not easily applicable in practice. In this contribution, similarly as in [8], we overcome this obstacle by obtaining designs minimizing the variability of the empirical zero.

Let the symbol A denote a probability measure describing the prior distribution of the zero and let us assume that A has a positive and continuous density $a(.)$ such that:

(A7) There exists $\delta > 0$ such that $a(x) > \delta$ for all $x \in \langle 0,1\rangle$.

The distribution of design points minimizing our (subjective) prior expectation of variability of empirical zero based on the nonparametric regression estimator with constant bandwidth (5) is derived in Proposition 2.

Proposition 2. *Assume that the assumptions of Proposition 1 and (A7) hold, $\sigma^2(.) = \sigma^2 w(.)$, where $w(.)$ is a known function and $0<\sigma^2<\infty$, $m^{(\nu+1)}(\xi_\nu) = m_1$ does not depend on the value of ξ_ν, and that the constand bandwidth $b_{0,n}(.)$ is given by (5).*

1. *Assuming that the product $w(.)a(.)$ satisfies assumption (A4), the density of design points $f_{V,w}(x) \propto \big\{w(x)a(x)\big\}^{1/2}$ minimizes the expectation of the asymptotic variance of the empirical zero, i.e., $\int \mathrm{Var}\big(\hat{\xi}_{n,b_n,\nu}|\xi_\nu = u\big) \times a(u)\,du$, with respect to the prior density $a(.)$.*
2. *Assuming that $\{w(.)\}^{2/3}\{a(.)\}^{4/3}$ satisfies assumption (A4), the density of design points $f_{L,w}(x) \propto \{w(x)\}^{1/3}\{a(x)\}^{2/3}$ minimizes the expected length of confidence intervals with respect to the prior density $a(.)$.*

Proof. The proof is analogous to the proof of Theorem 2 in [8]. □

Proposition 2 suggests that, using constant bandwidth, the density of design points minimizing the variability of the empirical zero is the same as the density of design points minimizing the variability of the empirical location of maximum; cf. [8, Theorem 2].

The main result is the following Theorem 1 where we derive the optimal distribution of design points for the empirical zero based on nonparametric regression estimator using local bandwidth.

Theorem 1. *Assume that the assumptions of Proposition 1 and (A7) hold,* $\sigma^2(x)=\sigma^2 w(x)$, *where* $w(x)$ *is a known function and* $0<\sigma^2<\infty$, $m^{(\nu+1)}(\xi_\nu)=m_1$ *does not depend on the value of the true zero* ξ_ν, *and that the local bandwidth* $b_{0,n,f,w}(.)$ *is given by* (6).

(1) *Assuming that the product* $\big\{w(x)\big\}^{(4k-4\nu)/(4k-2\nu+1)}\big\{a(x)\big\}^{(4k+2)/(4k-2\nu+1)}$ *satisfies (A4), the density of design points*

$$f_{V,w,l}(x) \propto \big\{w(x)\big\}^{(2k-2\nu)/(4k-2\nu+1)}\big\{a(x)\big\}^{(2k+1)/(4k-2\nu+1)}$$

minimizes the expectation of the asymptotic variance of the empirical zero,

$$\int \operatorname{Var}\left(\hat{\xi}_{n,b_n,\nu}|\xi_\nu = u\right) a(u)\, du,$$

with respect to the prior density $a(.)$.

(2) *Assuming that* $\big\{w(x)\big\}^{(4k-4\nu)/(3k-\nu+1)}\big\{a(x)\big\}^{(4k+2)/(3k-\nu+1)}$ *satisfies assumption (A4), the density of design points*

$$f_{L,w,l}(x) \propto \big\{w(x)\big\}^{(k-\nu)/(3k-\nu+1)}\big\{a(x)\big\}^{(2k+1)/(3k-\nu+1)}$$

minimizes the expected length of confidence intervals for the true zero with respect to the prior density $a(.)$.

Proof. We prove only part (1) because the proof of part (2) is very similar. Plugging the local bandwidth $b_{0,n,f,w}(.)$ into the asymptotic variance of the estimator provided by Proposition 1, we obtain that

$$\operatorname{Var}(\hat{\xi}_{n,b_n,\nu}) \propto \left\{\frac{w(\xi_\nu)}{f_X(\xi_\nu)}\right\}^{(2k-2\nu)/(2k+1)}$$

