

VARIANCE ESTIMATION FOR HIGH-DIMENSIONAL REGRESSION MODELS

SPOKOINY, V.

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ABSTRACT. The paper is concerned with the problem of variance estimation for a high-dimensional regression model. The results show that the accuracy $n^{-1/2}$ of variance estimation can be achieved only under some restrictions on smoothness properties of the regression function and on the dimensionality of the model. In particular, for a two times differentiable regression function, the rate $n^{-1/2}$ is achievable only for dimensionality smaller or equal to 8. For higher dimensional model, the optimal accuracy is $n^{-4/d}$ which is worse than $n^{-1/2}$. The rate optimal estimating procedure is presented.

1. Introduction

In this paper, we consider the problem of variance estimation for the regression model

$$Y_i = f(X_i) + \varepsilon_i \quad (1.1)$$

where X_1, \dots, X_n are deterministic design points in the Euclidean space \mathbb{R}^d , $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is an unknown regression function and $\varepsilon_1, \dots, \varepsilon_n$ are individual random errors which we assume independent and satisfying the conditions $\mathbf{E}\varepsilon_i = 0$, $\mathbf{E}\varepsilon_i^2 = \sigma^2$ and $\mathbf{E}\varepsilon_i^6 \leq C_6 < \infty$ for all $i \leq n$. We aim to estimate the unknown error variance σ^2 .

Wahba (1983) and Silverman (1985) proposed to use for estimating σ^2 usual non-parametric residuals obtained by subtracting an appropriately smoothed curve from the observations. Difference-based were thoroughly discussed in Gasser et al. (1986), Seifert et al. (1993) among other. Hall et al (1990) found asymptotically optimal differences. Choosing the curve estimation with respect to extracting residual variance has been studied by Buckley et al (1988) and Hall and Marron (1990). We refer to Seifert et al (1993) for more detailed descriptions and comparison of different procedures for variance estimation. Neumann (1994) discussed an application of data-driven procedure for non-parametric smoothing. Hall and Carroll (1989), Härdle and Tsybakov (1997), Ruppert et al (1997), Fan and Yao (1988) discussed the problem of estimating the heteroscedastic conditional variance.

The majority of the mentioned results focus on the mean squared error of the variance estimation in the univariate regression model and claim the possibility to estimate σ^2 at the rate $n^{-1/2}$. Some extensions to the two-dimensional case are discussed in Hall et al. (1991) and Seifert et al. (1993).

We show that this result can be extended to the case of a multivariate model but only if the dimension d is not too high, more precisely, if $d \leq 8$.

It is worth noting that the variance estimation is relatively rarely the target of statistical analysis. Typically it is used as a building block for further procedure like adaptive estimation (Rice, 1984; Gasser et al, 1991) of hypothesis testing (Hart, 1997), Spokoiny (1999), where some pilot variance estimation is required. This enforces to study not only

the risk of estimation but also some deviation probabilities which are presented in our results.

2. The estimate

Our approach is a multidimensional analog of the proposal from Hart (1997, p.123) which gives an unbiased estimate of the variance for a linear regression function. The idea is to construct for every design point X_i a locally linear fit $\widehat{f}(X_i)$ of the unknown regression function f and then to use the *pseudo-residuals* $\widehat{e}_i = Y_i - \widehat{f}(X_i)$ for variance estimation.

The main problem comes from design sparseness and non regularity in the multidimensional situation. This makes difficult the choice of the local neighborhood for constructing the locally linear fit. We propose below two approaches how this choice can be done. One utilizes a uniform bandwidth and another one allows the bandwidth to vary from point to point.

2.1. The locally linear fit

First we describe the locally linear fit we apply. Let $U_h(x)$ denote the ball with the center x and the radius h and $N_h(x)$ stand for the number of different design points in $U_h(x)$: $N_h(x) = \#\{X_i \in U_h(x)\}$.

Let K be the uniform kernel function $K(u) = \mathbf{1}(|u| \leq 1)$. Introduce linear functions $\psi_0(x) \equiv 1$, $\psi_\ell(x) = x_\ell$, $\ell = 1, \dots, d$.

Lemma 2.1. *For every $i \leq n$ and every $h > 0$ define the $(d+1) \times (d+1)$ matrix $\Psi_{i,h}$ with elements $\sum_{j=1}^n \psi_\ell(X_j) \psi_k(X_j) K\left(\frac{X_j - X_i}{h}\right)$, $\ell, k = 0, \dots, d$. If this matrix is non singular, then there exist coefficients $a_{ij,h}$, $j = 1, \dots, n$, depending on the design X_1, \dots, X_n only and such that $a_{ij,h} = 0$ if $|X_j - X_i| \geq h$ and*

$$\begin{aligned} \sum_{j=1}^n a_{ij,h} K\left(\frac{X_j - X_i}{h}\right) &= 1, \\ \sum_{j=1}^n a_{ij,h} \psi_\ell(X_j - X_i) K\left(\frac{X_j - X_i}{h}\right) &= 0, \quad \ell = 1, \dots, d. \end{aligned}$$

Proof. This is the system of $d+1$ linearly independent equations of n variables $a_{ij,h}$ and hence a solution exists (it is usually non-unique) provided that the corresponding characteristic matrix $\Psi_{i,h}$ is non degenerate. \square

Remark 2.1. The coefficients $a_{ij,h}$ can be calculated from the locally linear fit

$$\widehat{\theta}_h(X_i) = \underset{\theta \in \mathbb{R}^{d+1}}{\operatorname{arginf}} \sum_{j=1}^n \left(Y_j - \sum_{\ell=0}^d \theta_\ell \psi_\ell(X_j) \right)^2 K\left(\frac{X_j - X_i}{h}\right)$$

see Katkovnik (1985), Tsybakov (1986), Fan and Gijbels (1996). This is a quadratic optimization problem with respect to the vector of coefficients $\theta = (\theta_\ell)_{\ell=0,\dots,d}$ which can be solved explicitly and the solution is a linear combination of the observations Y_j with the deterministic coefficients depending on the design X_1, \dots, X_n only. In particular, the first coefficient can be represented in the form $\hat{\theta}_{0,h}(X_i) = \sum_{j=1}^n a_{ij,h} Y_j$ and it is easy to check that such defined coefficients $a_{ij,h}$ fulfill the conditions of Lemma 2.1.

