pyStoNED: A Python Package for Convex Regression and Frontier Estimation

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Abstract

Shape-constrained nonparametric regression is a growing area in econometrics, statistics, operations research, machine learning and related fields. In the field of productivity and efficiency analysis, recent developments in the multivariate convex regression and related techniques such as convex quantile regression and convex expectile regression have bridged the long-standing gap between the conventional deterministic-nonparametric and stochastic-parametric methods. Unfortunately, the heavy computational burden and the lack of powerful, reliable, and fully open access computational package has slowed down the diffusion of these advanced estimation techniques to the empirical practice. The purpose of the Python package pyStoNED is to address this challenge by providing a freely available and user-friendly tool for the multivariate convex regression, convex quantile regression, convex expectile regression, isotonic regression, stochastic nonparametric envelopment of data, and related methods. This paper presents a tutorial of the pyStoNED package and illustrates its application, focusing on the estimation of frontier cost and production functions.

Keywords: multivariate convex regression, nonparametric least squares, frontier estimation, efficiency analysis, stochastic noise, Python.

1. Introduction

Early contributions to nonparametric regression by Hildreth (1954), Brunk (1955), and Grenander (1956) built exclusively on the convexity and monotonicity constraints of the regression function. However, extending these approaches from the univariate setting to the more general multivariate regression proved a vexing challenge. Since the development of an explicit piecewise linear characterization of the multivariate convex nonparametric least squares (CNLS) by Kuosmanen (2008), convex regression has attracted growing interest in econometrics, statistics, operations research, machine learning and related fields (e.g., Magnani and Boyd, 2009; Seijo and Sen, 2011; Lim and Glynn, 2012; Hannah and Dunson, 2013; Mazumder, Choudhury, Iyengar, and Sen, 2019; Bertsimas and Mundru, 2021). The recent study by Yagi, Chen, Johnson, and Kuosmanen (2020) applies insights from convex regression to impose shape constraints on a local polynomial kernel estimator.

Convexity and monotonicity constraints are particularly relevant in the microeconomic ap-

plications where the duality theory of production and consumption directly implies certain monotonicity and convexity/concavity properties for many functions of interest (e.g., Afriat, 1967, 1972; Varian, 1982, 1984). For example, the cost function of the firm must be monotonic increasing and convex with respect to the input prices. Similar to the fact that a density function must be non-negative and its definite integral is equal to one, the cost function must satisfy the monotonicity and convexity properties implied by the theory, otherwise it is not really a cost function at all. The recent developments in the convex regression enable researchers to impose the concavity or convexity constraints implied by the theory to estimate the functions of interest without any parametric functional form assumptions.

In recent years, convex regression and related techniques are increasingly utilized in the estimation of frontier cost and production functions in the field of productivity and efficiency analysis, a multidisciplinary field that is widely applied in such areas as agriculture, banking, education, environment, health care, energy, manufacturing, transportation, and utilities (e.g., Kuosmanen, Johnson, and Saastamoinen, 2015; Johnson and Kuosmanen, 2015). Traditionally, this field was divided between two competing paradigms: Data Envelopment Analysis (DEA) (Charnes, Cooper, and Rhodes, 1978) and Stochastic Frontier Analysis (SFA) (Aigner, Lovell, and Schmidt, 1977; Meeusen, Van, and Broeck, 1977). DEA is a deterministic, fully nonparametric approach whereas SFA is a probabilistic, fully parametric approach. To bridge the gap between these two paradigms, Stochastic nonparametric envelopment of data (StoNED) (Kuosmanen, 2006; Kuosmanen and Kortelainen, 2012) was proposed as a unified framework that combines virtues of DEA and SFA, encompassing both approaches as its restricted special cases.

In practice, convex regression and StoNED are computationally demanding approaches, requiring a user to solve a mathematical programming problem subject to a large number of linear constraints. For example, the additive CNLS formulation by Kuosmanen (2008) is a quadratic programming (QP) problem, whereas the multiplicative logarithmic formulation first considered by Kuosmanen and Kortelainen (2012) requires solving a nonlinear programming (NLP) problem. Therefore, most empirical applications published thus far make use of commercial QP and NLP solvers, which can be coded using high-level mathematical computing languages such as GAMS (GAMS Development Corporation, 2013) or MATLAB (The Mathworks, Inc., 2017). Johnson and Kuosmanen (2015) present detailed examples of how to implement the most basic CNLS and StoNED formulations in MATLAB and GAMS. Recently, the Benchmarking package (Bogetoft and Otto, 2010) implemented in R (R Core Team, 2020) includes a new function StoNED() to estimate the CNLS/StoNED model, however, the R implementation is currently restricted to the additive CNLS QP formulation model.

The lack of a comprehensive, powerful, reliable, and fully open access computational package for the CNLS, StoNED, and related methods has slowed down the diffusion of these techniques to the empirical practice, which still heavily relies on the simple DEA and SFA techniques that either assume away noise or rely on restrictive functional form assumptions.¹ To lower

¹A plethora of computational tools, packages and resources are available for the conventional DEA and SFA. In the open access environment (R), one could use **Benchmarking** (Bogetoft and Otto, 2010), **FEAR** (Wilson, 2008), **rDEA** (Simm and Besstremyannaya, 2020), **nonparaeff** (Oh, DH and Suh, D, 2013), **npsf** (Badunenko, Mozharovskyi, and Kolomiytseva, 2020), and **frontiles** (Daouia and Laurent, 2013), among many others, for solving different types of DEA models. For the SFA models, there exist **frontier** (Coelli and Henningsen, 2020), **sfa** (Straub, 2014), and **sfaR** (Dakpo, Desjeux, and Latruffe, 2021). Other free packages such as **pyDEA** (Raith, Perederieieva, Fauzi, Harton, Lee, Lin, Priddey, and Rouse, 2021) and **DataEnvelopmentAnalysis** (Barbero and Zoffo, 2021) are available to implement efficiency analysis. Further, there are also a plenty of DEA and

the barrier for applied researchers and practitioners to apply more advanced techniques that help to relax unnecessarily restrictive assumption, the Python package **pyStoNED** was first introduced in April 2020 to prove a freely available and user-friendly tool for the multivariate CNLS and StoNED methods. Its latest edition 0.5.2 also includes modules for the convex quantile regression, convex expectile regression, isotonic regression, and graphical illustration. It also facilitates efficiency measurement using the conventional DEA and free disposable hull (FDH) approaches. The **pyStoNED** package allows practitioners to estimate these models in an open access environment under a GPL-3.0 License. The project, including source code, internal data, notebook tutorials, and web documentation, is publicly available at GitHub.²

The purpose of this paper is to present a tutorial of the **pyStoNED** package, briefly review the alternative models supported, and illustrate its application. We focus on the estimation of frontier cost and production functions, which currently forms the main application area of these techniques, emphasizing that the various modules of the **pyStoNED** package are directly applicable for (semi-)nonparametric regression analysis in any other contexts as well. We emphasize that the **pyStoNED** package is an ongoing development by the users for the users: further model specifications and methodological advances will be implemented and added to the **pyStoNED** package on a continuous basis.

The paper is organized as follows. Section 2 describes the basic setups of the **pyStoNED** package, and Section 3 introduces the structures of example data and the attributes of different models. Section 4 describes the first step of the StoNED model (e.g., the CNLS estimator) to estimate the conditional mean and some other commonly used extensions. The Python code for the CNLS estimator and these extensions are included. Section 5 demonstrates the rest of the steps of the StoNED model and related codes. Section 6 illustrates how to implement the CNLS-G algorithm to calculate the CNLS estimator using the developed **pyStoNED** package. The plot of the estimated function can be found in Section 7. Section 8 concludes this paper. The list of acronyms is presented in Appendix A. Appendices B and C present the estimated residuals for a same CNLS model solved by GAMS and **pyStoNED**, respectively.

2. Setup

2.1. Installation

The **pyStoNED** package supports Python 3.8 or later versions on Linux, macOS, and Windows, and is freely available on the Python Package Index (PyPI) at https://pypi.org/project/pystoned. The package can be installed by any of the following three approaches:

- Install from the PyPI pip install pystoned
- 2) Install from the GitHub repository pip install -U git+https://github.com/ds2010/pyStoNED

SFA codes and packages for MATLAB, GAMS, and other high-level mathematical computing languages (e.g., Kalvelagen, 2002; Ji and Lee, 2010; Belotti, Daidone, Ilardi, and Atella, 2013; Álvarez, Barbero, and Zofío, 2020).

²The pyStoNED package GitHub repository: https://github.com/ds2010/pyStoNED.

3) Clone developing branches and install with Python using the setup.py script (for developers)

```
git clone https://github.com/ds2010/pyStoNED.git
python setup.py install
```

The **pyStoNED** package is built based on a few existing dependencies.³ It is worth highlighting that **Pyomo** is a full-featured high-level programming language that provides a rich set of supporting libraries to program CNLS, StoNED, and various extensions. The other dependencies are also essential for **pyStoNED**. Specifically, **NumPy** and **pandas** are used to import input-output data, manipulate data, and export the estimation results. **SciPy** provides the algorithm to optimize the quasi-likelihood function. **Matplotlib** is then associated to plot the estimated functions.

2.2. Solvers

In the CNLS/StoNED framework, the existing models are either additive or multiplicative models, depending on the specification of the error term's structure. In the context of the optimization problems, the additive models are usually the QP problem with an exception of the CQR model, which is a linear programming (LP) problem, and all multiplicative models are the NLP problem. The attribute of models determines which type of solver will meet our needs, i.e., QP/LP-solver or NLP-solver. In the **pyStoNED** package, we can import these two kinds of solvers locally or remotely.

Remote Optimization

With the help of Network-Enabled Optimization System (NEOS) Server that freely provides a larger number of academic solvers such as **CPLEX** (Cplex, IBM ILOG, 2009), **MOSEK** (MOSEK ApS, 2021), **MINOS** (Murtagh and Saunders, 2003), and **KNITRO** (Byrd, Nocedal, and Waltz, 2006), pyStoNED has the ability to calculate the StoNED related models without installing the local solvers. Here we have a model optimizing remotely:

```
>>> model.optimize(email="email@address", solver='mosek')
```

The use of the remote optimization requiring email and solver as parameters.⁵ If the user leaves the parameter solver out (i.e., model.optimize(email="email@address")), the optimization job will be calculated by the default solver. That is, the additive and multiplicative models will be solved by MOSEK and KNITRO, respectively. The remote optimization is highly recommended for light computing jobs.

