CONSTRAINED NONPARAMETRIC KERNEL REGRESSION:
ESTIMATION AND INFEERENCE

JEFFREY S. RACINE, CHRISTOPHER F. PARMETER, AND PANG DU

ABSTRACT. Restricted kernel regression methods have recently received much well-deserved attention. Powerful methods have been proposed for imposing monotonicity on the resulting estimate, a condition often dictated by theoretical concerns; see Hall, Huang, Gifford & Gijbels (2001) and Hall & Huang (2001), among others. However, to the best of our knowledge, there does not exist a simple yet general approach towards constrained nonparametric kernel regression that allows practitioners to impose any manner and mix of constraints on the resulting estimate. In this paper we generalize Hall & Huang’s (2001) approach in order to allow for equality or inequality constraints on a nonparametric kernel regression model and its derivatives of any order. The proposed approach is straightforward, both conceptually and in practice. A testing framework is provided allowing researchers to thereby impose and test the validity of the restrictions. Theoretical underpinnings are provided, illustrative Monte Carlo results are presented, and an application is considered.

JEL Classification: C12 (Hypothesis testing), C13 (Estimation), C14 (Semiparametric and nonparametric methods)

1. Introduction and Overview

Kernel regression methods can be found in a range of application domains, and continue to grow in popularity. Their appeal stems from the fact that they are robust to functional misspecification that can otherwise undermine popular parametric regression methods. However, one complaint frequently levied against kernel regression methods is that, unlike their parametric counterparts, there does not exist a simple and general method for imposing a broad set of conventional constraints on the resulting estimate. One consequence of this is that when people wish to impose conventional constraints on a nonparametric regression model they must often leave the kernel smoothing framework and migrate towards, say, a series regression framework in which it is relatively straightforward to impose such constraints, or they resort to non-smooth convex programming methods.

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One particular constraint that has received substantial attention in kernel regression settings is that of monotonicity. In the statistics literature, the development of monotonic estimators dates back to the likelihood framework of Brunk (1955). This technique later came to be known as ‘isotonic regression’ and, while nonparametric in nature (min/max), produced curves that were not smooth. Notable contributions to the development of this method include Hanson, Pledger & Wright (1973) who demonstrated consistency in two dimensions (Brunk (1955) focused solely on the univariate setting) and Dykstra (1983), Goldman & Ruud (1992) and Ruud (1995) who developed efficient computational algorithms for the general class of restricted estimators to which isotonic regression belongs.1 Mukerjee (1988) and Mammen (1991) developed methods for kernel-based isotonic regression and both techniques consist of a smoothing step using kernels (as opposed to interpolation) and an isonotonization step which imposes monotonicity.2 A more recent alternative to these kernel-based isotonic methods employs constrained smoothing splines. The literature on constrained smoothing splines is vast and includes the work of Ramsay (1988), Kelly & Rice (1990), Li, Naik & Swetits (1996), Turlach (1997) and Mammen & Thomas-Agnan (1999), to name but a few.

Recent work on imposing monotonicity on a nonparametric regression function includes Pelckmans, Espinoza, Brabanter, Suykens & Moor (2005), Dette, Neumeyer & Pilz (2006) and Chernozhukov, Fernandez-Val & Galichon (2007). Each of these approaches is nonparametric in nature with the last two being kernel-based. Dette et al. (2006) and Chernozhukov et al. (2007) use a method known as ‘rearrangement’ which produces a monotonically constrained estimator derived from the probability integral transformation lemma. Essentially one calculates the cumulative distribution of the fitted values from a regression estimate to construct an estimate of the inverse of the monotonic function which is inverted to provide the final estimate. Pelckmans et al. (2005) construct a monotone function based on least squares using the Chebychev norm with a Tikhonov regularization scheme. This method involves solving a standard quadratic program and is comparable to the spline-based methods mentioned above. Braun & Hall (2001) propose a method closely related to rearrangement which they call ‘data sharpening’ that also involves rearranging the positions of data values, controlled by minimizing a measure of the total distance that the data

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1An excellent overview of isotonic regression can be found in Robertson, Wright & Dykstra (1988).
2The order of these two steps is irrelevant asymptotically.
are moved, subject to a constraint. Braun & Hall (2001) apply the method to render a density estimator unimodal and to monotonize a nonparametric regression; see also Hall & Kang (2005).

One of the most promising (and extensible) approaches for imposing monotonicity on a nonparametric regression model is that of Hall & Huang (2001) who proposed a novel approach towards imposing monotonicity constraints on a quite general class of kernel smoothers. Their monotonically constrained estimator is constructed by introducing probability weights for each response data point which can dampen or magnify the impact of any observation thereby imposing monotonicity. The weights are global with respect to the sample and are chosen by minimizing a preselected version of the power divergence metric of Cressie & Read (1984). The introduction of the weights in effect transforms the response variable in order to achieve monotonicity of the underlying regression function. Additionally, Hall & Huang (2001, Theorem 4.3) show that when underlying relationship is strictly monotonic everywhere the constrained estimator is consistent and equivalent to the unrestricted estimator.

Though Hall & Huang’s (2001) method delivers a smooth monotonically constrained nonparametric kernel estimator, unfortunately, probability weights and power divergence metrics are of limited utility when imposing the range of conventional constraints of the type we consider herein. But a straightforward generalization of Hall & Huang’s (2001) method will allow one to impose a broad class of conventional constraints, which we outline in the proceeding section.

Imposing a broad class of conventional constraints on nonparametric surfaces has not received anywhere near the attention as has imposing monotonicity, at least not in the kernel regression framework. Indeed, the existing literature dealing with constraints in a nonparametric framework appears to fall into three broad categories:

(i) Those that develop nonparametric estimators which satisfy a particular constraint (e.g., monotonically constrained estimators).

(ii) Those that develop nonparametric estimators which can satisfy general conventional constraints (e.g., constrained smoothing splines).

(iii) Those that develop tests of the validity of constraints (e.g., concavity).

Tests developed in (iii) can be further subdivided into statistical and nonstatistical tests. The nonstatistical tests ‘check’ for violations of economic theory, such as indifference curves crossing or isoquants having the wrong slope; see Hanoch & Rothschild (1972) and Varian (1985). The statistical tests propose a metric used to determine if the constraints are satisfied and then develop the asymptotic properties of the proposed metric. These metrics are typically constructed from measures of fit for the unrestricted and restricted models and do not focus on pure ‘economic’ violations.

Early nonparametric methods designed to impose general economic constraints include Gallant (1981), Gallant (1982), and Gallant & Golub (1984) who introduced the Fourier Flexible Form estimator (FFF) which is a series-based estimator whose coefficients can be easily restricted thereby imposing concavity, homotheticity and homogeneity in a nonparametric setting.4

The seminal work of Matzkin (1991, 1992, 1993, 1994), considers identification and estimation of general nonparametric problems with conventional economic constraints and is perhaps most closely related to the methods proposed herein. One of Matzkin’s key insights is that when nonparametric identification is not possible in general, imposing shape constraints tied to economic theory can deliver nonparametric identification where it otherwise would fail. This work lays the foundation for a general operating theory of constrained nonparametric estimation. Her methods focus on standard economic constraints (monotonicity, concavity, homogeneity, etc.) but can be generalized to allow for a wide range of conventional constraints on the function of interest. While the methods are completely general, she focuses mainly on the development of economically constrained estimators for the binary and polychotomous choice models.

Implementation of Matzkin’s constrained methods is of the two-step variety; see Matzkin (1999) for details. First, for the specified constraints, a feasible solution consisting of a finite number of points is determined through optimization of some criterion function (in the choice framework this is a pseudo-likelihood function). Second, the feasible points are interpolated or smoothed to construct the nonparametric surface that satisfies the constraints. The nonparametric least squares approach

4We note that monotonicity is not easily imposed in this setting.
of Ruud (1995) is similar in spirit to the work of Matzkin, but focuses primarily on monotonicity and concavity.\(^5\)

Yatchew & Bos (1997) develop a series-based estimator that can handle general constraints. This estimator is constructed by minimizing the sum of squared errors of a nonparametric function relative to an appropriate Sobolev norm. The basis functions that make up the series estimator are determined from a set of differential equations that provide ‘representors’. Yatchew & Bos (1997) begin by describing general nonparametric estimation and then show how to constrain the function space in order to satisfy given constraints. They also develop a conditional moment test to study the statistical validity of the constraints. Given that Matzkin’s early work did not focus on developing tests of economic constraints, Yatchew & Bos (1997) represents one of the first studies to simultaneously consider estimation and testing of economic constraints in a nonparametric (series) setting.

Contemporary work involving the estimation of smooth, nonparametric regression surfaces subject to derivative constraints includes Beresteanu (2004) and Yatchew & Härdle (2006). Beresteanu (2004) introduced a spline-based procedure that can handle multivariate data while imposing multiple, general, derivative constraints. His estimator is solved via quadratic programming over an equidistant grid created on the covariate space. These points are then interpolated to create a globally constrained estimator. Beresteanu (2004) also suggests testing the constraints using an \(L_2\) distance measure between the unrestricted and restricted function estimates. Thus, his work presents a general framework for constraining and testing a nonparametric regression function in a series framework, similar to the earlier work of Yatchew & Bos (1997). He employed his method to impose monotonicity and supermodularity of a cost function for the telephone industry.

The work of Yatchew & Härdle (2006) focuses on nonparametric estimation of an option pricing model where the unknown function must satisfy monotonicity and convexity along with the density

\(^5\)While Matzkin’s methods are novel and have contributed greatly to issues related to econometric identification, their use for constrained estimation in applied settings appears to be scarce and is likely due to the perceived complexity of the approach. For instance, statements such as those found in Chen & Randall (1997, p. 324) who note that “However, for those who desire the properties of a the distribution-free model, the empirical implementation can be difficult. […] To estimate the model using Matzkin’s method, a large constrained optimization needs to be solved.” underscore the perceived complexity of Matzkin’s approach. It should be noted that Matzkin has employed her methodology in an applied setting (see Briesch, Chintagunta & Matzkin (2002)) and her web page presents a detailed outline of both the methods and a working procedure for their use in economic applications (Matzkin (1999)).
of state prices being a true density. Their approach uses the techniques developed by Yatchew & Bos (1997). They too develop a test of their restrictions, but, unlike Beresteanu (2004), their test uses the residuals from the constrained estimate to determine if the covariates ‘explain’ anything else, and if they do the constraints are rejected.

Contemporary work involving the estimation of nonsmooth, constrained nonparametric regression surfaces includes Allon, Beenstock, Hackman, Passy & Shapiro (2007) who focused on imposing economic constraints for cost and production functions. Allon et al. (2007) show how to construct an estimator consistent with the nonparametric, nonstatistical testing device developed by Hanoch & Rothschild (1972). Their estimator employs a convex programming framework that can handle general constraints, albeit in a non-smooth setting. A nonstatistical testing device similar to Varian (1985) is discussed as well.