A necessary and usually sufficient condition for non singularity of the matrix $\Psi_{i,h}$ is that the ball $U_h(X_i)$ contains at least $d+1$ design points.

2.2. Procedure with a variable bandwidth

For every i , define the bandwidth h_i by the condition

$$h_i = \inf \{h : \Psi_{i,h} \text{ is non singular}\}$$

where $\Psi_{i,h}$ is the $(d+1) \times (d+1)$ matrix introduced in Lemma 2.1.

Next define the locally linear estimate

$$\hat{f}(X_i) = \hat{f}_{h_i}(X_i) = \sum_{j=1}^n a_{ij,h_i} Y_j$$

and *pseudo residuals* \hat{e}_i

$$\hat{e}_i = \hat{f}(X_i) - Y_i = \sum_{j=1}^n c_{ij} Y_j$$

with $c_{ij} = a_{ij,h_i}$ for $j \neq i$ and $c_{ii} = a_{ii,h_i} - 1$. Finally we set

$$\begin{aligned} s_i^2 &= \sum_{j=1}^n c_{ij}^2, \quad i = 1, \dots, n, \\ \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n \frac{|\hat{e}_i|^2}{s_i^2}. \end{aligned} \tag{2.1}$$

2.3. Procedure with a fixed bandwidth

Define the subset \mathcal{X}_h of the set X_1, \dots, X_n by

$$\mathcal{X}_h = \{X_i : \Psi_{i,h} \text{ is non singular}\}$$

and let M_h stand for the number of design points in \mathcal{X}_h : $M_h = \#\mathcal{X}_h$. Then, with a given $\alpha \geq 1/2$, we define the bandwidth h as the minimal value which satisfies the condition

$$M_h \geq n\alpha,$$

that is, there are at least $n\alpha$ points X_i , for which $\Psi_{i,h}$ is non singular. Next we define the locally linear estimate $\hat{f}(X_i)$ by $\hat{f}(X_i) = \sum_{j=1}^n a_{ij,h} Y_j$ and the *pseudo residuals* \hat{e}_i by

$$\widehat{e}_i = \widehat{f}(X_i) - Y_i = \sum_{j=1}^n c_{ij} Y_j$$

with $c_{ij} = a_{ij,h}$ for $j \neq i$ and $c_{ii} = a_{ii,h} - 1$. Finally the variance estimate $\widehat{\sigma}^2$ is defined by

$$s_i^2 = \sum_{j=1}^n c_{ij}^2,$$

$$\widehat{\sigma}_v^2 = \frac{1}{M_h} \sum_{i: X_i \in \mathcal{X}_h} \frac{\widehat{e}_i^2}{s_i^2}.$$

3. Properties

In this section we state some useful properties of the estimate $\widehat{\sigma}^2$ from (2.1). The estimate $\widehat{\sigma}_v^2$ can be studied similarly. First we present the result for the case of Gaussian errors ε_i and then we discuss the general case.

The estimate $\widehat{\sigma}^2$ assumes some smoothness of the regression function f at a small neighborhood of each design point X_i . When formulating the result, this local smoothness will be characterized by the value

$$L_i = 0.5 \sup_{u \in \mathbb{R}^d} \sup_{x \in U_{h_i}(X_i)} \frac{u^\top f''(x) u}{|u|^2}$$

where f'' denotes the $d \times d$ matrix of second derivatives of f .

Theorem 3.1. *Let the observations Y_1, \dots, Y_n follow the regression model (1.1) with i.i.d. Gaussian errors $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ and a two times differentiable regression function f . Introduce $n \times n$ -matrix R with elements*

$$r_{ij} = \frac{1}{n s_i s_j} \sum_{k=1}^n c_{ik} c_{jk}, \quad i, j = 1, \dots, n,$$

and define the values Δ and S^2 by

$$\Delta^2 = \frac{1}{n} \sum_{i=1}^n L_i^2 h_i^4 s_i^{-2} \left(\sum_{j \neq i} |c_{ij}| \right)^2,$$

$$S^2 = 2 \operatorname{tr} R^2 = 2 \sum_{i=1}^n \sum_{j=1}^n r_{ij}^2.$$

Then for every nonnegative λ with $\lambda^2 \leq \frac{\operatorname{tr} R^2}{2 \|R\|^2}$ and any $t > 0$, the variance estimate $\widehat{\sigma}^2$ fulfills

$$\mathbf{P} \left(\pm(\widehat{\sigma}^2 - \sigma^2) > \Delta^2 + \lambda \Delta S^{1/2} \sigma + (\lambda + t) S \sigma^2 \right) \leq 2e^{-\lambda^2/4 - \lambda t/2}. \quad (3.1)$$

Let also

$$\tilde{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n s_i^{-2} \left(\sum_{j=1}^n c_{ij} \varepsilon_j \right)^2 \quad (3.2)$$

be the variance estimate corresponding to the "no-response" model with the vanishing regression function $f(x) \equiv 0$ and hence, $Y_i = \varepsilon_i$. Then for any $\lambda \geq 1$

$$\mathbf{P} \left(\pm(\hat{\sigma}^2 - \tilde{\sigma}^2) > \Delta^2 + \lambda \Delta S^{1/2} \sigma \right) \leq e^{-\lambda^2/2}. \quad (3.3)$$

Remark 3.1. The norm of the matrix R can be very roughly estimated as follows:

$$\|R\|^2 \leq \max_{i=1, \dots, n} \sum_{j=1}^n r_{ij}^2.$$

3.1. The rate of estimation

Here we discuss some corollaries of Theorem 3.1 concerning the rate of estimation. For this we have to bound the quantities Δ and S . This can be easily done for a regular (equispaced) or random design. So we consider here two different model assumptions widely used in applications.

RD (Random design) The design points X_1, \dots, X_n are i.i.d. random variables from a distribution with a density $p(x)$ which is supported on a compact set \mathcal{X} and it is continuous and positive on \mathcal{X} .

ED (Equispaced design) The design points X_1, \dots, X_n form the regular grid in the unit cube $[0, 1]^d$ with the step δ_n such that δ_n^{-1} is an integer number and $\delta_n^{-d} = n$.

Recall that each bandwidth h_i is defined as the smallest radius h providing a non degenerated linear fit in the ball $U_h(X_i)$. This implies that the number $N_h(X_i)$ of design points in the ball $U_h(X_i)$ is at least $d + 1$. Define $\bar{N} = \max_i N_{h_i}(X_i)$. The following technical result is straightforward.