³List of dependencies used in **pyStoNED**: **NumPy** (Harris, Millman, van der Walt, Gommers, Virtanen, Cournapeau, Wieser, Taylor, Berg, Smith, Kern, Picus, Hoyer, van Kerkwijk, Brett, Haldane, del Río, Wiebe, Peterson, Gérard-Marchant, Sheppard, Reddy, Weckesser, Abbasi, Gohlke, and Oliphant, 2020), **pandas** (The pandas development team, 2020), **SciPy** (Virtanen, Gommers, Oliphant, Haberland, Reddy, Cournapeau, Burovski, Peterson, Weckesser, Bright, van der Walt, Brett, Wilson, Millman, Mayorov, Nelson, Jones, Kern, Larson, Carey, Polat, Feng, Moore, VanderPlas, Laxalde, Perktold, Cimrman, Henriksen, Quintero, Harris, Archibald, Ribeiro, Pedregosa, van Mulbregt, and SciPy 1.0 Contributors, 2020), **Matplotlib** (Hunter, 2007), and **Pyomo** (Bynum, Hackebeil, Hart, Laird, Nicholson, Siirola, Watson, and Woodruff, 2021). All the dependencies will be automatically added when installing the **pyStoNED** package.

⁴NEOS Server: State-of-the-Art Solvers for Numerical Optimization, https://neos-server.org/neos

⁵Replace with your own email address required by NEOS server, see https://neos-guide.org/content/
FAQ#email

Local Optimization

We can resort to the local solver pre-installed by ourselves to estimate the StoNED related models (e.g., MOSEK and CPLEX). The parameter OPT_LOCAL is added in the function .optimize(...) to indicate that the model optimizes locally. Here is an example of optimizing the additive model with local solver MOSEK.⁶

```
>>> model.optimize(OPT_LOCAL, solver='mosek')
```

Since the free and stable NLP solver remains scant, the **pyStoNED** package does not support the multiplicative model estimation locally at present. Hence, we recommend the user solve their multiplicative models remotely. We will update the package immediately when the free and stable NLP solver is available.

3. Data structures and dataset

3.1. Data structures

Data pre-processing is the first step to use the developed package, and thus the user must prepare the dataset based on the data structures of **pyStoNED**. In all CNLS/StoNED models, two common vectors or matrix are required: input variables \mathbf{x}_i and output variables \mathbf{y}_i for observed Decision Making Units (DMU) $i = 1, 2, \dots, n$. For a model considering operational conditions and practices, contextual variables \mathbf{z}_i are required. The directional distance function (DDF) based models handle the multi-dimensional inputs and outputs with given directional vectors \mathbf{g}^x and \mathbf{g}^y , respectively. The DDF based models also take undesired outputs \mathbf{b}_i and its directional vector \mathbf{g}^b into consideration. Table 1 summarizes the data structures used in all the CNLS/StoNED models.

Symbol	Model	Description
\overline{x}	All models	Input variables
$oldsymbol{y}$	All models	Output variables
\boldsymbol{z}	Contextual based models	Contextual variables
\boldsymbol{b}	DDF based models	Undesirable outputs
$oldsymbol{g}^x$	DDF based models	The direction of inputs
\boldsymbol{g}^y	DDF based models	The direction of outputs
\boldsymbol{g}^b	DDF based models	The direction of undesirable outputs

Table 1: Data structures.

The inputs of the estimation functions support two forms: matrix from NumPy and list from Python. The outputs (i.e., final estimates) are retrieved by using the corresponding functions .get_xxx() provided by pyStoNED, all of which are in the form of ndarray from NumPy.

⁶The tutorial of the MOSEK installation is available at https://pystoned.readthedocs.io/en/latest/install/index.html.

3.2. Internal data

To illustrate the application of the **pyStoNED** package, four commonly used datasets are attached:

1) Regulation of Finnish electricity distribution firms (load_Finnish_electricity_firm) The data of the regulation of Finnish electricity distribution firms are collected from Kuosmanen (2012) and Kuosmanen, Saastamoinen, and Sipiläinen (2013). The data consist of seven variables: three different expenditures are used as inputs (i.e., OPEX, CAPEX, and TOTEX); Energy, Length, and Customers are considered as outputs; Further, PerUndGr is denoted as the contextual variable. Table 2 presents the description of the dataset.

Variable	Unit	Description
OPEX	Thousand Euro	Controllable operational expenditure
CAPEX	Thousand Euro	Total capital expenditure
TOTEX	Thousand Euro	Total expenditure
Energy	Gigawatt Hours	Weighted amount of energy transmitted
Length	Kilometer	Length of the network
Customers	Person	Customers connected to the network
PerUndGr	Percentage	Proportion of underground cabling

Table 2: The regulation of Finnish electricity distribution firms.

2) GHG abatement cost of OECD countries (load_GHG_abatement_cost)
The data of the Greenhouse gas (GHG) abatement cost of OECD countries are provided by Kuosmanen, Zhou, and Dai (2020). The data contain two input variables (i.e., CPNK and HRSN), one good output variable (i.e., VALK), and one undesirable output variable (i.e., GHG). Table 3 describes the dataset in detail.

Variable	Unit	Description
CPNK	Billion Euro ²⁰¹⁰	Net capital stock
HRSN	Billion hours	Hours worked by total engaged
VALK	Billion Euro ²⁰¹⁰	Value added
GHG	Million tons of CO ₂ equivalents	Total GHG emissions

Table 3: The GHG abatement cost of OECD countries.

3) Data provided with Tim Coelli's Frontier 4.1 (load_Tim_Coelli_frontier)
The classic 60 firms dataset attached in Frontier 4.1 (Coelli, 1996) includes two input variables (i.e., capital and labour) and one output variable (i.e., output) (see Table 4).

Variable	Unit	Description
firm	Quantity	Firm ID
output	Quantity Index	Output quantity
capital	Quantity Index	Capital input
labour	Quantity Index	Labour input

Table 4: The data provided with Tim Coelli's Frontier 4.1.

⁷Note that $\mathtt{TOTEX} = \mathtt{OPEX} + \mathtt{CAPEX}$. It is possible to use \mathtt{TOTEX} as an aggregate input, or model \mathtt{OPEX} and \mathtt{CAPEX} as two separate input variables.

4) Rice Production in the Philippines (load_Philipines_rice_production)
The Rice Production in the Philippines dataset collected from Coelli, Rao, O'Donnell, and
Battese (2005) consists of 17 different variables. The different variables can be organized
into diversified combinations for target models. Table 5 summarizes the variables of the

Variable	Unit	Description
YEARDUM	Year	Time period
FMERCODE	Quantity	Farmer code
PROD	Tonnes	Toones of freshly threshed rice
AREA	Hactares	Area planted
LABOR	Mandays	Labour used
NPK	Kilogram	Fertiliser used
OTHER	Laspeyres index	Other inputs used
PRICE	Pesos/kilogram	Output price
AREAP	Pesos/hectare	Rental price of land
LABORP	Pesos/day	Labour price
NPKP	Pesos/kilogram	Fertiliser price
OTHERP	Implicit price index	Price of other inputs
AGE	Years	Age of the household head
EDYRS	Years	Education of the household head
HHSIZE	Quantity	Household size
NADULT	Quantity	Number of adults in the household
BANRAT	Percentage	Percentage of area classified as upland fields

Table 5: The rice production in the Philippines.

These datasets can be imported through the module dataset of **pyStoNED**. The variables in Tables 2–5 are used as parameters of dataset to load the input data. The following example demonstrates how to load the input-output data from the regulation of Finnish electricity distribution firms dataset. We first import the dataset module using the function load_Finnish_electricity_firm (i.e., Line 1), then define the x and y according to the imported dataset (Line 2). We can check the input and output data using the function print(...) (Lines 3 and 4). The parameters x_select, y_select, and z_select in load_Finnish_electricity_firm(x_select, y_select, z_select) are used to select the inputs, outputs, and contextual variables, respectively.

⁸In addition to the presented example, we can load other datasets using the corresponding dataset module, e.g., loading the GHG data: from pystoned.dataset import load_GHG_abatement_cost.

Note that the parameters in the module dataset can be defined according to the user's purpose. For example, if the target model only consists of two inputs (e.g., Energy and Customers) and one output (e.g., TOTEX), then the data selection in Line 2 should be

3.3. External data

In practice, the user's own dataset is the main input of **pyStoNED**. We present an example to show how to import the user's own data. Assume that Table 6 is the input-output data stored in Excel file table1.xlsx, the following code utilizes the **pandas** to read the Excel file and organize the data with **NumPy**. The input variable x is a matrix and the output variable y is then an array.

id	output	input1	input2
1	120	10	55
2	80	30	49
•	•	•	•
•		•	
100	90	25	72

Table 6: An example of user's own dataset.

In the following case, we first import the packages **NumPy** and **pandas** in Lines 1 and 2. Line 3 is used to read the Excel data file and the rest of the lines define the input and output variables. See more similar examples in Section 6.

```
>>> import numpy as np
>>> import pandas as pd
>>> df=pd.read_excel("table1.xlsx")
>>> y=df['output']
>>> x1=df['input1']
>>> x1=np.asmatrix(x1).T
```

```
>>> x2= df['input2']
>>> x2=np.asmatrix(x2).T
>>> x=np.concatenate((x1, x2), axis=1)
```

4. Shape-constrained nonparametric regression

Consider a standard multivariate, cross-sectional model in production economics:

$$y_i = f(\mathbf{x}_i) + \varepsilon_i$$

$$= f(\mathbf{x}_i) + v_i - u_i \quad \forall i$$
(1)

where y_i is the output of the DMU $i, f: R_+^m \to R_+$ is the production (cost) function that characterizes the production (cost) technology, and $\mathbf{x}_i = (x_{i1}, x_{i2}, \cdots, x_{im})'$ denotes the input vector of unit i. Similar to the literature in SFA, for production function, the presented composite error term $\varepsilon_i = v_i - u_i$ consists of the inefficiency term $u_i > 0$ and stochastic noise term v_i . Note that by setting $u_i = 0$ we have the standard nonparametric regression model as a special case. To estimate the function f, one could resort to the parametric and nonparametric methods or neoclassical and frontier models, which are classified based on the specifications of f and error term ε (see Kuosmanen and Johnson, 2010). In this paper, we assume certain axiomatic properties (e.g., monotonicity, concavity) instead of a priori functional form for the function f and apply the following nonparametric methods to estimate the function f.

