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Generalized quantile and expectile properties for shape constrained nonparametric estimation

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A B S T R A C T

Convex quantile regression (CQR) is a fully nonparametric approach to estimating quantile functions, which has proved useful in many applications of productivity and efficiency analysis. Importantly, CQR satisfies the quantile property, which states that the observed data is split into proportions by the CQR frontier for any weight in the unit interval. Convex expectile regression (CER) is a closely related nonparametric approach, which has the following expectile property: the relative share of negative deviations is equal to the weight of negative deviations. The first contribution of this paper is to extend these quantile and expectile properties to the general set of shape constrained nonparametric functions. The second contribution is to relax the global concavity assumptions of the CQR and CER estimators, developing the isotonic nonparametric quantile and expectile estimators. Our third contribution is to compare the finite sample performance of the CQR and CER approaches in the controlled environment of Monte Carlo simulations.

1. Introduction

Convex quantile regression (CQR) introduced by Wang et al. (2014) is a fully nonparametric approach to estimating quantile functions, which has proved useful in many applications of productivity and efficiency analysis due to its robustness against random noise, heteroscedasticity, and outliers. One of the prime application areas has been shadow pricing of undesirable outputs such as greenhouse gas emissions (see, e.g., Dai et al., 2020; Kuosmanen et al., 2020; Quinn et al., 2022; Zhao & Qiao, 2022).

In practice, CQR employs a convenient linear programming (LP) formulation that minimizes the weighted sum of positive and negative deviations from the frontier, which has the deterministic data envelopment analysis (DEA) as the limiting special case where the weight of positive deviations τ approaches to one.[1] Wang et al. (2014) formally show that the CQR production function satisfies the quantile property, which states that the observed data is split into proportions τ below and $1 - \tau$ above the CQR frontier for any weight τ in the unit interval. Kuosmanen & Zhou (2021) further

extend the quantile property to the multiple-input multiple-output setting using the directional distance function.

Convex expectile regression (CER) is a closely related nonparametric approach, which differs from CQR in that the weighted sum of squared deviations is minimized instead of the weighted sum of absolute deviations.[2] Kuosmanen et al. (2015) motivate the use of squared deviations by noting that the CER frontier is always unique, whereas the CQR frontier is not necessarily unique if there are ties in the data (i.e., $\mathbf{x}_i = \mathbf{x}_j$ for some pair of observations i, j). Kuosmanen & Zhou (2021) formally show that CER satisfies the expectile property, which states that the relative share of negative deviations in the total sum of deviations is always equal to the weight $\tilde{\tau}$ of negative deviations.

Thus far, the quantile property of CQR and the expectile property of CER have been established in the canonical case of monotonic increasing and globally concave production function. However, the literature on shape constrained nonparametric regression and frontier estimation includes many other relevant specifications, including the constant, non-increasing, or non-decreasing returns to scale (e.g., Kuosmanen et al., 2015) and the isotonic regression (e.g., Keshvari & Kuosmanen, 2013) that relaxes the concavity/convexity assumption. Besides single output production func-

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[1] Banker et al. (1991) consider a very similar approach to CQR, referring to it as "stochastic DEA".

[2] In the parametric stream of literature, Aigner et al. (1976) pioneer the expectile regression approach.

tions, the joint production of multiple outputs is routinely modeled using the cost functions and distance functions. Finally, additional regularizations such as the L_1 norm, L_2 norm, or the Lipschitz norm are used to alleviate overfitting and the curse of dimensionality (e.g., Dai, 2023; Mazumder et al., 2019). It is not immediately obvious whether and to what extent the quantile property of CQR or the expectile property of CER carries over to these relevant extensions. The first contribution of this paper is to state and prove the generalized quantile and expectile properties that apply to any shape constrained nonparametric estimators.

The second contribution of this paper is to relax the concavity assumptions of CQR and CER, building on the work by Keshvari & Kuosmanen (2013). Importantly, the generalized quantile and expectile properties established in this paper also apply to the resulting *isotonic convex quantile regression* and *isotonic convex expectile regression*, respectively. Our main motivation for relaxing the concavity constraints is to facilitate the comparison of the CQR and CER approaches with other commonly used quantile frontier approaches in the literature. For example, Aragon et al. (2005) propose the widely used order-α estimator, where no concavity/convexity assumptions are usually imposed.[3] In contrast to the direct CQR and indirect CER approaches, the order-α estimator first estimates the quantile of the empirical distribution of deviations from the best practice frontier and then converts it to the corresponding quantile function. Wang et al. (2014) suggest that the performance of this procedure heavily depends on the assumptions on the distribution of the composite error term and the functional form of the underlying regression function (e.g., production, cost, or distance function). Thus far, the finite sample performance of the direct CQR, the indirect CER, and the order-α estimators has not been systematically examined in the controlled environment of Monte Carlo simulations.

Our third contribution is to compare the finite sample performance of the direct CQR estimation versus the indirect CER estimation of quantiles. While the quantile and expectile functions differ (see, e.g., Newey & Powell, 1987), one can easily convert expectiles to quantiles, and vice versa, using a well-established transformation (e.g., Efron, 1991; Waltrup et al., 2015). In the present context, Kuosmanen & Zhou (2021) hypothesize that the indirect estimation of quantile frontiers by first estimating multiple CER frontiers and subsequently converting them to relevant quantile functions can help to improve statistical performance compared to the direct CQR estimation. The Monte Carlo evidence presented in this paper supports this hypothesis.

We stress that our main focus is on the further development of the CQR and CER estimators. Our main motivation for including the order-α estimator in our Monte Carlo simulations is to put the finite sample performance of CQR and CER into an appropriate perspective. While a thorough review of the well-established order-α estimator falls beyond the scope of this paper, our simulations might provide interesting evidence regarding the finite sample performance of the order-α estimator as well. For example, we document that the order-α frontier does not necessarily satisfy the quantile property, particularly at low quantile.

The rest of this paper is organized as follows. Section 2 describes the theory on shape constrained nonparametric quantile and expectile regression. Section 3 introduces the operational implementation of quantile function estimation. Section 4 performs a Monte Carlo study to compare the finite sample performance

among nonparametric quantile frontier estimators. To illustrate and visualize the estimated quantile functions, an empirical application to a dataset of U.S. electric power plants is presented in Section 5. Section 6 concludes this paper with suggested avenues for future research. Formal proof and additional Monte Carlo simulation evidence are provided in Appendices A and B.

2. Theory

This section introduces the shape constrained quantile regression and states the generalized quantile property in Section 2.1. The shape constrained expectile regression and the generalized expectile property are introduced in Section 2.2. Since the main use of these methods has thus far been in the context of productivity and efficiency analysis, we phrase the results in the context of a stochastic nonparametric production model. However, the generalized quantile and expectile properties introduced in this section apply more broadly in shape constrained nonparametric estimation in any context.

2.1. Shape constrained nonparametric quantile regression

Consider the following nonparametric regression model

$$y_i = f(\boldsymbol{x}_i) + \varepsilon_i, \quad \text{for } i = 1, \ldots, n, \tag{1}$$

where $\boldsymbol{x} \in \mathbb{R}^d$ is the d-dimensional input vector and $y \in \mathbb{R}$ is the single output, respectively.[4] $f : \mathbb{R}^d \to \mathbb{R}$ is a nonparametric frontier production function and the composite error term ε consists of the random noise term v and the inefficiency term u according to $\varepsilon = v - u$. The nonparametric model (1) does not assume any specific functional form for the regression function f, but rather assumes that f satisfies certain axiomatic properties (e.g., monotonicity, concavity/convexity). As such, one can readily use this nonparametric model to characterize a production function by imposing shape constraints for all values of x in the support of $\boldsymbol{x}$ (see, e.g., Kuosmanen, 2008; Kuosmanen & Johnson, 2010; Yagi et al., 2020).

Assume a real valued data set $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ and let F be the joint distribution function of $(\boldsymbol{x}, y)$ and $F_{\boldsymbol{x}}(x)$ be the associated marginal distribution function of x (Aragon et al., 2005). Given the quantile $\tau \in (0, 1)$, the corresponding quantile function is defined as

$$Q(\tau \mid \boldsymbol{x}) := F^{-1}(\tau \mid \boldsymbol{x}) = \inf\{y \geq 0 \mid F(y \mid \boldsymbol{x}) \geq \tau\} \tag{2}$$

where $F(y \mid \boldsymbol{x}) = F(\boldsymbol{x}, y)/F_{\boldsymbol{x}}(x)$ and it is the conditional distribution function of y given $\boldsymbol{x} \leq x$. If the distribution function $F(y \mid \boldsymbol{x})$ is strictly increasing, then $Q(\tau \mid \boldsymbol{x}) = F^{-1}(\tau \mid \boldsymbol{x})$, where $F^{-1}(\tau \mid \boldsymbol{x})$ is the inverse of $F(y \mid \boldsymbol{x})$.

Note that when the data are generated according to Eq. (1) and the inputs are exogenous in the sense that $\mathsf{E}(\varepsilon|x) = \mathsf{E}(u)$, then the quantile function (2) can be equivalently stated as

$$Q(\tau \mid \boldsymbol{x}_i) = f(\boldsymbol{x}_i) + F_{\varepsilon_i}^{-1}(\tau) \tag{3}$$

where F_ε is the cumulative distribution function of the composite error term ε.

The objective of the shape constrained nonparametric regression is to find the best-fit function f within the set of functions $\mathcal{F}$. For example, f could be specified as a production function as in Wang et al. (2014), penalized production function as in Dai (2023), directional distance function as in Kuosmanen & Zhou (2021), or some other functions (e.g., cost function). Set $\mathcal{F}$ could include the classes of monotonic increasing/decreasing, concave/convex, and/or

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[3] Of course, one can subsequently convexify the estimated step function, similar to Ferreira & Marques (2020) and Polemis et al. (2021). Note that although the order-α estimator assumes monotonicity, the conditional estimator does not necessarily satisfy monotonicity (see Section 5 for an illustration). The recent paper by Daouia et al. (2017) avoids this problem by proposing an alternative unconditional order-α estimator.

[4] In this paper, we focus on the single output case (i.e., $y \in \mathbb{R}$), noting that CQR/CER and their nonconvex counterparts can also handle multiple outputs, see, e.g., Kuosmanen & Zhou (2021).

homogenous functions, possibly subject to other restrictions as well.