Lemma 3.1. *Under RD, it holds $\mathbf{P}(\bar{N} = d + 1) = 1$. Under ED, it holds $\bar{N} = 2d + 1$.*

Further, let h_i be the smallest radius providing at least $d + 1$ point in the ball $U_{h_i}(X_i)$ with the center at X_i , and let $\bar{h} = \left(n^{-1} \sum_{i=1}^n h_i^4 \right)^{1/4}$. Under ED, one clearly has $h_i = n^{-1/d}$ for all i , so that $\bar{h} = n^{-1/d}$. Under RD, the following result can be proved:

Lemma 3.2. *Under RD, it holds for some positive constant $\kappa \geq 1$ depending on d and design density $p(x)$ only such that*

$$\mathbf{P} \left(\bar{h} \leq \kappa n^{-1/d} \right) \leq n^{-1}.$$

Next, since $s_i^2 = \sum_j c_{ij}^2$, the Cauchy-Schwarz inequality implies

$$\left(\sum_{j \neq i} |c_{ij}| \right)^2 \leq N_{h_i}(X_i) \sum_{j \neq i} c_{ij}^2 \leq N_{h_i}(X_i) s_i^2$$

and hence, if the function f has a bounded second derivative, i.e. if $\|f''\| \leq L$, then $L_i \leq L$ for all i and

$$\Delta^2 \leq \frac{1}{n} \sum_{i=1}^n L_i^2 h_i^4 N_{h_i}(X_i) \leq \frac{L^2 \bar{N}}{n} \sum_{i=1}^n h_i^4 = L^2 \bar{h}^4 \bar{N} \leq \kappa^2 L^2 n^{-4/d}$$

with κ from Lemma 3.2.

Further we bound S . The definition of the stochastic terms ξ_i implies $\mathbf{E}\xi_i = 0$ and

$$\mathbf{E}\xi_i^2 = n^{-1} s_i^{-2} \mathbf{E} \left(\sum_{j=1}^n c_{ij} \varepsilon_j \right)^2 = \frac{\sigma^2}{n}.$$

Therefore, for all i, j , it holds $v_{ij} = \mathbf{E}\xi_i \xi_j \leq \sigma^2/n$ and moreover, if $|X_j - X_i| > h_i + h_j$, then ξ_i and ξ_j are independent and $\mathbf{E}\xi_i \xi_j = 0$. This implies for every $i \leq n$

$$\sum_{j=1}^n v_{ij}^2 \leq N_i n^{-2} \sigma^4$$

with

$$N_i = \#\{X_j : |X_j - X_i| < h_i + h_j\}.$$

Similarly to Lemmas 3.1 and 3.2 one can bound under ED

$$\frac{1}{n} \sum_{i=1}^n N_i \leq N^*$$

with some fixed constant N^* depending on d only. Under RD, a similar bound holds with a probability exponentially close to 1 and the constant N^* depends also on the design density. Therefore,

$$S^2 = 2\sigma^{-4} \sum_{i=1}^n \sum_{j=1}^n v_{ij}^2 \leq \frac{2N^*}{n}.$$

On the other side,

$$\sum_{i=1}^n \sum_{j=1}^n v_{ij}^2 \geq \sum_{i=1}^n v_{ii}^2 = \sigma^4 n^{-1}$$

that is, $2 \leq nS^2 \leq 2N^*$. This and the inequality $\Delta \leq L\kappa n^{-2/d}$ yield in view of (3.1) the following rate of estimation: with a probability at least $1 - e^{-\lambda^2/4 - \lambda t/2}$

$$\begin{aligned} \pm (\hat{\sigma}^2 - \sigma^2) &\leq \Delta^2 + \lambda \Delta S^{1/2} \sigma + (\lambda + t) S \sigma^2 \\ &\leq \kappa^2 L^2 n^{-4/d} + \lambda \kappa L (2N^*)^{1/4} \sigma n^{-2/d-1/4} + (\lambda + t) \sigma^2 \sqrt{2N^*} n^{-1/2}. \end{aligned}$$

We observe that for $d < 8$, the first two summands in this bound are smaller in rate than the last one which is $O(n^{-1/2})$. If $d = 8$, then all three summands are of order $n^{-1/2}$ and for $d > 8$, the first term (which is of order $n^{-4/d}$) starts to dominate. Given a loss function w , define the risk of estimation

$$R(\hat{\sigma}^2) = \begin{cases} \mathbf{E}w(n^{1/2}\sigma^{-2}(\hat{\sigma}^2 - \sigma^2)), & d \leq 8, \\ \mathbf{E}w(n^{4/d}\sigma^{-2}(\hat{\sigma}^2 - \sigma^2)), & \text{otherwise.} \end{cases}$$

The above considerations lead to the following

Theorem 3.2. *Let $\hat{\sigma}^2$ be the variance estimate from (2.1). Let the quantities Δ and S defined in Theorem 3.1 and depending on n , the design X_1, \dots, X_n and on the smoothness properties of the regression function f , satisfy the conditions*

$$\begin{aligned} \Delta &\leq Bn^{-2/d}, \\ S^2 &\leq \frac{2N^*}{n} \end{aligned}$$

with some fixed constants B, N^* . Then for every continuously differentiable loss function w which obeys the conditions $w(0) = 0$, $w(x) = w(-x)$, $w'(x) \geq 0$ for $x > 0$ and $\int w'(x)e^{-\alpha x} dx < \infty$ for every $\alpha > 0$, the corresponding risk $R(\hat{\sigma}^2)$ remains bounded by some constant $C = C(B, N^*, w)$ depending on B, N^* and the function w only:

$$R(\hat{\sigma}^2) \leq C(B, N^*, w).$$

3.2. Non-Gaussian case

Here we discard the assumption that the errors ε_i are normally distributed. Instead we assume that they are independent identically distributed with 6 finite moments.

