Asymptotics for M-type smoothing splines with non-smooth objective functions

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Abstract
M-type smoothing splines are a broad class of spline estimators that include the popular least-squares smoothing spline but also spline estimators that are less susceptible to outlying observations and model misspecification. However, available asymptotic theory only covers smoothing spline estimators based on smooth objective functions and consequently leaves out frequently used resistant estimators such as quantile and Huber-type smoothing splines. We provide a general treatment in this paper and, assuming only the convexity of the objective function, show that the least-squares (super-)convergence rates can be extended to M-type estimators whose asymptotic properties have not been hitherto described. We further show that auxiliary scale estimates may be handled under significantly weaker assumptions than those found in the literature and we establish optimal rates of convergence for the derivatives, which have not been obtained outside the least-squares framework. A simulation study and a real-data example illustrate the competitive performance of non-smooth M-type splines in relation to the least-squares spline on regular data and their superior performance on data that contain anomalies.

Keywords Robust nonparametric regression · Smoothing splines · M-estimators · Reproducing kernel Hilbert spaces

Mathematics Subject Classification 62G08 · 62G35 · 62G20

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1 Introduction

Based on data \((t_1, Y_1), \ldots, (t_n, Y_n)\) with non-random \(t_i \in [0, 1]\), consider the classical nonparametric regression model

\[
Y_i = f_o(t_i) + \epsilon_i, \quad (i = 1, \ldots, n),
\]

where \(f_o\) is a sufficiently smooth function that we would like to estimate and the \(\epsilon_i, i = 1, \ldots, n\), are independent and identically distributed error terms, commonly assumed to have zero mean and finite variance \(\sigma^2\).

A popular estimation method involves restricting \(f_o\) to the Hilbert–Sobolev space of smooth functions denoted by \(W^{m,2}([0, 1])\) and defined as

\[
W^{m,2}([0, 1]) = \{f : [0, 1] \to \mathbb{R}, f \text{ has } m - 1 \text{ absolutely continuous derivatives}
\]

\[
f^{(1)}, \ldots, f^{(m-1)} \text{ and } \int_0^1 |f^{(m)}(x)|^2 dx < \infty\},
\]

and finding \(\hat{f}_n \in W^{m,2}([0, 1])\) which minimizes

\[
\frac{1}{n} \sum_{i=1}^n |Y_i - f(t_i)|^2 + \lambda \int_0^1 |f^{(m)}(x)|^2 dx,
\]

for some \(\lambda > 0\) that governs the trade-off between smoothness and goodness-of-fit. The problem is well-defined for \(n \geq m\) and its solution is a 2\(m\)th-order natural spline with knots at \(t_1, \ldots, t_n\). The subsequent least-squares smoothing spline can be computed very efficiently with the Kimeldorf-Wahba representer theorem and can be shown to attain the optimal rates of convergence, under the usual Gauss–Markov conditions on the error term. The interested reader is referred to Wahba (1990), Green and Silverman (1994) and Eubank (1999) for detailed theoretical developments and illustrative examples.

The focus of this paper is theoretical, as we aim show that, under weak assumptions, \(f_o\) may be optimally estimated even if the error lacks finite moments. The estimator in consideration is the M-type smoothing spline introduced by Huber (1979) and defined as a solution of

\[
\inf_{f \in W^{m,2}([0, 1])} \left[ \frac{1}{n} \sum_{i=1}^n \rho(Y_i - f(t_i)) + \lambda \int_0^1 |f^{(m)}(x)|^2 dx \right],
\]

for some convex non-negative function \(\rho\) that is symmetric about zero and satisfies \(\rho(0) = 0\). Clearly, the least-squares smoothing spline fulfils these conditions, but the benefit of the above formulation is that it allows for more general loss functions that reduce the effect of large residuals and make for resistant estimation of \(f_o\). Popular
examples include the resistant absolute value loss $|x|$ and Huber’s function

$$
\rho_k(x) = \begin{cases} 
\frac{x^2}{2}, & |x| \leq k \\
 k(|x| - k/2), & |x| > k 
\end{cases}
$$

where the tuning parameter $k$ controls the blending of square and absolute losses. It is shown below that under general conditions a solution to (3) in $W^{m,2}([0,1])$ exists, although, as Cox (1983) and Eggermont and LaRiccia (2009) remark, it may not be unique unless $\rho$ is strictly convex. Similarly to the least-squares setting, if $n \geq m$ then this minimizer must be a $2m$th-order natural spline with knots at the design points.

Traditionally in robust regression the losses are standardized with an equivariant scale estimator $\hat{\sigma}$ in order to achieve scale equivariance of the regression estimator. The M-type smoothing spline estimator defined in (3) cannot, in general, be scale equivariant even after this standardization on account of the penalty term. Nevertheless, we may define an "approximately" equivariant estimator as the solution of

$$
\inf_{f \in W^{m,2}([0,1])} \left[ \frac{1}{n} \sum_{i=1}^n \rho \left( \frac{Y_i - f(t_i)}{\hat{\sigma}} \right) + \lambda \int_0^1 |f^{(m)}(x)|^2 dx \right].
$$

Originally, Huber (1979) proposed simultaneous scale estimation, but nowadays it is recognized that preliminary scale estimates tend to perform better (see, e.g., Maronna et al. 2019). Such scale estimates may be obtained either from preliminary model fitting, that is, from fitting a robust regression estimator to the data and computing a robust scale from its residuals, or from robust scale estimates involving linear combinations of the $Y_i$s (Cunningham et al. 1991; Ghement et al. 2008). Inclusion of $\hat{\sigma}$ adds a new theoretical layer to the smoothing spline problem, and its asymptotic properties influence those of the smoothing spline estimator.