In general, the shape constrained nonparametric estimator of the quantile function (3) can be stated as

$$\hat{Q}(\tau \mid \boldsymbol{x}_i) = \underset{f_\tau \in \mathcal{F}}{\arg\min} \, \tau \sum_{i=1}^n \rho_\tau (y_i - f_\tau(\boldsymbol{x}_i)) \qquad (4)$$

where $\rho_\tau(t) = (\tau - \mathbb{1}\{t < 0\})t$ is the check function (Koenker & Bassett, 1978). Using Eq. (3), the estimator can be obtained as the optimal solution to the following optimization problem

$$\min \, \tau \sum_{i=1}^n \varepsilon_i^+ + (1 - \tau) \sum_{i=1}^n \varepsilon_i^- \qquad (5)$$

$$s.t. \quad y_i = Q(\tau \mid \boldsymbol{x}_i) + \varepsilon_i^+ - \varepsilon_i^- \quad \forall i$$
$$Q \in \mathcal{F}$$

Note that the error term ε_i in (1) is now decomposed into two non-negative components $\varepsilon_i^+ \geq 0$ and $\varepsilon_i^- \geq 0$ such that $\varepsilon_i = \varepsilon_i^+ - \varepsilon_i^-$.

Definition 1 (Quantile property). For any $\tau \in (0, 1)$, the number of strict positive residuals ($\hat{\varepsilon}_i^+ > 0$) denoted by n_τ^+ and the number of strict negative residuals ($\hat{\varepsilon}_i^- > 0$) denoted by n_τ^- satisfy the inequalities: $\frac{n_\tau^+}{n} \leq 1 - \tau$ and $\frac{n_\tau^-}{n} \leq \tau$, where n is the total number of observations.

Theorem 1. *For any real-valued data and non-empty set of functions $\mathcal{F}$, residuals $\hat{\varepsilon}_i^+$ and $\hat{\varepsilon}_i^-$, $i = 1, \ldots, n$ obtained as the optimal solution to (5) satisfy the quantile property.*

Proof. See Appendix A. □

This result generalizes the previous quantile properties established by Wang et al. (2014) and Kuosmanen & Zhou (2021) to any arbitrary shape constrained nonparametric quantile estimator that can be stated as a special case of the generic formulation (5). The practical benefit of this generalization is that it is no longer necessary to prove the quantile property every time one adds or deletes constraints. Note that the set $\mathcal{F}$ can include not only production axioms such as the weak or strong disposability, concavity/convexity, or alternative returns to scale assumptions, it can also include weight restrictions or regularization such as Lipschitz continuity, which can be useful to alleviate overfitting and/or the curse of dimensionality of the quantile estimator.

2.2. Shape constrained nonparametric expectile regression

Newey & Powell (1987) introduce linear expectile regression as an alternative method that relies on asymmetric least squares. Kuosmanen et al. (2015) are the first to consider asymmetric least squares in the present context of shape constrained nonparametric regression. Formally, for expectile $\tilde{\tau} \in (0, 1)$, the expectile function is defined as

$$\Gamma(\tilde{\tau} \mid \boldsymbol{x}_i) = f(\boldsymbol{x}_i) + F_{\varepsilon_i}^{-1}(\tau) \qquad (6)$$

The shape constrained nonparametric estimator of the expectile function (6) is formulated as

$$\hat{\Gamma}(\tilde{\tau} \mid \boldsymbol{x}_i) = \underset{f_{\tilde{\tau}} \in \mathcal{F}}{\arg\min} \, \tilde{\tau} \sum_{i=1}^n \rho_{\tilde{\tau}}(y_i - f_{\tilde{\tau}}(\boldsymbol{x}_i))^2 \qquad (7)$$

where $\rho_{\tilde{\tau}}(t) = (\tilde{\tau} - \mathbb{1}\{t < 0\})t^2$ is the "check function" in expectile regression (Newey & Powell, 1987). Using Eq. (3), the expectile estimator can be obtained as the optimal solution to the following optimization problem

$$\min \, \tilde{\tau} \sum_{i=1}^n (\varepsilon_i^+)^2 + (1 - \tilde{\tau}) \sum_{i=1}^n (\varepsilon_i^-)^2 \qquad (8)$$

$$s.t. \quad y_i = \Gamma(\tilde{\tau} \mid \boldsymbol{x}_i) + \varepsilon_i^+ - \varepsilon_i^- \qquad \forall i$$
$$\Gamma \in \mathcal{F}$$

Definition 2 (Expectile property). For any $\tilde{\tau} \in (0, 1)$, the number of strict positive residuals ($\hat{\varepsilon}_i^+ > 0$) and the number of strict negative residuals ($\hat{\varepsilon}_i^- > 0$) satisfy $\tilde{\tau} = \sum_{i=1}^n \hat{\varepsilon}_i^- / (\sum_{i=1}^n \hat{\varepsilon}_i^+ + \sum_{i=1}^n \hat{\varepsilon}_i^-)$.

Theorem 2. *For any real-valued data and non-empty set of functions $\mathcal{F}$, residuals $\hat{\varepsilon}_i^+$ and $\hat{\varepsilon}_i^-$, $i = 1, \ldots, n$ obtained as the optimal solution to (8) satisfy the expectile property.*

Proof. See Appendix A. □

This result generalizes the result by Kuosmanen & Zhou (2021) to any arbitrary shape constrained expectile estimator. Note that the expectile property is similar to the quantile property, but not exactly the same. This is because the expectile function is different from the quantile function (see, e.g., Newey & Powell, 1987; Waltrup et al., 2015). Beyond the discrepancy between the quantiles and expectiles, both approaches can be connected by a unique one-to-one mapping from quantile τ to expectile $\tilde{\tau}$. There exists a bijective function such that $\Gamma_{\tilde{\tau}} = Q_\tau$, where expectile $\tilde{\tau}$ is defined as below (De Rossi & Harvey, 2009)

$$\tilde{\tau} = \frac{\int_{-\infty}^{Q_\tau} (z - Q_\tau) dF(z)}{\int_{-\infty}^{Q_\tau} (z - Q_\tau) dF(z) - \int_{Q_\tau}^{\infty} (z - Q_\tau) dF(z)},$$

where $\int_{-\infty}^{Q_\tau} (z - Q_\tau) dF(z)$ and $\int_{Q_\tau}^{\infty} (z - Q_\tau) dF(z)$ are the lower and upper partial moments, respectively, and $F(z)$ is the cumulative distribution function of z. Therefore, we can always convert the expectile based quantile estimates $\hat{\Gamma}_{\tilde{\tau}}$ from the quantile estimates $\hat{Q}_\tau$, and vice versa. The estimator (7) can thus be treated as an indirect estimation of quantiles through expectile regression.

In practice, a simple procedure suggested by Efron (1991) is first to estimate the expectile and then indirectly determine the corresponding quantile by counting the number of negative residuals ε_i^- that take strictly positive values. More recently, Waltrup et al. (2015) propose a similar but more efficient approach by using the linear interpolation method. Note that all alternative transformation procedures rely on the quantile property. In another context, the estimated expectile function has been suggested to be more sensitive to outliers than the estimated quantile function (Daouia et al., 2020; Waltrup et al., 2015), which, however, is not supported by our Monte Carlo simulations (see Appendix B).

However, the effectiveness of indirect estimation of quantiles through expectile regression has not been tested in the present context of CER. Moreover, as an alternative to the direct quantile regression, we really do not know about the finite sample performance of CER. In Section 4, we will systematically compare the performance of these two approaches through Monte Carlo simulations.

3. Estimation

This section discusses the operational implementation of shape constrained quantile regression. Section 3.1 discusses the direct quantile estimation in the canonical case of monotonic increasing and concave production functions (Wang et al., 2014). Section 3.2 discusses the indirect estimation of quantiles based on CER (Kuosmanen & Zhou, 2021). In Sections 3.3 and 3.4 we relax the concavity assumption following Keshvari & Kuosmanen (2013), introducing the isotonic versions of CQR and CER, respectively.

3.1. Direct CQR

If the regression function f is assumed to be a family of continuous, monotonic increasing, and globally concave functions, we

can apply the direct CQR approach or the indirect CER approach to estimate quantile functions. Specifically, we solve problem (4) to obtain the estimated quantile function by converting it to the following LP problem (Wang et al., 2014)

$$\min_{\alpha, \boldsymbol{\beta}, \varepsilon^+, \varepsilon^-} \tau \sum_{i=1}^n \varepsilon_i^+ + (1 - \tau) \sum_{i=1}^n \varepsilon_i^- \tag{9}$$

$$s.t. \quad y_i = \alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i + \varepsilon_i^+ - \varepsilon_i^- \quad \forall i$$
$$\alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i \leq \alpha_h + \boldsymbol{\beta}_h' \boldsymbol{x}_i \quad \forall i, h$$
$$\boldsymbol{\beta}_i \geq \boldsymbol{0} \quad \forall i$$
$$\varepsilon_i^+ \geq 0, \ \varepsilon_i^- \geq 0 \quad \forall i$$

where the objective function is convex but not strictly convex on $\mathbb{R}^n$. The first set of constraints can be interpreted as a multivariate regression equation. The second set of constraints, i.e., a system of Afriat inequalities, imposes concavity. The third set of constraints imposes monotonicity, and the last refers to the sign constraints on the decomposed error terms.

Since it was proposed by Wang et al. (2014), convex quantile regression (CQR), as formulated in (9), has been applied to a number of studies because of its appealing features (e.g., Jradi & Ruggiero, 2019; Kuosmanen et al., 2015; Kuosmanen & Zhou, 2021). For example, the CQR estimator aims to estimate the conditional median or other quantiles of the response variable, and thus is more robust to random noise and heteroscedasticity than other central tendency estimators such as convex nonparametric least squares (Kuosmanen, 2008) and penalized convex regression (Dai et al., 2022). Furthermore, the CQR estimator is relatively computationally simple due to its LP formulation. In practice, problem (9) can be solved by standard algorithms for LP such as CPLEX or MOSEK.

One notable drawback of CQR is that the optimal solution to problem (9) is not necessarily unique, which also affects the estimated intercepts and slope coefficients (i.e., $\hat{\alpha}_i$ and $\hat{\beta}_{ij}$). This non-uniqueness problem of quantile regression could be assumed away if the inputs $\boldsymbol{x}$ are randomly drawn from a continuous distribution. However, the data will likely contain ties if the inputs are randomly drawn from a discrete distribution (consider, e.g., binomial or Poisson distribution). Empirical data are always rounded to a limited number of decimal digits, so the data tend to be discrete even when the underlying input distribution is continuous. Finally, firms optimize their inputs and outputs to maximize profit (or some other objective function), so the assumption of randomly drawn data is also debatable.

The coefficients α and $\boldsymbol{\beta}$ in problem (9) characterize the subgradients of the estimated nonparametric quantiles. Having solved problem (9), the τth quantile function can be expressed as (see, e.g., Kuosmanen, 2008; Seijo & Bodhisattva, 2011)

$$\hat{Q}(\tau \mid \boldsymbol{x}_i) = \min_{i=1,\dots,n} \left\{ \hat{\alpha}_i^\tau + \hat{\boldsymbol{\beta}}_i^{\tau'} \boldsymbol{x} \right\}.$$

This representor function allows us to 1) built an explicit representation for the quantile function $\hat{Q}$, which helps assess marginal properties, connect to the intuitive economic interpretations, and forecast and model *ex-post* economic events; 2) transform the infinite dimensional regression problem (4) into a finite dimensional LP problem (9), which also apply to the general multiple regression setting.