Our variance estimate allows for the following representation, cf. (2.1):

$$\hat{\sigma}^2 = \sum_{i=1}^n \left[\sum_{j=1}^n \alpha_{ij} \{f(X_j) + \varepsilon_j\} \right]^2 = \sum_{i=1}^n \left(b_i + \sum_{j=1}^n \alpha_{ij} \varepsilon_j \right)^2$$

where the coefficients α_{ij} satisfy $\sum_{j=1}^n \alpha_{ij}^2 = 1/n$ so that $\sum_{i=1}^n \sum_{j=1}^n \alpha_{ij}^2 = 1$, and $\sum_{i=1}^n b_i^2 \leq \Delta^2$, see the proof of Theorem 3.1. Clearly

$$\hat{\sigma}^2 = \sum_{i=1}^n b_i^2 + 2 \sum_{i=1}^n \sum_{j=1}^n \alpha_{ij} b_i \varepsilon_j + \sum_{i=1}^n \sum_{j=1}^n \beta_{ij} \varepsilon_i \varepsilon_j$$

with

$$\beta_{ij} = \sum_{k=1}^n \alpha_{ki} \alpha_{kj}.$$

Theorem 3.3. *Let the errors ε_i from (1.1) be i.i.d. random variables with $\mathbf{E}\varepsilon_i = 0$, $\mathbf{E}\varepsilon_i^2 = \sigma^2$, $\mathbf{E}(\varepsilon_i^2 - \sigma^2)^2 \leq C_4^2\sigma^4$ and $\mathbf{E}|\varepsilon_i^2 - \sigma^2|^3 \leq C_6\sigma^6$ for all i . Let also value C_A be such that*

$$\frac{n \max_{i=1, \dots, n} \sum_{j=1}^n \beta_{ij}^2}{\sum_{i=1}^n \sum_{j=1}^n \beta_{ij}^2} \leq C_A, \quad \frac{n \max_{i=1, \dots, n} \beta_{ii}^2}{\sum_{i=1}^n \beta_{ii}^2} \leq C_A.$$

Then there exists an absolute constant C such that for every $\lambda \geq 0$ with $\lambda^2 \leq \frac{n}{2C_A}$ every $t \geq 0$ and every δ with $0 < \delta \leq 1$

$$\begin{aligned} \mathbf{P} \left(\pm(\hat{\sigma}^2 - \sigma^2) > \Delta^2 + 2\Delta S^{1/2}\sigma + (\lambda + t + \delta)S\sigma^2 + (\lambda + t)S''\sigma^2 \right) \\ \leq 2e^{-\lambda^2/4 - \lambda t/2} + Cn^{-1/2}\delta^{-3} \end{aligned}$$

where $|S''|^2 = \sum_{i=1}^n \beta_{ii}^2$ and the constant C depends on C_4, C_6 and C_A only.

This result clearly implies an analog of Theorem 3.2 for non-Gaussian errors under the conditions of Theorem 3.3.

3.3. Rate optimality

Here we show that the critical dimension $d = 8$ appears not only for our particular estimator. Actually, no estimator achieves the rate $n^{-1/2}$ for $d > 8$ uniformly over any class of smooth functions with the smoothness degree 2.

To simplify the construction, we suppose hereafter that $n^{1/d}$ is an integer number, and X_1, \dots, X_n form the regular grid in the unit cube $[0, 1]^d$. Define the following Sobolev type class $\mathcal{F}_n(2, L)$:

$$\mathcal{F}_n(2, L) = \left\{ f : \frac{1}{n} \sum_{i=1}^n \sup_{x: |x - X_i| \leq n^{-1/d}} \|f''(x)\|^2 \leq L^2 \right\}.$$

Let \mathbf{P}_{f, σ^2} denote the measure on the observation space which corresponds to a regression function f and the variance σ^2 and let \mathbf{E}_{f, σ^2} denote the expectation w.r.t. \mathbf{P}_{f, σ^2} .

Theorem 3.4. *Let X_1, \dots, X_n be the equispaced design in the unit cube $[0, 1]^d$ and the observations Y_1, \dots, Y_n be generated from the regression model (1.1) with i.i.d. Gaussian errors $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$. For $d \geq 8$, sufficiently large L and for every continuous bounded loss function w ,*

$$\liminf_{n \rightarrow \infty} \sup_{\tilde{\sigma}_n^2} \sup_{f \in \mathcal{F}_n(2, L)} \sup_{\sigma^2 \in \Sigma_n} \mathbf{E}_{f, \sigma^2} w \left(n^{4/d} (\tilde{\sigma}_n^2 - \sigma^2) \right) = r > 0$$

where the infimum is taken over the set of all possible estimates of the parameter σ^2 and Σ_n is the three points set of the form $\Sigma_n = \{1, 1 + n^{-4/d}, 1 + 2n^{-4/d}\}$.

4. Proofs

In this section we gather the proofs of Theorem 3.1 through 3.4.

4.1. Proof of Theorem 3.1

Define

$$f_{h_i}(X_i) = \sum_{j=1}^n a_{ij,h_i} f(X_j)$$

so that

$$\sum_{j=1}^n c_{ij} f(X_j) = \sum_{j=1}^n a_{ij,h_i} f(X_j) - f(X_i) = f_{h_i}(X_i) - f(X_i).$$

The model equation (1.1) implies for every $i \leq n$

$$\begin{aligned} \hat{e}_i &= \sum_{j=1}^n c_{ij} Y_j \\ &= \sum_{j=1}^n c_{ij} \{f(X_j) + \varepsilon_j\} \\ &= \sum_{j=1}^n c_{ij} f(X_j) + \sum_{j=1}^n c_{ij} \varepsilon_j \end{aligned}$$

which leads to the following representation for the estimate $\hat{\sigma}^2$:

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n \frac{|\hat{e}_i|^2}{s_i^2} = \sum_{i=1}^n (b_i + \xi_i)^2$$

with

$$\begin{aligned} b_i &= n^{-1/2} s_i^{-1} \{f_{h_i}(X_i) - f(X_i)\}, \\ \xi_i &= n^{-1/2} s_i^{-1} \sum_{j=1}^n c_{ij} \varepsilon_j. \end{aligned}$$