Notwithstanding these recent developments, there does not yet exist a methodology grounded in kernel methods that can impose general constraints and statistically test the validity of these constraints. We bridge this gap by providing a method for imposing general constraints in nonparametric kernel settings delivering a smooth constrained nonparametric estimator and we provide a simple bootstrapping procedure to test the validity of the constraints of interest. Our approach is achieved by modifying and extending the approach of Hall & Huang (2001) resulting in a simple yet general multivariate, multi-constraint procedure. As noted by Hall & Huang (2001, p. 625), the use of splines does not hold the same attraction for users of kernel methods, and the fact that Hall & Huang’s (2001) method is rooted in a conventional kernel framework naturally appeals to the community of kernel-based researchers. Furthermore, recent developments that permit the kernel smoothing of categorical and continuous covariates can dominate spline methods; see Li & Racine (2007) for some examples. Nonsmooth methods, either the fully nonsmooth methods of Allon et al. (2007) or the interpolated methods of Matzkin (1991, 1992), may fail to appeal to kernel users for the same reasons. As such, to the best of our knowledge, there does not yet exist a simple and easily implementable procedure for imposing and testing the validity of conventional

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6 This paper is closely related to our idea of imposing general derivative constraints as their approach focuses on the first three derivatives of the regression function.

7 When we use the term nonsmooth we are referring to methods that either do not smooth the nonparametric function or smooth the constrained function after the constraints have been imposed.
constraints on a regression function estimated using kernel methods that is capable of producing smooth constrained estimates.

The rest of this paper proceeds as follows. Section 2 outlines the basic approach then lays out a general theory for our constrained estimator in the presence of linear constraints and presents a simple test of the validity of the constraints. Section 3 considers a number of simulated applications, examines the finite-sample performance of the proposed test, and presents an empirical application involving technical efficiency on Indonesian rice farms. Section 4 presents some concluding remarks. Appendix A presents proofs of lemmas and theorems presented in Section 2, Appendix B presents details on the implementation for the specific case of monotonicity and concavity which may be of interest to some readers, while Appendix C presents R code (R Development Core Team (2008)) to replicate the simulated illustration presented in Section 3.1.

2. The Constrained Estimator and its Theoretical Properties

2.1. The Estimator. In what follows we let \( \{Y_i, X_i\}_{i=1}^n \) denote sample pairs of response and explanatory variables where \( Y_i \) is a scalar, \( X_i \) is of dimension \( r \), and \( n \) denotes the sample size. The goal is to estimate the unknown average response \( g(x) \equiv E(Y|X = x) \) subject to constraints on \( g^{(s)}(x) \) where \( s \) is an \( r \)-vector corresponding to the dimension of \( x \). In what follows, the elements of \( s \) represent the order of the partial derivative corresponding to each element of \( x \). Thus \( s = (0,0,\ldots,0) \) represents the function itself, while \( s = (1,0,\ldots,0) \) represents \( \partial g(x)/\partial x_1 \). In general, for \( s = (s_1,s_2,\ldots,s_r) \) we have

\[
g^{(s)}(x) = \frac{\partial^{s_1}g(x)}{\partial x_1^{s_1}}, \ldots, \frac{\partial^{s_r}g(x)}{\partial x_r^{s_r}}.
\]

We consider the class of kernel regression smoothers that can be written as linear combinations of the response \( Y_i \), i.e.,

\[
\hat{g}(x) = \sum_{i=1}^n A_i(x)Y_i,
\]

where \( A_i(x) \) is a local weighting matrix. This class of kernel smoothers includes the Nadaraya-Watson estimator (Nadaraya (1965),Watson (1964)), the Priestley-Chao estimator (Priestley &
Chao (1972)), the Gasser-Müller estimator (Gasser & Müller (1979)) and the local polynomial estimator (Fan (1992)), among others.

We presume that the reader wishes to impose constraints on the estimate \( \hat{g}(x) \) of the form

\[
(3) \quad l(x) \leq \hat{g}^{(s)}(x) \leq u(x)
\]

for arbitrary \( l(\cdot), u(\cdot), \) and \( s \), where \( l(\cdot) \) and \( u(\cdot) \) represent (local) lower and upper bounds, respectively. For some applications, \( s = (0, \ldots, 0, 1, 0, \ldots, 0) \) would be of particular interest, say for example when the partial derivative represents a budget share and therefore must lie in \([0, 1]\). Or, \( s = (0, 0, \ldots, 0) \) might be of interest when an outcome must be bounded (i.e., \( \hat{g}(x) \) could represent a probability hence must lie in \([0, 1]\) but this could be violated when using, say, a local linear smoother). Or, \( l(\cdot) = u(\cdot) \) might be required (i.e., equality rather than inequality constraints) such as when imposing adding up constraints, say, when the sum of the budget shares must equal one, or when imposing homogeneity of a particular degree, by way of example. The approach we describe is quite general. It is firmly embedded in a conventional multivariate kernel framework, and admits arbitrary combinations of constraints (i.e., for any \( s \) or combination thereof) subject to the obvious caveat that the constraints must be internally consistent.

Following Hall & Huang (2001), we consider a generalization of \( \hat{g}(x) \) defined in (2) given by

\[
(4) \quad \hat{g}(x|p) = \sum_{i=1}^{n} p_i A_i(x) Y_i,
\]

and for what follows \( \hat{g}^{(s)}(x|p) = \sum_{i=1}^{n} p_i A_i^{(s)}(x) Y_i \) where \( A_i^{(s)}(x) = \frac{\partial^{s_1} A_i(x)}{\partial x_1^{s_1}}, \ldots, \frac{\partial^{s_r} A_i(x)}{\partial x_r^{s_r}} \) for real-valued \( x \). Again, in our notation \( s \) represents a \( r \times 1 \) vector of nonnegative integers that indicate the order of the partial derivative of the weighting function of the kernel smoother.

We first consider the mechanics of the proposed approach, and by way of example use (4) to generate an unrestricted Nadaraya-Watson estimator. In this case we would set \( p_i = 1/n, \) \( i = 1, \ldots, n, \) and set

\[
(5) \quad A_i(x) = \frac{nK_\gamma(X_i, x)}{\sum_{j=1}^{n} K_\gamma(X_j, x)}.
\]
where \( K_\gamma(\cdot) \) is a generalized product kernel that admits both continuous and categorical data, and \( \gamma \) is a vector of bandwidths; see Racine & Li (2004) for details. When \( p_i \neq 1/n \) for some \( i \), then we would have a restricted Nadaraya-Watson estimator (the selection of \( p \) satisfying particular restrictions is discussed below). Note that one uses the same bandwidths for the constrained and unconstrained estimator hence bandwidth selection proceeds using standard methods, i.e., cross-validation on the sample data.

We now consider how one can impose particular restrictions on the estimator \( \hat{g}(x|p) \). Let \( p_u \) be an \( n \)-vector with elements \( 1/n \) and let \( p \) be the vector of weights to be selected. In order to impose our constraints, we choose \( p \) to minimize some distance measure from \( p \) to the uniform weights \( p_i = 1/n \) \( \forall i \) as proposed by Hall & Huang (2001). This is appealing intuitively since the unconstrained estimator is that for which \( p_i = 1/n \) \( \forall i \), as noted above. Whereas Hall & Huang (2001) consider probability weights (i.e., \( 0 \leq p_i \leq 1, \sum_i p_i = 1 \)) and distance measures suitable for probability weights (i.e., Hellinger), we need to relax the constraint that \( 0 \leq p_i \leq 1 \) and will instead allow for both positive and negative weights (while retaining \( \sum_i p_i = 1 \)), and shall also therefore require alternative distance measures. To appreciate why this is necessary, suppose one simply wished to constrain a surface that is uniformly positive to have negative regions. This could be accomplished by allowing some of the weights to be negative. However, probability weights would fail to produce a feasible solution as they are non-negative, hence our need to relax this condition.

We also have to forgo the power divergence metric of Cressie & Read (1984) which was used by Hall & Huang (2001) since it is only valid for probability weights. For what follows we select the well-worn \( L_2 \) metric \( D(p) = (p_u - p)'(p_u - p) \) which has a number of appealing features in this context, as will be seen. Our problem therefore boils down to selecting those weights \( p \) that minimize \( D(p) \) subject to \( l(x) \leq \hat{g}^{(s)}(x|p) \leq u(x) \) (and perhaps additional constraints of a similar form), which can be cast as a general nonlinear programming problem. For the illustrative constraints we consider below we have (in)equalities that are linear in \( p \),\(^8\) which can be solved using standard quadratic programming methods and off-the-shelf software. For example, in the R language (R Development Core Team (2008)) it is solved using the quadprog package, in GAUSS it is solved using the qprog

\(^8\)Common economic constraints that satisfy (in)equalities that are linear in \( p \) include monotonicity, supermodularity, additive separability, homogeneity, diminishing marginal returns/products, bounding of derivatives of any order, necessary conditions for concavity, etc.
command, and in MATLAB the quadprog command. Even when \( n \) is quite large the solution is computationally fast using any of these packages. Code in the \( \text{R} \) language is available from the authors upon request; see Appendix C for an example. For (in)equalities that are nonlinear in \( p \) we can convert the nonlinear programming problem into a quadratic programming problem that can again be solved using off-the-shelf software albeit with modification (iteration); see Appendix B for an example.

The next two subsections outline the theoretical underpinnings of the constrained estimator and present a framework for inference.

### 2.2. Theoretical Properties

Theorem 2.1 below provides conditions under which a unique set of weights exist that satisfy the constraints defined in (3). Theorem 2.2 below states that for nonbinding constraints the constrained estimator converges to the unconstrained estimator with probability one in the limit, for constraints that bind with equality on an interior hyperplane subset (defined below) the order in probability of the difference between the constrained and unconstrained estimates is obtained, while in a shrinking neighborhood where the constraints bind the ratio of the restricted and unrestricted estimators is approximately constant.

Hall & Huang (2001) demonstrate that a vector of weights always exists that satisfy the monotonicity constraint when the response is assumed to be positive for all observations.\(^9\) Moreover, they show that when the function is weakly monotonic at a point on the interior of the support of the data the difference between the restricted and unrestricted kernel regression estimates is \( O_p(h^{5/4}) \) on an interval of length \( h \) around this point; \( h \) here is the bandwidth employed for univariate kernel regression. For what follows we focus on linear (in \( p \)) restrictions which are quite general and allow for the equivalent types of constraint violations albeit in a multidimensional setting.\(^{10}\)

To allow for multiple simultaneous constraints we express our restrictions as follows:

\[
\sum_{i=1}^{n} p_i \left[ \sum_{s \in S} \alpha_s A_i^{(s)}(x) \right] Y_i - c(x) \geq 0,
\]

\(^9\)This assumption, however, is too restrictive for the framework we envision.
\(^{10}\)See Appendix B for an example of how to implement our method with constraints that are nonlinear in \( p \) and Henderson & Parmeter (2009) for a more general discussion of imposing arbitrary nonlinear constraints on a non-parametric regression surface, albeit with probability weights and the power divergence metric of Cressie & Read (1984).
where the inner sum is taken over all vectors $S$ that correspond to our constraints and $\alpha_s$ is a set of constants used to generate various constraints. In what follows we presume, without loss of generality, that for all $s$, $\alpha_s \geq 0$ and $c(x) \equiv 0$, since $c(x)$ is a known function. For what follows $c(x)$ equals either $l(x)$ or $-u(x)$ and since we admit multiple constraints our proofs cover both lower bound, upper bound, and equality constraint settings. To simplify the notation, we define a differential operator $m \mapsto m^{[d]}$ such that $m^{[d]}(x) = \sum_{s \in S} \alpha_s m^{(s)}(x)$ and let $\psi_i(x) = A_i^{[d]}(x)Y_i$.

Before considering the theoretical properties of the proposed constrained estimator we first provide an existence theorem.