In stark contrast to least-square smoothing splines, where numerous theoretical results have been obtained ranging from equivalent kernels to convergence rates of the derivatives, only a few works have delved into the theory of general M-type smoothing splines. Cox (1983) and Oh et al. (2007) obtained an asymptotic linearization of M-type estimators with $\rho$ functions in $C^3(\mathbb{R})$ and used this to show that smooth M-type estimators attain the least-squares convergence rates. Cunningham et al. (1991) complemented the work of the first author by showing that for the special case of $m = 2$ the optimal rates of convergence are retained if one uses a root-n preliminary scale provided that the error term possesses a first moment. van de Geer (2002) was able to reduce the smoothness requirements to a Lipschitz condition on $\rho$, but her work does not address either the case of auxiliary scale estimates or estimation of derivatives. Finally, Eggermont and LaRiccia (2009) study the least-absolute deviations smoothing spline in detail, but only under the assumption that it is asymptotically contained in a ball around $f_o$.

We provide a unified treatment of the M-type smoothing spline problem in this paper, including preliminary scale estimation and estimation of derivatives. Our main assumptions center around a convex loss function, two mild regularity conditions on the errors $\epsilon_i$ that have been widely used in the non-penalized case, and approximate
uniformity of the design points. For well-chosen loss functions, these conditions do not require the existence of any moments of the error allowing for very heavy-tailed distributions, under which the least-squares estimator may fail to be consistent. Furthermore, we show that these conditions barely change with the inclusion of auxiliary scale estimates constructed either from pseudo-residuals or preliminary regression estimates. Our treatment is potentially of independent mathematical interest, as it relies on the theory of reproducing kernel Hilbert spaces instead of the nowadays commonly used theory of empirical processes (van de Geer 2000, 2002).

2 Main results: existence of solutions and rates of convergence

We begin by introducing some useful notation. We denote the standard $L^2([0, 1])$ inner product by $\langle \cdot, \cdot \rangle_2$. Its associated norm $\| \cdot \|_2$ is given by $\langle f, f \rangle_2^{1/2}$ for any $f \in L^2([0, 1])$. Throughout, we endow $W^{m,2}([0, 1])$ with the inner product given by

$$\langle f, g \rangle_{m, \lambda} = \langle f, g \rangle_2 + \lambda \langle f^{(m)}, g^{(m)} \rangle_2,$$

for any $f, g \in W^{m,2}([0, 1])$. The associated norm is denoted by $\| \cdot \|_{m, \lambda}$. Norms depending on the smoothing parameter have also been used by Silverman (1996) and Eggermont and LaRiccia (2009), for example. Denoting the M-type smoothing spline by $\hat{f}_n$, we shall see that an advantage of this norm is that establishing rates of convergence with respect to $\| \hat{f}_n - f_0 \|_{m, \lambda}$ will semi-automatically yield rates of convergence for the derivatives with respect to $\| \cdot \|_2$.

By an extension of the Sobolev embedding theorem, Eggermont and LaRiccia (2009) showed that for all $x \in [0, 1]$, all $f \in W^{m,2}([0, 1])$ and all $\lambda \in (0, 1)$, there exists a constant $c_m$, depending only on $m$, such that

$$|f(x)| \leq \frac{c_m}{\lambda^{1/4m}} \| f \|_{m, \lambda}.$$  

This result implies that point evaluation is a continuous linear functional with inner product (5). It follows that $W^{m,2}([0, 1])$ is a reproducing kernel Hilbert space and there exists a symmetric function $R_{m, \lambda}(x, \cdot)$, the reproducing kernel, such that $R_{m, \lambda}(x, \cdot) \in W^{m,2}([0, 1])$ for every $x \in [0, 1]$ and for every $f \in W^{m,2}([0, 1])$,

$$f(x) = \langle f, R_{m, \lambda}(x, \cdot) \rangle_{m, \lambda}.$$  

Consequently, by (6),

$$\sup_{x \in [0, 1]} \| R_{m, \lambda}(x, \cdot) \|_{m, \lambda} \leq \frac{c_m}{\lambda^{1/4m}},$$

with the same constant $c_m$. The above bounds will play a key role in the establishment of our results.

We first deal with the existence of the M-type smoothing spline and show that problem (3) is well-defined, in the sense that it possesses at least one solution in
We consider $\mathcal{W}^{m,2}([0, 1])$. The theorem requires only a weak form of continuity of $\rho$ and may therefore be useful in other settings as well.

**Theorem 1** If $\rho$ is a non-negative, lower semicontinuous loss function and $n \geq m$, the minimization problem

$$
\inf_{f \in \mathcal{W}^{m,2}([0,1])} \left[ \frac{1}{n} \sum_{i=1}^{n} \rho \left( Y_i - f(t_i) \right) + \lambda \left\| f^{(m)} \right\|^2_2 \right],
$$

has a solution in $\mathcal{W}^{m,2}([0, 1])$.

Arguing in a standard way now shows that a minimizer may be found in the $n$-dimensional space of natural splines of order $2m$ with knots at $t_1, \ldots, t_n$. Convex $\rho$-functions satisfy the condition of Theorem 1, being continuous. It is worth noting, however, that the conditions of the theorem are satisfied much more broadly, e.g., by bounded $\rho$-functions such as Tukey’s bisquare. As mentioned previously, existence can be strengthened to uniqueness if one uses a strictly convex $\rho$-function, such as the logistic $\rho$-function. See Proposition 2.1 of Cox (1983).