The smoothness assumption on the function f implies for every j with $|X_j - X_i| \leq h_i$

$$|f(X_j) - f(X_i) - f'(X_i)(X_j - X_i)| \leq L_i h_i^2.$$

The properties $\sum_{j=1}^n c_{ij} = 0$ and $\sum_{j=1}^n c_{ij}(X_j - X_i) = 0$ provide

$$\begin{aligned} |f_{h_i}(X_i) - f(X_i)| &= \left| \sum_{j=1}^n c_{ij} f(X_j) - f(X_i) \sum_{j=1}^n c_{ij} - f'(X_i) \sum_{j=1}^n c_{ij}(X_j - X_i) \right| \\ &= \left| \sum_{j=1}^n c_{ij} \{f(X_j) - f(X_i) - f'(X_i)(X_j - X_i)\} \right| \\ &\leq L_i h_i^2 \sum_{j \neq i} |c_{ij}|. \end{aligned}$$

Therefore

$$\sum_{i=1}^n b_i^2 \leq \frac{1}{n} \sum_{i=1}^n L_i^2 h_i^4 s_i^{-2} \left(\sum_{j \neq i} |c_{ij}| \right)^2 = \Delta^2. \quad (4.1)$$

We now apply the following general statement from Spokoiny (1999, Proposition 6.2). Let V denote the covariance matrix of the vector $\xi = (\xi_1, \dots, \xi_n)$, that is, $V = (\mathbf{E} \xi_i \xi_j, i, j = 1, \dots, n)$. Then for every positive $\gamma > 0$ with $\gamma \leq \|V\|^{-1} \sqrt{\text{tr } V^2 / 2}$ and every $t \geq 0$

$$\mathbf{P} \left(\pm \left(\sum_{i=1}^n |\xi_i|^2 - \text{tr } V \right) > (\gamma + t) \sqrt{2 \text{tr } V^2} \right) \leq e^{-\gamma^2/4 - \gamma t/2} \quad (4.2)$$

and

$$\begin{aligned} \mathbf{P} \left(\pm \left(\sum_{i=1}^n |b_i + \xi_i|^2 - \|b\|^2 - \text{tr } V \right) > \gamma \|b\| (2 \text{tr } V^2)^{1/4} + (\gamma + t) \sqrt{2 \text{tr } V^2} \right) \\ \leq 2e^{-\gamma^2/4 - \gamma t/2}. \end{aligned}$$

Here $\|b\|^2 = \sum_{i=1}^n b_i^2$ and $\text{tr } V$ (resp. $\text{tr } V^2$) denotes the trace of the matrix V (resp. V^2). Since $\mathbf{E} \xi_i^2 = \sigma^2/n$, then clearly

$$\text{tr } V = \sum_{i=1}^n \mathbf{E} \xi_i^2 = \sigma^2.$$

Next, for $i \neq j$

$$\mathbf{E} \xi_i \xi_j = \frac{\sigma^2}{n s_i s_j} \sum_{k=1}^n c_{ik} c_{jk} = \sigma^2 r_{ij}$$

so that

$$2 \text{tr } V^2 = 2 \sum_{i=1}^n \sum_{j=1}^n (\mathbf{E} \xi_i \xi_j)^2 = 2\sigma^4 \sum_{i=1}^n \sum_{j=1}^n r_{ij}^2 = \sigma^4 S^2.$$

This implies the required assertion in view of (4.1).

4.2. Proof of Theorem 3.2

This result is an easy corollary of Theorem 3.1. Indeed, application of this result with $d \leq 8$, $\gamma = 1$ and varying t yields

$$\mathbf{P} \left(n^{1/2} \sigma^{-2} |\hat{\sigma}^2 - \sigma^2| > C + t\sqrt{2N^*} \right) \leq 2e^{-t/2}.$$

where $C = B^2 \sigma^{-2} + B(2N^*)^{1/4} \sigma^{-1} + \sqrt{2N^*}$. Therefore

$$\begin{aligned} R(\hat{\sigma}^2) &= \mathbf{E} w \left(n^{1/2} \sigma^{-2} (\hat{\sigma}^2 - \sigma^2) \right) \\ &\leq - \int_0^\infty w(x) d\mathbf{P} \left(n^{1/2} \sigma^{-2} |\hat{\sigma}^2 - \sigma^2| > x \right) \\ &\leq w(C) + \int_0^\infty w'(t+C) \mathbf{P} \left(n^{1/2} \sigma^{-2} |\hat{\sigma}^2 - \sigma^2| > t+C \right) dt \\ &\leq w(C) + \int_0^\infty w'(t+C) \exp \left(-\frac{t}{2\sqrt{2N^*}} \right) dt \end{aligned}$$

and the assertion follows. The case of $d > 8$ can be treated similarly.

4.3. Proof of Theorem 3.3

Since $\sum_{i=1}^n \beta_{ii} = \sum_{i=1}^n \sum_{j=1}^n \alpha_{ij}^2 = 1$, the difference $\hat{\sigma}^2 - \sigma^2$ can be represented in the form

$$\begin{aligned} \hat{\sigma}^2 - \sigma^2 &= \sum_{i=1}^n b_i^2 + 2 \sum_{i=1}^n \left(\sum_{j=1}^n \alpha_{ij} b_j \right) \varepsilon_i + \sum_{i=1}^n \beta_{ii} (\varepsilon_i^2 - \sigma^2) + \sum_{i=1}^n \sum_{j \neq i}^n \beta_{ij} \varepsilon_i \varepsilon_j \\ &= \sum_{i=1}^n b_i^2 + Q_2 + Q_3 + Q_4. \end{aligned}$$

We now estimate separately each term in this expression. Note first that

$$\sum_{i=1}^n b_i^2 \leq \Delta^2$$

see the proof of Theorem 3.1.

Let $\tilde{\varepsilon}_1, \dots, \tilde{\varepsilon}_n$ be a sequence of i.i.d. random variables from the normal law $\mathcal{N}(0, \sigma^2)$. Define the sums $\tilde{Q}_2, \tilde{Q}_3, \tilde{Q}_4$ similarly to Q_2, Q_3, Q_4 with $\tilde{\varepsilon}_i$'s in place of ε_i 's. The idea is to show that the distribution of every Q_k only weakly depends on the particular distribution of ε_i 's and therefore, the bounds for \tilde{Q}_k are valid for Q_k as well (in some asymptotic sense if n is large enough), $k = 2, 3, 4$.