3.2. Indirect CER

Following Kuosmanen & Zhou (2021), we can indirectly estimate monotonic and concave quantile functions through expectile regression by transforming problem (7) into the following

quadratic programming (QP) problem

$$\min_{\alpha, \boldsymbol{\beta}, \varepsilon^+, \varepsilon^-} \tilde{\tau} \sum_{i=1}^n (\varepsilon_i^+)^2 + (1 - \tilde{\tau}) \sum_{i=1}^n (\varepsilon_i^-)^2 \tag{10}$$

$$s.t. \quad y_i = \alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i + \varepsilon_i^+ - \varepsilon_i^- \quad \forall i$$
$$\alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i \leq \alpha_h + \boldsymbol{\beta}_h' \boldsymbol{x}_i \quad \forall i, h$$
$$\boldsymbol{\beta}_i \geq \boldsymbol{0} \quad \forall i$$
$$\varepsilon_i^+ \geq 0, \ \varepsilon_i^- \geq 0 \quad \forall i$$

where the CER problem now minimizes the asymmetric squared deviations instead of the absolute deviations in (9).[5] The quadratic objective function in (10) guarantees the uniqueness of estimated quantile functions. Note that solving the CER problem requires QP, and that standard solvers such as CPLEX or MOSEK can effectively handle QP problems as well.

While the estimated quantile function is always unique in the CER estimation, the feasible set of problem (10) could be unbounded. That is, there may exist multiple combinations of shadow prices ($\hat{\beta}_{ij}$) leading to the same optimal value of the objective function (Dai, 2023). The non-unique estimates in both CQR and CER may further cause a longstanding problem of quantile crossing in quantile estimation. Dai et al. (2022) propose to address this problem by introducing additional regularization. By Theorem 2, such regularization does not violate the expectile property.

3.3. Direct isotonic CQR

Since the current methodological toolbox does not include a nonconvex quantile regression method, we propose to extend the approach by relaxing the convexity assumption and relying on the monotonicity assumption only. For both CQR and CER, we propose isotonic CQR and isotonic CER as their nonconvex counterparts. We then can resort to the direct isotonic CQR or indirect isotonic CER approach to estimate the monotonic quantile function.

Consider the production function f is isotonic with respect to a partial ordering: if for any pair $\boldsymbol{x}_i$ and $\boldsymbol{x}_h$, $\boldsymbol{x}_i \preccurlyeq \boldsymbol{x}_h$, the estimated production function $\hat{f}(\boldsymbol{x}_i) \in \mathcal{M}$, where $\mathcal{M} := \{ f \in \mathbb{R}^d : f(\boldsymbol{x}_i) \leq f(\boldsymbol{x}_h) \}$. When the partial ordering is defined as the dominance relation (i.e., $\boldsymbol{x}_i \preccurlyeq \boldsymbol{x}_j$ if $\boldsymbol{x}_i \leq \boldsymbol{x}_j$), the non-decreasing production function satisfies monotonicity (i.e., free disposability of inputs); that is, isotonicity is equivalent to monotonicity. However, the partial ordering could also be defined by other criteria (e.g., revealed preference information), where isotonicity is not exactly the same as monotonicity. In this paper, we follow the general isotonic notation given above but note that monotonicity is an important special case of isotonicity.

For a given set of data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ and quantile τ, for a given quantile τ, convex quantile regression over the class $\mathcal{M}$ is

$$\hat{Q}(\tau \mid \boldsymbol{x}_i) = \arg\min_{f_\tau \in \mathcal{M}} \sum_{i=1}^n \rho_\tau (y_i - f_\tau(\boldsymbol{x}_i)) \tag{11}$$

where the isotonic CQR problem (11) selects the best-fit isotonic quantile function from the class $\mathcal{M}$. In practice, however, it is impossible to directly search for the optimal solution from this infinite problem. Following Barlow & Brunk (1972), we can harmlessly replace the class of isotonic quantile functions $\mathcal{M}$ by the step functions $\mathcal{G} = \left\{ Q : \mathbb{R}_+^d \to \mathbb{R}_+ \mid Q(\tau \mid \boldsymbol{x}) = \sum_{i=1}^n \delta_i \mathcal{Z}(\tau \mid \boldsymbol{x}_i) \right\}$ where $\mathcal{Z}(\tau \mid \boldsymbol{x}_i)$ is an indicator function at a given quantile τ and

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[5] The convex nonparametric least squares (CNLS) estimator (Kuosmanen, 2008) is the special case of the CER estimator (10) when $\tilde{\tau} = 0.5$, that is, when the equal weight $\tilde{\tau}$ is given to both positive and negative deviations.
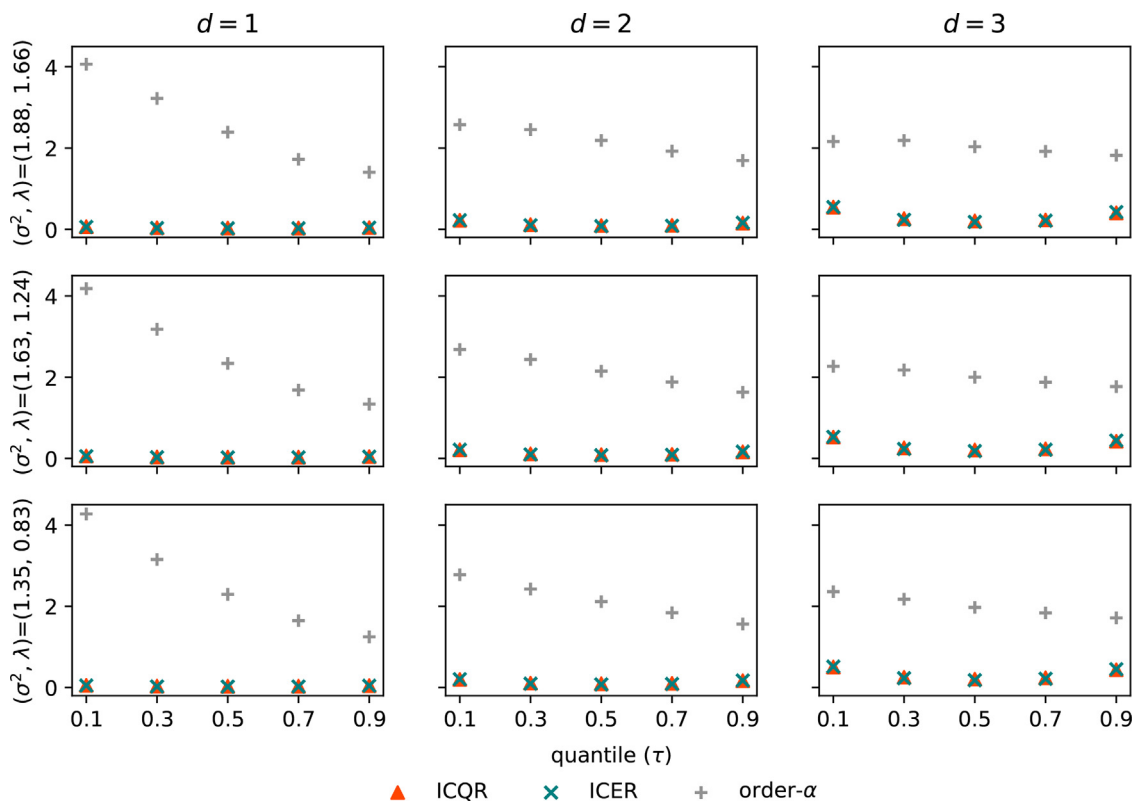
Fig. 1. MSE results of the order-α, isotonic CQR, and isotonic CER estimators with $n = 1000$.

is formulated as

$$\mathcal{Z}(\tau \mid \boldsymbol{x}_i) = \begin{cases} 1 & \text{if } \boldsymbol{x}_i \preccurlyeq \boldsymbol{x}, \\ 0 & \text{otherwise.} \end{cases}$$

and $\delta_i > 0$ is the parameter to characterize the step height. Note that the step functions $\mathcal{G}$ are a subset of the isotonic functions $\mathcal{M}$ (i.e., $\mathcal{G} \subset \mathcal{M}$), which helps to transform the infinite problem (11) to a finite problem (see, e.g., Barlow & Brunk, 1972; Keshvari & Kuosmanen, 2013).

The infinite problem (11) can be solved via the following finite dimensional isotonic CQR approach

$$\min_{\alpha, \boldsymbol{\beta}, \varepsilon^+, \varepsilon^-} \quad \tau \sum_{i=1}^{n} \varepsilon_i^+ + (1 - \tau) \sum_{i=1}^{n} \varepsilon_i^- \qquad (12)$$

$$\begin{aligned}
s.t. \quad & y_i = \alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i + \varepsilon_i^+ - \varepsilon_i^- && \forall i \\
& p_{ih}\left(\alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i\right) \leq p_{ih}\left(\alpha_h + \boldsymbol{\beta}_h' \boldsymbol{x}_i\right) && \forall i, h \\
& \boldsymbol{\beta}_i \geq \boldsymbol{0} && \forall i \\
& \varepsilon_i^+ \geq 0, \ \varepsilon_i^- \geq 0 && \forall i
\end{aligned}$$

where isotonic CQR requires an additional preprocessing step to determine the value of p_{ih} that represents the partial order between observation i and h. If $p_{ih} = 0$, the concavity constraint on the production function f is relaxed in isotonic CQR, that is, the Afriat inequality constraints are eliminated from isotonic CQR (12); otherwise, the isotonic CQR estimator is reduced to the original CQR estimator (9). Note that all the notations but p_{ih} in problem (12) are the same as those in problem (9). Therefore, the isotonic CQR estimator provides an alternative way to model the class of

nonparametric isotonic quantile regressions, which is computationally convenient and provides a clear link to CQR.[6]

To determine the value of p_{ih} in (12), we need to define a binary matrix $\boldsymbol{P} = \left[p_{ih}\right]_{n \times n}$

$$p_{ih} = \begin{cases} 1 & \text{if } \boldsymbol{x}_i \preccurlyeq \boldsymbol{x}_h, \\ 0 & \text{otherwise.} \end{cases}$$

The matrix $\boldsymbol{P}$ converts the partial order relations between two observations into binary values and the value of p_{ih} is determined by the standard dominance relations, which can be simply detected by an enumeration procedure suggested by Keshvari & Kuosmanen (2013). Further, the matrix $\boldsymbol{P}$ can be interpreted as a preference matrix if the partial ordering denotes the preference of a decision maker.