**Theorem 2.1.** If one assumes that

(i) A sequence $\{i_1, \ldots, i_k\} \subseteq \{1, \ldots, n\}$ exists such that for each $k$, $\psi_{i_k}(x)$ is strictly positive and continuous on $(L_{i_k}, U_{i_k}) \equiv \prod_{i=1}^{r} (L_{i_k}, U_{i_k}) \subset \mathbb{R}^r$, and vanishes on $(\infty, L_{i_k}]$ (where $L_{i_k} < U_{i_k}$),

(ii) Every $x \in I \equiv [c, d] = \prod_{i=1}^{r} [c_i, d_i]$ is contained in at least one interval $(L_{i_k}, U_{i_k})$,

(iii) For $1 \leq i \leq n$, $\psi_{i_k}(x)$ is continuous on $(-\infty, \infty)$,

then there exists a vector $p = (p_1, \ldots, p_n)$ such that the constraints are satisfied for all $x \in I$.

**Proof of Theorem 2.1.** This result is a straightforward extension of the induction argument provided in Theorem 4.1 of Hall & Huang (2001) which we therefore omit. $\square$

We note that the above conditions are sufficient but not necessary for the existence of a set of weights that satisfy the constraints for all $x \in I$. For example, if for some sequence $j_n$ in $\{1, \ldots, n\}$ $\text{sgn} \psi_{j_n}(x) = 1 \forall x \in I$ and for another sequence $l_n$ in $\{1, \ldots, n\}$ $\text{sgn} \psi_{l_n}(x) = -1 \forall x \in I$, then for those observations that switch signs $p_i$ may be set equal to zero, while $p_{j_n} > 0$ and $p_{l_n} < 0$ is sufficient to ensure existence of a set of $p$s satisfying the constraints. Moreover, since the forcing matrix $(I_n)$ in the quadratic portion of our $L_2$ norm, $p' I_n p$, is positive semidefinite, if our solution satisfies the set of linear equality/inequality constraints then it is the unique, global solution to the problem (Nocedal & Wright (2000, Theorem 16.4)). Positive semi-definiteness guarantees that our objective function is convex which is what yields a global solution.\(^{11}\)

For the theorems and proofs that follow we invoke the following assumptions:

\(^{11}\)When the forcing matrix is not convex, multiple solutions may exist and these types of problems are referred to as ‘indefinite quadratic programs’.
Assumption 2.1.

(i) The sample $X_i$ either form a regularly spaced grid on a compact set $\mathcal{I}$ or constitute independent random draws from a distribution whose density $f$ is continuous and nonvanishing on $\mathcal{I}$; the $\varepsilon_i$ are independent and identically distributed with zero mean and are independent of the $X_i$; the kernel function $K(\cdot)$ is a symmetric, compactly supported density with a Hölder-continuous derivative on $J \equiv [a, b] = \prod_{i=1}^{r} [a_i, b_i] \subset \mathcal{I}$.

(ii) $E (|\varepsilon_i|^t)$ is bounded for sufficiently large $t > 0$.

(iii) $\partial f^{[d]} / \partial x$ and $\partial g^{[d]} / \partial x$ are continuous on $J$.

(iv) The bandwidth associated with each explanatory variable, $h_j$, satisfies $h_j \propto n^{-1/(r+4)}$, $1 \leq j \leq r$.

Assumption 2.1 (i) is standard in the kernel regression literature. Assumption 2.1 (ii) is a sufficient condition required for the application of a strong approximation result which we invoke in Lemma A.3, while Assumption 2.1 (iii) assures requisite smoothness of $f^{[d]}$ and $g^{[d]}$ ($f$ is the design density). The bandwidth rate in Assumption 2.1 (iv) is the standard optimal rate. Note that when the bandwidths all share the same optimal rate, one can rescale each component of $x$ to ensure a uniform bandwidth $h \propto n^{-1/(r+4)}$ for all components which simplifies the notation in the proofs somewhat without loss of generality. In the proofs that follow we will therefore use $h^r$ rather than $\prod_{j=1}^{r} h_j$ purely for notational simplicity.

Define a hyperplane subset of $J = \prod_{i=1}^{r} [a_i, b_i]$ to be subset of the form $S = \{ x_{0k} \times \prod_{i \neq k} [a_i, b_i] \}$ for some $1 \leq k \leq r$ and some $x_{0k} \in [a_k, b_k]$. We call $S$ an interior hyperplane subset if $x_{0k} \in (a_k, b_k)$. For what follows, $g^{[d]} (g)$ is the true data generating process (DGP), $\hat{p}$ is the optimal weight vector satisfying the constraints, $\hat{g}^{[d]} (\cdot | \hat{p}) (\hat{g} (\cdot | \hat{p}))$ is the constrained estimator defined in (4), and $\tilde{g}^{[d]} (\tilde{g})$ is the unconstrained estimator defined in (2). Additionally, we define $|s| = \sum_{i=1}^{r} s_i$ as the order for a derivative vector $s = (s_1, \ldots, s_r)$. We say a derivative $s_1$ has a higher order than $s_2$ if $|s_1| > |s_2|$. For technical reasons outlined in the proof of Lemma A.2, in the case of tied orders we also treat derivative vectors with all even components as having a higher order than those with at least one odd component. For example, $(2, 2)$ is considered to be of higher order than $(1, 3)$. With a slight abuse of notation, let $d$ be a derivative with the “maximum order” among all the derivatives in the constraint (6). In the case of ties, such as $\{(2, 2), (0, 4), (1, 3), (3, 1)\}$, $d$ can be either $(2, 2)$ or...
For notational ease in what follows we define a constant \( \delta_d = 1 \) if \( d \) has at least one odd component and 0 otherwise.

**Theorem 2.2.** Assume 2.1(i)-(iv) hold.

(i) If \( g^{[d]} > 0 \) on \( J \) then, with probability 1, \( \hat{p} = 1/n \) for all sufficiently large \( n \) and \( \hat{g}^{[d]}(\cdot|\hat{p}) = \tilde{g}^{[d]} \) on \( J \) for all sufficiently large \( n \). Hence, \( \hat{g}(\cdot|\hat{p}) = \tilde{g} \) on \( J \) for all sufficiently large \( n \).

(ii) Suppose that \( g^{[d]} > 0 \) except on an interior hyperplane subset \( X_0 \subset J \) such that \( g^{[d]}(x) = 0, \forall x \in X_0 \) and for any \( x_0 \in X_0 \), and suppose that \( g^{[d]} \) has two continuous derivatives in the neighborhood of \( x_0 \) with \( \partial g^{[d]} / \partial x(x_0) = 0 \) and with \( \partial^2 g^{[d]} / \partial x \partial x^T(x_0) \) nonsingular; then \( |\hat{g}(\cdot|\hat{p}) - \tilde{g}| = O_p \left( h^{3/8 - \delta_d/4} \right) \) uniformly on \( J \).

(iii) Under the same conditions given in (ii) above, there exist random variables \( \Theta = \Theta(n) \) and \( Z_1 = Z_1(n) \geq 0 \) satisfying \( \Theta = O_p \left( h^{3/8 - \delta_d/4} \right) \) and \( Z_1 = O_p(1) \) such that \( \hat{g}(x|\hat{p}) = (1 + \Theta)\tilde{g}(x) \) uniformly for \( x \in J \) with \( \inf_{x_0 \in X_0} |x - x_0| > Z_1 h^{3/8 - \delta_d/4} \). The latter property reflects the fact that, for a random variable \( Z_2 = Z_2(n) \geq 0 \) satisfying \( Z_2 = O_p(1) \), we have \( \hat{p}_i = n^{-1}(1 + \Theta) \) for all indices \( i \) such that both \( \inf_{x_0 \in X_0} |X_i - x_0| > Z_2 h^{3/8 - \delta_d/4} \) and \( A_i(x) \neq 0 \) for some \( x \in J \).

The proof of Theorem 2.2 is rather lengthy and invokes a number of lemmas, therefore it is relegated to Appendix A. Theorem 2.2 is the multivariate, multiconstraint, hyperplane subset generalization of the univariate, single constraint, single point violation setting considered in Hall & Huang (2001) having dispensed with probability weights and power divergence distance measures of necessity. However, the theory in Hall & Huang (2001) lays the foundation for several of the results that we obtain, for which we are indebted. We obtain the same rates in parts (ii) and (iii) of Theorem 2.2 above as Hall & Huang (2001, Theorem 4.3(c)) obtain in their single interior point setting, and point out that the key to proving part (iii) of Theorem 2.2 is the utilization of a strong approximation theorem of Komlós, Major & Tusnády (1975, 1976) known as the Hungarian Embedding (van der Vaart (2000, page 269)) which we use in Lemma A.3. As this powerful theorem is not commonplace in the econometrics literature (Burridge & Guerre (1996), Wang, Lin & Gulati (2003)) we highlight its use here.

We briefly discuss the types of constraint violations addressed in Theorem 2.2. First, if the constraints are not violated then, for a large enough sample, there will be no need to impose the
constraints. However, if the constraints are only weakly satisfied then parts (ii) and (iii) state that we have nonconstant weights within a neighborhood of radius $O\left(h^{1/2}\right)$ and the ratio of the constrained and unconstrained kernel estimates is constant within this neighborhood. Additionally, the nonempty $\partial X_0 \setminus \partial J$ requirement\textsuperscript{12} eliminates the case where $X_0$ lies completely on the boundary of $J$ which is of less interest but in this setting can be handled directly.

Were we to instead allow for arbitrary violations of the constraints (as opposed to weak violations), the ratio of the constrained and unconstrained functions will no longer be constant which would require us to place a bound on the unknown function as opposed to assuming $\frac{\partial g}{\partial x}(x_0) = 0$ (Lemma A.2 in Appendix A could be modified to handle this case). For these types of arbitrary constraint violations we cannot say anything about the relative magnitudes of the restricted and unrestricted estimators on the set where the constraints are erroneously imposed. However, a rate similar to that in (ii) in Theorem 2.2 for the two estimators on an appropriately defined set where the constraints are valid could be obtained.\textsuperscript{13}

### 2.3. Inference

As noted in Section 1, there exists a growing literature on testing restrictions in nonparametric settings. This literature includes Abrevaya & Jiang (2005), who test for curvature restrictions and provide an informative survey, Epstein & Yatchew (1985), who develop a nonparametric test of the utility maximization hypothesis and homotheticity, Yatchew & Bos (1997), who develop a conditional moment test for a broad range of smoothness constraints, Ghosal, Sen & van der Vaart (2000), who develop a test for monotonicity, Beresteanu (2004), who as mentioned above outlines a conditional mean type test for general constraints, and Yatchew & Härdle (2006), who employ a residual-based test to check for monotonicity and convexity. The tests of Yatchew & Bos (1997) and Beresteanu (2004) are the closest in spirit to the method we adopt below, having the ability to test general smoothness constraints. One could easily use the same test statistic as Yatchew & Bos (1997) and Beresteanu (2004) but replace the series estimator with a kernel estimator if desired. Aside from the test of Yatchew & Bos (1997), most existing tests check for specific

\textsuperscript{12} We let $\partial$ denote the boundary of a set, and we let $\setminus$ denote complement of a set.

\textsuperscript{13} An additional benefit of the theory provided here is that our generalization of the results of Hall & Huang (2001) that instead employs a quadratic criterion is amenable to quadratic programming solvers rather than nonlinear programming solvers hence our approach can be applied using off-the-shelf software.
constraints. This is limiting in the current setting as our main focus is on a smooth, arbitrarily restricted estimator.