We may now treat the asymptotics of M-type estimators with scale either known or, more realistically, not needed. The required regularity conditions on $\rho$, the error term and the design points $t_1, \ldots, t_n$ are as follows.

(A1) The loss function $\rho(x)$ is absolutely continuous and convex with $\psi(x)$ any choice of its subgradient.

(A2) There exist finite constants $\kappa$ and $M_1$ such that for all $x \in \mathbb{R}$ and $|y| < \kappa$,

$$
|\psi(x + y) - \psi(x)| \leq M_1.
$$

(A3) There exists a finite constant $M_2$ such that

$$
\sup_{|r| \leq h} \mathbb{E}[|\psi(\epsilon_1 + r) - \psi(\epsilon_1)|^2] \leq M_2|h|,
$$

as $h \to 0$.

(A4) $\mathbb{E}[|\psi(\epsilon_1)|^2] \leq \tau^2 < \infty$, $\mathbb{E}[\psi(\epsilon_1)] = 0$ and there exists a constant $\xi > 0$ such that

$$
\mathbb{E}\{\psi(\epsilon_1 + t)\} = \xi t + o(t), \quad \text{as} \quad t \to 0.
$$

(A5) The family of the design points $\{t_i\}_{i=1}^{n}$ is quasi-uniform in the sense of Eggermont and LaRiccia (2009), that is, there exists a constant $M_3$ such that, for all $n \geq 2$ and all $f \in \mathcal{W}^{1,1}([0, 1])$,

$$
\left| \frac{1}{n} \sum_{i=1}^{n} f(t_i) - \int_{0}^{1} f(t)dt \right| \leq \frac{M_3}{n} \int_{0}^{1} |f'(t)|dt
$$

Condition (A1) is standard in the asymptotic theory of M-estimators for unpenalized linear models (see, for example, Yohai and Maronna 1979; Bai and Wu 1994).
Condition (A2) requires that $\psi$ has uniformly bounded local increments and is the only condition that is imposed directly on $\psi$. This needs to be contrasted with the restrictive smoothness conditions of Cox (1983), Cunningham et al. (1991) and Oh et al. (2007), all of whom assumed a twice-differentiable $\psi$-function with bounded second derivative. In the same spirit, conditions (A3)–(A4) trade differentiability of $\psi$ with some regularity of the distribution of the error term. They are very mild. Condition (A3) is a mean-square continuity condition on $m(t) := \psi(\epsilon_1 + t)$ and holds quite generally. For example, Bai and Wu (1994) demonstrated that in some cases it may be possible to have the much tighter bound $M_2|h|^2$ on the right-hand side of the inequality, even for $\psi$-functions that have jumps. See also Welsh (1989) for this point. Condition (A4) ensures the Fisher-consistency of the estimates and has been widely used for many types of M-estimators (see Huber and Ronchetti 2009; Maronna et al. 2019) for relevant discussions. A number of interesting estimators can be covered by condition (A4), as we now show.

Example 1 (LAD and quantile regression). Consider M-estimation with $\rho(x) = |x|$. Then, provided that $\epsilon_1$ has a distribution function $F$ that is symmetric about zero and a positive density $f$ on an interval about zero,

$$
\mathbb{E}\{|\text{sign}(\epsilon_1 + t)|\} = 2f(0) + o(t), \quad \text{as} \quad t \to 0.
$$

(cfr. Pollard 1991). This generalizes easily to M-estimation with $\rho_\alpha(x) = |x| + (2\alpha - 1)x$, provided that in this case one views the regression function as the $\alpha$-quantile function, that is, $\text{Pr}(Y_i \leq f_o(t_i)) = \alpha$.

Example 2 (Huber). For $k > 0$, $\psi_k(x) = \max\{-k, \min\{x, k\}\}$ and we may assume that $F$ is absolutely continuous and symmetric about zero so that

$$
\mathbb{E}\{\psi_k(\epsilon_1 + t)|\} = (2F(k - 1) - 1) + o(t), \quad \text{as} \quad t \to 0.
$$

The term $2F(k) - 1$ is strictly positive for all $k > 0$ under these assumptions.

Example 3 ($L^p$ regression estimates with $1 < p < 2$). Clearly, $\psi_p(x) = p|x|^{p-1}\text{sign}(x)$ and if we assume that $F$ is symmetric about zero, $\mathbb{E}\{|\epsilon_1|^{p-1}\} < \infty$ and $\mathbb{E}\{|\epsilon|^{p-2}\} < \infty$ then

$$
\mathbb{E}\{\psi_p(\epsilon_1 + t)|\} = p(p-1)\mathbb{E}\{|\epsilon|^{p-2}\}t + o(t), \quad \text{as} \quad t \to 0,
$$

(see Arcones 2000). The latter expectation is finite, if, e.g., $F$ possesses a Lebesgue density $f$ that is bounded at an interval about zero.

Example 4 (Expectile regression). As an alternative to the check loss, consider the expectile loss $\rho_\alpha(x) = x^2/2|\alpha - \mathbb{I}(x \leq 0)|$ with $\alpha \in (0, 1)$, such that $\psi_\alpha(x) = (1 - \alpha)x\mathbb{I}(x \leq 0) + \alpha x \mathbb{I}(x > 0)$. Assuming that there exists an interval about zero on which $F$ has no atoms, we have

$$
\mathbb{E}\{\psi_\alpha(\epsilon_1 + t)|\} = [\alpha + (1 - 2\alpha)F(0)]t + o(t), \quad \text{as} \quad t \to 0.
$$

Therefore, assumption (A4) holds with $\xi = \alpha + (1 - 2\alpha)F(0)$ and this is bounded away from zero and infinity for all $\alpha \in (0, 1)$. 