First we estimate the sum

$$Q_2 = 2 \sum_{i=1}^n \sum_{j=1}^n b_i \alpha_{ij} \varepsilon_j = 2 \sum_{j=1}^n c_j \varepsilon_j$$

with $c_j = \sum_{i=1}^n \alpha_{ij} b_i$. Define the $n \times n$ -matrix A with elements α_{ij} and the vectors b (resp. c) with elements b_i (resp. c_i) and note that

$$\sum_{j=1}^n c_j^2 = |A^T b|^2 = b^T A A^T b \leq \|A A^T\| |b|^2 \leq \|A A^T\| \Delta^2.$$

Note also that $\|A A^T\| = \|A^T A\| = \|R\|$ with the matrix R defined in Theorem 3.1. By the Cauchy-Schwarz inequality

$$\mathbf{P} \left(\left| \sum_{i=1}^n c_i \varepsilon_i \right| > \Delta S^{1/2} \sigma \right) \leq \frac{\sigma^2 \sum_{i=1}^n c_i^2}{\Delta^2 S \sigma^2} \leq \frac{\|R\|}{S}$$

and by the conditions of the theorem, see also Remark 3.1, $n\|R\|^2/S^2 \leq C_A$, so that

$$\mathbf{P} \left(|Q_2| > 2\Delta S^{1/2} \sigma \right) \leq 4C_A^{1/2} n^{-1/2}.$$

Next, it holds for Q_3

$$\mathbf{E} Q_3^2 = \mathbf{E} \left(\sum_{i=1}^n \beta_{ii} (\varepsilon_i^2 - \sigma^2) \right)^2 = C_4^2 \sigma^4 \sum_{i=1}^n \beta_{ii}^2$$

and the Berry-Essen inequality, see Petrov (1975), applied to Q_3 yields with $S'' = \sigma^{-2} \sqrt{\mathbf{E} Q_3^2}$

$$\begin{aligned} \mathbf{P} (Q_3 > x S'' \sigma^2) &\leq \mathbf{P} (\tilde{Q}_3 > x S'' \sigma^2) + \rho \delta^{-3} \frac{1}{S''^3 \sigma^6} \sum_{i=1}^n \mathbf{E} |\beta_{ii} (\varepsilon_i^2 - \sigma^2)|^3 \\ &\leq \mathbf{P} (\tilde{Q}_3 > (x - \delta) S'' \sigma^2) + C_6 \rho \delta^{-3} (S'')^{-3} \sum_{i=1}^n |\beta_{ii}|^3. \end{aligned}$$

The conditions of the theorem provide

$$\sum_{i=1}^n |\beta_{ii}|^3 \leq \max_{i=1, \dots, n} \beta_{ii} \sum_{i=1}^n |\beta_{ii}|^2 \leq C_A S''^3 n^{-1/2}$$

and hence

$$\mathbf{P} (Q_3 > x S'' \sigma^2) \leq \mathbf{P} (\tilde{Q}_3 > x S'' \sigma^2) + C_6 \rho \delta^{-3} C_A n^{-1/2}.$$

In addition, the use of (4.2) yields for every λ with $\lambda^2 \leq \frac{n}{2C_A}$

$$\mathbf{P} (\tilde{Q}_3 > (\lambda + t) S'' \sigma^2) \leq e^{-\lambda^2/4 - \lambda t/2}.$$

For estimating Q_4 , we apply the following general result from Spokoiny (1999, Corollary 6.2). Let $U = (u_{ij}, i, j = 1, \dots, n)$ be a $n \times n$ symmetric matrix with $u_{ii} = 0$ for all i . By $U(\varepsilon_1, \dots, \varepsilon_n)$ we denote the corresponding quadratic form of i.i.d. random variables $\varepsilon_1, \dots, \varepsilon_n$, that is,

$$U(\varepsilon_1, \dots, \varepsilon_n) = \sum_{i=1}^n \sum_{j \neq i}^n u_{ij} \varepsilon_i \varepsilon_j.$$

Let also $\tilde{\varepsilon}_1, \dots, \tilde{\varepsilon}_n$ be a sequence of independent Gaussian r.v.'s with $\mathbf{E}\tilde{\varepsilon}_i = 0$ and $\mathbf{E}\tilde{\varepsilon}_i^2 = \sigma^2$, $i = 1, \dots, n$. Define another quadratic form

$$U(\tilde{\varepsilon}_1, \dots, \tilde{\varepsilon}_n) = \sum_{i=1}^n \sum_{j \neq i}^n u_{ij} \tilde{\varepsilon}_i \tilde{\varepsilon}_j.$$

Clearly $\mathbf{E}U(\tilde{\varepsilon}_1, \dots, \tilde{\varepsilon}_n) = 0$ and $\mathbf{E}|U(\tilde{\varepsilon}_1, \dots, \tilde{\varepsilon}_n)|^2 = \mathbf{E}|U(\varepsilon_1, \dots, \varepsilon_n)|^2$.

Proposition 4.1. *Let $\mathbf{E}\varepsilon_i^4 \leq C_4\sigma^4$ for some fixed constant $C_4 \geq 3$. Let, for a symmetric matrix U with $u_{ii} = 0$ for $i = 1, \dots, n$, and for a normalizing constant G , the value C_U be defined by*

$$C_U = \max_{i=1, \dots, n} nG^{-2}\sigma^4 \sum_{j=1}^n u_{ij}^2.$$

Then, for each $\delta > 0$ and every x

$$\mathbf{P}(G^{-1}U(\varepsilon_1, \dots, \varepsilon_n) > x) \leq \mathbf{P}(G^{-1}U(\tilde{\varepsilon}_1, \dots, \tilde{\varepsilon}_n) > x - \delta) + \rho(C_4 C_U)^{3/2} n^{-1/2} \delta^{-3}$$

with an absolute constant ρ .