For what follows we adopt a testing approach similar to that proposed by Hall et al. (2001) which is predicated on the objective function \( D(\hat{p}) \). This approach involves estimating the constrained regression function \( \hat{g}(x|p) \) based on the sample realizations \( \{Y_i, X_i\} \) and then rejecting \( H_0 \) if the observed value of \( D(\hat{p}) \) is too large. We use a resampling approach for generating the null distribution of \( D(\hat{p}) \) which involves generating resamples for \( y \) drawn from the constrained model via \( \text{iid} \) residual resampling (i.e., conditional on the sample \( \{X_i\} \)), which we denote \( \{Y_i^*, X_i\} \). These resamples are generated under \( H_0 \), hence we recompute \( \hat{g}(x|p) \) for the bootstrap sample \( \{Y_i^*, X_i\} \) which we denote \( \hat{g}(x|p^*) \) which then yields \( D(p^*) \). We then repeat this process \( B \) times. Finally, we compute the empirical \( P \) value, \( P_B \), which is simply the proportion of the \( B \) bootstrap resamples \( D(p^*) \) that exceed \( D(\hat{p}) \), i.e.,

\[
P_B = 1 - \hat{F}(D(\hat{p})) = \frac{1}{B} \sum_{j=1}^{B} I(D(p^*) > D(\hat{p})),
\]

where \( I(\cdot) \) is the indicator function and \( \hat{F}(D(\hat{p})) \) is the empirical distribution function of the bootstrap statistics. Then one rejects the null hypothesis if \( P_B \) is less than \( \alpha \), the level of the test. For an alternative approach involving kernel smoothing of \( F(\cdot) \), see Racine & MacKinnon (2007a).

Before proceeding further, we note that there exist three situations that can occur in practice:

(i) Impose non-binding constraints (they are ‘correct’ de facto)
(ii) Impose binding constraints that are correct
(iii) Impose binding constraints that are incorrect

We only consider (ii) and (iii) in the Monte Carlo simulations in Section 3 below since, as noted by Hall et al. (2001, p 609), “For those datasets with \( D(\hat{p}) = 0 \), no further bootstrapping is necessary […] and so the conclusion (for that dataset) must be to not reject \( H_0 \).” The implication in the current paper is simply that imposing non-binding constraints does not alter the estimator and the unconstrained weights will be \( \hat{p}_i = 1/n \forall i \) hence \( D(\hat{p}) = 0 \) and the statistic is degenerate. Of course, in practice this simply means that we presume people are imposing constraints that bind, which is a reasonable presumption. In order to demonstrate the flexibility of the constrained estimator, in
Section 3 below we consider testing for two types of restrictions. In the first case we impose the restriction that the regression function \( g(x) \) is equal to a known parametric form \( g(x, \beta) \), while in the second case we test whether the first partial derivative is constant and equal to the value one for all \( x \) (testing whether the first partial equals zero would of course be a test of significance).

We now demonstrate the flexibility and simplicity of the approach by first imposing a range of constraints on a simulated dataset using a large number of observations thereby showcasing the feasibility of this approach in substantive applied settings, and then consider some Monte Carlo experiments that examine the finite-sample performance of the proposed test.

3. Simulated Illustrations, Finite-Sample Test Performance, and an Application

For what follows we simulate data from a nonlinear multivariate relationship and then consider imposing a range of restrictions by way of example. We consider a 3D surface defined by

\[
Y_i = \frac{\sin\left(\sqrt{X_{i1}^2 + X_{i2}^2}\right)}{\sqrt{X_{i1}^2 + X_{i2}^2}} + \varepsilon_i, \quad i = 1, \ldots, n,
\]

where \( x_1 \) and \( x_2 \) are independent draws from the uniform \([-5,5]\). We draw \( n = 10,000 \) observations from this DGP with \( \varepsilon \sim N(0, \sigma^2) \) and \( \sigma = 0.1 \). As we will demonstrate the method by imposing restrictions on the surface and also on its first and second partial derivatives, we use the local quadratic estimator for what follows as it delivers consistent estimates of the regression function and its first and second partial derivatives. Figure 1 presents the unrestricted regression estimate whose bandwidths were chosen via least squares cross-validation.\(^{14}\)

3.1. A Simulated Illustration: Restricting \( \hat{g}^{(0)}(x) \).

Next, we arbitrarily impose the constraint that the regression function lies in the range \([0,0.5]\). A plot of the restricted surface appears in Figure 2.

Figures 1 and 2 clearly reveal that the regression surface for the restricted model is both smooth and satisfies the constraints.

\(^{14}\)In all of the restricted illustrations to follow we use the same cross-validated bandwidths.
3.2. A Simulated Illustration: Restricting $\hat{g}^{(1)}(x)$. We consider the same DGP given above, but now we arbitrarily impose the constraint that the first derivatives with respect to both $x_1$ and $x_2$ lie in the range $[-0.1,0.1]$.$^{15}$ A plot of the restricted surface appears in Figure 3.

$^{15}$s = (1, 0) and t = (0, 1).
Figure 3. Restricted nonparametric estimate of (7) where the restriction is defined over \( g^{(s)}(x), s \in \{(1, 0), (0, 1)\}, (-0.1 \leq \partial \hat{g}(x|p)/\partial x_1 \leq 0.1, -0.1 \leq \partial \hat{g}(x|p)/\partial x_2 \leq 0.1), n = 10,000. \)

Figure 3 clearly reveals that the regression surface for the restricted model possesses derivatives that satisfy the constraints everywhere and is smooth.

3.3. A Simulated Illustration: Restricting \( \hat{g}^{(2)}(x) \). We consider the same DGP given above, but now we arbitrarily impose the constraint that the second derivatives with respect to both \( x_1 \) and \( x_2 \) are positive (negative), which is a necessary (but not sufficient) condition for concavity and convexity; see Appendix B for details on imposing concavity or convexity using our approach. As can be seen from figures 4 and 5 the shape of the restricted function changes drastically depending on the curvature restrictions placed upon it.

We could as easily impose restrictions defined perhaps jointly on, say, both \( \hat{g}(x) \) and \( \hat{g}^{(1)}(x) \), or perhaps on cross-partial derivatives if so desired. We hope that these illustrative applications reassure the reader that the method we propose is powerful, fully general, and can be applied in large-sample settings.

3.4. Finite-Sample Test Performance: Testing Correct Parametric Specification. By way of example we consider testing the restriction that the nonparametric model \( g(x) \) is equivalent to a specific parametric functional form (i.e., we impose an equality restriction on \( \hat{g}(x) \), namely
that $\hat{g}(x)$ equals $x'\hat{\beta}$ where $x'\hat{\beta}$ is the parametric model). Note that we could consider any number of tests for illustrative purposes and consider another application in the following subsection. We
consider the following DGP:

\[ Y_i = g(X_{i1}, X_{i2}) + \varepsilon_i = 1 + X_{i1}^2 + X_{i2} + \varepsilon_i, \]

where \( X_{ij}, j = 1, 2 \) are uniform \([-2, 2]\) and \( \varepsilon \sim N(0, 1/2) \).

We then impose the restriction that \( g(x) \) is of a particular parametric form, and test whether this restriction is valid. When we generate data from this DGP and impose the correct model as a restriction (i.e., that given by the DGP, say, \( \beta_0 + \beta_1 x_{i1}^2 + \beta_2 x_{i2} \)) we can assess the test’s size, while when we generate data from this DGP and impose an incorrect model that is in fact linear in variables we can assess the test’s power.

We conduct \( M = 1,000 \) Monte Carlo replications from our DGP, and consider \( B = 99 \) bootstrap replications; see Racine & MacKinnon (2007b) for details on determining the appropriate number of bootstrap replications. Results are presented in Table 1 in the form of empirical rejection frequencies for \( \alpha = (0.10, 0.05, 0.01) \) for samples of size \( n = 25, 50, 75, 100, 200 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \alpha = 0.10 )</th>
<th>( \alpha = 0.05 )</th>
<th>( \alpha = 0.01 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.100</td>
<td>0.049</td>
<td>0.010</td>
</tr>
<tr>
<td>50</td>
<td>0.074</td>
<td>0.043</td>
<td>0.011</td>
</tr>
<tr>
<td>75</td>
<td>0.086</td>
<td>0.034</td>
<td>0.008</td>
</tr>
<tr>
<td>100</td>
<td>0.069</td>
<td>0.031</td>
<td>0.006</td>
</tr>
<tr>
<td>200</td>
<td>0.093</td>
<td>0.044</td>
<td>0.007</td>
</tr>
<tr>
<td>Power</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.391</td>
<td>0.246</td>
<td>0.112</td>
</tr>
<tr>
<td>50</td>
<td>0.820</td>
<td>0.665</td>
<td>0.356</td>
</tr>
<tr>
<td>75</td>
<td>0.887</td>
<td>0.802</td>
<td>0.590</td>
</tr>
<tr>
<td>100</td>
<td>0.923</td>
<td>0.849</td>
<td>0.669</td>
</tr>
<tr>
<td>200</td>
<td>0.987</td>
<td>0.970</td>
<td>0.903</td>
</tr>
</tbody>
</table>

Table 1 indicates that the test appears to be correctly sized while power increases with \( n \).

3.5. Finite-Sample Performance: Testing an Equality Restriction on a Partial Derivative. For this example we consider a simple linear DGP given by

\[ Y_i = g(X_i) + \varepsilon_i = \beta_1 X_i + \varepsilon_i, \]
where $X_i$ is uniform $[-2, 2]$ and $\varepsilon \sim N(0, 1)$.

We consider testing the equality restriction $H_0 : g^{(1)}(x) = 1$ where we take the first order derivative (i.e., $g^{(1)}(x) = dg(x)/dx_1$), and let $\beta_1$ vary from 1 through 2 in increments of 0.1. Note that the test of significance would be a test of the hypothesis that $g^{(1)}(x) = 0$ almost everywhere rather than $g^{(1)}(x) = 1$ which we consider, so clearly we could also perform a test of significance in the current framework. The utility of the proposed approach lies in its flexibility as we could as easily test the hypothesis that $g^{(1)}(x) = \xi(x)$ where $\xi(x)$ is an arbitrary function. Significance testing in nonparametric settings has been considered by a number of authors; see Racine (1997) and Racine, Hart & Li (2006) for alternative approaches to testing significance in a nonparametric setting.

When $\beta_1 = 1.0$ we can assess size while when $\beta_1 \neq 1.0$ we can assess power. We construct power curves based on $M = 1,000$ Monte Carlo replications, and we compute $B = 99$ bootstrap replications. The power curves corresponding to $\alpha = 0.05$ appear in Figure 6.

![Figure 6](image-url)

**Figure 6.** Power curves for $\alpha = 0.05$ for sample sizes $n = (25, 50, 75, 100)$ based upon the DGP given in (8). The dashed horizontal line represents the test’s nominal level ($\alpha$).

Figure 6 reveals that for small sample sizes (e.g., $n = 25$) there appears to be a small size distortion, however, the distortion appears to fall rather quickly as $n$ increases. Furthermore, power increases with $n$. Given that the sample sizes considered here would typically be much
smaller than those used by practitioners adopting nonparametric smoothing methods, we expect that the proposed test would possess reasonable size in empirical applications.