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Example 5 (Smooth ρ-functions). All monotone everywhere differentiable score functions \( \psi \) with bounded second derivative \( \psi''(x) \), resulting, for example, from \( \rho(x) = \log(\cosh(x)) \), satisfy the second part of assumption (A4) provided that \( \mathbb{E}\{\psi'(\epsilon_i)\} > 0 \). This is a classical Fisher-consistency for M-estimators based on differentiable score functions (see Maronna et al. 2019).

It should be noted that although for convenience (A3) and (A4) are stated here with independent and identically distributed errors in mind, these conditions can be weakened to include solely independent errors. In that case we would require some shared regularity of the errors and restate (A3) as

\[
\sup_n \max_{1 \leq i \leq n} \mathbb{E}\{|\psi(\epsilon_i + t) - \psi(\epsilon_i)|^2\} \leq M_2|h|,
\]

for some finite \( M_2 \), as \( h \to 0 \). Similarly, to extend (A4) to independent errors we would require

\[
\sup_n \max_{1 \leq i \leq n} \mathbb{E}\{|\psi(\epsilon_i)|^2\} \leq \tau^2, \quad \mathbb{E}\{|\psi(\epsilon_i)|\} = 0, \quad \mathbb{E}\{|\psi(\epsilon_i + t)|\} = \xi_i t + o(t),
\]

as \( t \to 0 \) for \( i = 1, \ldots, n \), with

\[
0 < \inf_n \min_{1 \leq i \leq n} \xi_i \leq \sup_n \max_{1 \leq i \leq n} \xi_i < \infty.
\]

Finally, condition (A5) ensures that the responses are observed at a sufficiently regular grid. It is a quite weak assumption that can be shown to hold for all frequently employed designs such as \( t_i = i/n \) or \( t_i = 2i/(2n+1) \). Call \( G_n \) the distribution function that jumps \( n^{-1} \) at each \( t_i \). An integration by parts argument shows

\[
\frac{1}{n} \sum_{i=1}^{n} f(t_i) - \int_{0}^{1} f(x)dx = \int_{0}^{1} \{x - G_n(x)\} f'(x)dx,
\]

and (A5) is satisfied, if, for example, \( G_n \) approximates well the uniform distribution function in the Kolmogorov metric.

It should also be noted that none of the loss functions in examples 1–4 are covered by the theory of Cox (1983) and Oh et al. (2007), while the Lipschitz condition employed by van de Geer (2002) leaves out \( L^p \) and expectile smoothing spline estimators, among others. Our first asymptotic result is Theorem 2, which establishes the optimality of general M-type smoothing splines, provided that the smoothing parameter \( \lambda \) decays to zero a little more slowly than in the typical least-squares smoothing spline problem.

**Theorem 2** Assume (A1)–(A5), \( \lambda \to 0 \) and \( n\lambda^{3/2m-1/4m^2} \to \infty \), as \( n \to \infty \). Then there exists a sequence of M-type smoothing splines \( \hat{f}_n \) satisfying

\[
||\hat{f}_n - f_o||_{m,\lambda}^2 = O_P \left( \lambda + (n\lambda^{1/2m})^{-1} \right).
\]

The limit requirements of Theorem 2 replace the least-squares requirements \( \lambda \to 0 \) and \( n\lambda^{1/2m} \to \infty \), as \( n \to \infty \). For \( \lambda \asymp n^{-2m/(2m+1)} \) these conditions are met and we are lead to

\[
||\hat{f}_n - f_o||_{m,\lambda}^2 = O_P(n^{-2m/(2m+1)}),
\]

which is the optimal rate of convergence for \( f_o \in \mathcal{W}_m^2([0, 1]) \) (Stone 1982). Thus, a broad class of smoothing spline estimators
is theoretically optimal. Moreover, for such $\lambda$, Sobolev embedding theorem (6) allows us to deduce that $||\hat{f}_n - f||_\infty = O_P(n^{(1-2m)/(2m+1)})$, which implies that convergence can be made uniform.

Corollary 1 establishes (optimal) rates of convergence for the derivatives $\hat{f}_n^{(j)}$ for $j = 1, \ldots, m - 1$ and tightness of $\hat{f}_n^{(m)}$ in the $L^2([0, 1])$ metric.

**Corollary 1** Assume the conditions of Theorem 2 hold. Then, for any $\lambda \asymp n^{-2m/(2m+1)}$ the M-type sequence $\hat{f}_n$ of Theorem 2 satisfies

$$||\hat{f}_n^{(j)} - f^{(j)}||_2 = O_P\left(n^{-2(m-j)/(2m+1)}\right).$$

As noted previously, with the exception of the work of Eggermont and LaRiccia (2009) on the least-absolute deviations smoothing spline, we are unaware of results concerning derivatives of general M-type estimates. Corollary 1 serves to remedy this deficiency.

A rather interesting feature of the least-squares smoothing spline is the possibility for a bias reduction, under certain boundary conditions on the derivatives of $f_o$ (see, e.g., Rice and Rosenblatt 1981; Eubank 1999). This phenomenon leads to superior convergence rates and is known as super-convergence. As Corollary 2 shows, super-convergence carries over to the general M-case.