We now apply this result to Q_4 with $u_{ij} = \beta_{ij}$, $i \neq j$ and

$$G = \sigma^2 \left(\sum_{i=1}^n \sum_{j=1}^n \beta_{ij}^2 \right)^{1/2}.$$

Since

$$\sum_{i=1}^n \sum_{j=1}^n \beta_{ij}^2 = \text{tr}(AA^\top)^2 = \text{tr}R^2 = S^2$$

we derive

$$\mathbf{P}(Q_4 > (\lambda + t + \delta)\sigma^2 S) \leq \mathbf{P}(\tilde{Q}_4 > (\lambda + t)\sigma^2 S) + \rho(C_4 C_A)^{3/2} n^{-1/2} \delta^{-3}.$$

The bound (4.2) applied to \tilde{Q}_4 provides for every λ with $\lambda^2 \leq \frac{n}{2C_A}$ and every $t > 0$

$$\mathbf{P}(\tilde{Q}_4 > (\lambda + t)\sigma^2 S) \leq e^{-\lambda^2/4 - \lambda t/2}.$$

Summing up everything, what we have got so far, leads to the bound

$$\begin{aligned} & \mathbf{P}\left(\pm(\hat{\sigma}^2 - \sigma^2) > \Delta^2 + 2\Delta S^{1/2}\sigma + (\lambda + t + \delta)S\sigma^2 + (\lambda + t)S''\sigma^2\right) \\ & \leq \mathbf{P}\left(|Q_2| > 2\Delta S^{1/2}\sigma\right) + \mathbf{P}\left(\pm Q_3 > (\lambda + t)S''\sigma^2\right) + \mathbf{P}\left(\pm Q_4 > (\lambda + t + \delta)S\sigma^2\right) \\ & \leq 2e^{-\lambda^2/4 - \lambda t/2} + Cn^{-1/2}\delta^{-3} \end{aligned}$$

where C depends on C_4, C_6 and C_A only.

4.4. Proof of Theorem 3.4

The idea of the proof is as follows. We first change the minimax statement for a Bayes one. For a prior measure π on the set \mathcal{F} , define the corresponding marginal measure $\mathbf{P}_{\pi, \sigma^2}$ by

$$\mathbf{P}_{\pi, \sigma^2}(A) = \int \mathbf{P}_{f, \sigma^2}(A) \pi(\mathrm{d}f).$$

We intend to show that there exists a sequence of random functions f_n with prior distributions π_n satisfying $\pi_n(\mathcal{F}_n(2, L)) \rightarrow 1$ and such that

$$\mathbf{E}_{\pi_n, \sigma^2} w\left(n^{4/d}(\tilde{\sigma}_n^2 - \sigma^2)\right) = r > 0$$

for n large enough. For the latter, it suffices to show that the measures $\mathbf{P}_{\pi_n, \sigma_0^2}$ with $\sigma_0^2 = 1$ and $\mathbf{P}_{\pi_n, \sigma_n^2}$ with $\sigma_n^2 = \sigma_0^2 + n^{-4/d}$ are not asymptotically separable.

The priors π_n are selected on the base of the following consideration. We define the values of random functions f_n either identically zero or i.i.d. normally distributed at each design point X_i . If d is sufficiently large and if the variance of this distribution is small enough, then this random function will be with a large probability in the class $\mathcal{F}_n(2, L)$. Then clearly this random function f_n introduce some additional noise in the observations Y_i and we cannot distinguish whether this noise comes from the errors ε_i only (this would be the case when $f_n \equiv 0$) or there is some contribution from the random regression function f_n . More precisely, let ξ_1, \dots, ξ_n be i.i.d. standard Gaussian r.v.'s and $\delta_n = n^{-2/d}$. We will show that there exist random functions g_n with $g_n(X_i) = \delta_n \xi_i$ and with $\mathbf{P}(g_n \in \mathcal{F}_n(2, L)) \rightarrow 1$ as $n \rightarrow \infty$ for $d \geq 8$. The random functions f_n are constructed as follows. With probability $1/2$, we set $f_n = 0$ and with probability $1/2$, the function f_n coincides with g_n . Then, for $\sigma = \sigma_0$ the marginal distribution of the observations $Y_i = f(X_i) + \sigma \varepsilon_i$ is with probability $1/2$ i.i.d. from $\mathcal{N}(0, \sigma_0^2)$ and with probability $1/2$ i.i.d. from $\mathcal{N}(0, \sigma_n^2)$. Similarly, for $\sigma = \sigma_n$, the marginal distribution of the observations Y_i corresponds with probability $1/2$ an i.i.d. sample from $\mathcal{N}(0, \sigma_n^2)$ and with probability $1/2$ an i.i.d. sample from $\mathcal{N}(0, \sigma_n^2 + n^{-4/d})$. Hence, with a positive probability, these two marginal distributions coincide and therefore any estimate has a non-vanishing risk.

Now we present a formal description. Let $h = n^{-1/d}$. Define for every grid point X_i a function ϕ_i of the form

$$\phi_i(x) = \prod_{\ell=1}^d Q\left(\frac{x_\ell - X_{i,\ell}}{h}\right)$$

where Q is a smooth symmetric nonnegative function supported on $[-1, 1]$. Clearly all functions ϕ_i have non-overlapping supports and for every i

$$\begin{aligned} |\phi_i(x)| &\leq 1, \\ \left| \frac{\partial \phi_i(x)}{\partial x_\ell} \right| &\leq \frac{\|Q'\|}{h}, \\ \left| \frac{\partial^2 \phi_i(x)}{\partial x_\ell \partial x_k} \right| &\leq \frac{\max\{\|Q'\|^2, \|Q''\|\}}{h^2} \end{aligned}$$

so that

$$\|\phi_i''(x)\| \leq \frac{C_Q}{h^2} \quad (4.3)$$

with $C_Q = \sqrt{d} \max\{\|Q'\|^2, \|Q''\|\}$.

Let also $\{\xi_i, i = 1, \dots, n\}$ be a collection of independent standard Gaussian random variables. Define the random function g_n of the form

$$g_n(x) = \delta_n \sum_{i=1}^n \xi_i \phi_i(x).$$

Finally, for an independent of g_n Bernoulli random variable ν_n with $\mathbf{P}(\nu_n = 0) = \mathbf{P}(\nu_n = 1) = 1/2$, define

$$f_n = \nu_n g_n.$$

The property (4.3) provides for every $i \leq n$

$$\sup_{x: |x - X_i| \leq n^{-1/d}} \|g_n''(x)\|^2 \leq C_Q h^{-4} \delta_n^2 \max_{j: X_j \in U_h(X_i)} \xi_j^2 \leq C_Q \sum_{j: X_j \in U_h(X_i)} \xi_j^2$$

and hence, using $N_h(X_i) \leq 2d + 1$

$$\frac{1}{n} \sum_{i=1}^n \sup_{x: |x - X_i| \leq n^{-1/d}} \|g_n''(x)\|^2 \leq \frac{C_Q}{n} (2d + 1) \sum_{i=1}^n \xi_i^2$$

so that, for $L^2 > (2d + 1)C_Q$, by the law of large numbers,

$$\mathbf{P} \left(\frac{1}{n} \sum_{i=1}^n \sup_{x: |x - X_i| \leq n^{-1/d}} \|g_n''(x)\|^2 > L^2 \right) \rightarrow 0, \quad n \rightarrow \infty.$$

This means that the random functions g_n belong to $\mathcal{F}_n(2, L)$ with a probability close to 1 if $L^2 > (2d + 1)C_Q$ and clearly the same holds for f_n 's.