3.6. Application: Imposing Constant Returns to Scale for Indonesian Rice Farmers.
We consider a production dataset that has been studied by Horrace & Schmidt (2000) who analyzed technical efficiency for Indonesian rice farms. We examine the issue of returns to scale, focusing on one growing season’s worth of data for the year 1977, acknowledged to be a particularly wet season. Farmers were selected from six villages of the production area of the Cimanuk River Basin in West Java, and there were 171 farms in total. Output is measured as kilograms of rice produced, and inputs included seed (kg), urea (kg), trisodium phosphate (TSP) (kg), labour (hours), and land (hectares). Table 2 presents some summary statistics for the data. Of interest here is whether or not the technology exhibits constant returns to scale (i.e., whether or not the sum of the partial derivatives equals one). We use log transformations throughout.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Mean</th>
<th>StdDev</th>
</tr>
</thead>
<tbody>
<tr>
<td>log(rice)</td>
<td>6.9170</td>
<td>0.9144</td>
</tr>
<tr>
<td>log(seed)</td>
<td>2.4534</td>
<td>0.9295</td>
</tr>
<tr>
<td>log(urea)</td>
<td>4.0144</td>
<td>1.1039</td>
</tr>
<tr>
<td>log(TSP)</td>
<td>2.7470</td>
<td>1.4093</td>
</tr>
<tr>
<td>log(labor)</td>
<td>5.6835</td>
<td>0.8588</td>
</tr>
<tr>
<td>log(land)</td>
<td>-1.1490</td>
<td>0.9073</td>
</tr>
</tbody>
</table>

We estimate the production function using a nonparametric local linear estimator with cross-validated bandwidth selection. Figure 7 presents the unrestricted and restricted partial derivative sums for each observation (i.e., farm), where the restriction is that the sum of the partial derivatives equals one. The horizontal line represents the restricted partial derivative sum (1.00) and the points represent the unrestricted sums for each farm. An examination of Figure 7 reveals that the estimated returns to scale lie in the interval \([0.98, 1.045]\).

Figures 8 and 9 present the unrestricted and restricted partial mean plots, respectively. Notice the change in the partial mean plot of log(urea) across the restricted and unrestricted models. It is clear that the bulk of the restricted weights are targeting this input’s influence on returns to scale.

\[^{16}\text{A 'partial mean plot' is simply a 2D plot of the outcome } y \text{ versus one covariate } x_j \text{ when all other covariates are held constant at their respective medians/modes.}\]
The remaining partial mean plots are unchanged visually across the unrestricted and restricted models.

In order to test whether the restriction is valid we apply the test outlined in Section 2.3. We conducted $B = 99$ bootstrap replications and test the null that the technology exhibits constant returns to scale. The empirical $P$ value is $P_B = 0.131$, hence we fail to reject the null at all conventional levels. We are encouraged by this fully nonparametric application particularly as it involves a fairly large number of regressors (five) and a fairly small number of observations ($n = 171$).

4. Concluding Remarks

We present a framework for imposing and testing the validity of conventional constraints on the $s$th partial derivatives of a nonparametric kernel regression function, namely, $l(x) \leq g^{(s)}(x) \leq u(x)$, $s = 0, 1, \ldots$. The proposed approach nests special cases such as imposing monotonicity, concavity (convexity) and so forth while delivering a seamless framework for general restricted nonparametric kernel estimation and inference. Illustrative simulated examples are presented, finite-sample performance of the proposed test is examined via Monte Carlo simulations, and an
illustrative application is undertaken. An open implementation in the R language (R Development Core Team (2008)) is available from the authors.
One interesting extension of this methodology would be to the cost system setup popular in production econometrics (Kumbhakar & Lovell (2001)). There, the derivatives of the cost function are estimated along with the function itself in a system framework. Currently, Hall & Yatchew (2007) have proposed a method for estimating the cost function based upon integrating the share equations, resulting in an improvement in the rate of convergence relative to direct nonparametric estimation of the cost function. It would be interesting to determine the merits of restricting the first order partial derivatives of the cost function using the approach described here to estimate the cost function in a single equation framework. We also note that the procedure we outline is valid for a range of kernel estimators in addition to those discussed herein. Semiparametric models such as the partially linear, single index, smooth coefficient, and additively separable models could utilize this approach towards constrained estimation. Nonparametric unconditional and conditional density and distribution estimators, as well as survival and hazard functions, smooth conditional quantiles and structural nonparametric estimators including auction methods could also benefit from the framework developed here. We leave this as a subject for future research.
References


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URL: http://www.r-project.org/


Appendix A. Proofs

For the proofs that follow we first establish some technical lemmas. Lemma A.1 partitions the weights into two sets, one where individual weights are identical and one where they are a set of fixed constants (that may differ), and is used exclusively in Theorem 2.2 (iii). Lemma A.2 establishes that there exist a set of weights that guarantee that the constraint is satisfied with probability approaching one in the limit. These weights do not have to equal the optimal weights, but are used to bound the distance metric evaluated at the optimal weights. Lemma A.2 is used in Theorem 2.2 (ii) and (iii). Lemma A.3 establishes that with probability approaching one in the limit the unrestricted estimate \( \tilde{g} \) satisfies \( \tilde{g}^{[d]}(x) > \frac{1}{3}g^{[d]}(x) \) for any point \( x \) lying a given distance from \( X_0 \). It is used to determine the requisite distance from \( X_0 \) for a point \( x \) to satisfy \( \hat{g}^{[d]}(x|\tilde{p}) > 0 \), which is then used to derive the orders of \( Z_1 \) and \( Z_2 \) in Theorem 2.2 (iii).

Lemma A.1. If \( A \) and \( B \) are complementary subsets of the integers 1, \ldots, \( n \) and if \( p_i \), for \( i \in A \) are fixed, then the values of \( p_j \) for \( j \in B \) that minimize \( L_2(p) \) are identical, and are uniquely determined by the constraint that their sum should equal \( 1 - \sum_{i \in A} p_i \).

Proof of Lemma A.1. We find the optimal \( p_j \)s by minimizing \( \sum (p_j - 1/n)^2 \) subject to \( \sum_{j \in B} p_j = 1 - \sum_{i \in A} p_i \). Without loss of generality, assume \( n \in B \). By incorporating the constraint directly into our distance metric we obtain

\[
\min_{p_j, j \in B \setminus \{n\}} \left[ \sum_{j \in B \setminus \{n\}} (p_j - 1/n)^2 + \left( 1 - \sum_{i \in A} p_i - \sum_{j \in B \setminus \{n\}} p_j - 1/n \right)^2 \right],
\]

which yields the first order conditions, for \( j \in B \setminus \{n\} \), \( p_j = 1 - \sum_{i \in A} p_i - \sum_{k \in B \setminus \{n\}} p_k \). Since \( \sum_{k \in B \setminus \{n\}} p_k \) is fixed we see that all \( p_j, j \in B \setminus \{n\} \), are identical. Moreover, the excluded \( p_n \) is also equal to \( 1 - \sum_{j \in A} p_j - \sum_{k \in B \setminus \{n\}} p_k \) which proves Lemma A.1. \( \square \)

Lemma A.2. For each \( \delta > 0 \) there exists a \( \tilde{p} = \tilde{p}(\delta) \) satisfying

\[
(A1) \quad P \left\{ g^{[d]}(x|\tilde{p}) > 0 \quad \forall x \in J \right\} > 1 - \delta
\]

for all sufficiently large \( n \). Moreover, this yields \( L_2(\tilde{p}) = O_p \left( n^{-1}h_2^{2d|d|+2r-\delta_4+1/2} \right) \).
Proof of Lemma A.2. Choose any $x_0 \in X_0$. Define

\begin{align*}
(A2) \quad \tilde{p}_i &= n^{-1} \left\{ 1 + \Delta + h^{j_1} g(X_i)^{-1} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) \right\},
\end{align*}

where $\Delta$ is a constant defined by $\sum_{i=1}^{n} \tilde{p}_i = 1$, $j_1$ is a constant to be determined later in the proof, and $L(x) = \sum_{j=1}^{r} L_j(x_j)$ with each $L_j$ being a fixed, compactly supported and twice differentiable function. Then

\begin{align*}
\hat{g}^{[d]}(x | \tilde{p}) &= \sum_{i=1}^{n} \tilde{p}_i A_i^{[d]}(x) Y_i \\
&= (1 + \Delta) n^{-1} \sum_{i=1}^{n} p_i A_i^{[d]}(x) Y_i + n^{-1} \sum_{i=1}^{n} \left[ h^{j_1} g(X_i)^{-1} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) A_i^{[d]}(x) Y_i \right] \\
(A3) &= (1 + \Delta) \hat{g}^{[d]}(x) + h^{j_1} B_1(x) + h^{j_1} B_2(x),
\end{align*}

where,

\begin{align*}
B_1(x) &= n^{-1} \sum_{i=1}^{n} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) A_i^{[d]}(x) \\
B_2(x) &= n^{-1} \sum_{i=1}^{n} g(X_i)^{-1} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) A_i^{[d]}(x) \varepsilon_i.
\end{align*}

The compactness of $L(\cdot)$ gives us

\begin{align*}
(A4) \quad n^{-1} \sum_{i=1}^{n} g(X_i)^{-1} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) &= O_p \left( h^{1/2} \right)
\end{align*}

and we have $\sum_{i=1}^{n} \tilde{p}_i = 1 + \Delta + h^{j_1} O_p \left( h^{1/2} \right)$, which implies $\Delta = O_p \left( h^{j_1 + 1/2} \right)$.

Since a higher order derivative $(j)$ implies a higher order for $A^{(j)}(x)$, we have $B_1(x) = O_p \left( \tilde{B}_1(x) \right)$ and $B_2(x) = O_p \left( \tilde{B}_2(x) \right)$ with

\begin{align*}
\tilde{B}_1(x) &= n^{-1} \sum_{i=1}^{n} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) A_i^{(d)}(x), \\
\tilde{B}_2(x) &= n^{-1} \sum_{i=1}^{n} g(X_i)^{-1} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) A_i^{(d)}(x) \varepsilon_i.
\end{align*}
where only the highest order derivative is included for both terms. We can then bound $\tilde{B}_1(x)$ and $\tilde{B}_2(x)$ as follows.

Note that $\tilde{B}_2(x)$ is the sum of $n$ i.i.d. random variables with mean zero and variance

$$
\text{Var} \left( g(X_i)^{-1} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) A_i^{(d)}(x) \varepsilon_i \right) = E \left[ g(X_i)^{-2} L \left( \frac{x_0 - X_i}{h^{1/2}} \right)^2 A_i^{(d)}(x)^2 \right] E[\varepsilon_i^2] \\
= O_p \left( h^{-2(|d|+2r-1/2)} \right),
$$

where the independence of $\varepsilon_i$ and $X_i$ is used in the first equality. Hence

$$
\sup_{x \in J} |B_2(x)| = O_p \left( \left( nh^{2|d|+2r-1/2} \right)^{-1/2} \right) = O_p \left( h^{\frac{d}{2} - |d| - \frac{r}{2}} \right).
$$

For $\tilde{B}_1(x)$, without loss of generality, we have the following

$$
\tilde{B}_1(x) = h^{-(|d|+r)} \sum_{i=1}^{n} K^{(d)} \left( \frac{x - X_i}{h} \right) L \left( \frac{x_0 - x}{h^{1/2}} + \frac{x - X_i}{h^{1/2}} \right) \\
= h^{-(|d|+r-1)} \int K^{(d)}(y)L \left( \frac{x_0 - x}{h^{1/2}} + h^{1/2}y \right) dy + O_p(1),
$$

where the last equality follows from the definition of the integral.