**Corollary 2** Assume the conditions of Theorem 2 hold and further that $f_o \in W^{2m,2}([0, 1])$ and $f_o^{(s)}(0) = f_o^{(s)}(1) = 0$ for all $m \leq s \leq 2m - 1$. Then, there exists a sequence of M-type smoothing splines $\hat{f}_n$ satisfying

$$||\hat{f}_n - f_o||_{m, \lambda} = O_P\left(\lambda^2 + (n^{1/2m})^{-1}\right).$$

A consequence of this corollary is that if $\lambda \asymp n^{-2m/(4m+1)}$ then $f_o$ can be estimated with an integrated squared error decaying like $n^{-4m/(4m+1)}$ asymptotically. Of course, had we suspected that $f_o \in W^{2m,2}([0, 1])$ then an appropriate modification of the penalty would also yield the rate $n^{-4m/(4m+1)}$. In this light, as Eubank (1999, p. 259) notes, the higher rate of convergence may be viewed as a bonus of the smoothing-spline estimator for some situations where the regression function is smoother than anticipated.

We now turn to the problem of M-type smoothing splines with an auxiliary scale estimate. We aim to extend Theorem 2 and its corollaries to this case under suitable assumptions on $\rho$, $\epsilon$ and $\hat{\sigma}$. The revised set of assumptions is as follows.

(B1) $\rho$ is a convex function on $\mathbb{R}$ with derivative $\psi$ that exists everywhere and is Lipschitz. Further, for any $\epsilon > 0$ there exists $M_\epsilon$ such that

$$|\psi(tx) - \psi(sx)| \leq M_\epsilon |t - s|,$$

for any $t > \epsilon$, $s > \epsilon$ and $-\infty < x < \infty$. 

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(B2) For any $\alpha > 0$, $E\{\psi(\epsilon_1/\alpha)\} = 0$ and

$$E \left\{ \psi \left( \frac{\epsilon_1}{\alpha} + t \right) \right\} = \xi(\alpha)t + o(t), \quad \text{as} \quad t \to 0,$$

for some function $\xi(\alpha)$ such that $0 < \inf_{|\sigma - \alpha| \leq \delta} \xi(\alpha) \leq \sup_{|\sigma - \alpha| \leq \delta} \xi(\alpha) < 0$ for some $\delta > 0$.

(B3) $n^{m/(2m+1)}(\hat{\sigma} - \sigma) = O_P(1)$, for some $\sigma > 0$ that need not be the standard deviation of $\epsilon_1$.

(B4) Assume (B1)–(B4) and further that $\lambda \to 0$ and $n\lambda^{1/m} \to \infty$, as $n \to \infty$.

Then there exists a sequence of M-type smoothing splines $\hat{f}_{n,\hat{\sigma}}$ satisfying

$$||\hat{f}_{n,\hat{\sigma}} - f_0||^2_{m,\lambda} = O_P \left( \lambda + (n\lambda^{1/(2m)})^{-1} \right).$$

Since the proofs of Corollaries 1 and 2 regarding optimal estimation of derivatives and bias reduction do not depend on the existence of a scale estimate, they carry over immediately to this setting.

As requested by a reviewer, we may also seek conditions ensuring the extension of the above results to the case of a random design, that is, to the case where $t_i, i = 1, \ldots, n$, are i.i.d. random variables with distribution $G$. The main complication in this setting is that (A5) may fail to hold due to the comparatively lower rate of convergence of the empirical distribution to its population counterpart in the uniform metric. Nevertheless, inspection of the proofs reveals that such an extension is indeed
possible after the modification of (A5) given below. To better indicate the randomness of the design points we now write \( T_1, \ldots, T_n \) instead of the previous \( t_1, \ldots, t_n \).

\( (A5)' \) The design variables \( T_1, \ldots, T_n \) are independent and identically distributed with Lebesgue density \( g \) that is bounded away from zero and infinity on \([0, 1]\), and are also independent of the errors \( \epsilon_1, \ldots, \epsilon_n \).

The assumption of a bounded density goes back at least to Stone (1985) and has been extensively used in nonparametric regression. With this assumption in place, Theorem 4 now replaces Theorem 2.

**Theorem 4** Assume (A1)–(A4), (A5′), \( \lambda \to 0 \) and \( n\lambda^{3/2m - 1/4m^2} \to \infty \), as \( n \to \infty \). Then there exists a sequence of M-type smoothing splines \( \hat{f}_n \) satisfying

\[
||\hat{f}_n - f_o||^2_{m, \lambda} = O_P \left( \lambda + (n\lambda^{1/2m})^{-1} \right).
\]

An extension of Theorem 3 to the present setting is now completely analogous under the understanding that (B5) there is replaced with condition (A5′), as are the extensions of Corollary 1 and Corollary 2. We omit the details.

### 3 Computation and smoothing parameter selection

As discussed in Sect. 2, there exists at least one solution of (3) in the space of natural splines of order \( 2m \) with knots at the unique \( t_i \). Thus we may restrict attention to the linear subspace of natural splines for the computation of the estimator. Here, we assume that the scale is known and equal to one; if that is not true, the scale can be absorbed into the \( \rho \)-function and all the arguments of this section still apply. Assume for simplicity that all \( t_i \) are distinct and let \( a = \min_i t_i > 0 \) and \( b = \max_i t_i < 1 \). Then the natural spline \( f \) has \( n \) interior knots and we may write

\[
f(t) = \sum_{k=1}^{n+2m} f_k B_k(t),
\]

where \( f_k \) are scalar coefficients and the \( B_k(\cdot) \) are the B-spline basis functions of order \( 2m \) supported by the knots at \( t_i \). It is well-known that the space of natural splines with \( n \) interior knots is \( n \)-dimensional on account of the boundary conditions that force the natural spline to be a polynomial of order \( m \) outside \([a, b]\), but for the moment we operate in the larger \((n + 2m)\)-dimensional spline subspace. This is computationally convenient due to the local support and numerical stability of B-splines. As we explain below, the penalty automatically imposes the boundary conditions (see also Hastie et al. 2009, pp. 161–162).