leading the minimization problem

$$\begin{aligned} f_{V,w,l} &= \arg\min_{f_X} \int_0^1 \operatorname{Var}\left(\hat{\xi}_{n,b_{0,n,f,w}(x),\nu}|\xi_\nu = x\right) a(x\,)\, dx \\ &= \arg\min_{f_X} \int_0^1 \big\{f_X(x)\big\}^{-(2k-2\nu)/(2k+1)}\big\{w(x)\big\}^{(2k-2\nu)/(2k+1)} a(x)\, dx \end{aligned}$$

that belongs to standard calculus of variations. Denoting

$$\begin{aligned} F(x,y,y') &= F(x,F_X,f_x) \\ &= \big\{f_X(x)\big\}^{-(2k-2\nu)/(2k+1)}\big\{w(x)\big\}^{(2k-2\nu)/(2k+1)}a(x), \end{aligned}$$

the necessary condition for an extreme of

$$I(f_X) = I(y') = \int_0^1 F(x,y,y')\,dx$$

is

$$F'_y - \frac{\mathrm{d}}{\mathrm{d}x}F'_{y'} = 0,$$

see, e.g., [13], [19]. In our setup, $F'_y = 0$ and

$$F'_{y'}(x) \propto -f_X^{-(4k-2\nu+1)/(2k+1)}(x)\big\{w(x)\big\}^{(2k-2\nu)/(2k+1)}a(x)$$

and the optimal density of design points $f_{V,w,l}(.)$ thus has to satisfy

$$\big\{f_{V,w,l}(x)\big\}^{-(4k-2\nu+1)/(2k+1)}\big\{w(x)\big\}^{(2k-2\nu)/(2k+1)}a(x) = \text{constant}.$$

The proof may now be finished similarly as the proof of Theorem 2 in [8]. $\square$

In Table 1, we summarize the powers of the prior density defining optimal nonparametric regression designs concerning the regression function and its first two derivatives in a homoscedastic situation (i.e., $w(.) \equiv 1$) with $k = \nu + 2$.

TABLE 1. Powers of the prior density defining the optimal experiment design for estimators of zeros of the regression function and its first and second derivative for homoscedastic random errors.

	Constant bandwidth			Local bandwidth		
	$m(.)$	$m'(.)$	$m^{(2)}(.)$	$m(.)$	$m'(.)$	$m^{(2)}(.)$
$r_{\text{opt}}(\text{MSE})$	1/2	1/2	1/2	$5/9 \doteq 0.56$	$7/11 \doteq 0.63$	$9/13 \doteq 0.69$
$r_{\text{opt}}(\text{MAD})$	2/3	2/3	2/3	$5/7 \doteq 0.71$	$7/9 \doteq 0.78$	$9/11 \doteq 0.82$

We have already remarked that, using constant bandwidth, exactly the same designs are obtained in [8] for the location of maximum. Using local bandwidth, it can be shown that the optimal design for the location of maximum of $m^{(\nu)}(.)$ is also optimal for estimation of the zero of the $(\nu+1)$th derivative $m^{(\nu+1)}(.)$.

Comparing our results with the AIMSE optimal design (7), we note that MSE optimal design for the empirical zero is also AIMSE optimal with $h(.)$ replaced by the prior density $a(.)$; cf. [10].

3. Simulations

The simulation study was implemented in the statistical computing environment R [15]. All simulation results are based on GM estimator using the quartic kernel ($\nu = 0$, $k = 2$) and 1000 simulations.

Notice that bandwidths (5) and (6) are asymptotically optimal for estimation of zeros of a regression function ($\nu = 0$) if $m^{(2)}(\xi_0) \neq 0$. For example, if $m(.)$ is a linear function, more precise estimators of ξ_0 could be obtained by over--smoothing, see also [8] for a similar observation concerning estimators of the location of maximum of a symmetric unimodal regression function.

In order to guarantee that

$$m^{(2)}(\xi_0) \neq 0,$$

we use the nonlinear regression function

$$m(x) = \big\{(x + 0.05)^2 - (\xi_0 + 0.05)^2\big\}(x + 0.05)^{-1}.$$

Notice also that the first derivative $m^{(1)}(\xi_0)$ does not depend on ξ_0. For simplicity, we assume homoscedasticity ($w(.) \equiv 1$) and write the local bandwidth (6) as

$$b_{0,n,f,w}(x) = b\big\{f_X(x)\big\}^{-1/(2k+1)}$$

so that b remains the only bandwidth parameter used in the remaining part of this section.