A Taylor expansion of $L$ gives

$$
L \left( \frac{x_0 - x}{h^{1/2}} + h^{1/2}y \right) = L \left( \frac{x_0 - x}{h^{1/2}} \right) + h^{1/2}y L^{(1)} \left( \frac{x_0 - x}{h^{1/2}} \right) + O_p(h), \tag{A6}
$$

where $1$ is a vector having all elements equal to one. Due to the component-wise symmetry of $K(\cdot)$, we have $\int K^{(d)}(y)dy = 0$ if at least one of the $d_i$, $1 \leq i \leq r$, is odd. Given (A6), we treat two separate cases: (i) at least one of the $d_i$, $1 \leq i \leq r$, is odd and (ii) all the $d_i$, $1 \leq i \leq r$, are even.

Let’s consider case (i) first. Substituting (A6) into (A5), we have

$$
\tilde{B}_1(x) = h^{-(|d|+r-3/2)}c_K^T L^{(1)} \left( \frac{x_0 - x}{h^{1/2}} \right) + O_p \left( h^{2-|d|-r} \right) + O_p(1),
$$

where $c_K = \int K^{(d)}(y)dy$. This gives us

$$
\tilde{g}^{[d]}(x|\hat{p}) = \tilde{g}^{[d]}(x) + h^{j_1-|d|-r+3/2}c_K^T L^{(1)} \left( \frac{x_0 - x}{h^{1/2}} \right) + B_3(x), \tag{A7}
$$

where $B_3(x) = o_p(h^{1/2})$ uniformly in $x \in J$. 


For a subset $S \subset J$, define

$$B(S, \delta) = \left\{ x \in J : \inf_{y \in S} |x - y| \leq \delta \right\}.$$ 

Consider any point $x \in J \setminus B(X_0, Ch^{1/2})$. Let $y_0 \in X_0$ be the point such that $|x - y_0| = \inf_{y \in X_0} |x - y|$. The existence of such a $y_0$ is guaranteed by the fact that $X_0$ is a closed subset. Since $\partial g^{[d]}/\partial x$ is continuous, we must have $\partial g^{[d]} / \partial x (y_0) = 0$. Hence, the Taylor expansion at $y_0$ gives $g^{[d]}(x) = \frac{1}{2} (x - y_0)^T \frac{\partial^2 g^{[d]}}{\partial x \partial x^T} (y_0)(x - y_0) + O_p(h^{3/2})$. Since $\tilde{g}$ is a consistent estimate of $g$, for sufficiently large $n$ and $C > 0$ we have

$$(A8) \quad P \left\{ \tilde{g}^{[d]}(x) > 3h, \quad \forall x \in J \setminus B(X_0, Ch^{1/2}) \right\} > 1 - \frac{1}{3} \delta.$$ 

In (A7), when $x$ is in the neighborhood of $x_0$, $\tilde{g}^{[d]}(x) = O_p(h^2) = o_p(h)$. Hence, for such an $x$, we need to have a positive dominating second term in (A7) in order to claim

$$(A9) \quad P \left\{ \tilde{g}^{[d]}(x) + h^{(j_1 - |d| - r + 3/2)} c_K^T L^{(1)} \left( \frac{x_0 - x}{h^{1/2}} \right) > 2h, \quad \forall x \in B(X_0, Ch^{1/2}) \right\} > 1 - \frac{1}{3} \delta.$$ 

Given (A8), we must also have

$$(A10) \quad h^{(j_1 - |d| - r + 3/2)} c_K^T L^{(1)} \left( \frac{x_0 - x}{h^{1/2}} \right) > -h, \quad \forall x \in J \setminus B(X_0, Ch^{1/2}).$$ 

To ensure the right order in (A9) and (A10), we need to have $j_1 - |d| - r + 3/2 = 1$ which implies $j_1 = |d| + r - 1/2$. To further guarantee (A9) and (A10), given both $C$ and $\delta$, we may choose $L$ such that each component is linearly increasing or decreasing, depending on the positivity of the corresponding component of $c_K$, at a sufficiently fast rate on a sufficiently wide interval containing the origin and returning sufficiently slowly to 0 on either side of the interval where it is linearly increasing or decreasing. Note that our restrictions on $X_0$ play a role here. A point in the neighborhood of $X_0$ will have at least one coordinate (the $k$th coordinate) falling in the neighborhood of the corresponding coordinate of the chosen point $x_0$ in (A2). This is critical for guaranteeing that $L^{(1)} \left( \frac{x_0 - x}{h^{1/2}} \right)$ in (A9) has at least one non-zero component for any $x \in B(X_0, Ch^{1/2})$.

Lastly, for all $C, \delta > 0$, we have,

$$(A11) \quad P \{ B_3(x) > -h, \quad \forall x \in J \} > 1 - \frac{1}{3} \delta.$$
The derivation in (A7) with the above set probabilities yields

\[(A12) \quad P \left\{ \hat{g}^{[d]}(x|\bar{p}) > 0, \quad \forall x \in J \right\} > 1 - \delta,\]

which establishes (A1) for the case where at least one of the \(d_i\) is odd, \(1 \leq i \leq r\). When all the \(d_i\) are even, \(1 \leq i \leq r\), a similar derivation with \(j_1 = |d| + r\) and a suitably chosen \(L\) will also yield (A1). Combining the two cases, we have \(j_1 = |d| + r - \delta d/2\).

Next, we will show that \(L_2(\hat{p}) = O_p \left( n^{-1}h^{2j_i+1/2} \right)\). This follows from \(\Delta = O_p \left( h^{2j_i+1/2} \right)\) and

\[(A13) \quad n^{-1} \sum_{i=1}^{n} g(X_i)^{-2} L \left( \frac{x_0 - X_i}{h^{1/2}} \right)^2 = O_p \left( h^{1/2} \right),\]

which follows from the compactness of \(L(\cdot)\). Replacing \(p_i\) with \(\tilde{p}_i\) yields

\[
\sum_{i=1}^{n} (n\tilde{p}_i - 1)^2 = \sum_{i=1}^{n} \left[ \Delta + h^{j_1} \sum_{i=1}^{n} g(X_i)^{-1} L \left( \frac{x_0 - X_i}{h^{1/2}} \right) \right]^2 \\
\leq 2 \sum_{i=1}^{n} \left[ \Delta^2 + h^{2j_1} g(X_i)^{-2} L \left( \frac{x_0 - X_i}{h^{1/2}} \right)^2 \right] \\
= 2n \Delta^2 + 2nh^{2j_1} \cdot n^{-1} \sum_{i=1}^{n} g(X_i)^{-2} L \left( \frac{x_0 - X_i}{h^{1/2}} \right)^2 \\
= O_p \left( nh^{2j_1+1} \right) + O_p \left( nh^{2j_1+1/2} \right) = O_p \left( nh^{2j_1+1/2} \right) .
\]

Since \(\hat{p}\) minimizes \(L_2(p)\) subject to nonnegativity of \(\hat{g}^{[d]}\) on \(J\), this implies that for all sufficiently large \(n\),

\[P \{ L_2(\hat{p}) \leq L_2(\tilde{p}) \} > 1 - \delta.\]

Hence \(L_2(\hat{p}) = O_p \left( n^{-1}h^{2j_i+1/2} \right) = O_p \left( n^{-1}h^{2|d|+2r-\delta a+1/2} \right). \)

**Lemma A.3.** For each \(\delta > 0\), there exists \(C = C(\delta)\) such that, for all sufficiently large \(n\),

\[(A14) \quad P \left\{ \hat{g}^{[d]}(x) > \frac{1}{3} g^{[d]}(x), \forall x \text{ such that } \inf_{x_0 \in X_0} |x - x_0| \geq Ch^{1/2} \right\} > 1 - \delta.\]
Proof of Lemma A.3. Define \( \mathcal{X} = \{X_1, \ldots, X_n\} \) and \( \mu = E[\tilde{g}|\mathcal{X}] \). Let

\[
(A15) \quad A_n = \sup \left\{ M > 0 : \mu^{|d|}(x) < \frac{2}{3}g^{|d|}(x), \forall x \text{ such that } \inf_{x_0 \in \mathcal{X}_0} |x - x_0| \leq M \right\},
\]

\[
(A16) \quad B_n = \sup \left\{ M > 0 : |\tilde{g}^{|d|}(x) - \mu^{|d|}(x)| > \frac{1}{3}g^{|d|}(x), \forall x \text{ such that } \inf_{x_0 \in \mathcal{X}_0} |x - x_0| \leq M \right\},
\]

and \( C_n = \max(A_n, B_n) \). Then, for any \( x \) such that \( \inf_{x_0 \in \mathcal{X}_0} |x - x_0| \geq C_n \), we have \( \mu^{|d|}(x) \geq \frac{2}{3}g^{|d|}(x) \) and \( |\tilde{g}^{|d|}(x) - \mu^{|d|}(x)| \leq \frac{1}{3}g^{|d|}(x) \). Thus,

\[
\tilde{g}^{|d|}(x) > \frac{1}{3}g^{|d|}(x), \forall x \text{ such that } \inf_{x_0 \in \mathcal{X}_0} |x - x_0| \geq C_n.
\]

Therefore, we only need to show that

\[
(A17) \quad A_n = O_p \left( h^{1/2} \right) \quad \text{and} \quad B_n = O_p \left( h^{1/2} \right).
\]

Define the stochastic processes \( \gamma_1 = \mu^{|d|} - g^{|d|} \) and \( \gamma_2 = \tilde{g}^{|d|} \). For an integer \( j \geq 0 \), let

\[
\mathcal{J}_j = \left\{ x \in \mathcal{C}(\mathcal{J} \setminus \mathcal{X}_0) : jh^{1/2} \leq \inf_{x_0 \in \mathcal{X}_0} |x - x_0| \leq (j + 1)h^{1/2} \right\},
\]

where \( \mathcal{C}(S) \) is the closure of a subset \( S \subset \mathcal{J} \). Let \( J = \max\{j : \mathcal{J}_j \neq \emptyset\} \). Define \( \gamma_{kj}(x) = h^{|d|} + \hat{\sigma}_k^{|d|} \gamma_k(x) \) on \( \mathcal{J}_j \) for each \( 0 \leq j \leq J \). We want to show that

\[
(A18) \quad \sup_j P \left\{ \sup_{x \in \mathcal{J}_j} |\lambda_j(x)| > v \right\} \leq C_1(1 + v)^{-2}
\]

for all \( v \in [0, C_2h^{-1/2}] \), where \( \lambda_j \) stands for \( \gamma_{1j} \) or \( \gamma_{2j} \) and the constants \( C_1, C_2 > 0 \) do not depend on \( n \).