4.1. Convex Nonparametric Least Square

Additive CNLS model

Hildreth (1954) is the first to consider the nonparametric regression subject to monotonicity and concavity constraints in the case of a single input variable x. Afriat (1972) also proposes methods to impose convexity on the estimation of a production function. Kuosmanen (2008) extends Hildreth's approach to the multivariate setting with the multidimensional input x, and refers it to as the CNLS. CNLS builds upon the assumption that the true but unknown production function f belongs to the set of continuous, monotonic increasing and globally concave (convex) functions, imposing the same production axioms as standard DEA (see further discussion in Kuosmanen and Johnson, 2010). The additive multivariate CNLS formulations are defined as

⁹In this paper, we focus on introducing the CNLS/StoNED and other related models and illustrating how to apply the **pyStoNED** to solve these models. Of course, one can use this package to solve other nonparametric models such as DEA and FDH. See more tutorials about DEA and FDH estimations at https://pystoned.readthedocs.io.

• Estimating production function (i.e., regression function f is concave and increasing)

$$\min_{\alpha,\beta,\varepsilon} \sum_{i=1}^{n} \varepsilon_{i}^{2}$$
s.t. $y_{i} = \alpha_{i} + \beta'_{i} \mathbf{x}_{i} + \varepsilon_{i} \quad \forall i$

$$\alpha_{i} + \beta'_{i} \mathbf{x}_{i} \leq \alpha_{j} + \beta'_{j} \mathbf{x}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} \geq \mathbf{0} \quad \forall i$$
(2)

• Estimating cost function (i.e., regression function f is convex and increasing)

$$\min_{\alpha,\beta,\varepsilon} \sum_{i=1}^{n} \varepsilon_{i}^{2}$$
s.t. $y_{i} = \alpha_{i} + \beta'_{i} x_{i} + \varepsilon_{i} \quad \forall i$

$$\alpha_{i} + \beta'_{i} x_{i} \ge \alpha_{j} + \beta'_{j} x_{i} \quad \forall i, j, \text{ and } i \ne j$$

$$\beta_{i} \ge \mathbf{0} \quad \forall i$$
(3)

where α_i and β_i define the intercept and slope parameters of tangent hyperplanes that characterize the estimated piecewise linear frontier, respectively. ε_i denotes the regression residual. The first constraint can be interpreted as a multivariate regression equation, the second constraint imposes convexity (concavity), and the third constraint imposes monotonicity. Similar to the DEA specification, other standard specifications of returns to scale can be imposed by an additional constraint on the intercept term α_i . If $\alpha_i = 0$, then Problems (2) and (3) are the constant returns to scale (CRS) model, otherwise they are the variable returns to scale (VRS) model. Note that both Problems (2) and (3) are the QP problem and hence can be solved by **MOSEK** and **CPLEX**.

The basic additive CNLS model can be estimated in **pyStoNED** using the module CNLS(y, x, ...) with the contextual variable z parameter set to None (default) and the type of model cet parameter set to CET_ADDI (additive model; default). The type of estimated function can be classified by setting the fun parameter to FUN_PROD (production function; default) or FUN_COST (cost function). The returns to scale assumption can be specified by setting the rts parameter to RTS_VRS (VRS model; default) or RTS_CRS (CRS model). The results can be displayed in the screen directly using the .display_alpha() (i.e., display the coefficients $\hat{\alpha}_i$) or stored in the memory using the .get_alpha().

We first present an example to solve the VRS production model and store the estimates as the following Lines 12-14.

```
>>>
>>> model.display_alpha()
>>> model.display_beta()
>>> model.display_residual()
>>>
>>> alpha = model.get_alpha()
>>> beta = model.get_beta()
>>> residuals = model.get_residual()
alpha : alpha
   Size=89, Index=I
   Key : Lower : Value
                                     : Upper : Fixed : Stale : Domain
     0 : None : -22.935939927355427 :
                                        None : False : False :
          None: -22.98683384275405:
                                        None : False : False :
                                                                Reals
    88 :
          None : -22.860373724764905 : None : False : False :
beta : beta
   Size=178, Index=beta_index
            : Lower : Value
                                            : Upper : Fixed : Stale : Domain
               0.0:
                        0.13585845731547977 :
                                               None : False : False :
                                                                       Reals
     (0, 1):
                                               None : False : False :
               0.0:
                       0.011273984231181894 :
                                                                       Reals
     (1, 0):
               0.0:
                        0.13637662344803758 :
                                               None : False : False :
                                                                       Reals
     (1, 1):
               0.0:
                       0.010903786808952633 : None : False : False :
                                                                       Reals
    (88, 0):
               0.0:
                        0.13561549262636433 : None : False : False :
                                                                       Reals
                       0.011417220278201383 : None : False : False :
    (88, 1):
               0.0:
epsilon : residual
   Size=89, Index=I
   Key : Lower : Value
                                     : Upper : Fixed : Stale : Domain
     0 : None : -2.8024040090178914 : None : False : False :
          None: 1.4140528128759229: None: False: False: Reals
    88 : None : -0.885163858119256 : None : False : False : Reals
```

In this example, Lines 1-3 import the CNLS module, parameter setting modules, and dataset module. Line 4 defines the input and output variables using the Finnish electricity distribution firm data. Lines 5-6 define the CNLS production model with a user-defined name (e.g., model) and solve the production model using the local off-the-shelf solver (i.e., MOSEK).¹⁰ Lines 8-10 directly display the estimated coefficients (i.e., $\hat{\alpha}_i$, $\hat{\beta}_{ij}$, and $\hat{\varepsilon}_i$) on screen, and Lines 12-14

¹⁰The name of estimated model is free to be assigned, e.g., CNLS_model=CNLS.CNLS(y=data.y, x=data.x, z=None, cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS). Correspondingly, the Line 6 in this example should be replaced by CNLS_model.optimize(OPT_LOCAL), and Line 8 now is CNLS_model.display_alpha().

store the estimates in memory with a special variable name (e.g, alpha). Appendix C presents the full estimated CNLS residuals that are equivalent to those in GAMS (cf. Appendix B). Note that the estimated alpha and beta in **pyStoNED** may be slightly different from those in GAMS due to non-uniqueness in CNLS estimation (see Kuosmanen, 2008; Dai, 2021).

Multiplicative CNLS model

Similar to the existing SFA literature, the Cobb-Douglas and translog functions are commonly assumed to be the functional form for the function f, where inefficiency u and noise v affect production in a multiplicative fashion. We, thus, further consider the multiplicative specification in the nonparametric models. Note that the assumption of CRS would also require a multiplicative error structure. Under the multiplicative composite error structure, the function (1) is rephrased as

$$y_i = f(\mathbf{x}_i) \cdot \exp(\varepsilon_i) = f(\mathbf{x}_i) \cdot \exp(v_i - u_i)$$
 (4)

Applying the log-transformation to Eq.(4), we obtain

$$ln y_i = ln f(\mathbf{x}_i) + v_i - u_i$$
(5)

To estimate Eq.(5), we reformulate the additive production model (2) and obtain the following log-transformed CNLS formulation:

$$\min_{\alpha,\beta,\phi,\varepsilon} \sum_{i=1}^{n} \varepsilon_{i}^{2}$$

$$s.t. \quad \ln y_{i} = \ln(\phi_{i} + 1) + \varepsilon_{i} \quad \forall i$$

$$\phi_{i} = \alpha_{i} + \beta'_{i} \mathbf{x}_{i} - 1 \quad \forall i$$

$$\alpha_{i} + \beta'_{i} \mathbf{x}_{i} \leq \alpha_{j} + \beta'_{j} \mathbf{x}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} > \mathbf{0} \quad \forall i$$
(6)

where $\phi_i + 1$ is the CNLS estimator of $\mathsf{E}[y_i \,|\, x_i]$. The value of one is added here to make sure that the computational algorithms do not take the logarithm of zero. The first equality can be interpreted as the log-transformed regression equation (using the natural logarithm function $\ln(\cdot)$). The rest of the constraints are the same as those of the additive models. The use of ϕ_i allows the estimation of a multiplicative relationship between output and input while assuring convexity of the production possibility set in the original input-output space. Note that one could not apply the log transformation directly to the input data x due to the fact that the piece-wise log-linear frontier does not satisfy the axiomatic property (i.e., concavity or convexity) of the function f. Since the multiplicative model (6) is a nonlinear programming (NLP) problem, we need to use the nonlinear solvers, e.g., MINOS, KNITRO. We next demonstrate the estimation of both VRS and CRS multiplicative cost function models. Let the type of model cet parameter be CET_MULT (multiplicative model). Note that the following NLP models are remotely solved by KNITRO solver via the NEOS Server.

- >>> from pystoned import CNLS
- >>> from pystoned.constant import CET_MULT, FUN_COST, RTS_VRS, RTS_CRS
- >>> from pystoned.dataset import load_Finnish_electricity_firm

```
>>> data = load_Finnish_electricity_firm(x_select=['Energy','Length','Customers'],
       y_select=['TOTEX'])
>>> model1=CNLS.CNLS(y=data.y, x=data.x, z=None,
        cet=CET_MULT, fun=FUN_COST, rts=RTS_VRS)
>>> model1.optimize('email@address')
>>> model2=CNLS.CNLS(y=data.y, x=data.x, z=None,
        cet=CET_MULT, fun=FUN_COST, rts=RTS_CRS)
>>> model2.optimize('email@address')
>>>
>>> model1.display_residual()
>>> model2.display_residual()
epsilon : residual
   Size=89, Index=I
   Key: Lower: Value
                                        : Upper : Fixed : Stale : Domain
     0 : None :
                   0.03795367428994332 : None : False : False :
          None :
                  0.030099796252526297 : None : False : False :
    88 : None :
                   0.04860152062781719 : None : False : False : Reals
epsilon : residual
   Size=89, Index=I
   Key : Lower : Value
                                         : Upper : Fixed : Stale : Domain
     0 : None :
                    0.03591704717267953 :
                                           None : False : False :
          None:
                   0.026035484542682643 : None : False : False :
                                                                    Reals
    88:
          None :
                    0.07738478945809676 : None : False : False :
```

Corrected CNLS model

Corrected convex nonparametric least squares (C²NLS) is a variant of the corrected ordinary least squares (COLS) model, in which nonparametric least squares subject to monotonicity and concavity constraints replace the first-stage parametric ordinary least squares (OLS) regression. To estimate the production function, the C²NLS model assumes that the regression f is monotonic increasing and globally concave production function, the inefficiencies ε are identically and independently distributed with mean μ and a finite variance σ^2 , and that the inefficiencies ε are uncorrelated with inputs \boldsymbol{x} .