Let now $\mathbf{P}_\sigma^{(n)}$ denote the product measure in \mathbb{R}^n corresponding to the model $Y_i = \sigma \varepsilon_i$ with i.i.d. standard normal errors ε_i . Then clearly

$$\begin{aligned} \mathbf{P}_{f_n, \sigma_0^2} &= \left(\mathbf{P}_{\sigma_0}^{(n)} + \mathbf{P}_{\sigma_n}^{(n)} \right) / 2, \\ \mathbf{P}_{f_n, \sigma_n^2} &= \left(\mathbf{P}_{\sigma_n}^{(n)} + \mathbf{P}_{s_n}^{(n)} \right) / 2 \end{aligned}$$

with $s_n^2 = \sigma_n^2 + n^{-4/d} = \sigma_0^2 + 2n^{-4/d}$. Next we show that all three sequences of measures $(\mathbf{P}_{\sigma_0}^{(n)})$, $(\mathbf{P}_{\sigma_n}^{(n)})$ and $(\mathbf{P}_{s_n}^{(n)})$ are pairwise asymptotically singular, if $d > 8$. Then the required assertion follows from the next general result.

Lemma 4.1. *Let three sequences $P_j^{(n)}$, $j = 0, 1, 2$, of probability measures be pairwise asymptotically singular, that is,*

$$Z_{k,j}^{(n)} = \frac{dP_k^{(n)}}{dP_j^{(n)}} \xrightarrow{P_j^{(n)}} 0, \quad n \rightarrow \infty, \quad k \neq j.$$

Then for any continuous bounded function $u(x)$, it holds

$$H_n = \frac{1}{2} \int u \left(\frac{dP_0^{(n)} + dP_1^{(n)}}{dP_1^{(n)} + dP_2^{(n)}} \right) d(P_1^{(n)} + P_2^{(n)}) \rightarrow \{u(0) + u(1)\} / 2, \quad (4.4)$$

that is, the likelihood $\frac{dP_0^{(n)} + dP_1^{(n)}}{dP_1^{(n)} + dP_2^{(n)}}$ converges weakly to the Bernoulli distribution with parameter $1/2$.

Proof. One obviously has

$$2H_n = \int u \left(\frac{Z_{0,1}^{(n)} + 1}{Z_{2,1}^{(n)} + 1} \right) dP_1^{(n)} + \int u \left(\frac{Z_{0,2}^{(n)} + Z_{1,2}^{(n)}}{Z_{1,2}^{(n)} + 1} \right) dP_2^{(n)} \rightarrow u(1) + u(0)$$

as required. \square

It remains to check (4.4) for the sequences $\mathbf{P}_\sigma^{(n)}$ with $\sigma \in \{\sigma_0, \sigma_n, s_n\}$. We consider the derivative $Z_{0,1}^{(n)} = d\mathbf{P}_{\sigma_0}^{(n)} / d\mathbf{P}_{\sigma_n}^{(n)}$, the other cases can be treated similarly.

The definition $\sigma_n^2 = \sigma_0^2 + \delta_n^2 = 1 + \delta_n^2$ clearly yields

$$L_{0,1}^{(n)} := \log \frac{d\mathbf{P}_{\sigma_0}^{(n)}}{d\mathbf{P}_{\sigma_n}^{(n)}} = n \log(\sigma_n / \sigma_0) - \sum_{i=1}^n \frac{Y_i^2}{2\sigma_0^2} + \sum_{i=1}^n \frac{Y_i^2}{2\sigma_n^2} = \frac{n}{2} \log \frac{\sigma_0^2 + \delta_n^2}{\sigma_0^2} - \sum_{i=1}^n \frac{Y_i^2 \delta_n^2}{2\sigma_0^2 \sigma_n^2}.$$

Under the measure $\mathbf{P}_{\sigma_n}^{(n)}$, it holds $Y_i = \sigma_n \zeta_i$ with i.i.d. standard normal r.v.'s ζ_i . Therefore

$$\begin{aligned} L_{0,1}^{(n)} &= \frac{n}{2} \log(1 + \delta_n^2) - \frac{\delta_n^2}{2} \sum_{i=1}^n \zeta_i^2 \\ &= \frac{n}{2} \log(1 + \delta_n^2) - \frac{n\delta_n^2}{2} - \frac{\sqrt{n}\delta_n^2}{2} \frac{1}{\sqrt{n}} \sum_{i=1}^n (\zeta_i^2 - 1) \\ &= \frac{n}{2} \log(1 + \delta_n^2) - \frac{n\delta_n^2}{2} - \frac{\sqrt{n}\delta_n^2}{2} \eta_n \\ &= \frac{\sqrt{n}\delta_n^2}{2} (r_n - \eta_n) \end{aligned}$$

where the random variables $\eta_n = \frac{1}{\sqrt{n}} \sum_{i=1}^n (\zeta_i^2 - 1)$ are asymptotically standard normal and

$$r_n = \frac{\sqrt{n}}{\delta_n^2} \log(1 + \delta_n^2) - \sqrt{n} \leq -\sqrt{n} \left\{ \frac{\delta_n^2}{2} - \frac{\delta_n^4}{3} \right\} = -\sqrt{n} \left\{ \frac{n^{-4/d}}{2} - \frac{n^{-8/d}}{3} \right\} \rightarrow -\infty$$

if $d > 8$. Since also $\sqrt{n}\delta_n^2 = n^{1/2-4/d} \rightarrow \infty$, this implies $L_{0,1}^{(n)} \rightarrow -\infty$ and hence $Z_{0,1}^{(n)} = \exp L_{0,1}^{(n)} \rightarrow 0$ as required.

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WEIERSTRASS INSTITUTE FOR APPLIED ANALYSIS AND STOCHASTICS, MOHRENSTR. 39, 10117
BERLIN, GERMANY

E-mail address: spokoiny@wias-berlin.de