For this purpose, we need to use a strong approximation result found in Komlós, Major & Tusnády (1975), generally referred to as the Hungarian embedding. Let \( z_i, i = 1, \ldots, n \) be a sequence of independent and identically distributed random variables with \( E[z_i] = 0 \) and \( E[z_i^2] = \sigma^2 \), and let \( S_n = \sum_{i=1}^n z_i \). Then the Hungarian embedding result says that there exists a sequence \( T_n \) with the same distribution as \( S_n \) and a sequence of a standard Brownian bridge \( B_n(t) \) such that

\[
\sup_{0 \leq t \leq 1} \left| T_{nt} - \sigma \sqrt{n} B_n(t) \right| = O_p(\log n),
\]

where \( \lfloor x \rfloor \) signifies the integer part of \( x \).
Again, we only need to prove (A18) for the highest order derivative $d$. To economize on notation, we now use $\gamma_1 = \mu^{(d)} - g^{(d)}$ and $\gamma_2 = g^{(d)} - \mu^{(d)}$. Due to the independence between $\varepsilon_i = Y_i - g(X_i)$ and $X_i$, we have $\mu^{(d)}(x) = \frac{1}{n} \sum_{i=1}^{n} A_i^{(d)}(x) g(X_i)$. Hence

\[(A19) \quad \gamma_1(x) = \frac{1}{n} \sum_{i=1}^{n} \left\{ A_i^{(d)}(x) g(X_i) - g^{(d)}(x) \right\} \quad \text{and} \quad \gamma_2(x) = \frac{1}{n} \sum_{i=1}^{n} A_i^{(d)}(x) \varepsilon_i.\]

Note that $\text{Var}(\gamma_k(x)) = (nh^2)^{-1} C_k g(x) + o((nh^2)^{-1})$, where $C_1, K$ and $C_2, K$ are both constants depending only on $K(\cdot)$. Also, the fact that $K(\cdot)$ is compactly supported indicates that both sums in (A19) essentially have only $\lfloor nC_{x,h} \rfloor$ terms, where $C_{x,h} = P\{X \in B(x, Ch)\}$ for some constant $C$. Now applying the Hungarian embedding result to each $\sqrt{n}\gamma_k(x)$ yields

$$\sup_{x \in J} |\lambda_j(x)| \leq \sup_{x \in J} \left| \sqrt{C_{k,K} g(x)} B_n(C_{x,h}) \right| + O_p \left( \frac{\log n}{\sqrt{n}} \right).$$

Then (A18) follows from the modulus of continuity for a Brownian bridge; see e.g., Csörgő & Révész (1981, Chapter 1).

Therefore, letting $w_j \equiv (3h)^{-1} \inf_{x \in J} g^{(d)}(x)$ and $v_j \equiv \min(w_j, C_2h^{-1/2})$, we have

\[P \left\{ |\gamma(t)| > \frac{1}{3} g^{(d)}(t) \right\} \leq \sum_{j=0}^{J} \left( \sum_{j=0}^{J} P \left\{ |\gamma(t)| > \frac{1}{3} g^{(d)}(t) \right\} \right) \leq \sum_{j=0}^{J} P \left\{ \sup_{x \in J} |\lambda_j(x)| > v \right\} \leq \sum_{j=0}^{J} C_1(1 + v_j)^{-2},\]

where $\gamma$ represents either $\gamma_1$ or $\gamma_2$. For any $x \in J$, let $x_0 = \arg\min_{y_0 \in \mathcal{X}_0} |x - y_0| \in \partial \mathcal{X}_0 \setminus \partial J$ and $e = (x - x_0)/|x - x_0|$ be a unit vector. Then there exists a constant $0 \leq u \leq 1$ such that $x = x_0 + (j + u)h^{1/2}e$. The conditions imposed on $g$ in the theorem imply that

$$g^{(d)}(x_0 + (j + u)h^{1/2}e) = \frac{1}{2}(j + u)^2 h \nabla^T \partial g^{(d)} / \partial x_0 (x_0) e + O_p \left( h^{3/2} \right).$$

Hence, $w_j \geq C_3 j^2$ and $v_j \geq \min(C_3 j^2, C_4 h^{-1/2})$, where $C_3, C_4 > 0$ do not depend on $n$. Since $\sum_{j=0}^{J} (1 + C_3 j^2)^{-2} \to 0$ as $j_0 \to \infty$ and $\sum_{j=0}^{J} (1 + C_4 h^{-1/2})^{-2} = O_p(Jh) = O_p(h^{1/2})$, it now
follows from (A20) that
\[
\lim_{C \to \infty} \limsup_{n \to \infty} P \left\{ \tilde{g}^{[d]}(x) > \frac{1}{3} g^{[d]}(x), \text{ for some } x \text{ such that } \inf_{x_0 \in X_0} |x - x_0| \geq C h^{1/2} \right\} = 0.
\]

Applying the results to the respective versions of \( \gamma \) we obtain (A14).

**Proof of Theorem 2.2.** We prove each part of Theorem 2.2 in turn.

(i) For \( n \) sufficiently large the uniform weights will automatically satisfy the constraints. In this case the constrained estimator will be equivalent to the unconstrained estimator.

(ii) By the Cauchy-Schwarz inequality,
\[
\left| \hat{g}^{(j)}(x|\hat{p}) - \tilde{g}^{(j)}(x) \right| \leq \left| n^{-1} \sum_{i=1}^{n} (n\hat{p}_i - 1)^2 \right|^{1/2} \left| n^{-1} \sum_{i=1}^{n} A_i^{(j)}(x) Y_i^2 \right|^{1/2}
\]
\[
\leq O_p \left( n^{-1} h^{2|d|+2r-\delta_d+1/2} \right)^{1/2} O_p \left( h^{-(2r+2)|j|^{-1}} \right)^{1/2} = O_p \left( h^{j_d} \right),
\]
where \( j_d = |d| - |j| - \delta_d/2 + 3/4 \). The last inequality follows from Lemma A.2 and the fact that \( K(\cdot) \) is compactly supported. Note that (A21) indicates that when \( j \) is of lower order than \( d \),
\[
\sup_{x \in J} \left| \hat{g}^{(j)}(x|\hat{p}) - \tilde{g}^{(j)}(x) \right| \leq \sup_{x \in J} \left| \hat{g}^{(d)}(x|\hat{p}) - \tilde{g}^{(d)}(x) \right| = O_p \left( h^{j_d} \right).
\]
We used Lemma A.2 to establish the final order of the above difference. In particular, \( \sup_{x \in J} \left| \hat{g}(x|\hat{p}) - \tilde{g}(x) \right| = O_p \left( h^{d-\delta_d/2+3/4} \right) \). This proves part (ii) of Theorem 2.2.

(iii) Since \( K(\cdot) \) is compactly supported, there exists a constant \( M \) such that
\[
A_i(x) = 0 \quad \text{if } |x - X_i| \geq M h.
\]

Let \( Z_2 \) be a random variable such that
\[
Z_2 h^{j_d/2} = \inf \left\{ z > 0 : \hat{p}_i = n^{-1}(1 + \Theta), \forall i \text{ such that } \inf_{x_0 \in X_0} |x_0 - X_i| \geq z \right\},
\]
where \( j_d \) is the order in (A22) and \( \Theta \) is a random variable not depending on \( i \). This infinitum is well defined given Lemma A.1. Given (A23), any \( x \) such that \( \inf_{x_0 \in X_0} |x - x_0| \geq
\( Mh + Z_2h^{j_a/2} \) implies \( \hat{\rho}_i = n^{-1}(1 + \Theta) \), \( \forall i \) such that \( A_i(x) \neq 0 \), which in turn implies that \( \hat{g}(x|\hat{\rho}) = (1 + \Theta)\hat{g}(x) \).

Then Lemma A.3 yields

\[
(A24) \quad P \left\{ \hat{g}^{[d]}(x|\hat{\rho}) > \frac{1}{3}(1 + \Theta)g^{[d]}(x) > 0, \forall x \text{ such that} \right. \\
\left. \inf_{x_0 \in X_0} |x - x_0| \geq \max (Ch^{1/2}, Mh + Z_2h^{j_a/2}) \right\} > 1 - \delta.
\]

Using (A22) along with the convergence rate of \( \hat{g}^{[d]} \) gives us \( \hat{g}^{[d]}(x|\hat{\rho}) = g^{[d]}(x) + O_p(h^{j_a}) \) for any \( x \in J \). In particular, let \( x = x_0 + (Ch^{1/2} + Z_2h^{j_a/2}) \epsilon \in J \setminus X_0 \), where \( x_0 = \arg\min_{y_0 \in X_0} |x - y_0| \in \partial J \) and \( \epsilon = (x - x_0)/||x - x_0|| \) is a vector of unit length. Using \( Z(h^{1/2}) = Ch^{1/2} + Z_2h^{j_a/2} \) and a Taylor expansion gives

\[
\hat{g}^{[d]}(x_0 + Z(h^{1/2}) \epsilon|\hat{\rho}) = \frac{1}{2} Z(h^{1/2})^2 e^T \frac{\partial^2 g^{[d]}}{\partial x \partial x^T}(x_0) e + O_p(h^{j_a}) + o_p\left(Z(h^{1/2})^2\right) \\
= O_p(h^1) + O_p\left(Z_2^2h^{j_a}\right) + O_p(h^{j_a}).
\]

Clearly, we should have \( Z_2 = O_p(1) \) in order to guarantee (A24). Hence, \( \hat{\rho}_i \) is identically equal to \( n^{-1}(1 + \Theta) \) for some random variable \( \Theta \) and for all \( i \) such that \( |X_i - x_0| \geq Z_2h \), where \( Z_2 = O_p(1) \). Now we can define a random variable \( Z_1 \) such that

\[
Z_1h^{j_a/2} = \inf \left\{ z \geq 0 : \forall x \in J \text{ for which} \right. \\
\left. \inf_{x_0 \in X_0} |x - x_0| \geq z, \right. \\
\left. A_i(x) = 0 \text{ whenever} \hat{\rho}_i \neq n^{-1}(1 + \Theta) \right\}.
\]

Clearly \( Z_1 = O_p(1) \) and \( \hat{g}(x|\hat{\rho}) = (1 + \Theta)\hat{g}(x) \) for all values \( x \in J \) such that \( \inf_{x_0 \in X_0} |x - x_0| \geq Z_1h^{j_a/2} \). Recall that \( j_d = 3/4 - \delta_d/2 \). Hence this establishes the second part of (iii) of Theorem 2.2.

The order of \( \Theta \) is derived as follows. From Lemma A.1 we have that the weights \( \hat{\rho}_i \) are identical to \( n^{-1}(1 + \Theta) \) for indices \( i \) that lie a distance \( O(h^{1/2}) \) from \( x_0 \). Let there be \( N \) such indices that \( \hat{\rho}_i = n^{-1}(1 + \Theta) \), and let \( A \) be the set of remaining indices. Then
This establishes the first part of (iii) of Theorem 2.2. □
Appendix B. The Quadratic Program for Joint Monotonicity and Concavity

The method outlined in this paper requires the solution of a standard quadratic programming problem when the (in)equality constraints are linear in $p$. When our set of constraints is nonlinear in $p$, we can modify the problem to still allow for the use of standard off-the-shelf quadratic programming methods, which is computationally appealing. This appendix spells out in greater detail how to implement an appropriate quadratic program to solve for a vector of weights that will ensure a regression function is both monotonic (a constraint that is linear in $p$) and concave (a constraint that is nonlinear in $p$). For a more general overview of the procedures used to determine a set of weights when a user imposes nonlinear (in $p$) constraints on a regression function we refer the reader to Henderson & Parmeter (2009), though they restrict attention to probability weights and the power divergence metric of Cressie & Read (1984) whose limitations in the current setting are discussed in Section 1.