3.4. Indirect isotonic CER

Similarly, the indirect approach to fitting the isotonic quantile function is formulated as

$$\hat{\Gamma}(\tilde{\tau} \mid \boldsymbol{x}_i) = \operatorname*{arg\,min}_{f_{\tilde{\tau}} \in \mathcal{M}} \sum_{i=1}^{n} \rho_{\tilde{\tau}}(y_i - f_{\tilde{\tau}}(\boldsymbol{x}_i))^2 \qquad (13)$$

We also convert the infinite dimensional problem (13) to the following tractable QP problem to guarantee the unique expectile estimation and derive the isotonic CER approach

$$\min_{\alpha, \boldsymbol{\beta}, \varepsilon^+, \varepsilon^-} \quad \tilde{\tau} \sum_{i=1}^{n} (\varepsilon_i^+)^2 + (1 - \tilde{\tau}) \sum_{i=1}^{n} (\varepsilon_i^-)^2 \qquad (14)$$

$$s.t. \quad y_i = \alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i + \varepsilon_i^+ - \varepsilon_i^- \qquad \forall i$$

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[6] As an extension of CQR, isotonic CQR remains in the class of convex regression, even though the resulting step function is typically neither convex nor concave. Note that the estimated step function envelops a union of n convex sets.
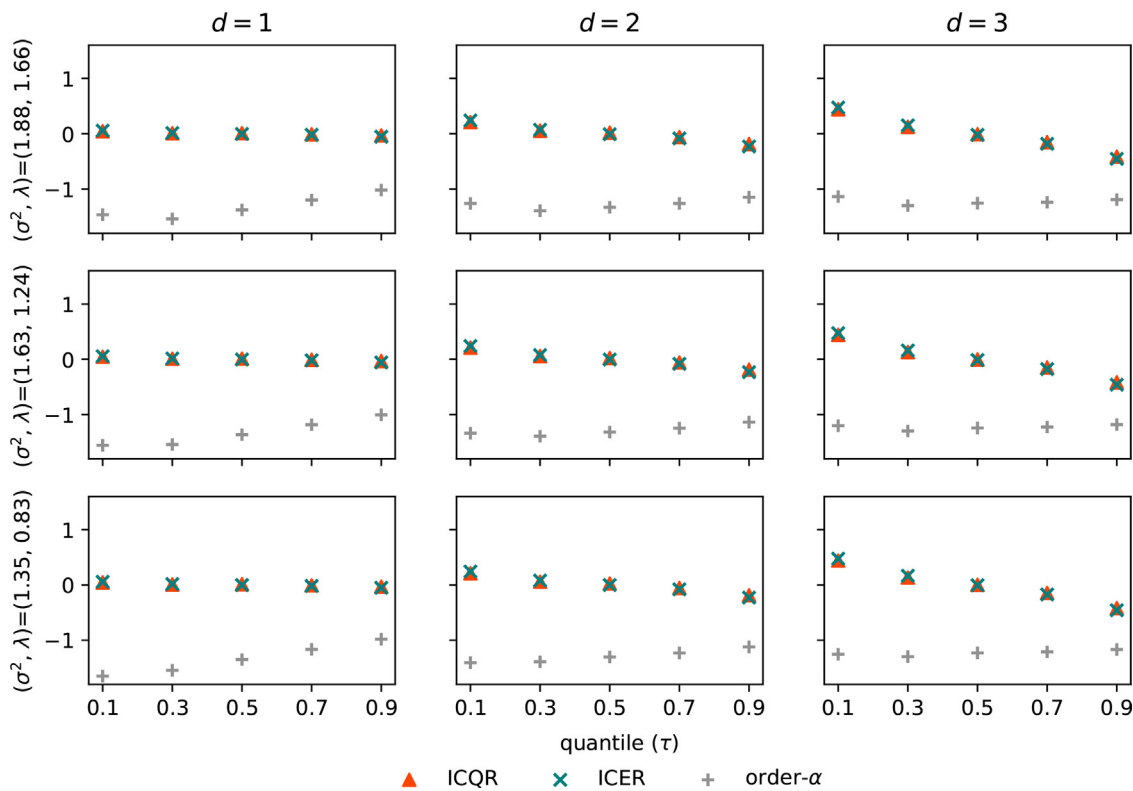
Fig. 2. Bias results of the order-α, isotonic CQR, and isotonic CER estimators with $n = 1000$.

$$p_{ih}\left(\alpha_i + \boldsymbol{\beta}'_i \boldsymbol{x}_i\right) \leq p_{ih}\left(\alpha_h + \boldsymbol{\beta}'_h \boldsymbol{x}_i\right) \quad \forall i, h$$

$$\boldsymbol{\beta}_i \geq \boldsymbol{0} \qquad \forall i$$

$$\varepsilon_i^+ \geq 0, \ \varepsilon_i^- \geq 0 \qquad \forall i$$

where the parameter p_{ih} is also predetermined by the standard dominance relation between the pairs of observations i and h. If $p_{ih} = 1$, problem (14) is reduced to problem (10), whereas problem (14) can be more easily solved in comparison with the original CER estimator (10). Furthermore, when the quadratic objective function is applied, we can connect the isotonic CER estimator with the standard FDH approach as a special case (i.e., $\tilde{\tau} = 0.5$). Note that the shape constrained quantile and expectile regression estimators can be extended to handle multiple outputs by introducing the directional distance function (see, e.g., Kuosmanen & Zhou, 2021).

In the context of efficiency analysis, the estimated quantile production functions can also serve as a better benchmark than the conventional full frontier for a unit's production structure analysis. Following Lai et al. (2018) we can easily measure the quantile technical efficiency for the evaluated units and even can extend the quantile efficiency analysis to meta-frontier analysis. For a given quantile τ, the estimated quantile technical efficiency for a specific unit could be greater than 1 (i.e., "super efficient"), equal to 1 (i.e., "efficient"), or less than 1 (i.e., "inefficient"), which are the same as the efficiency interpretation in the order-α estimator. Furthermore, as explained by Kuosmanen & Zhou (2021), quantile regression estimators are more appropriate for shadow pricing undesirable outputs (e.g., pollutants, CO_2 emissions).

Considering that CQR (9) and CER (10) are the restricted special cases of isotonic CQR (12) and isotonic CER (14), we could resort to isotonic CQR and isotonic CER to examine concavity for their convex counterparts (i.e., CQR and CER). Specifically, we can apply the standard F-test to test if the sum of weighted absolute residuals of the CQR problem is significantly smaller than that of the

isotonic CQR problem.[7] Note that the degree of freedom for those shape constrained nonparametric regression estimators can be determined by a data-driven approach (see Chen et al., 2020). Another possible approach to testing the shape (i.e., concavity and even monotonicity) is to apply the wild bootstrap methods (see, e.g., Yagi et al., 2020). While such a testing procedure is promising and straightforward, the computational efficiency is a serious concern, especially with a large sample size (Dai, 2023).

The curse of dimensionality is not a problem in the proposed quantile regression estimators. A recent study by Dai (2023) proposes the penalized CQR/CER approaches by introducing L_0-norm regularization and showed their high effectiveness in the dimensionality reduction of variables (or inputs). The same regularization can directly be applied to isotonic CQR/CER to ameliorate the effect of the curse of dimensionality. However, the rate of convergence of CQR/CER and isotonic CQR/CER has not been formally investigated in the literature, which warrants further research.

4. Monte Carlo study

The main objective of our simulations is to investigate the finite sample performance of those approaches and whether the generalized quantile and expectile properties are retained in the estimation of quantile functions.

4.1. Setup

We generate data according to the following additive Cobb-Douglas production function with d inputs and one output

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[7] In the expectile case, we can replace the sum of weighted absolute residuals with the sum of weighted squared residuals.

(cf. Lee et al., 2013; Yagi et al., 2020),

$$y_i = \prod_{d=1}^{D} \pmb{x}_{d,i}^{\frac{0.8}{D}} + \varepsilon_i,$$

where the input variables $\pmb{x}_i \in \mathbb{R}^{n \times d}$ are randomly and independently drawn from $U[1, 10]$ and the error term ε_i has three specifications: $\varepsilon_i = v_i$, $\varepsilon_i = -u_i$, and $\varepsilon_i = v_i - u_i$, where v_i and u_i are generated independently from $N(0, \sigma_v^2)$ and $N^+(0, \sigma_u^2)$, respectively. The variance parameters σ_v^2 and σ_u^2 are determined once we set signal to noise ratio (SNR) λ and variance σ^2, where $\lambda = \sigma_u/\sigma_v$ and $\sigma^2 = \sigma_u^2 + \sigma_v^2$. Following Aigner et al. (1977), $(\sigma^2, \lambda) = (1.88, 1.66)$, $(1.63, 1.24)$, and $(1.35, 0.83)$ are selected which allow for investigating whether those quantile-like estimators are robust to a wide range of SNR values.

To assess the finite sample performance of the quantile-like estimators, we utilize the standard mean squared error (MSE) and bias statistics to evaluate how the estimated quantile function deviates from the true conditional quantile function. The MSE and bias statistics can be defined as

$$\text{MSE} = \frac{1}{n} \sum_{i}^{n} \left(\hat{Q}(\tau \mid \pmb{x}_i) - Q(\tau \mid \pmb{x}_i) \right)^2,$$

$$\text{bias} = \frac{1}{n} \sum_{i}^{n} \left(\hat{Q}(\tau \mid \pmb{x}_i) - Q(\tau \mid \pmb{x}_i) \right),$$

where $\hat{Q}$ denotes the estimated conditional quantile function and Q represents the true conditional quantile function; the latter can be estimated based on the known inverse cumulative distribution function of the error term ε_i, i.e., $F_{\varepsilon_i}^{-1}(\tau)$. The MSE is always greater than or equal to zero, with zero indicating perfect precision; while the bias can be negative, positive, or zero, suggesting whether the estimated conditional quantile function $\hat{Q}$ systematically underestimates (bias < 0), overestimates (bias > 0), or provides an unbiased estimate of (bias = 0) the true conditional quantile function.

In all experiments that follow, we resort to Julia/JuMP to solve the CQR/CER and isotonic CQR/CER estimators with the commercial off-the-shelf solver MOSEK (9.3).[8] The standard and convexified order-α estimators are computed using the R packages "frontiles" (Daouia et al., 2020) and "Benchmarking" (Bogetoft & Otto, 2010). All experiments are run on Aalto University's high-performance computing cluster Triton with Xeon @2.8 GHz processors, one CPU, and 3 GB of RAM per task.