Working in the unrestricted spline subspace, the solution to (3) or (4) may be written as \( \hat{f}_n = \sum_{k=1}^{n+2m} \hat{f}_k B_k(t) \) where \( \hat{f} = (\hat{f}_1, \ldots, \hat{f}_{n+2m})^\top \) satisfies

\[
\hat{f} = \arg\min_{f \in \mathbb{R}^{n+2m}} \left[ \frac{1}{n} \sum_{i=1}^{n} \rho \left( Y_i - B_i^\top f \right) + \lambda f^\top P f \right],
\]

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with \( \mathbf{B}_i = (B_1(t_i), \ldots, B_{n+2m}(t_i))^\top \) and \( \mathbf{P} = \langle B_k^{(m)}, B_l^{(m)} \rangle \), \( k, l = 1, \ldots, n + 2m \).

Initially, it may seem that this formulation ignores the boundary constraints that govern natural splines, but it turns out the penalty term automatically imposes them. The reasoning is as follows: if that were not the case, it would always be possible to find a \( 2m \)-th order natural interpolating spline of the form of (9) that leaves the first term in (3) unchanged, but due to it being a polynomial of order \( m \) outside of \([a, b] \subset [0, 1]\) the penalty semi-norm would be strictly smaller. Hence, any minimizer in the form of (9) incorporates the boundary conditions.

The solution to (10) may be expediently found through minor modification of the penalized iteratively reweighted least-squares algorithm found in, e.g., Maronna (2011). The algorithm consists of solving a weighted penalized least-squares problem at each iteration until convergence, which is guaranteed irrespective of the starting values and yields a stationary point of (3), under mild conditions on \( \rho \) that include the boundedness of \( \rho'(x)/x \) near zero (Huber and Ronchetti 2009). For the quantile loss, this condition fails on account of the kink at the origin. Nevertheless, the easily implementable recipe of Nychka et al. (1995) may be used in order to obtain an approximate solution of (3). In particular, in the algorithm the loss function can be replaced by the smooth approximation

\[
\tilde{\rho}_\alpha(x) = \begin{cases} 
\rho_\alpha(x) & \text{if } |x| \geq \epsilon \\
\alpha x^2/\epsilon & 0 \leq x < \epsilon \\
(1-\alpha)x^2/\epsilon & -\epsilon < x \leq 0,
\end{cases}
\]

for some small \( \epsilon > 0 \). The objective function \( \tilde{\rho}_\alpha \) allows to easily calculate an approximate quantile smoothing spline estimate with this algorithm, without the need of a more computationally burdensome quadratic program. Whenever such a modification of the objective function is not feasible, we recommend utilizing a convex-optimization program in order to identify a minimizer of (10), as given, for example, by Fu et al. (2020).

In order to select the smoothing parameter \( \lambda \) we propose to use the weighted generalized cross-validation criterion proposed by Cunningham et al. (1991). That is, we propose to select \( \lambda \) as the minimizer of

\[
\text{GCV}(\lambda) = \frac{n^{-1} \sum_{i=1}^{n} W_i (\hat{f}_n)(r_i(\hat{f}_n))^2}{|1-n^{-1} \text{Tr} \mathbf{H}(\lambda)|^2},
\]

where \( r_i(\hat{f}_n) = Y_i - \hat{f}_n(t_i) \), \( W_i(\hat{f}_n) = \psi(r_i(\hat{f}_n))/r_i(\hat{f}_n) \), \( i = 1, \ldots, n \), and \( \mathbf{H}(\lambda) \) is the pseudo-influence matrix obtained upon convergence. Throughout the simulation experiments and real-data examples to follow we have adopted a two-step approach in order to identify the minimizer of GCV(\( \lambda \)). First, we have determined the approximate location of the minimizer by evaluating GCV(\( \lambda \)) on a grid and afterward employed a numerical optimizer based on golden section search and parabolic interpolation (Nocedal and Wright 2006). Such a hybrid approach is often advisable due to the possible local minima and near-flat regions of the GCV criterion, particularly for non-smooth loss functions.
4 A Monte Carlo study

In our simulation experiments we compare the performance of the Huber-type smoothing spline with tuning parameter equal to 1.345 corresponding to 95% efficiency in the location model, the least-absolute deviation smoothing spline and the least-squares smoothing spline in a variety of shapes of the regression function and tails of the error. For the Huber-type estimator we compute the scale in two ways, reflecting the asymptotic considerations of Sect. 2.

On the one hand, we use a robust scale constructed from consecutive differences of the response variables, as proposed by Ghement et al. (2008). In particular, we use the M-scale estimator \( \hat{\sigma} \) obtained as the solution of

\[
\frac{1}{n-1} \sum_{i=1}^{n-1} \rho \left( \frac{Y_{i+1} - Y_i}{2^{1/2}\hat{\sigma}} \right) = \frac{3}{4},
\]

where \( \rho \) is the Tukey loss function with tuning parameter equal to 0.704. The constants \( 2^{1/2} \) and \( 3/4 \) ensure Fisher-consistency of the estimator at the Gaussian distribution and maximal breakdown value, respectively. On the other hand, call \( r \) the residual vector that results from an initial \( L_1 \)-type smoothing spline fit to the data. A robust scale that converges slower than root-\( n \) is

\[
\hat{\sigma}_{PR} = \tau(r),
\]

where \( \tau(\cdot) \) stands for the \( \tau \)-scale introduced by Yohai and Zamar (1988). In our implementation we used the Tukey bisquare loss function and cutoff constants equal to 4.5 and 3 for the biweighting of the mean and the \( \rho \)-function, respectively, as recommended by Maronna and Zamar (2002). As discussed in introduction, the least-absolute deviations smoothing spline does not require an auxiliary scale estimate. We denote the resulting smoothing splines by \( \hat{f}_{HPS} \) and \( \hat{f}_{HPR} \), respectively, while we use \( \hat{f}_{LAD} \) and \( \hat{f}_{LS} \) as abbreviations for the least-absolute deviations smoothing spline and the least-squares smoothing spline, respectively.