Similarly as in [8], the prior distribution of the zero, $a_S(.)$, is a mixture of Uniform, $U(0, 1)$, and Normal distribution, $N\big(\mu_\xi, \sigma_\xi^2\big)$, restricted to $\langle 0, 1\rangle$, i.e.,

$$a_S(\xi) \propto (1 - p)\phi_{\mu_\xi,\sigma_\xi^2}\big(\xi|\xi \in \langle 0, 1\rangle\big) + p,$$

where $\phi\big(.|\langle 0, 1\rangle\big)$ denotes the density of a $N\big(\mu_\xi, \sigma_\xi^2\big)$ distribution restricted to the interval $\langle 0, 1\rangle$. In this simulation, we set $\mu_\xi = 0.4$, $\sigma_\xi = 0.1$, and $p = 0.1$.

The density of design points is controlled by a parameter r such that for fixed value of r, the density of design points, $f_{X,r}(.)$, is proportional to $a_S^r(.)$, i.e.,

$$f_{X,r}(x) \propto a_S^r(x).$$

The value $r = 0$ leads uniformly distributed design points

$$f_{X,0}(x) = I\big(x \in \langle 0, 1\rangle\big),$$

the value $r = 1$ means that the density of design points is equal to the prior density of the zero

$$f_{X,1}(x) = a_S(x).$$

In general, higher values of the parameter r mean that design points are more concentrated in the neighborhood of the mode of the prior density $a_S(.)$.

We choose somewhat higher number of observations, $n = 800$, because all theoretical results are asymptotic. We assume homoscedasticity and set $\sigma = 0.5$.

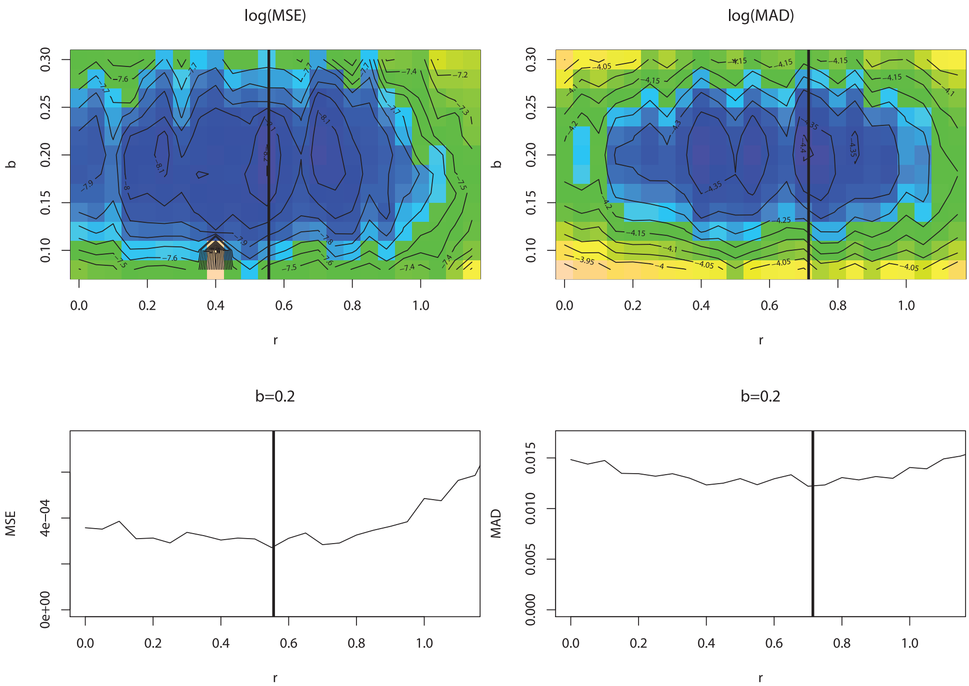

FIGURE 1. Simulations for local bandwidth: $n = 800$, $\sigma = 0.5$, thick vertical lines denote the MSE optimal value $r_{\text{opt}}(\text{MSE}) = 5/9 \doteq 0.56$ and the MAD optimal value $r_{\text{opt}}(\text{MAD}) = 7/9 \doteq 0.71$.

Logarithms of simulated MSE and MAD of the empirical zero on a grid for the bandwidth parameter b and the design density parameter r are plotted in contour- and heatplots in the upper part of Figure 1: the optimal bandwidth parameter seems to be $b = 0.2$ and, for this bandwidth, the simulation agrees very well with the theoretically optimal values.

The improvement of using the optimal distribution of design points is displayed in the lower part of Figure 1 only for $b = 0.2$. Both MSE and MAD do not change much for the parameter $r \in (0.4, 0.8)$ and even the uniformly distributed design points, i.e., $r = 0$, do not perform much worse than the optimal design.

Similarly as in [8], we may conclude by saying that the choice of appropriate bandwidth is much more important than the distribution of the design points. From practical point of view, it looks that uniformly distributed design points are not much worse than the asymptotically optimal design.

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