4.2. Experiment with monotonic estimators

In the first group of experiments, we explore whether the non-convex quantile estimator (i.e., isotonic CQR/CER) has better finite sample performance than the nonconvex order-α estimator in estimating the quantile production functions. We consider 225 scenarios with different numbers of observations (50, 100, 200, 500, and 1000), input dimensions (1, 2, and 3), SNRs (1.66, 1.24, and 0.83), and quantiles (0.1, 0.3, 0.5, 0.7, and 0.9). Each scenario is replicated 1000 times to calculate the MSE and bias statistics. For the sake of comparison, the expectiles $\tilde{\tau}$ are transformed into their corresponding quantiles τ based on the empirical inverse quantile function of the error term ε_i.

Table 1 reports the effect of sample size on the performance of each estimator in the case of $\tau = 0.9$, a commonly used parameter value in the robust frontier estimation. The results show that the finite sample performance of the isotonic CQR and isotonic CER

Table 1

Performance in estimating monotonic quantile function with $\sigma^2 = 1.88$ and $\tau = 0.9$. ICQR = Isotonic CQR, ICER = Isotonic CER.

d	n	MSE			Bias		
		ICQR	ICER	Order-α	ICQR	ICER	Order-α
1	50	0.368	0.406	1.470	−0.284	−0.385	−0.969
	100	0.215	0.231	1.479	−0.166	−0.252	−1.000
	200	0.132	0.135	1.419	−0.097	−0.156	−1.003
	500	0.069	0.067	1.409	−0.051	−0.086	−1.012
	1000	0.042	0.039	1.404	−0.031	−0.054	−1.018
2	50	0.933	0.989	1.777	−0.671	−0.731	−1.076
	100	0.639	0.692	1.784	−0.522	−0.591	−1.121
	200	0.416	0.454	1.742	−0.387	−0.454	−1.131
	500	0.236	0.255	1.712	−0.261	−0.313	−1.146
	1000	0.150	0.160	1.692	−0.186	−0.231	−1.150
3	50	1.479	1.519	1.959	−0.912	−0.944	−1.115
	100	1.152	1.197	1.901	−0.787	−0.827	−1.129
	200	0.875	0.920	1.882	−0.668	−0.714	−1.158
	500	0.572	0.602	1.849	−0.514	−0.558	−1.181
	1000	0.405	0.425	1.820	−0.415	−0.455	−1.191

estimators is superior to that of the order-α estimator in terms of both MSE and bias statistics. Further, the performance of each estimator improves with a larger sample size n, as expected. Specifically, the MSE and bias statistics of isotonic CQR and isotonic CER estimators get closer to zero as n increases, which suggests that both estimators are consistent. The MSE of the order-α estimator also generally falls as the sample size increases, whereas the bias does not diminish as the sample size increases due to losing the $\sqrt{n}$-consistency (Aragon et al., 2005).

Next, consider the choice of quantiles τ. Fig. 1 depicts the MSE results in estimating the quantile functions for different input dimensions and SNR specifications, while keeping the sample size fixed at $n = 1000$. In all scenarios considered, the isotonic CQR and isotonic CER estimators have far smaller MSE values than the order-α estimator. However, the difference in terms of MSE between isotonic CQR and isotonic CER is quite small. Another interesting observation is that when the quantile τ becomes smaller, the MSE of the order-α estimator sees a systematic increasing trend.

We note that the MSE of each estimator generally increases as more input variables are introduced. This is because a larger dimensionality increases the data sparsity, which degrades the performance of each estimator, *ceteris paribus*. For example, when $\tau = 0.9$ and $\sigma^2 = 1.88$, the MSE of the order-α estimator increases from 1.40 in the one-input case to 1.69 in the two-input case to 1.82 in the three-input case, and isotonic CQR's and isotonic CER's MSE values rise from 0.04 to 0.15 to 0.40 and from 0.04 to 0.16 to 0.42, respectively. A similar curse of dimensionality also exists in the DEA simulation studies, where the performance of DEA deteriorates when the number of inputs increases, *ceteris paribus* (see, e.g., Cordero et al., 2015; Pedraja-Chaparro et al., 1999).

Fig. 2 displays the bias results. The isotonic CQR and isotonic CER estimators yield both positive and negative biases. The bias gets greater (in terms of the absolute value) when τ deviates from 0.5: it becomes a larger positive value when τ decreases from 0.5 and, on the opposite, a smaller negative value when τ increases from 0.5. By contrast, the order-α estimator yields only negative biases. Since the order-α frontier converges to the FDH full frontier in a finite sample when $\tau \to 1$, the observed negative bias of the order-α estimator for each quantile τ is due to the small sample bias, similar to FDH. Moreover, the bias of the order-α estimator becomes larger as τ decreases because the effective sample size gets smaller.

Furthermore, we obtain similar results about the MSE and bias statistics and the sample size effect in additional experiments
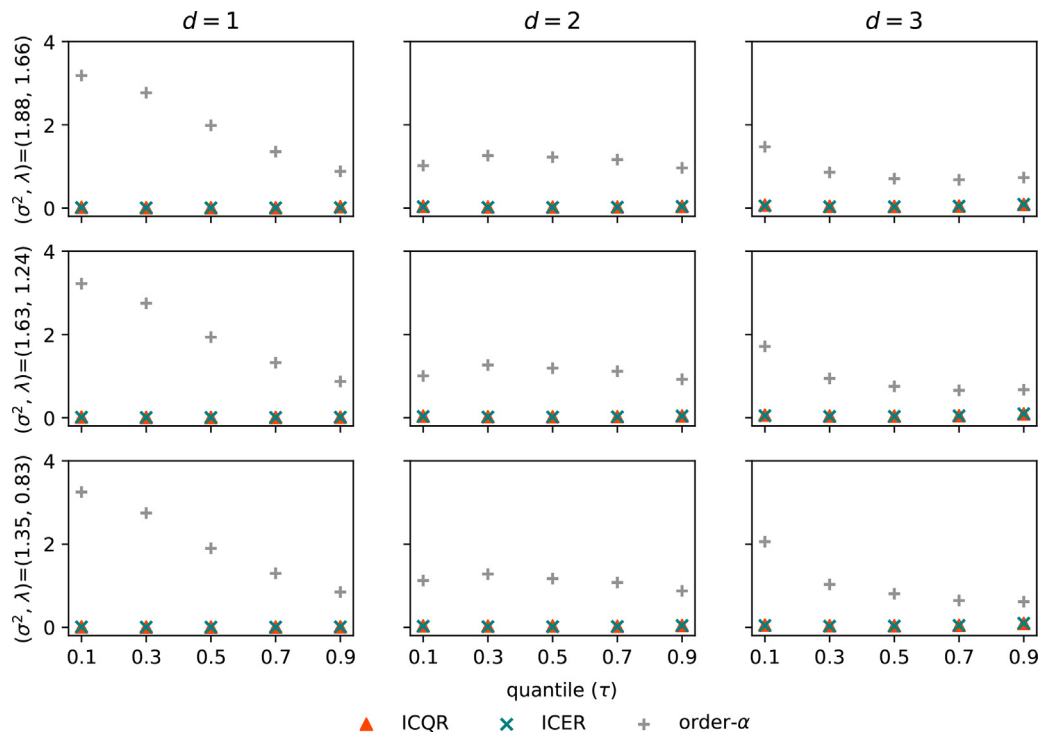
Fig. 3. MSE results of the convexified order-α, CQR, and CER estimators with $n = 1000$.

where the composite error term ε_i contains either inefficiency ($\varepsilon_i = -u_i$) or noise ($\varepsilon_i = v_i$) (see Appendix B.1). We also investigate the estimators' performance in the presence of functional form misspecification and find that the isotonic CQR and isotonic CER estimator outperform the order-α estimator in terms of both MSE and bias statistics (see Appendix B.2). To examine the robustness of each estimator, we consider additional scenarios with outliers. The results suggest that the isotonic CER estimator is superior in all scenarios, and the isotonic CER and isotonic CQR estimators are more robust than the order-α estimator due to the fact that the order-α estimator does not satisfy the quantile property (see Appendix B.3).

Another point worth noting is that the order-α estimator is found to perform relatively poorly at low quantiles. Thus, we further investigate the frequency of violations of the quantile property in 1000 replications. Our simulations confirm that both isotonic CQR and isotonic CER satisfy the quantile property with the violation rates being zero. In contrast, the quantile property is systematically violated in the order-α estimator at low quantiles, particularly at the 10% quantile (see Table 2). The observed violations are due to the fact that the order-α estimator relies on the quantiles of an appropriate distribution based on a subset of the sample. However, for high quantiles (i.e., $\tau > 0.5$), the violation rates in the order-α estimator are also equal to zero, suggesting that the order-α estimator can satisfy the quantile property for large τ. This is consistent with the findings from the MSE and bias comparisons. In conclusion, the Monte Carlo simulations presented in this subsection demonstrate that the true quantile estimators perform notably better than the order-α estimator in the nonconvex case.

4.3. Experiment with monotonic and convex estimators

We next conduct the second group of experiments to compare the performance of the convex estimators (i.e., CQR, CER, and convexified order-α) using the same scenarios as in Section 4.2. Table 3 presents the effects of sample size and dimensionality on the MSE and bias statistics for $\tau = 0.9$. Figs. 3 and 4 display the

MSE and bias statistics of the convexified order-α, CQR, and CER estimators as we alternate the values of τ and SNR, while keeping the sample size constant at $n = 1000$.

The simulation results reported in Table 3 suggest that both CQR and CER estimators exhibit superior performance compared to the convexified order-α estimator both in terms of MSE and bias. Further, the MSE and bias of CQR and CER converge towards zero as the sample size n increases, while this is not the case for the convexified order-α estimator when the dimensionality $d = 1, 2$.

Comparing Figs. 1 and 3, we notice that the MSE statistic for each estimator decreases to a great extent once imposing the concavity constraint, especially for the order-α estimator. For instance, in the one-input case with $\sigma = 1.88$, the average MSE of the convexified order-α estimator for the five estimated quantiles decreases by more than 160% compared to its original counterpart. This finding confirms that the power of the CQR, CER, and convexified order-α estimators derives from their global shape constraints, including monotonicity and convexity/concavity (Kuosmanen et al., 2020).

While the performance of the order-α estimator increases after imposing the concavity constraint, the CQR and CER estimators continue to outperform the convexified order-α estimator in all cases considered. However, the relative MSE ratio between the convexified order-α estimator and CQR (or CER) decreases as the input dimensionality or the quantile τ increases. Regarding the effect of different SNRs, the smaller the value of λ, the higher the difference in MSE between the quantile and order-α estimators. However, the difference in MSE among the three SNRs is close to zero when the quantile τ approaches 1.