Similar to COLS, the C²NLS method includes two stages, which can be stated as follows:

- Estimate $\mathsf{E}[y_i \,|\, x_i]$ by solving the CNLS model, e.g., Problem (2). Denote the CNLS residuals by ε_i^{CNLS} .
- Shift the residuals analogous to the COLS procedure; the C^2NLS efficiency estimator is

$$\hat{\varepsilon}_i^{C2NLS} = \varepsilon_i^{CNLS} - \max_i \varepsilon_j^{CNLS}$$

where values of $\hat{\varepsilon_i}^{C2NLS}$ range from $[0, +\infty]$ with 0 indicating efficient performance. Similarly, we adjust the CNLS intercepts α_i as

$$\hat{\alpha}_i^{C2NLS} = \alpha_i^{CNLS} + \max_j \varepsilon_j^{CNLS}$$

where α_i^{CNLS} is the optimal intercept for firm i in above CNLS problem and $\hat{\alpha}_i^{C2NLS}$ is the C²NLS estimator. Slope coefficients β_i for C²NLS are obtained directly as the optimal solution to the CNLS problem.

To solve the C²NLS model (e.g., additive production model), we only need to introduce two new functions: .get_adjusted_residual() and .get_adjusted_alpha(). After completing the first-stage estimation, we use these two functions to obtain the adjusted residuals and intercept terms.

```
>>> from pystoned import CNLS
>>> from pystoned.constant import CET ADDI, FUN PROD, OPT LOCAL, RTS VRS
>>> from pystoned.dataset import load_Finnish_electricity_firm
   data = load_Finnish_electricity_firm(x_select=['OPEX', 'CAPEX'],
        y_select=['Energy'])
   model=CNLS.CNLS(y=data.y, x=data.x, z=None,
        cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
   model.optimize(OPT_LOCAL)
>>>
>>>
>>> print(model.get_adjusted_residual())
>>> print(model.get_adjusted_alpha())
                                -701.60761871 -1030.2948489
[ -682.18627782
                -677.969821
  -693.08377375
                                -685.44491325 -680.26903767]
Γ 656.44793389
                              656.51998647
                656.39703997
                                            712.844865
  656.44540447
                              656.38925598
                                            656.52350009]
```

4.2. Convex Quantile and Expectile Regression

While CNLS estimates the conditional mean $E(y_i | x_i)$, quantile regression aims at estimating the conditional median or other quantiles of the response variable (Koenker and Bassett, 1978; Koenker, 2005) and provides an overall picture of the conditional distributions. The quantile τ splits the observations τ % above and $(1-\tau)$ % below. In this subsection, we extend CNLS problem to estimate CQR (Wang, Wang, Dang, and Ge, 2014; Kuosmanen et al., 2015) and convex expectile regression (CER) (Kuosmanen et al., 2020; Dai, Zhou, and Kuosmanen, 2020; Kuosmanen and Zhou, 2021). Note that both quantile and expectile estimations are more robust to outliers and heteroscedasticity than the CNLS estimation.

Convex quantile regression

Given a pre-specified quantile $\tau \in (0,1)$, the CQR model is formulated as

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

$$s.t. \quad y_{i} = \alpha_{i} + \beta_{i}' \mathbf{x}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \forall i$$

$$\alpha_{i} + \beta_{i}' \mathbf{x}_{i} \leq \alpha_{j} + \beta_{j}' \mathbf{x}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} \geq \mathbf{0} \qquad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0 \qquad \forall i$$

$$(7)$$

where ε_i^+ and ε_i^- denote the two non-negative components. The objective function in (7) minimizes the asymmetric absolute deviations from the function rather than the symmetric quadratic deviations. The last set of constraints is the sign constraint of the error terms. The other constraints are the same as those of the CNLS problem (2).

Convex expectile regression

Convex quantile regression (7) may suffer from non-uniqueness due to that Problem (7) is a linear programming (LP) problem (Kuosmanen *et al.*, 2015). To address this problem, Kuosmanen *et al.* (2015) purpose a CER approach, where a quadratic objective function is used to ensure unique estimates of the quantile functions. Consider the following QP problem

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

$$s.t. \quad y_{i} = \alpha_{i} + \beta_{i}' \mathbf{x}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \quad \forall i$$

$$\alpha_{i} + \beta_{i}' \mathbf{x}_{i} \leq \alpha_{j} + \beta_{j}' \mathbf{x}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} \geq \mathbf{0} \quad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0 \quad \forall i$$
(8)

where the expectile $\tilde{\tau} \in (0,1)$ can be converted from/to the quantile τ (Kuosmanen and Zhou, 2021).

The alternative module CQER includes the function CQR(y, x, ...) that is designed for solving CQR problem and the function CER(y, x, ...) that is for CER problem. Therefore, we use the CQER.CQR() and CQER.CER() to define the CQR problem (see Line 5 in following example) and the CER problem, respectively. The other parameters settings are similar to those in module CNLS(y, x, ...). To display the estimated ε_i^+ and ε_i^- , the functions .display_positive_residual() and .display_negative_residual() are designed in the new module CQER.¹¹ The following additive CQR model is presented to estimate a quantile production function.

>>> from pystoned import CQER

>>> from pystoned.constant import CET_ADDI, FUN_PROD, OPT_LOCAL, RTS_VRS

¹¹Note that as shown in Problem 8, both residuals ε_i^+ and ε_i^- are larger than 0. The function names, positive and negative residuals, are simply used to keep the consistency with the math notations in Problem 8.

```
>>> from pystoned import dataset as dataset
>>> data=dataset.load_GHG_abatement_cost(x_select=['HRSN','CPNK','GHG'],
       y_select=['VALK'])
>>> model=CQER.CQR(y=data.y, x=data.x, tau=0.5, z=None,
       cet=CET ADDI, fun=FUN PROD, rts=RTS VRS)
>>> model.optimize(OPT_LOCAL)
>>>
>>> model.display_alpha()
>>> model.display_beta()
>>> model.display_positive_residual()
>>> model.display_negative_residual()
alpha : alpha
   Size=168, Index=I
   Key : Lower : Value
                            : Upper : Fixed : Stale : Domain
     0 : None : -1306.0485023191532 : None : False : False : Reals
     1 : None : -1306.0485023191268 : None : False : False : Reals
   167 : None : 170680.2112574062 : None : False : False : Reals
beta : beta
   Size=504, Index=beta_index
        : Lower : Value
                                             : Upper : Fixed : Stale : Domain
     (0, 0) : 0.0 :
                          21.043360329998244 : None : False : False :
                0.0:
     (0, 1):
                          0.1758315887019594 : None : False : False :
                                                                       Reals
     (0, 2) : 0.0 :
                                         0.0 : None : False : False : Reals
    (167, 0):
                          13.22794884204182 : None : False : False : Reals
                0.0:
    (167, 1):
                0.0:
                         0.11023334987523721 : None : False : False : Reals
    (167, 2) : 0.0 :
                          645.5693304144419 : None : False : False : Reals
epsilon_plus : positive error term
   Size=168, Index=I
   Key : Lower : Value
                                   : Upper : Fixed : Stale : Domain
     0:
          0.0:
                               0.0 : None : False : False : Reals
     1:
           0.0:
                               0.0 : None : False : False : Reals
   167: 0.0: 98359.68518583104: None: False: False: Reals
epsilon_minus : negative error term
   Size=168, Index=I
   Key : Lower : Value
                                   : Upper : Fixed : Stale : Domain
     0 : 0.0 : 16157.82681402145 : None : False : False : Reals
     1 : 0.0 : 7158.090538541088 : None : False : False : Reals
```

•

167 : 0.0 :

0.0 : None : False : False : Reals

4.3. Contextual Variables

A firm's ability to operate efficiently often depends on operational conditions and practices, such as the production environment and the firm-specific characteristics (i.e., technology selection and managerial practices). Johnson and Kuosmanen (2011, 2012) refer to both variables that characterize operational conditions and practices as contextual variables.

- Contextual variables are often (but not always) external factors that are beyond the control of firms
 - Examples: competition, regulation, weather, location
 - Need to adjust efficiency estimates for the operating environment
 - Policymakers may influence the operating environment
- Contextual variables can also be internal factors
 - Examples: management practices, ownership
 - Better understanding of the impacts of internal factors can help the firm to improve performance

By introducing the contextual variables z_i , the multiplicative model (5) is reformulated as a partial log-linear model to take the operational conditions and practices into account.

$$\ln y_i = \ln f(\boldsymbol{x}_i) + \boldsymbol{\lambda}' \boldsymbol{z}_i + v_i - u_i \tag{9}$$

where parameter vector $\lambda = (\lambda_1, \dots, \lambda_r)$ represents the marginal effects of contextual variables on output. All other variables maintain their previous definitions. Similarly, we can also introduce the contextual variables to the additive model. In this subsection, we consider the multiplicative production model as our starting point.

CNLS with z variables

Following Johnson and Kuosmanen (2011), we incorporate the contextual variables in the multiplicative CNLS model and redefine it as follows:

$$\min_{\alpha, \beta, \lambda, \varepsilon} \sum_{i=1}^{n} \varepsilon_{i}^{2}$$

$$s.t. \quad \ln y_{i} = \ln(\phi_{i} + 1) + \lambda' z_{i} + \varepsilon_{i} \forall i$$

$$\phi_{i} = \alpha_{i} + \beta'_{i} x_{i} - 1 \qquad \forall i$$

$$\alpha_{i} + \beta'_{i} x_{i} \leq \alpha_{j} + \beta'_{j} x_{i} \qquad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} \geq \mathbf{0} \qquad \forall i$$
(10)

Denote by $\hat{\lambda}$ the coefficients of the contextual variables obtained as the optimal solution to the above nonlinear problem. Johnson and Kuosmanen (2011) examine the statistical properties of this estimator in detail, showing its unbiasedness, consistency, and asymptotic efficiency.

The contextual variables z have been integrated into the modules CNLS() and CQER(). Further, the function <code>.display_lamda()</code> is used to display the marginal effect of contextual variable. In the following example, we estimate a log-transformed cost function model with z-variable. Note that we assume that the firms are constant returns to scale in this example.