We investigate the performance of the estimators in the regression model \( Y_i = f(t_i) + \epsilon_i \) where \( t_i = (i - 1/2)/n \) and \( f_o \) is each of the following three functions

1. \( f_1(t) = \cos(2\pi t) \),
2. \( f_2(t) = 1/(1 + \exp(-20(t - 0.5))) \),
3. \( f_3(t) = \sin(2\pi t) + e^{-3(t-0.5)^2} \).

All three regression functions are smooth; the first regression function is bowl-shaped, the second is a sigmoid and the third is essentially a shifted sinusoid with more variable slope. We shall estimate these functions with cubic smoothing splines, that is, with \( m = 2 \). In order to assess the effect of outliers on the estimates different distributions for the error term were considered. Other than the standard Gaussian distribution, we have complemented our setup with a t-distribution with 3 degrees of freedom, a right-skewed t-distribution with 3 degrees of freedom and non-centrality parameter equal to 2, a mixture of mean-zero Gaussians with standard deviations equal to 1.
Table 1  Means and standard errors of 1000 MSEs with $n = 60$ of the Huber-type estimator with preliminary scale, the Huber-type estimator with scale computed from robust regression residuals, the least-absolute deviations estimator and the least-squares estimator

| $f$ | Dist.  | $\hat{f}_{HPS}$ |  | $\hat{f}_{HPR}$ |  | $\hat{f}_{LAD}$ |  | $\hat{f}_{LS}$ |  |
|-----|--------|-----------------|---|-----------------|---|-----------------|---|-----------------|---|
|     |        | Mean | SE | Mean | SE | Mean | SE | Mean | SE | Mean | SE |
| $f_1$ | Gaussian | 0.087 | 0.002 | 0.086 | 0.002 | 0.114 | 0.002 | 0.082 | 0.002 |
|      | $t_3$   | 0.125 | 0.003 | 0.125 | 0.003 | 0.137 | 0.003 | 0.216 | 0.016 |
|      | $st_{3,2}$ | 0.771 | 0.008 | 0.794 | 0.008 | 0.649 | 0.008 | 1.108 | 0.014 |
|      | M. Gaussian | 0.138 | 0.004 | 0.139 | 0.003 | 0.146 | 0.004 | 0.719 | 0.020 |
|      | Slash | 0.520 | 0.013 | 0.515 | 0.012 | 0.389 | 0.009 | 766.6 | 352.9 |
| $f_2$ | Gaussian | 0.064 | 0.001 | 0.064 | 0.001 | 0.081 | 0.002 | 0.065 | 0.001 |
|      | $t_3$ | 0.091 | 0.002 | 0.090 | 0.002 | 0.101 | 0.002 | 0.153 | 0.056 |
|      | $st_{3,2}$ | 0.767 | 0.008 | 0.765 | 0.008 | 0.635 | 0.007 | 1.107 | 0.014 |
|      | M. Gaussian | 0.097 | 0.004 | 0.095 | 0.004 | 0.106 | 0.003 | 0.562 | 0.019 |
|      | Slash | 0.345 | 0.011 | 0.331 | 0.011 | 0.286 | 0.008 | 7997 | 6934 |
| $f_3$ | Gaussian | 0.117 | 0.003 | 0.117 | 0.003 | 0.166 | 0.002 | 0.099 | 0.002 |
|      | $t_3$ | 0.182 | 0.003 | 0.183 | 0.003 | 0.192 | 0.003 | 0.234 | 0.005 |
|      | $st_{3,2}$ | 0.793 | 0.008 | 0.816 | 0.008 | 0.721 | 0.008 | 1.134 | 0.015 |
|      | M. Gaussian | 0.203 | 0.004 | 0.204 | 0.004 | 0.203 | 0.003 | 0.734 | 0.019 |
|      | Slash | 0.518 | 0.011 | 0.512 | 0.010 | 0.418 | 0.008 | 1e+08 | 1e+08 |

and 9 and weights equal to 0.85 and 0.15, respectively, as well as Tukey’s Slash distribution defined as the quotient of independent standard Gaussian and uniform random variables.

All computations were carried out in the freeware R (R Core Team 2018). For ease of comparison all smoothing spline estimators were computed using custom-made functions implementing the method outlined in Sect. 3. For all smoothing spline estimators the penalty parameter was selected via the GCV criterion given in Sect. 3. A link to the implementations used in this experiment is given at the end of this paper. The mean-squared errors of the experiment are summarized in Table 1 for sample sizes of 60 and 1000 replications.