Suppose one wished to impose monotonicity and concavity in a two variable regression setting which involves jointly imposing constraints that are linear and nonlinear in $p$. We wish to minimize $D(p) = (p_u - p)'(p_u - p)$ subject to $\partial \hat{g}(x|p)/\partial x_1 \geq 0$, $\partial \hat{g}(x|p)/\partial x_2 \geq 0$, $H(x)$ (the Hessian of the estimated regression function) being negative semi-definite $\forall x \in \mathbb{R}^2$ and $\sum_{i=1}^{n} p_i = 1$. The first two conditions imply monotonicity of the regression function for each covariate, while the third condition gives us concavity of the function. The set of linear constraints for the quadratic program can be represented in matrix form as

\[ B^T = \begin{bmatrix} 1 & 1 & \ldots & 1 \end{bmatrix}, \]

\[ C_1^T = \begin{bmatrix} A_1^{(1,0)}(x_1)Y_1 & \ldots & A_1^{(1,0)}(x_n)Y_1 \\ A_2^{(1,0)}(x_1)Y_2 & \ldots & A_2^{(1,0)}(x_n)Y_2 \\ \vdots & \ddots & \vdots \\ A_n^{(1,0)}(x_1)Y_n & \ldots & A_n^{(1,0)}(x_n)Y_n \end{bmatrix}, \]
The last constraint can to be linearized with respect to \( p \) and can be written in matrix form as

\[
C_2^T = \begin{bmatrix}
A_1^{(0,1)}(x_1)Y_1 & \cdots & A_1^{(0,1)}(x_n)Y_1 \\
A_2^{(0,1)}(x_1)Y_2 & \cdots & A_2^{(0,1)}(x_n)Y_2 \\
\vdots & \ddots & \vdots \\
A_n^{(0,1)}(x_1)Y_n & \cdots & A_n^{(0,1)}(x_n)Y_n
\end{bmatrix}.
\]

Solving the quadratic program subject to \( B^T p = 1 \) and \( C_1^T p \geq 0 \) and \( C_2^T p \geq 0 \) will impose the adding up constraint on the weights and monotonicity. However, guaranteeing concavity of the regression function requires a modified approach.

Recall that for a matrix to be negative semi-definite the signs of the determinants of the principal minors must alternate in sign, beginning with a negative or zero value. That is, we need \( |H_1^*| \leq 0 , |H_2^*| \geq 0, \ldots , |H_k^*| = |H| \geq 0 \) if \( k \) is even (\( \leq 0 \) if \( k \) is odd), where \( | \cdot | \) denotes determinant. Aside from the principal minors of order one, the determinant of the remaining principal minor is nonlinear in the \( ps \). In our two variable setting we therefore need to have \( \partial^2 g(x|p)/\partial x_1^2 \leq 0 , \partial^2 g(x|p)/\partial x_2^2 \leq 0 , \) and \( (\partial^2 g(x|p)/\partial x_1^2)(\partial^2 g(x|p)/\partial x_2^2) - (\partial^2 g(x|p)/\partial x_2 \partial x_1)^2 \geq 0 \). The first two constraints are linear in \( p \) and can be written in matrix form as

\[
C_3^T = \begin{bmatrix}
A_1^{(2,0)}(x_1)Y_1 & \cdots & A_1^{(2,0)}(x_n)Y_1 \\
A_2^{(2,0)}(x_1)Y_2 & \cdots & A_2^{(2,0)}(x_n)Y_2 \\
\vdots & \ddots & \vdots \\
A_n^{(2,0)}(x_1)Y_n & \cdots & A_n^{(2,0)}(x_n)Y_n
\end{bmatrix},
\]

and

\[
C_4^T = \begin{bmatrix}
A_1^{(0,2)}(x_1)Y_1 & \cdots & A_1^{(0,2)}(x_n)Y_1 \\
A_2^{(0,2)}(x_1)Y_2 & \cdots & A_2^{(0,2)}(x_n)Y_2 \\
\vdots & \ddots & \vdots \\
A_n^{(0,2)}(x_1)Y_n & \cdots & A_n^{(0,2)}(x_n)Y_n
\end{bmatrix}.
\]

The last constraint can to be linearized with respect to \( p \) and one could then iterate this procedure using sequential quadratic programming (see Nocedal & Wright (2000, Chapter 18)). Letting \( g_{rs}(x|p) = \sum_{i=1}^n A_i^{(r,s)}(x)Y_ip_i \), the linearized version of the determinant of the second order cross...
partial is

$$C_5^T = \begin{bmatrix}
  c_{11} & \cdots & c_{1n} \\
  c_{21} & \cdots & c_{2n} \\
  \vdots & \ddots & \vdots \\
  c_{n1} & \cdots & c_{nn}
\end{bmatrix},$$

where $c_{vw} = g_{11}(x_w|p)A_v^{(0,2)}(x_w)Y_v + g_{22}(x_w|p)A_v^{(2,0)}(x_w)Y_v - 2g_{12}(x_w|p)A_v^{(1,1)}(x_w)Y_v$. To solve for the vector of weights consistent with both monotonicity and concavity, the quadratic program would be solved using $B$ and $C_1$ through $C_5$ to obtain an initial solution. This solution would then augment the starting value of $p$ to become an updated solution. The process would then be iterated until convergence of the $p$'s occurs. See Henderson & Parmeter (2009) for a more detailed explanation of this process.
Appendix C. R code to replicate the example in Section 3.1

We provide R code (R Development Core Team (2008)) to replicate the example in Section 3.1. Ignoring the code that generates the data for this example, the approach requires only 12 simple commands involving straightforward code and a call to a short routine that follows which generates the weights necessary for solving the quadratic programming problem (the rest of the code is used to generate the estimation and evaluation data). To allow the user to test the code on a trivial dataset we have changed the number of observations to \( n = 250 \) and evaluate on a grid of size 25x25 (instead of 10,000 and 50x50 used in Section 3.1).

```r
library(np)
library(quadprog)

n <- 250
n.eval <- 25
x.min <- -5
x.max <- 5
lower <- 0.0
upper <- 0.5

## The following loads a simple function that will return the
## weight matrix multiplied by n
source("Aymat_train_eval.R")

## Generate a draw from the DGP
x1 <- runif(n,x.min,x.max)
x2 <- runif(n,x.min,x.max)
y <- sin(sqrt(x1^2+x2^2))/sqrt(x1^2+x2^2) + rnorm(n,sd=.1)
data <- data.frame(y,x1,x2)
rm(y,x1,x2)

## Create the evaluation data matrix
data.eval <- data.frame(y=0,expand.grid(x1=seq(x.min,x.max,length=n.eval),
                                x2=seq(x.min,x.max,length=n.eval)))

## Now that we have generated the data, here is the body of the code
## (12 commands excluding comments)

## Generate the cross-validated local linear bandwidth object
## using the np package, then compute the unrestricted model
```
and gradients using the np package

```r
bw <- npregbw(y~x1+x2,regtype="ll",tol=.1,ftol=.1,nmulti=1,data=data)
model.unres <- npreg(bws=bw,data=data,newdata=data.eval,gradients=TRUE)

## Start from uniform weights equal to 1/n, generate p, Dmat, and dvec
## which are fed to the quadprog() function

p <- rep(1/n,n)
Dmat <- diag(1,n,n)
dvec <- as.vector(p)

## Generate the weight matrix

Aymat.res <- Aymat(0,data,data.eval,bw)

## Create Amat which is fed to the quadprog() function. The first line
## contains the adding to one constraint, the next blocks contain the
## lower and upper bound weighting matrices.

Amat <- t(rbind(rep(1,n),Aymat.res,-Aymat.res))
rm(Aymat.res)

## Create bvec (the vector of constraints) which is fed to the
## quadprog() function

bvec <- c(0,(rep(lower,n.eval)-fitted(model.unres)),
          (fitted(model.unres)-rep(upper,n.eval)))

## Solve the quadratic programming problem

QP.output <- solve.QP(Dmat=Dmat,dvec=dvec,Amat=Amat,bvec=bvec,meq=1)

## That's it. Now extract the solution and update the uniform weights

p.updated <- p + QP.output$solution

## Now estimate the restricted model using the np package and you are done.

data.trans <- data.frame(y=p.updated*n*data$y,data[,2:ncol(data)])
model.res <- npreg(bws=bw,data=data.trans,newdata=data.eval,gradients=TRUE)

## You could then, say, plot the restricted estimate if you wished.

plot(model.res,data=data.trans)
```
Here is the Aymat code located in source("Aymat_train_eval.R") called by the above example. It returns the weight matrix for the local linear estimator and its derivatives multiplied by \( n \).

\[
\text{Aymat} \leftarrow \text{function}(j.\text{reg}=1,\text{mydata}\_\text{train},\text{mydata}\_\text{eval},\text{bw}) \{
\]

\[
y \leftarrow \text{mydata}\_\text{train}[,1]
\]

\[
n.\text{train}=\text{nrow}(\text{mydata}\_\text{train})
\]

\[
n.\text{eval}=\text{nrow}(\text{mydata}\_\text{eval})
\]

\[
X.\text{train} \leftarrow \text{as.data.frame}(\text{mydata}\_\text{train}[,-1])
\]

\[
\text{names}(X.\text{train}) \leftarrow \text{names}(\text{mydata}\_\text{train})[-1]
\]

\[
X.\text{eval} \leftarrow \text{as.data.frame}(\text{mydata}\_\text{eval}[,-1])
\]

\[
\text{names}(X.\text{eval}) \leftarrow \text{names}(\text{mydata}\_\text{eval})[-1]
\]

\[
k \leftarrow \text{ncol}(X.\text{train})
\]

\[
\text{Aymat} \leftarrow \text{matrix}(\text{NA},\text{nrow}=\text{n.eval},\text{ncol}=\text{n.train})
\]

\[
\text{iota} \leftarrow \text{rep}(1,\text{n.train})
\]

\[
\text{for}(j \text{ in } 1:\text{n.eval}) \{
\]

\[
\text{evalmat} \leftarrow \text{as.data.frame}(\text{t}(\text{matrix}(\text{as.numeric}(X.\text{eval}[j,]),k,\text{n.train})))
\]

\[
\text{names}(\text{evalmat}) \leftarrow \text{names}(X.\text{eval})
\]

\[
W \leftarrow \text{as.matrix}(\text{data.frame}(\text{iota},X.\text{train}-\text{evalmat}))
\]

\[
K \leftarrow \text{npksum}(\text{txdat}=\text{evalmat}[1,],
\]

\[
\text{exdat}=X.\text{train},
\]

\[
\text{bws}=\text{bw}\_\text{bw}$\_\text{ksum}$\]

\[
\text{Wmat}\.\text{sum}\.\text{inv} \leftarrow \text{solve}(\text{npksum}(\text{exdat}=\text{evalmat}[1,],
\]

\[
\text{txdat}=X.\text{train},
\]

\[
\text{tydat}=W,
\]

\[
\text{weights}=W,
\]

\[
\text{bws}=\text{bw}\_\text{bw}$\_\text{ksum}$[,1])
\]

\[
\text{Aymat}[j,] \leftarrow \text{sapply}(1:\text{n.train},
\]

\[
\text{function}(i)\{(\text{Wmat}\.\text{sum}\.\text{inv} \odot \odot W[i,] \* K[i] \* y[i])[(j.\text{reg}+1)]\}
\]

\[
\}
\]

\[
\text{return}(\text{n.train} \* \text{Aymat})
\]

\[
\}
\]