CER with z variables

Following Kuosmanen, Tan, and Dai (2021), we also incorporate the contextual variable in the multiplicative CER estimation. The reformulation of CER model is

$$\min_{\alpha,\beta,\lambda,\varepsilon^{+},\varepsilon^{-}} \tilde{\tau} \sum_{i=1}^{n} (\varepsilon_{i}^{+})^{2} + (1 - \tilde{\tau}) \sum_{i=1}^{n} (\varepsilon_{i}^{-})^{2}$$

$$s.t. \quad \ln y_{i} = \ln(\phi_{i} + 1) + \lambda' \mathbf{z}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \forall i$$

$$\phi_{i} = \alpha_{i} + \beta'_{i} \mathbf{x}_{i} - 1 \qquad \forall i$$

$$\alpha_{i} + \beta'_{i} \mathbf{x}_{i} \leq \alpha_{j} + \beta'_{j} \mathbf{x}_{i} \qquad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} \geq \mathbf{0} \qquad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0 \qquad \forall i$$

The following code is prepared to solve the CER model with z-variable. We now use the function CQER.CER() to model the CER with z-variable problem and assume that the expectile $\tilde{\tau}$ is equal to 0.5. In this example, we also estimate a CRS cost function.

```
>>> from pystoned import CQER
>>> from pystoned.constant import CET_MULT, FUN_COST, RTS_CRS
>>> from pystoned.dataset import load_Finnish_electricity_firm
>>> data=load_Finnish_electricity_firm(x_select=['Energy','Length','Customers'],
```

```
... y_select=['TOTEX'], z_select=['PerUndGr'])
>>> model=CQER.CER(y=data.y, x=data.x, z=data.z, tau=0.5,
... cet=CET_MULT, fun=FUN_COST, rts=RTS_CRS)
>>> model.optimize('email@address')
>>>
>>> model.display_lamda()

lamda : z coefficient
    Size=1, Index=K
    Key : Lower : Value : Upper : Fixed : Stale : Domain
    0 : None : 0.3609226375022837 : None : False : False : Reals
```

4.4. Multiple Outputs (DDF Formulation)

CNLS with multiple outputs

Until now, the convex regression approaches have been presented within the single output, multiple input framework. In this subsection, we describe the CNLS/CQR/CER approaches with the DDF to handle multiple-input multiple-output data (Chambers, Chung, and Färe, 1996, 1998).

Consider the following QP problem (Kuosmanen and Johnson, 2017)

$$\min_{\alpha,\beta,\gamma,\varepsilon} \sum_{i=1}^{n} \varepsilon_{i}^{2}$$
s.t. $\gamma_{i}' \mathbf{y}_{i} = \alpha_{i} + \beta_{i}' \mathbf{x}_{i} - \varepsilon_{i} \qquad \forall i$

$$\alpha_{i} + \beta_{i}' \mathbf{x}_{i} - \gamma_{i}' \mathbf{y}_{i} \leq \alpha_{j} + \beta_{j}' \mathbf{x}_{i} - \gamma_{j}' \mathbf{y}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\gamma_{i}' g^{y} + \beta_{i}' g^{x} = 1 \qquad \forall i$$

$$\beta_{i} \geq \mathbf{0}, \gamma_{i} \geq \mathbf{0} \qquad \forall i$$

where the residual ε_i represents the estimated value of d ($\vec{D}(x_i, y_i, g^x, g^y) + u_i$). In addition to the same notations as the CNLS estimator, we also introduce firm-specific coefficients γ_i that represent marginal effects of outputs to the DDF.

The first constraint defines the distance to the frontier as a linear function of inputs and outputs. The linear approximation of the frontier is based on the tangent hyperplanes, analogous to the original CNLS formulation. The second set of constraints is the system of Afriat inequalities that impose global concavity. The third constraint is a normalization constraint that ensures the translation property. The last two constraints impose monotonicity in all inputs and outputs. It is straightforward to show that the CNLS estimator of function d satisfies the axioms of free disposability, convexity, and translation property.

To perform the DDF related models, the **pyStoNED** includes the modules CNLSDDF(y, x, ...) and CQERDDF(y, x, ...), and takes the undesirable outputs into account. We first present the CNLS-DDF models in the following two examples and then describe the CQR/CER-DDF models in next subsection. To apply the module CNLSDDF(y, x, ...), we have to predefine the directional vector for the parameters gx, gb (None; default) and gy (i.e., Line 5:

```
gx=[1.0, 0.0], gb=None, gy=[0.0, 0.0, 0.0]). The module also reports the estimates
using .display_alpha(), .display_beta(), .display_gamma(), and .display_residual().
>>> from pystoned import CNLSDDF
>>> from pystoned.constant import FUN_PROD, OPT_LOCAL
>>> from pystoned.dataset import load Finnish_electricity_firm
>>> data=load_Finnish_electricity_firm(x_select=['OPEX','CAPEX'],
       y_select=['Energy','Length','Customers'])
>>> model=CNLSDDF.CNLSDDF(y=data.y, x=data.x, b=None, fun=FUN_PROD,
       gx=[1.0, 0.0], gb=None, gy=[0.0, 0.0, 0.0])
>>> model.optimize(OPT_LOCAL)
>>>
>>> model.display_alpha()
>>> model.display beta()
>>> model.display_gamma()
>>> model.display_residual()
alpha : alpha
   Size=89, Index=I
   Key : Lower : Value
                                     : Upper : Fixed : Stale : Domain
      0 : None : -231.06893282325376 : None : False : False :
                                                               Reals
      1 : None : -212.5240841137753 : None : False : False :
                                                               Reals
    88 : None : -330.8605696176572 : None : False : False : Reals
beta : beta
   Size=178, Index=beta_index
   Key : Lower : Value
                                            : Upper : Fixed : Stale : Domain
     (0, 0):
               0.0:
                                        1.0 : None : False : False : Reals
               0.0: 0.00027176268397506657: None: False: False: Reals
    (88, 0):
               0.0:
                                        1.0 : None : False : False :
                                                                      Reals
    (88, 1):
                        0.0526234540690525 : None : False : False : Reals
               0.0:
gamma : gamma
   Size=267, Index=gamma_index
         : Lower : Value
                                            : Upper : Fixed : Stale : Domain
     (0, 0):
               0.0:
                         3.806267544117393 : None : False : False : Reals
     (0, 1):
                         0.2311214613059167 : None : False : False :
               0.0:
                                                                      Reals
     (0, 2):
               0.0 : 0.004895753020650473 : None : False : False : Reals
    (88, 0):
               0.0:
                     0.015392372124732883 : None : False : False :
                                                                      Reals
    (88, 1):
               0.0 : 0.0029598467042669355 : None : False : False :
                                                                     Reals
    (88, 2):
               0.0:
                      0.06644931421296872 : None : False : False : Reals
```

When considering undesirable outputs, the CNLS-DDF problem (12) can be reformulated as

$$\min_{\alpha,\beta,\gamma,\delta,\varepsilon} \sum_{i=1}^{n} \varepsilon_{i}^{2}$$

$$s.t. \quad \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} = \alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{i}' \boldsymbol{b}_{i} - \varepsilon_{i} \qquad \forall i$$

$$\alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{i}' \boldsymbol{b}_{i} - \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} \leq \alpha_{j} + \boldsymbol{\beta}_{j}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{j}' \boldsymbol{b}_{i} - \boldsymbol{\gamma}_{j}' \boldsymbol{y}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\boldsymbol{\gamma}_{i}' g^{y} + \boldsymbol{\beta}_{i}' g^{x} + \boldsymbol{\delta}_{i}' g^{b} = 1 \qquad \forall i$$

$$\boldsymbol{\beta}_{i} \geq \mathbf{0}, \boldsymbol{\delta}_{i} \geq \mathbf{0}, \boldsymbol{\gamma}_{i} \geq \mathbf{0}$$

$$\forall i$$

where the coefficients δ_i denote marginal effects of undesirable outputs to the DDF.

We can also model the undesirable outputs (b) in the framework of DDF via the module CNLSDDF (Line 5; cf., the example above). The estimated coefficients can be displayed by using the function .display_delta().

```
>>> from pystoned import CNLSDDF
>>> from pystoned.constant import FUN_PROD, OPT_LOCAL
>>> from pystoned import dataset as dataset
>>> data = dataset.load GHG abatement cost()
>>> model = CNLSDDF.CNLSDDF(y=data.y, x=data.x, b=data.b,
        fun=FUN_PROD, gx=[0.0, 0.0], gb=-1.0, gy=1.0)
>>> model.optimize(OPT_LOCAL)
>>>
>>> model.display_delta()
delta : delta
   Size=168, Index=delta_index
                                           : Upper : Fixed : Stale : Domain
             : Lower : Value
                0.0 : 27.122300643881694 : None : False : False :
      (1, 0):
                0.0 : 31.329802702797316 : None : False : False :
    (167, 0):
                0.0:
                          6.10497985046203 : None : False : False : Reals
```

CQR/CER with multiple outputs

Similar to CNLS with DDF, we present another two approaches integrating DDF to convex quantile/expectile regression, and we also consider modeling the undesirable outputs.

- without undesirable outputs
 - 1) CQR-DDF model

$$\min_{\alpha,\beta,\gamma,\varepsilon^{+},\varepsilon^{-}} \tau \sum_{i=1}^{n} \varepsilon_{i}^{+} + (1-\tau) \sum_{i=1}^{n} \varepsilon_{i}^{-}$$

$$s.t. \quad \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} = \alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \qquad \forall i$$

$$\alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} - \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} \leq \alpha_{j} + \boldsymbol{\beta}_{j}' \boldsymbol{x}_{i} - \boldsymbol{\gamma}_{j}' \boldsymbol{y}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\boldsymbol{\gamma}_{i}' g^{y} + \boldsymbol{\beta}_{i}' g^{x} = 1 \qquad \forall i$$

$$\boldsymbol{\beta}_{i} \geq \mathbf{0}, \boldsymbol{\gamma}_{i} \geq \mathbf{0} \qquad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0 \qquad \forall i$$

2) CER-DDF model

$$\min_{\alpha,\beta,\gamma,\varepsilon^{+},\varepsilon^{-}} \tilde{\tau} \sum_{i=1}^{n} (\varepsilon_{i}^{+})^{2} + (1 - \tilde{\tau}) \sum_{i=1}^{n} (\varepsilon_{i}^{-})^{2}$$

$$s.t. \quad \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} = \alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \qquad \forall i$$

$$\alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} - \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} \leq \alpha_{j} + \boldsymbol{\beta}_{j}' \boldsymbol{x}_{i} - \boldsymbol{\gamma}_{j}' \boldsymbol{y}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\boldsymbol{\gamma}_{i}' g^{y} + \boldsymbol{\beta}_{i}' g^{x} = 1 \qquad \forall i$$

$$\boldsymbol{\beta}_{i} \geq \mathbf{0}, \boldsymbol{\gamma}_{i} \geq \mathbf{0} \qquad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0 \qquad \forall i$$

Similar to the module CNLSDDF, the module CQERDDF uses the same parameters and is applied to estimate the CQR/CER-DDF model. The results can be reported using the functions that have been introduced in module CQER.CQR(y, x, \ldots)/.CER(y, x, \ldots). For instance, the functions .display_positive_residual() and .display_negative_residual() are used to display the estimated residuals, respectively (Lines 8 and 9).

```
>>> from pystoned import CQERDDF
>>> from pystoned.constant import FUN_PROD, OPT_LOCAL
>>> from pystoned import dataset as dataset
>>> data = dataset.load_Finnish_electricity_firm(x_select=['OPEX', 'CAPEX'],
        y_select=['Energy', 'Length', 'Customers'])
>>> model = CQERDDF.CQRDDF(y=data.y, x=data.x, b=None, tau=0.9,
        fun = FUN_PROD, gx= [1.0, 0.0], gb=None, gy= [0.0, 0.0, 0.0])
>>> model.optimize(OPT_LOCAL)
>>>
>>> model.display_positive_residual()
>>> model.display_negative_residual()
epsilon_plus : positive error term
   Size=89, Index=I
   Key : Lower : Value
                                     : Upper : Fixed : Stale : Domain
                                 0.0 : None : False : False : Reals
     0 :
           0.0:
                                 0.0 : None : False : False : Reals
     1:
           0.0:
```

•

88 : 0.0 : 0.0 : None : False : False : Reals

epsilon_minus : negative error term

Size=89, Index=I

.