Recall that the biases of the order-α estimator in all considered scenarios are negative, indicating that the estimated order-α frontiers systematically underestimate the true quantile functions. After imposing the concavity constraint, for the three-input cases, the convexified order-α estimator does not only underestimate but can also overestimate the true quantile function. Moreover, the absolute bias of the convexified order-α estimator is larger than that of
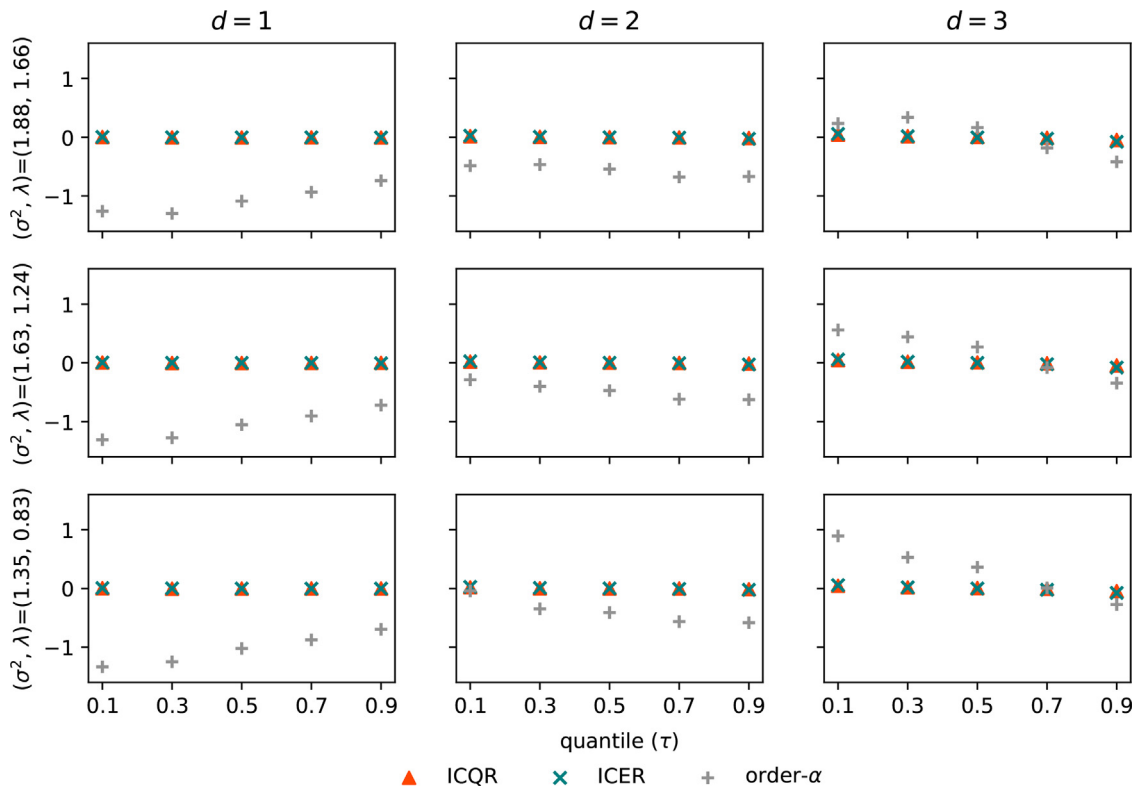
Fig. 4. Bias results of the convexified order-α, CQR, and CER estimators with $n = 1000$.
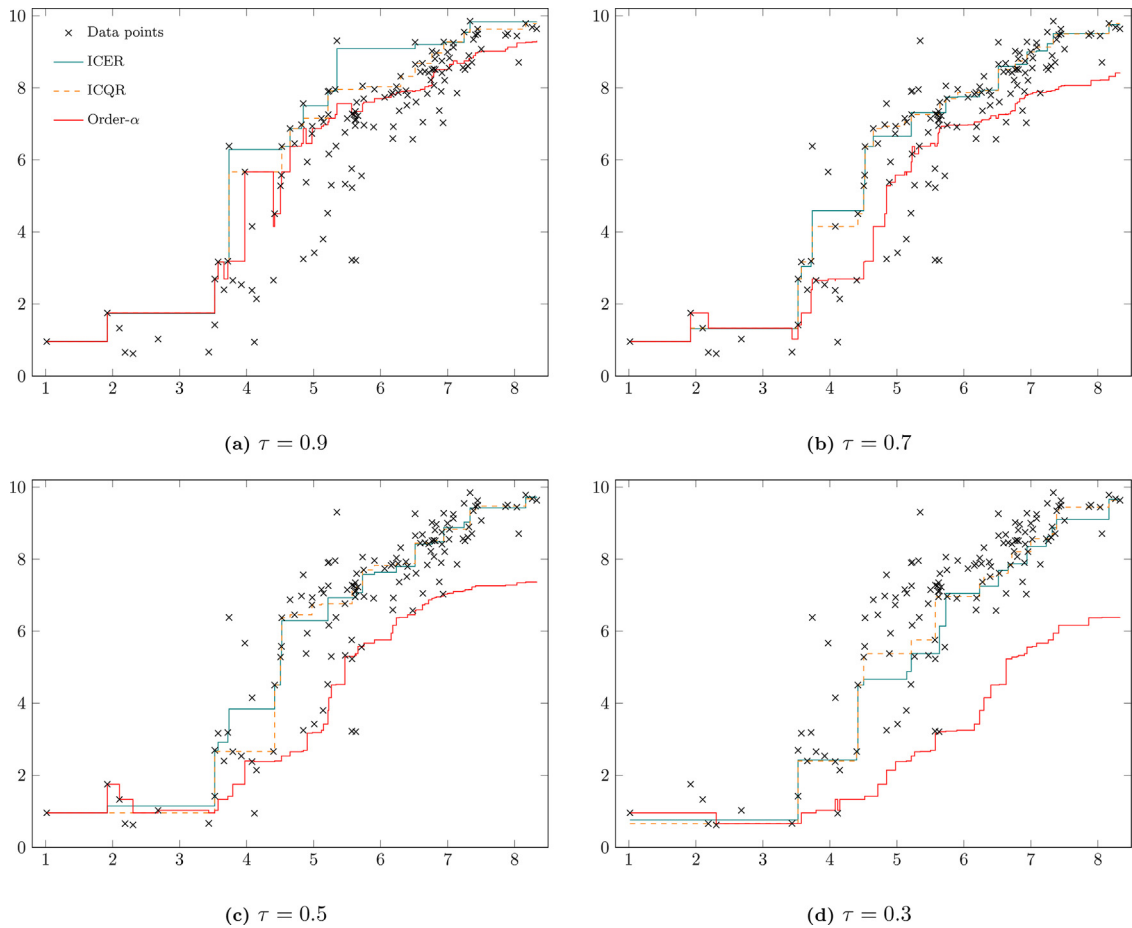

(a) $\tau = 0.9$

(b) $\tau = 0.7$

(c) $\tau = 0.5$

(d) $\tau = 0.3$

Fig. 5. Illustration of the estimated order-α, isotonic CQR, and isotonic CER functions. *X*-axis: ln(C), *Y*-axis: ln(G).

Table 2

Frequency of quantile property violations for the order-α estimator in 1000 replications.

n	d	(σ^2, λ)	τ			n	d	(σ^2, λ)	τ	
			0.1	0.3	0.5				0.1	0.3
50	1	(1.88, 1.66)	95.8%	0.3%		100	1	(1.88, 1.66)	99.6%	
		(1.63, 1.24)	90.3%	0.3%				(1.63, 1.24)	97.7%	
		(1.35, 0.83)	75.1%	0.4%				(1.35, 0.83)	86.7%	
	2	(1.88, 1.66)	89.6%	1.7%			2	(1.88, 1.66)	88.8%	
		(1.63, 1.24)	83.8%	1.6%				(1.63, 1.24)	76.8%	
		(1.35, 0.83)	79.7%	1.9%				(1.35, 0.83)	66.1%	0.1%
	3	(1.88, 1.66)	98.9%	7.6%	0.2%		3	(1.88, 1.66)	98.1%	0.5%
		(1.63, 1.24)	98.8%	8.2%	0.2%			(1.63, 1.24)	97.3%	0.7%
		(1.35, 0.83)	98.7%	7.1%	0.1%			(1.35, 0.83)	96.7%	0.5%
500	1	(1.88, 1.66)	100.0%			1000	1	(1.88, 1.66)	100.0%	
		(1.63, 1.24)	100.0%					(1.63, 1.24)	100.0%	
		(1.35, 0.83)	98.7%					(1.35, 0.83)	100.0%	
	2	(1.88, 1.66)	89.3%				2	(1.88, 1.66)	90.1%	
		(1.63, 1.24)	32.6%					(1.63, 1.24)	10.8%	
		(1.35, 0.83)	10.0%					(1.35, 0.83)	0.9%	
	3	(1.88, 1.66)	74.5%				3	(1.88, 1.66)	37.9%	
		(1.63, 1.24)	60.2%					(1.63, 1.24)	17.1%	
		(1.35, 0.83)	50.7%					(1.35, 0.83)	11.3%	

Note: The blanks in the columns of different quantiles denote zero violations.