The results in Table 1 indicate the extreme sensitivity of the least-squares estimator to even mild deviations from the ideal assumptions. In particular, the regular t-distribution with 3 degrees of freedom and the mixture-Gaussian distribution have finite second moments and first moments equal to zero, so that the least-squares assumptions are technically fulfilled. Nevertheless, in all three of our examples the performance of the least-squares estimator markedly deteriorates as one moves away from the Gaussian ideal. By contrast, the robust estimators almost match the performance of the least-squares estimator in ideal data and exhibit a large degree of resistance in the t- and mixture Gaussian distributions. Quite notably, the robust estimators seem somewhat vulnerable to asymmetric contamination, although they still outperform the least-squares estimator in this setting. Their performance also deteriorates with the
heavy-tailed Slash distribution but clearly not to the same extent as the performance of the least-squares estimator, which appears to suffer a catastrophic breakdown.

Comparing the robust estimators $\hat{f}_{HPS}$, $\hat{f}_{HPR}$ and $\hat{f}_{LAD}$ in detail, it is seen that the Huber estimators outperform the least-absolute deviation estimator in the case of Gaussian, $t_3$ and mixture Gaussian errors but get outperformed in turn under skewed-t and Slash errors. These facts indicate the resistance of the least-absolute deviations estimator both with respect to asymmetric contamination and gross outliers. The Huber estimators $\hat{f}_{HPS}$ and $\hat{f}_{HPR}$ overall exhibit similar performance, except in the case of heavy contamination where the latter estimator has a slight edge on account of its more robust scale. However, this advantage comes at the price of additional computational effort, as $\hat{f}_{HPR}$ depends on the computation of two robust smoothing spline estimators. Overall, the present experiment indicates that the computationally simple $\hat{f}_{HPS}$ presents a viable alternative to $\hat{f}_{LS}$ in clean data and to $\hat{f}_{HPR}$ in mildly contaminated data.

5 Real data example: urban air pollution in Italy

The present dataset consists of air pollution measurements from a gas multi-sensor device that was deployed in an undisclosed Italian city (De Vito et al. 2008). In particular, the dataset contains 7396 instances of hourly averaged responses from an array of 5 metal oxide chemical sensors embedded in the device. In this study we will focus on the effect of temperature on the concentration of benzene and nitrogen oxides in the atmosphere, the full dataset being available at http://archive.ics.uci.edu/ml/datasets/Air+quality. These gases are known carcinogens and are responsible for a series of acute respiratory conditions in high concentrations, so that the ability to forecast high concentrations may be helpful. Figure 1 presents the scatter plots of benzene concentrations versus temperature and nitrogen oxides concentration versus temperature on the left and right panel, respectively.
The scatter plots indicate the presence of several atypical observations in the form of abnormally high concentrations at certain temperature ranges. Specifically, the concentration of benzene seems more volatile in medium temperatures, while the concentration of nitrogen oxides seems more unpredictable in lower temperatures. Computing the least-squares and Huber-type with preliminary scale smoothing splines yields the solid red and solid blue curves, respectively. It may be immediately seen that although the resulting smoothing spline estimates do not qualitatively differ as to their main features, the least-squares estimate is more drawn toward these atypically high concentrations resulting in overestimation of the concentrations, particularly in the case of nitrogen oxides.

For a better understanding of the discrepancy between these estimates, Fig. 1 also includes a color and shape coding of the weights \( \psi(r_i)/r_i \) produced by the Huber estimator. Here, \( r_i \) stands for the ith residual, i.e., \( r_i = y_i - \hat{f}(t_i) \), \( i = 1, \ldots, n \). These weights demonstrate the usefulness of M-estimators with bounded score functions: while the least-squares estimator assigns equal weight to all observations and is thus unduly influenced by outliers, robust M-estimators significantly downweight observations sufficiently far from the center of the data resulting in resistant estimates. These atypical observations produce large residuals, which in turn allow for their detection. We may think of numerous examples in economics, medicine and other fields where resistant estimation combined with the possibility of outlier detection can be similarly useful.

Lastly, to examine the characteristics of the conditional distributions of the gases given the temperature, one may wish to obtain nonparametric estimates of the conditional quantiles. Figure 2 presents quantile smoothing spline estimates for the 10th, 30th, 50th, 70th and 90th percentiles. The estimates serve to confirm the extreme heavy-tailedness of the conditional distributions for medium and medium-low temperatures, casting doubt on the suitability of the least-squares estimator.
6 Concluding remarks

The asymptotic results of this paper indicate that there is little theoretical difference between least-squares smoothing splines and general M-type smoothing splines derived from convex but possibly non-smooth objective functions. In particular, under general conditions, M-type smoothing splines enjoy the same rates of convergence for the regression function as well as its derivatives. Furthermore, the presence of reasonable auxiliary scale estimates does not diminish these rates. In practice, M-type smoothing splines may be efficiently computed with the convenient B-spline representation and well-established iterative algorithms and may be used to good effect in either regular or contaminated datasets. Thus, this broad family of estimators provides a valuable tool for the applied scientist.

We believe that at least two extensions of the present paper would be of great interest to theoreticians and practitioners alike. The first concerns the problem of estimating the smoothing parameter $\lambda$, which was barely touched upon in this paper. We conjecture that the robust generalized cross-validation criterion proposed by Cunningham et al. (1991) would yield the optimal rate of decay for $\lambda$, but formal verification is required. Another useful extension would be to the case of dependent errors, which arise, for example, in mean estimation of discretely sampled functional data. We firmly believe that M-type smoothing spline estimators with repeated measurements would still enjoy the optimal rates, as derived by Cai and Yuan (2011), while also providing a considerably safer estimation method in the presence of atypical observations.

Supplementary material

The electronic supplementary material related to this article contains proofs of the theoretical results.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s11749-021-00782-y.

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Declarations

Software availability R-scripts reproducing the simulation experiments and real-data examples are available in https://github.com/ioanniskalogridis/Smoothing-splines.

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