88 : 0.0 : 224.05081364484738 : None : False : False : Reals

- with undesirable outputs
 - 1) CQR-DDF-b model

$$\min_{\alpha,\beta,\gamma,\delta,\varepsilon^{+},\varepsilon^{-}} \tau \sum_{i=1}^{n} \varepsilon_{i}^{+} + (1-\tau) \sum_{i=1}^{n} \varepsilon_{i}^{-}$$

$$s.t. \quad \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} = \alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{i}' \boldsymbol{b}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \qquad \forall i$$

$$\alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{i}' \boldsymbol{b}_{i} - \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} \leq \alpha_{j} + \boldsymbol{\beta}_{j}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{j}' \boldsymbol{b}_{i} - \boldsymbol{\gamma}_{j}' \boldsymbol{y}_{i} \qquad \forall i, j, \text{ and } i \neq j$$

$$\boldsymbol{\gamma}_{i}' g^{y} + \boldsymbol{\beta}_{i}' g^{x} + \boldsymbol{\delta}_{i}' g^{b} = 1 \qquad \forall i$$

$$\boldsymbol{\beta}_{i} \geq \mathbf{0}, \delta_{i} \geq \mathbf{0}, \boldsymbol{\gamma}_{i} \geq \mathbf{0} \qquad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0 \qquad \forall i$$

2) CER-DDF-b model

$$\min_{\alpha,\beta,\gamma,\boldsymbol{\delta},\varepsilon^{+},\varepsilon^{-}} \tilde{\tau} \sum_{i=1}^{n} (\varepsilon_{i}^{+})^{2} + (1 - \tilde{\tau}) \sum_{i=1}^{n} (\varepsilon_{i}^{-})^{2}$$

$$s.t. \quad \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} = \alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{i}' \boldsymbol{b}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \qquad \forall i$$

$$\alpha_{i} + \boldsymbol{\beta}_{i}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{i}' \boldsymbol{b}_{i} - \boldsymbol{\gamma}_{i}' \boldsymbol{y}_{i} \leq \alpha_{j} + \boldsymbol{\beta}_{j}' \boldsymbol{x}_{i} + \boldsymbol{\delta}_{j}' \boldsymbol{b}_{i} - \boldsymbol{\gamma}_{j}' \boldsymbol{y}_{i} \quad \forall i, j, \text{ and } i \neq j$$

$$\boldsymbol{\gamma}_{i}' g^{y} + \boldsymbol{\beta}_{i}' g^{x} + \boldsymbol{\delta}_{i}' g^{b} = 1 \qquad \forall i$$

$$\boldsymbol{\beta}_{i} \geq \mathbf{0}, \delta_{i} \geq \mathbf{0}, \boldsymbol{\gamma}_{i} \geq \mathbf{0} \qquad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0$$

The following code shows how to solve the CQR-DDF model when the data include the undesirable output (i.e., GHG emissions).

```
>>> from pystoned import CQERDDF
>>> from pystoned.constant import FUN_PROD, OPT_LOCAL
>>> from pystoned import dataset as dataset
>>> data = dataset.load_GHG_abatement_cost()
>>> model = CQERDDF.CQRDDF(y=data.y, x=data.x, b=data.b, tau=0.9,
... fun = FUN_PROD, gx= [0.0, 0.0], gb=[-1], gy=[1])
```

4.5. Relaxing convexity

Isotonic CNLS

This section introduces a variant of the CNLS estimator, Isotonic CNLS that relies only on the monotonicity assumption. To relax the concavity assumption in CNLS estimation (i.e., estimating a production function), we have to rephrase the Afriat inequality constraint in Problem (2).

Define a binary matrix $P = [p_{ij}]_{n \times n}$ to represent isotonicity (Keshvari and Kuosmanen, 2013) as follows.

$$p_{ij} = \begin{cases} 1 & \text{if } x_i \leq x_j \\ 0 & \text{otherwise} \end{cases}$$

Applying the enumeration method to define the elements of matrix P, we then solve the following QP problem

$$\min_{\alpha,\beta,\varepsilon} \sum_{i=1}^{n} \varepsilon_{i}^{2}$$

$$s.t. \quad y_{i} = \alpha_{i} + \beta'_{i} \mathbf{x}_{i} + \varepsilon_{i} \qquad \forall i$$

$$p_{ij}(\alpha_{i} + \beta'_{i} \mathbf{x}_{i}) \leq p_{ij}(\alpha_{j} + \beta'_{j} \mathbf{x}_{i}) \quad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} \geq \mathbf{0} \qquad \forall i$$
(18)

Note that the concavity constraints between units i and j are relaxed by the matrix $P_{ij} = 0$. If the $P_{ij} = 1$ for all i and j, then the above QP problem (i.e., ICNLS problem) reduces to the CNLS problem.

To calculate the monotonic models, the **pyStoNED** package provides the modules ICNLS(y, x, ...) and ICQER(y, x, ...), of which inherit the parameter settings from the modules CNLS(y, x, ...) and CQER(y, x, ...). Therefore, the usages of CNLS() and CQER() are similar to those of CNLS() and CQER(). Note that the matrix P is added in the module as the internal function. The readers could check the source code from the GitHub repository.

```
>>> from pystoned import ICNLS
>>> from pystoned.constant import CET_ADDI, FUN_PROD, OPT_LOCAL, RTS_VRS
>>> from pystoned.dataset import load_Finnish_electricity_firm
>>> data=load_Finnish_electricity_firm(x_select=['OPEX','CAPEX'],
         y select=['Energy'])
>>> model=ICNLS.ICNLS(y=data.y, x=data.x, z=None,
          cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> model.optimize(OPT_LOCAL)
>>>
>>> model.display_residual()
epsilon : residual
    Size=89, Index=I
    Key : Lower : Value
                                                    : Upper : Fixed : Stale : Domain
       0: None: 0.0006849098000571985: None: False: False: Reals
                          -3.833461767868812 : None : False : False : Reals
       1 : None :
      88 : None : 7.8890389440795445 : None : False : False : Reals
Isotonic CQR/CER
Similar to ICNLS, the Isotonic CQR and CER approaches are defined as follows:
   • ICQR estimator
                     \min_{\alpha,\beta,\varepsilon^+,\varepsilon^-} \tau \sum_{i=1}^n \varepsilon_i^+ + (1-\tau) \sum_{i=1}^n \varepsilon_i^-
                                                                                            (19)
                       s.t. y_i = \alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i + \varepsilon_i^+ - \varepsilon_i^-
                             p_{ij}(\alpha_i + \boldsymbol{\beta}_i' \boldsymbol{x}_i) \le p_{ij}(\alpha_j + \boldsymbol{\beta}_j' \boldsymbol{x}_i) \quad \forall i, j, \text{ and } i \ne j
                             \varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0
                                                                 \forall i
>>> from pystoned import ICQER
>>> from pystoned.constant import CET_ADDI, FUN_PROD, OPT_LOCAL, RTS_VRS
>>> from pystoned.dataset import load_Finnish_electricity_firm
>>> data=load_Finnish_electricity_firm(x_select=['OPEX','CAPEX'],
         y_select=['Energy'])
. . .
>>> model = ICQER.ICQR(y=data.y, x=data.x, tau = 0.9, z=None,
          cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> model.optimize(OPT_LOCAL)
```

>>>

>>> model.display_residual()

epsilon : error term Size=89, Index=I

88 : None : -25.00000000488575 : None : False : False : Reals

• ICER estimator

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

$$s.t. \quad y_{i} = \alpha_{i} + \beta_{i}' \mathbf{x}_{i} + \varepsilon_{i}^{+} - \varepsilon_{i}^{-} \qquad \forall i$$

$$p_{ij}(\alpha_{i} + \beta_{i}' \mathbf{x}_{i}) \leq p_{ij}(\alpha_{j} + \beta_{j}' \mathbf{x}_{i}) \quad \forall i, j, \text{ and } i \neq j$$

$$\beta_{i} \geq \mathbf{0} \qquad \forall i$$

$$\varepsilon_{i}^{+} \geq 0, \ \varepsilon_{i}^{-} \geq 0 \qquad \forall i$$

```
>>> from pystoned import ICQER
>>> from pystoned.constant import CET_ADDI, FUN_PROD, OPT_LOCAL, RTS_VRS
>>> from pystoned.dataset import load_Finnish_electricity_firm
>>> data=load_Finnish_electricity_firm(x_select=['OPEX','CAPEX'],
       y_select=['Energy'])
>>> model=ICQER.ICER(y=data.y, x=data.x, tau=0.9, z=None,
        cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> model.optimize(OPT_LOCAL)
>>>
>>> model.display_residual()
epsilon : error term
   Size=89, Index=I
   Key : Lower : Value
                                       : Upper : Fixed : Stale : Domain
     O : None : -17.735777393077573 : None : False : False :
          None : -30.733601094693068 : None : False : False :
    88 : None : -9.466741932963199 : None : False : False : Reals
```

5. Stochastic Nonparametric Envelopment of Data

Combining virtues of SFA and DEA in a unified framework, StoNED (Kuosmanen, 2006; Kuosmanen and Kortelainen, 2012) uses a composed error term to model both inefficiency u and noise v without assuming a functional form of f. Analogous to the COLS/C²NLS estimators, the StoNED estimator consists of the following four steps:

• Step 1: Estimating the conditional mean $E[y_i | x_i]$ using CNLS estimator

- Step 2: Estimating the expected inefficiency μ based on the residual ε_i^{CNLS}
- Step 3: Estimating the StoNED frontier \hat{f}^{StoNED} based on the $\hat{\mu}$
- Step 4: Estimating firm-specific inefficiencies $\mathsf{E}[u_i \mid \varepsilon_i^{CNLS}]$

Besides the CNLS estimator, we can apply other convex regression approaches such as IC-NLS and CNLS-DDF to estimate the conditional mean in the first step (see Keshvari and Kuosmanen, 2013; Kuosmanen and Johnson, 2017). However, the quantile and expectile related estimators introduced in Section 4 can not be integrated into the StoNED framework at present.