(a) $\tau = 0.9$ **(b)** $\tau = 0.7$

(c) $\tau = 0.5$ **(d)** $\tau = 0.3$
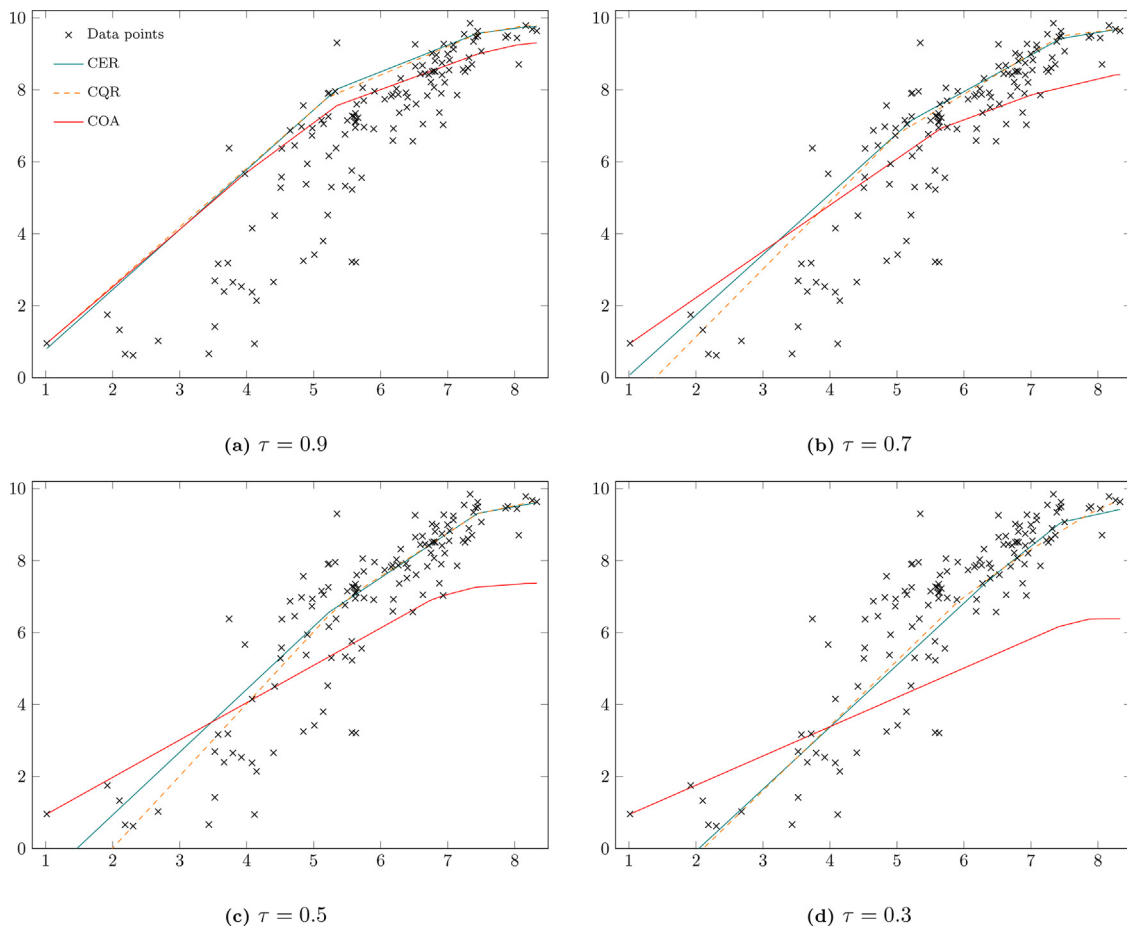
Fig. 6. Illustration of the estimated convexified order-α, CQR, and CER functions. *X*-axis: $\ln(C)$, *Y*-axis: $\ln(G)$.

CQR/CER in all scenarios. Note that CQR and CER can better fit the true quantile functions with lower MSE and bias values compared to the monotonic estimators in Section 4.2.

The simulation results in Sections 4.2 and 4.3 reveal that the indirect estimation of quantiles using expectiles improves the performance in most scenarios considered, particularly for the concave quantile functions. Table 4 reports the percentage of simulation rounds where the MSE of the indirect expectile estimators is lower than that of the direct quantile estimators. Compared to isotonic CQR, isotonic CER has smaller MSE values for most quantiles considered except for those extreme quantiles (e.g., the 10% and 90% quantiles). Further, when we impose the concavity constraint, the CER estimator outperforms the CQR estimator in a larger proportion of scenarios (e.g., all scenarios at the 10% and 50% quantiles). The observation from Table 4 suggests that the indirect estimation of quantiles through expectiles performs better when τ is

Table 3
Performance in estimating monotonic and concave quantile function with $\sigma^2 = 1.88$ and $\tau = 0.9$. COA = Convexified order-α.

d	n	MSE			Bias		
		CQR	CER	COA	CQR	CER	COA
1	50	0.170	0.169	0.635	−0.056	−0.110	−0.497
	100	0.094	0.088	0.704	−0.023	−0.056	−0.574
	200	0.050	0.050	0.757	−0.009	−0.023	−0.636
	500	0.022	0.021	0.831	−0.005	−0.010	−0.694
	1000	0.031	0.011	0.880	−0.005	−0.005	−0.738
2	50	0.377	0.395	0.838	−0.194	−0.308	−0.574
	100	0.231	0.239	0.854	−0.106	−0.186	−0.601
	200	0.133	0.137	0.880	−0.056	−0.102	−0.621
	500	0.067	0.069	0.934	−0.027	−0.048	−0.654
	1000	0.039	0.039	0.964	−0.013	−0.026	−0.668
3	50	0.632	0.671	0.857	−0.406	−0.502	−0.574
	100	0.412	0.438	0.741	−0.249	−0.344	−0.485
	200	0.263	0.280	0.709	−0.152	−0.229	−0.440
	500	0.141	0.150	0.722	−0.082	−0.126	−0.427
	1000	0.087	0.091	0.732	−0.046	−0.078	−0.419

close to 0.5, whereas the direct quantile estimation remains competitive when τ is very small or very large.

5. Empirical illustration

To gain an intuition of what the quantile production functions look like, we proceed to illustrate those estimators with a real cross-sectional dataset used in Kuosmanen & Zhou (2021) and Dai et al. (2022). It covers plant-level data on 130 U.S. electric power plants in 2014. A very similar dataset has been repeatedly used in the empirical demonstration of newly developed frontier estimators (see, e.g., Gijbels et al., 1999; Martins-Filho & Yao, 2008).

Following Gijbels et al. (1999) and Martins-Filho & Yao (2008), we consider a univariate case where the output $y = \ln(G)$ with G being the net generation of each power plant and the input $x = \ln(C)$ with C being the sum of fixed cost and variable cost of electricity production. See Kuosmanen & Zhou (2021) for a detailed discussion of the data sources and descriptive statistics.

Since there exists a one-to-one mapping between quantiles and expectiles, we estimate a number of expectiles (i.e., $\tilde{\tau} = 0.001$, 0.002, ..., 0.999) and then determine the corresponding quantile τ by counting the number of negative residuals ε_i that take strictly positive values (Efron, 1991). Fig. 5 depicts the estimated monotonic quantile and expectile functions by the order-α, isotonic CQR, and isotonic CER estimators at $\tau = 0.9$, 0.7, 0.5, and 0.3, respectively.

For the sake of illustration, the order-α estimator (Aragon et al., 2005), one of the most notable partial frontier estimators, is applied and compared in all the application and simulations. Further, the thorough comparisons also include the convexified order-α estimator, where we first utilize the order-α estimator to estimate the order-α production frontier and then apply the standard DEA-

VRS (variable returns to scale) estimator to the estimated output on the order-α production frontier (Polemis et al., 2021). Note that the order-α estimator has been extended to the multivariate setting (Daouia & Simar, 2007; Daouia et al., 2017), hyperbolic orientation (Wheelock & Wilson, 2009), and directional measures (Simar & Vanhems, 2012). Meanwhile, the standard order-α estimator and its extensions have been widely applied in the context of productivity and efficiency analysis (see, e.g., Carvalho & Marques, 2014; Kounetas et al., 2021; Polemis et al., 2021; Wheelock & Wilson, 2013).

The estimated isotonic CQR and isotonic CER functions are step functions enveloping exactly $100\tau\%$ of the observations for each quantile τ. In contrast, the estimated order-α frontier does not necessarily envelope $100\tau\%$ of the observations, but rather less than $100\tau\%$ of the observations especially when the quantile τ gets smaller such as $\tau = 0.3$ (see Fig. 5d). This observation suggests that the order-α estimator cannot guarantee the quantile property, especially for the low quantile estimation. This is because the order-α estimator is geared towards estimating high quantiles but deteriorates when τ decreases. Further, the standard order-α estimator does not even satisfy monotonicity, which is its only assumed shape constraint. The violation of monotonicity occurs in all cases—the estimated order-α frontier (red line) is not strictly increasing but can also decrease, as shown in Fig. 5 (see also Figs. 2 and 3 in Daouia & Simar 2007).

Fig. 6 illustrates the direct CQR and indirect CER quantile estimates when global concavity is imposed and the estimated convexified order-α frontier. All three estimators yield a concave piecewise linear curve which can be useful in applications where shadow pricing of non-market inputs and/or outputs is the main object of interest. In this respect, it is worth noting that the slope of the order-α frontier is similar to those of CQR and CER for $\tau = 0.9$, but the slope decreases rapidly as τ decreases. The slope coefficients of CQR and CER, which are important for estimating the marginal products and elasticities, are much more robust across different values of τ in this illustrative example.

This example also illustrates that indirect estimation of quantiles using expectiles can be a good alternative to estimate monotonic concave quantile functions and even monotonic step quantile functions. For each quantile τ, the indirectly estimated quantile function using expectile regression (teal line) is quite close to the directly estimated quantile function (orange dashed line) (see Figs. 5 and 6). Of course, a single example does not allow one to judge which approach performs better.

6. Conclusions

In this paper we have extended the theory and methodology of shape constrained quantile and expectile regression in three directions. First, we have stated and proved the generalized quantile and expectile properties that apply to any shape constrained nonparametric estimators. Examples of such estimators include the

Table 4
Percentage of scenarios where the indirect CER estimator has smaller MSE than the direct CQR estimator.

Model specification	τ	$\varepsilon = v - u$	$\varepsilon = v$	$\varepsilon = -u$	No. scenarios
Monotonicity	all quantiles	65.8%	63.1%	57.3%	225
	0.1	22.2%	13.3%	26.7%	45
	0.5	100.0%	100.0%	100.0%	45
	0.9	13.3%	13.3%	13.3%	45
+ Concavity	all quantiles	88.0%	88.0%	89.8%	225
	0.1	100.0%	100.0%	100.0%	45
	0.5	100.0%	100.0%	100.0%	45
	0.9	40.0%	40.0%	55.6%	45

isotonic regression that relaxes the global concavity or convexity assumptions. Our result also implies that the quantile and expectile properties carry over to the constant, non-increasing, or non-decreasing returns to scale technologies, the cost function and distance function specifications, as well as additional regularizations, which are increasingly used in applications to alleviate overfitting and the curse of dimensionality.

Second, we have extended the toolbox of shape constrained quantile and expectile estimation by introducing the isotonic convex quantile regression and isotonic convex expectile regression, respectively. These new variants of CQR and CER enable us to relax the concavity assumptions of CQR and CER, similar to isotonic regression.

Third, we have provided new evidence of the finite sample performance of the CQR, CER, and their isotonic counterparts in the controlled environment of Monte Carlo simulations. To compare CQR and CER, we converted the expectiles estimated by CER to quantiles using a transformation suggested by Efron (1991). Our simulations confirm that the indirect estimation of quantile frontiers by first estimating multiple CER frontiers and subsequently converting them to relevant quantile functions improves finite sample performance compared to the direct CQR estimation.

Our simulations also included the widely used order-α estimator to place the excellent finite sample performance of the CQR and CER methods into a proper perspective. Our simulations demonstrate that the standard order-α estimator does not necessarily satisfy the quantile property, particularly at low quantile. In this sense, the interpretation of the order-α frontier as the quantile function seems debatable. Of course, improving the robustness of efficiency measurement and benchmarking is frequently cited as the primary motivation for using the order-α estimator as well as other similar partial frontier approaches.