5.1. Estimating the expected inefficiency

After obtaining the residuals (e.g., ε_i^{CNLS}) from the convex regression approaches, one can estimate the expected value of the inefficiency term $\mu = E(u_i)$. In practice, three commonly used methods are available to estimate the expected inefficiency μ : method of moments (Aigner et al., 1977), quasi-likelihood estimation (Fan, Li, and Weersink, 1996), and kernel deconvolution estimation (Hall and Simar, 2002). We next briefly review these three approaches and demonstrate the application of **pyStoNED**; see more detailed theoretical introduction in Kuosmanen et al. (2015).

Method of moments

The method of moments requires some additional parametric distributional assumptions. Following Kuosmanen *et al.* (2015), under the maintained assumptions of half-normal inefficiency (i.e., $u_i \sim N^+(0, \sigma_u^2)$) and normal noise (i.e., $v_i \sim N(0, \sigma_v^2)$), the second and third central moments of the composite error (i.e., ε_i) distribution are given by

$$M_2 = \left[\frac{\pi - 2}{\pi}\right] \sigma_u^2 + \sigma_v^2$$
$$M_3 = \left(\sqrt{\frac{2}{\pi}}\right) \left[1 - \frac{4}{\pi}\right] \sigma_u^2$$

The second and third central moments can be estimated by using the CNLS residuals, i.e., $\hat{\varepsilon}_i^{CNLS}$:

$$\hat{M}_2 = \sum_{i=1}^n (\hat{\varepsilon}_i - \bar{\varepsilon})^2 / n$$

$$\hat{M}_3 = \sum_{i=1}^n (\hat{\varepsilon}_i - \bar{\varepsilon})^3 / n$$

Note that the third moment M_3 (which measures the skewness of the distribution) only depends on the standard deviation parameter σ_u of the inefficiency distribution. Thus, given the estimated \hat{M}_3 (which should be positive in the case of a cost frontier), we can estimate

the parameters σ_u and σ_v by

$$\hat{\sigma}_u = \sqrt[3]{\frac{\hat{M}_3}{\left(\sqrt{\frac{2}{\pi}}\right)\left[1 - \frac{4}{\pi}\right]}}$$

$$\hat{\sigma}_v = \sqrt[2]{\hat{M}_2 - \left[\frac{\pi - 2}{\pi}\right]\hat{\sigma}_u^2}$$

To estimate the unconditional expected inefficiency μ and firm-specific inefficiencies, we provide a module StoNED() that inherits the parameter setting from the module CNLS(). We estimate the conditional expected inefficiency through the presented example below. Following the calculation procedure of StoNED estimator, we first utilize the module CNLS() to estimate the conditional mean $\mathsf{E}[y_i \mid \boldsymbol{x}_i]$ (i.e., Lines 5-6), then apply the module StoNED(model), where the parameter model is defined as the name of CNLS model (cf. footnote 10), to decompose the estimated residuals (i.e., Line 8). We develop and import the parameter RED_MOM (i.e., Line 3) to decompose the residuals by using the method of moment. We finally resort to the function .get_unconditional_expected_inefficiency(RED_MOM)) included in the module StoNED() to retrieve the expected inefficiency $\hat{\mu}$.

0.028561358246550088

Quassi-likelihood estimation

Quasi-likelihood approach is an alternative approach to decomposing σ_u and σ_v suggested by Fan *et al.* (1996). Given the shape of the CNLS curve, we apply the standard maximum likelihood method to estimate the parameters σ_u and σ_v . The quasi-likelihood function is formulated as

$$\ln L(\lambda) = -n \ln(\hat{\sigma}) + \sum \ln \Phi \left[\frac{-\hat{\varepsilon}_i \lambda}{\hat{\sigma}} \right] - \frac{1}{2\hat{\sigma}^2} \sum \hat{\varepsilon}_i^2$$

where

$$\hat{\varepsilon}_i = \hat{\varepsilon}_i^{CNLS} - (\sqrt{2}\lambda\hat{\sigma})/[\pi(1+\lambda^2)]^{1/2}$$

$$\hat{\sigma} = \left\{ \frac{1}{n} \sum (\hat{\varepsilon}_i^{CNLS})^2 / \left[1 - \frac{2\lambda^2}{\pi(1+\lambda^2)} \right] \right\}.$$

Note that the quasi-likelihood function only consists of a single parameter λ (i.e., the signal-to-noise ratio $\lambda = \sigma_u/\sigma_v$). The symbol Φ represents the cumulative distribution function of the standard normal distribution. In the **pyStoNED** package, we use the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm provided by **SciPy** to estimate the maximum likelihood function.

Since we apply the quasi-likelihood estimation to decompose the residuals, we import the parameter RED_QLE in the module StoNED() (see Line 3).

0.05776223709846952

Kernel deconvolution estimation

While the method of moments and quasi-likelihood approaches require additional distributional assumptions for the inefficiency and noise terms, an alternative nonparametric estimation of the expected inefficiency μ is available by applying nonparametric kernel deconvolution proposed by Hall and Simar (2002). Note that the residual $\hat{\varepsilon}_i^{CNLS}$ is a consistent estimator of $e^o = \varepsilon_i + \mu$ (for production model). Following Kuosmanen and Johnson (2017), the density function of e^o is

$$\hat{f}_{e^o}(z) = (nh)^{-1} \sum_{i=1}^n K\left(\frac{z - e_i^o}{h}\right),$$

where $K(\cdot)$ is a compactly supported kernel, and h is a bandwidth. Hall and Simar (2002) show that the first derivative of the density function of the composite error term (f_{ε}') is proportional to that of the inefficiency term (f_u') in the neighborhood of μ . Therefore, a nonparametric estimator of expected inefficiency μ is obtained as

$$\hat{\mu} = \arg\max_{z \in C} (\hat{f'}_{e^o}(z)),$$

where C is a closed interval in the right tail of f_{e^o} .

We then import the parameter RED_KDE to decompose the estimated residuals, i.e., $\hat{\varepsilon}_i^{CNLS}$ (i.e., Line 3).

¹²Note the notation difference between signal-to-noise ratio λ and the marginal effect of contextual variable λ in Problems (10) and (11).

3.1932648065241334

5.2. Estimating firm-specific inefficiencies

After estimating the expected inefficiency μ using the methods of moment (MOM) or quasilikelihood estimation (QLE),¹³ we then employ JLMS estimator proposed by Jondrow, Lovell, Materov, and Schmidt (1982) to estimate the firm-specific inefficiencies (Johnson and Kuosmanen, 2015). Under the assumption of a normally distributed error term and a half-normally distributed inefficiency term, JLMS formulates the conditional distribution of inefficiency u_i , given $\hat{\varepsilon}_i$, and proposes the inefficiency estimator as the conditional mean $\mathsf{E}[u_i \mid \hat{\varepsilon}_i]$.

Following Kumbhakar and Lovell (2000), the conditional expected value of inefficiency $\mathsf{E}[u_i \,|\, \hat{\varepsilon}_i]$ for production function and cost function are shown as follows, respectively:

• Production function

$$\mathsf{E}[u_i \,|\, \hat{\varepsilon}_i] = \mu_{*i} + \sigma_* \Bigg[\frac{\phi(-\mu_{*i}/\sigma_*)}{1 - \Phi(-\mu_{*i}/\sigma_*)} \Bigg] = \sigma_* \Bigg[\frac{\phi(\varepsilon_i \lambda/\sigma)}{1 - \Phi(\varepsilon_i \lambda/\sigma)} - \frac{\varepsilon_i \lambda}{\sigma} \Bigg]$$

where $\mu_* = -\varepsilon \sigma_u^2/\sigma^2$, $\sigma_*^2 = \sigma_u^2 \sigma_v^2/\sigma^2$, $\lambda = \sigma_u/\sigma_v$, and $\sigma^2 = \sigma_u^2 + \sigma_v^2$. The symbol ϕ is the standard normal density function, and the symbol Φ denotes the cumulative distribution function of the standard normal distribution.

Cost function

$$\mathsf{E}[u_i \mid \hat{\varepsilon}_i] = \mu_{*i} + \sigma_* \left[\frac{\phi(-\mu_{*i}/\sigma_*)}{1 - \Phi(-\mu_{*i}/\sigma_*)} \right] = \sigma_* \left[\frac{\phi(\varepsilon_i \lambda/\sigma)}{1 - \Phi(-\varepsilon_i \lambda/\sigma)} + \frac{\varepsilon_i \lambda}{\sigma} \right]$$

where
$$\mu_* = \varepsilon \sigma_u^2 / \sigma^2$$
, $\sigma_*^2 = \sigma_u^2 \sigma_v^2 / \sigma^2$, $\lambda = \sigma_u / \sigma_v$, and $\sigma^2 = \sigma_u^2 + \sigma_v^2$.

The firm-level technical efficiency (TE) is then measured based on the estimated conditional mean. For other models, the technical efficiency can be estimated as follows.

 $^{^{13}}$ For the expected inefficiency μ estimated by kernel deconvolution, Dai (2016) proposes a non-parametric strategy where the Richardson–Lucy blind deconvolution algorithm is used to identify firm-specific inefficiencies. However, the **pyStoNED** package only supports the parametric estimation of firm-specific inefficiencies due to the fact that the parametric method is more widely used in efficiency analysis literature.

- Production function
 - Multiplicative model: TE = $\exp(-E[u_i \mid \varepsilon_i])$
 - Additive model: TE = $\frac{y \mathsf{E}[u_i|\varepsilon_i]}{y}$
- Cost function
 - Multiplicative model: $TE = \exp(E[u_i \mid \varepsilon_i])$
 - Additive model: $TE = \frac{y + E[u_i | \varepsilon_i]}{y}$

To calculate the firm-level technical efficiency, we resort to the function .get_technical_inefficiency(). We either set the parameter in function .get_technical_inefficiency() to RED_MOM (i.e., using the MOM approach to calculate the efficiency; Line 9) or to RED_QLE (i.e., using the quassi-likelihood estimation approach).

```
>>> from pystoned import CNLS, StoNED
>>> from pystoned.dataset import load_Finnish_electricity_firm
>>> from pystoned.constant import CET_MULT, FUN_COST, RTS_VRS, RED_MOM
>>> data=load_Finnish_electricity_firm(x_select=['Energy','Length','Customers'],
       y_select=['TOTEX'])
. . .
>>> model = CNLS.CNLS(data.y, data.x, z=None,
        cet=CET MULT, fun=FUN COST, rts=RTS VRS)
>>> model.optimize('email@address')
>>>
>>> rd = StoNED.StoNED(model)
>>> print(rd.get_technical_inefficiency(RED_MOM))
[1.02974326 1.029505
                       1.03407182 1.03011172 1.03285089 1.02624282
1.02854464 1.03305965 ...
                                  1.02883011 1.03059918 1.03003701]
```

Further, we can consider the effect of contextual variables (z) in the first-step estimation of the StoNED estimator (i.e., Line 5) when calculating the technical efficiency.