We conclude by noting that the attractive asymptotic properties of the order-α estimator did not carry over as excellent finite sample performance in our Monte Carlo simulations, even when the global concavity constraints were relaxed. Still, the rigorous statistical theory remains a key advantage of the order-α approach. While there has been notable progress in the statistical theory of convex regression (see, e.g., Lim, 2014; Lim & Glynn, 2012; Seijo & Bodhisattva, 2011), which is the special case of CER when $\tilde{\tau} = 0.5$, the asymptotic theory and statistical inference for the CQR, CER and their isotonic counterparts remains to be developed. We would like to suggest this as an interesting avenue for future research for competent mathematical statisticians.

Acknowledgments

Appendix A. Proofs

A1. Proof of Theorem 1

We can rewrite problem (5) as the equivalent problem according to the quantile regression definition (Koenker & Bassett, 1978).

Specifically, problem (5) can be reformulated as

$$\min \tau \sum_{i=1}^{n} \rho_\tau(y_i - Q) \tag{A1}$$

$$s.t. \quad Q \in \mathcal{F}$$

The quantile property for any nonparametric quantile regression function subject to shape constraints can be established by using the proof in Wang et al. (2014). Suppose that $(\hat{Q}_1, \ldots, \hat{Q}_n)$ is a feasible solution to problem (A1). For any $\alpha \in \mathbb{R}$, $(\hat{Q}_1 + \alpha, \ldots, \hat{Q}_n + \alpha)$ is also a feasible solution to problem (A1) as the new estimated quantile function is merely the parallel shift of the original one with level α (Wang et al., 2014). Note that $n_\tau^+ + n_\tau^- \le n$ and hence we introduce n_τ^0 to denote the number of the observations with $\varepsilon_i^+ = \varepsilon_i^- = 0$. We then have the equation $n = n_\tau^+ + n_\tau^- + n_\tau^0$.

The marginal effects of shifting the estimated quantile function on the objective function are calculated by

$$\frac{\partial \sum_{i=1}^{n} \rho_\tau(y_i - Q + \alpha)}{\partial \alpha} = \begin{cases} (1-\tau)(n_\tau^- + n_\tau^0) - \tau n_\tau^+ & \text{if } \alpha \ge 0, \\ (1-\tau)n_\tau^- - \tau(n_\tau^+ + n_\tau^0) & \text{otherwise.} \end{cases}$$

Given that n_τ^0 may be positive (i.e., $n_\tau^0 > 0$), we have

$$\begin{cases} (1-\tau)(n_\tau^- + n_\tau^0) - \tau n_\tau^+ \ge 0 \\ (1-\tau)n_\tau^- - \tau(n_\tau^+ + n_\tau^0) \le 0 \end{cases}$$

Reorganizing the above two inequalities leads to

$$\begin{cases} (1-\tau)n - n_\tau^+ \ge 0 \\ n_\tau^- - \tau n \le 0 \end{cases} \Rightarrow \begin{cases} \dfrac{n_\tau^+}{n} \le 1 - \tau \\ \dfrac{n_\tau^-}{n} \le \tau \end{cases}$$

Therefore, Theorem 1 is proved. That is, the quantile property can be applied to any nonparametric quantile function subject to shape constraints. □

A2. Proof of Theorem 2

We rewrite problem (8) by the following equivalent problem (Newey & Powell, 1987)

$$\min \tilde{\tau} \sum_{i=1}^{n} \rho_{\tilde{\tau}}(y_i - \Gamma)^2 \tag{A2}$$

$$s.t. \quad \Gamma \in \mathcal{F}$$

The expectile property for any nonparametric expectile regression function subject to shape constraints can be established following Kuosmanen & Zhou (2021). Similar to the proof of Theorem 1, the marginal effect of shifting the estimated expectile function on the objective function is

$$\frac{\partial \sum_{i=1}^{n} \rho_{\tilde{\tau}}(y_i - \Gamma + \alpha)^2}{\partial \alpha} = 2(1-\tilde{\tau}) \sum_{i=1}^{n} \hat{\varepsilon}_i^- - 2\tilde{\tau} \sum_{i=1}^{n} \hat{\varepsilon}_i^+$$

By reorganizing the first-order condition, we have

$$2(1-\tilde{\tau}) \sum_{i=1}^{n} \hat{\varepsilon}_i^- - 2\tilde{\tau} \sum_{i=1}^{n} \hat{\varepsilon}_i^+ = 0$$

The expectile property in Theorem 2 is immediately proved as we have $\tilde{\tau} = \sum_{i=1}^{n} \hat{\varepsilon}_i^- / (\sum_{i=1}^{n} \hat{\varepsilon}_i^+ + \sum_{i=1}^{n} \hat{\varepsilon}_i^-)$.

Appendix B. Additional experimental results

B1. Experiment with different error specifications

Table B1
Performance in estimating the quantile function when $\varepsilon_i = v_i$ and $\varepsilon_i = -u_i$ with $n = 1000$ and $d = 1$, respectively. ICQR = Isotonic CQR, ICER = Isotonic CER, COA = Convexified order-α.

ε		τ	ICQR		ICER		COA	
			Bias	MSE	Bias	MSE	Bias	MSE
σ_v	0.708	0.1	0.040	0.032	0.048	0.029	−1.900	4.895
		0.3	0.016	0.021	0.017	0.016	−1.593	3.352
		0.5	0.017	0.020	0.002	0.014	−1.310	2.191
		0.7	−0.005	0.021	−0.014	0.016	−1.053	1.358
		0.9	−0.029	0.031	−0.047	0.029	−0.800	0.761
	0.801	0.1	0.041	0.038	0.057	0.035	−1.856	4.687
		0.3	0.018	0.025	0.017	0.020	−1.571	3.257
		0.5	0.017	0.023	0.002	0.017	−1.315	2.206
		0.7	−0.006	0.025	−0.014	0.019	−1.082	1.435
		0.9	−0.030	0.037	−0.049	0.035	−0.843	0.855
	0.894	0.1	0.044	0.044	0.052	0.041	−1.814	4.499
		0.3	0.019	0.030	0.017	0.023	−1.553	3.177
		0.5	0.019	0.028	0.003	0.020	−1.319	2.220
		0.7	−0.005	0.029	−0.015	0.023	−1.107	1.508
		0.9	−0.032	0.043	−0.051	0.041	−0.884	0.955
σ_u	1.174	0.1	0.044	0.050	0.055	0.045	−1.670	4.468
		0.3	0.009	0.028	0.012	0.019	−1.639	3.582
		0.5	0.009	0.020	−0.005	0.013	−1.427	2.551
		0.7	−0.015	0.015	−0.022	0.009	−1.157	1.587
		0.9	−0.040	0.010	−0.048	0.008	−0.773	0.748
	0.994	0.1	0.041	0.039	0.051	0.035	−1.818	4.810
		0.3	0.009	0.022	0.011	0.015	−1.674	3.694
		0.5	0.007	0.016	−0.006	0.010	−1.411	2.493
		0.7	−0.014	0.012	−0.020	0.007	−1.104	1.450
		0.9	−0.037	0.008	−0.044	0.007	−0.695	0.580
	0.742	0.1	0.037	0.026	0.045	0.023	−1.983	5.371
		0.3	0.008	0.015	0.010	0.010	−1.717	3.860
		0.5	0.006	0.010	−0.005	0.007	−1.383	2.403
		0.7	−0.013	0.008	−0.019	0.005	−1.028	1.264
		0.9	−0.034	0.006	−0.040	0.005	−0.598	0.414

B2. Experiment with model misspecification

Table B2
Performance in estimating quantile function over noncovex set.

n	(σ^2, λ)	ICQR		ICER		COA	
		Bias	MSE	Bias	MSE	Bias	MSE
50	(1.88, 1.66)	0.075	0.401	−0.028	0.353	−4.510	31.867
	(1.63, 1.24)	0.087	0.405	−0.016	0.355	−4.485	31.640
	(1.35, 0.83)	0.096	0.411	−0.008	0.355	−4.463	31.448
100	(1.88, 1.66)	0.067	0.270	−0.022	0.228	−4.637	32.881
	(1.63, 1.24)	0.076	0.273	−0.014	0.229	−4.614	32.639
	(1.35, 0.83)	0.082	0.277	−0.008	0.229	−4.593	32.432
200	(1.88, 1.66)	0.056	0.180	−0.010	0.147	−4.691	33.218
	(1.63, 1.24)	0.062	0.182	−0.004	0.148	−4.668	32.975
	(1.35, 0.83)	0.069	0.185	0.000	0.148	−4.648	32.779
500	(1.88, 1.66)	0.036	0.100	−0.009	0.079	−4.733	33.649
	(1.63, 1.24)	0.040	0.101	−0.005	0.080	−4.710	33.400
	(1.35, 0.83)	0.044	0.102	−0.002	0.080	−4.690	33.192
1000	(1.88, 1.66)	0.024	0.064	−0.007	0.049	−4.750	33.751
	(1.63, 1.24)	0.027	0.064	−0.004	0.050	−4.728	33.507
	(1.35, 0.83)	0.029	0.065	−0.002	0.050	−4.709	33.307

DGP: $y_i = x_i + 0.1x_i^2 + v_i - u_i$, where $x_i \sim U[1, 10]$, $v_i \overset{\text{i.i.d.}}{\sim} N(0, \sigma_v^2)$, and $u_i \overset{\text{i.i.d.}}{\sim} N^+(0, \sigma_u^2)$.

B3. Experiment with outliers

Table B3
Performance in estimating the quantile function with three outliers.

(σ^2, λ)	d	ICQR		ICER		COA	
		Bias	MSE	Bias	MSE	Bias	MSE
(1.88, 1.66)	1	0.029	0.104	−0.011	0.081	−1.844	19.823
	2	0.032	0.105	−0.007	0.082	−1.828	19.748
	3	0.034	0.105	−0.006	0.082	−1.814	19.686
(1.63, 1.24)	1	0.035	0.232	−0.021	0.202	−1.760	19.840
	2	0.044	0.236	−0.012	0.203	−1.743	19.781
	3	0.050	0.238	−0.005	0.203	−1.727	19.732
(1.35, 0.83)	1	0.011	0.408	−0.033	0.370	−1.618	19.691
	2	0.024	0.411	−0.018	0.371	−1.598	19.639
	3	0.035	0.414	−0.006	0.372	−1.582	19.592

DGP: $y_i = \prod_{d=1}^{D} X_{d,i}^{\frac{0.8}{d}} + v_i - u_i$, where $X = (x1, x2)'$, $x1_m \sim U[1, 10]$ $(m = 1, \ldots, 200)$, $x2_n \sim U[90, 100]$ $(n = 1, \ldots, 3)$, $v_i \overset{\text{i.i.d.}}{\sim} N(0, \sigma_v^2)$, and $u_i \overset{\text{i.i.d.}}{\sim} N^+(0, \sigma_u^2)$.

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