6. CNLS-G Algorithm

Since convex regression approaches shape the convexity (concavity) of function using the Afrait inequality, the estimation becomes excessively expensive due to the $O(n^2)$ linear constraints. For example, if the data samples have 500 observations, the total number of linear constraints is equal to 250,000. To speed up the computational time, Lee, Johnson, Moreno-Centeno, and Kuosmanen (2013) propose a more efficient generic algorithm, CNLS-G, which uses the relaxed Afriat constraint set and iteratively adds violated constraints to the relaxed model as necessary. See further discussions in Lee et al. (2013).

To illustrate the CNLS-G algorithm, we follow Lee *et al.* (2013) to generate the input and output variables. In this section, we assume an additive production function with two-input and one-output, $y = x_1^{0.4} \times x_2^{0.4} + u$. We randomly draw the inputs x_1 and x_2 from a uniform distribution, $x \sim U[1, 10]$, and the error term u from a normal distribution, $u \sim N(0, 0.7^2)$. Based on these settings, we generate 500 artificial observations, estimate the CNLS problem (2) and the CER problem (8), and calculate the firm-level technical efficiency using the CNLS-G algorithm.

6.1. Solving CNLS model

We first compare the running time of original CNLS and CNLS-G algorithm in the same computation environment. Line 1 imports the modules CNLSG() that is designed to perform the CNLS-G algorithm and CNLS() from the package pyStoNED. Note that the module CNLSG() has the same parameters as the module CNLS(). Line 3 imports the numPy to provide multidimensional array and functions for linear algebra. We use the numPy to provide multime for CNLS estimation (i.e., Lines 4, 9, 12) and employ the function numPy to directly obtain the running time for CNLS-G algorithm (i.e., Line 16). To replicate the experiment, we set a random seed using the numPy random seed(). Lines 6-8 generate the variables numPy, and numPy model1 and numPy model2 are the normal CNLS model and CNLS-G model, respectively. To count the number of constraints included in the CNLS-G algorithm, the module CNLSG() provides an internal function numPy number of constraints included in the CNLS-G algorithm, the

```
>>> from pystoned import CNLSG, CNLS
>>> from pystoned.constant import CET_ADDI, FUN_PROD, OPT_LOCAL, RTS_VRS
>>> import numpy as np
>>> import time
>>> np.random.seed(0)
>>> x=np.random.uniform(low=1, high=10, size=(500, 2))
>>> u=np.random.normal(loc=0, scale=0.7, size=500)
>>> y=x[:, 0]**0.4*x[:, 1]**0.4+u
>>> t1=time.time()
>>> model1=CNLS.CNLS(y, x, z=None,
        cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> model1.optimize(OPT_LOCAL)
>>> CNLS time = time.time()-t1
>>> model2=CNLSG.CNLSG(y, x, z=None,
        cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> model2.optimize(OPT_LOCAL)
```

```
>>>
>>> print("The running time with algorithm is ", model2.get_runningtime())
>>> print("The running time without algorithm is ", CNLS_time)
>>>
>>> print("The total number of constraints is ", model2.get_totalconstr())
The running time with algorithm is 20.35739278793335
The running time without algorithm is 30.252474308013916
The total number of constraints is 9700.0
```

6.2. Solving CER model

We next demonstrate a CER model solved by the CNLS-G algorithm prepared in module CQERG(). The other experimental settings are similar to those in Section 6.1. Note that the CQR model can also be solved by the CNLS-G algorithm via the function CQERG.CQRG(y, x, ...) (cf. Line 14).

```
>>> from pystoned import CQERG, CQER
>>> from pystoned.constant import CET_ADDI, FUN_PROD, OPT_LOCAL, RTS_VRS
>>> import numpy as np
>>> import time
>>> np.random.seed(0)
>>> x=np.random.uniform(low=1, high=10, size=(500, 2))
>>> u=np.random.normal(loc=0, scale=0.7, size=500)
>>> y=x[:, 0]**0.4*x[:, 1]**0.4+u
>>> tau=0.5
>>> t1=time.time()
>>> model1=CQER.CER(y, x, tau, z=None,
        cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> model1.optimize(OPT_LOCAL)
>>> CER time=time.time()-t1
>>> model2=CQERG.CERG(y, x, tau, z=None,
        cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> model2.optimize(OPT_LOCAL)
>>>
>>> print("The running time with algorithm is ", model2.get_runningtime())
>>> print("The running time without algorithm is ", CER_time)
>>> print("The total number of constraints in CER model is ",
        model2.get_totalconstr())
. . .
The running time with algorithm is 22.845768451690674
The running time without algorithm is 29.961899280548096
The total number of constraints in CER model is 9701.0
```

6.3. Calculating firm-level efficiency

We can apply the CNLS-G algorithm to calculate the firm-level efficiency more efficiently. In

the first step of StoNED() estimator, we use the module CNLSG(y, x, ...) as a substitute for the module CNLS(y, x, ...) (Lines 1 and 5). The other settings are similar to those in Section 5.

7. Graphical illustration of estimated function

To illustrate how the estimated function looks like, the **pyStoNED** package provides the functions plot.plot2d() and plot.plot3d() to plot two- and three-dimensional (2D and 3D) estimated functions. Similar to the usage of the module StoNED(y, x, ...), we first estimate the nonparametric regression such as CNLS, CQR, and ICNLS and then apply the plot function to draw the figures. In this section, we use the internal data provided with Tim Coelli's Frontier 4.1 to demonstrate the plotting process.

7.1. One-input and One-output

In the one-input and one-output case, we present two different estimated functions: the CNLS function and the CQR function. Therefore, we import the modules CNLS and CQER in Line 1 as the estimators, the plotting module plot2d (Line 2), and the example dataset (Line 4). Lines 6 and 7 and Lines 10 and 11 define and solve the CNLS and CQR models. Lines 8 and 12 are used to plot the estimated function. There are four parameters in the module plot2d(...): the first is the model's name (see footnote 10), the second parameter x_select defines which is the selected input x, the third and last are the given names of the legend and generated picture, respectively.

```
>>> from pystoned import CNLS, CQER
>>> from pystoned.plot import plot2d
>>> from pystoned.constant import CET_ADDI, FUN_PROD, OPT_LOCAL, RTS_VRS
>>> from pystoned.dataset import load_Tim_Coelli_frontier
>>> data=load_Tim_Coelli_frontier(x_select=['labour'],y_select=['output'])
>>> CNLS_model=CNLS.CNLS(y=data.y, x=data.x, z=None,
... cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
```

Figure 1 depicts the functions estimated by the CNLS and CQR model (with $\tau = 0.5$).

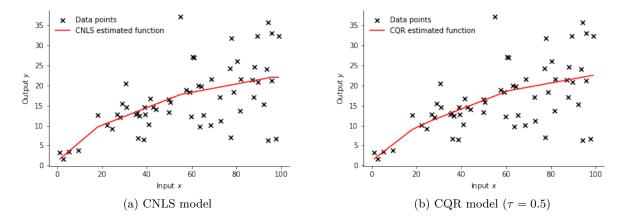


Figure 1: Estimated function by CNLS/CQR model.

7.2. Two-input and One-output

In the two-input and one-output case, we use linear interpolation to obtain the 3D surface due to the fact that CNLS estimates hyperplanes at the observation points. ¹⁴ The function plot3d(model, x_select_1, x_select_2, fig_name=None, line_transparent=False, pane_transparent=False) includes six parameters: the first is the name of the estimated model, the second and third define the selected input, the fourth is the name of generated figure, the last two are the basic settings for the figure (False; default). We import function plot3d(...) in Line 2 and plot the figure in Line 8. Figure 2 presents the estimated 3D estimated function.

¹⁴Note that the CNLS estimator includes linear programming as the second stage estimation to find the minimum extrapolated production function (Kuosmanen and Kortelainen, 2012).

```
... cet=CET_ADDI, fun=FUN_PROD, rts=RTS_VRS)
>>> CNLS_model.optimize(OPT_LOCAL)
>>> plot3d(CNLS_model,x_select_1=0, x_select_2=1, fig_name="CNLS_3d")
```

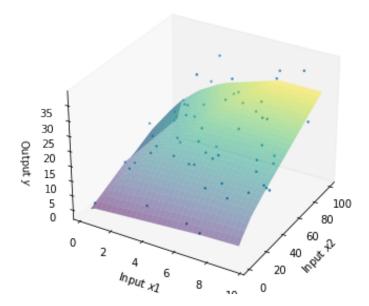


Figure 2: Estimated function by CNLS model.

8. Conclusions

Convex regression and related methods provide an appealing way to impose shape constraints implied by the theory without making restrictive functional form assumptions. As these techniques are becoming increasingly popular, there is a great demand for a powerful, reliable, and fully open access computational package. The Python package **pyStoNED** aims to address this need, providing a comprehensive set of functions for estimating CNLS, StoNED, and their numerous variants. For more information, see its developed repository on GitHub at https://github.com/ds2010/pyStoNED and documentation at https://pystoned.readthedocs.io.

This paper has reviewed the models and specifications currently supported by **pyStoNED**, and demonstrated its use by empirical examples taken from the literature of productivity and efficiency analysis. All modules are implemented in a fully open access environment. We encourage the users to utilize **pyStoNED** to further develop their own packages for specific estimation purposes.

In the future, our plan is to include further extensions to **pyStoNED** on a continuous basis. One interesting avenue of ongoing research is to include additional penalty terms to the objective function of the CNLS/CQR/CER problems to alleviate overfitting and the curse of dimensionality (e.g., Lee and Cai, 2020). More efficient computational algorithms such as the CNLS-A proposed by Dai (2021) are under active development, and will be included in the future editions of **pyStoNED**.

We hope that the **pyStoNED** package could contribute to raising the standards of empirical applications of productivity and efficiency analysis, and facilitate more meaningful and rele-

vant applications that influence the managerial and policy decisions. The basic idea of the StoNED approach is to enable applied researchers and practitioners of efficiency analysis to incorporate existing tools and techniques from different domains such as econometrics, statistics, operational research, and machine learning to a logically consistent unified framework, but also to facilitate further methodological development in a multi-disciplinary environment. The purpose of the **pyStoNED** package is to support this development.

While we have phrased this review and the **pyStoNED** modules in terms of the cost and production function, most of the modules are readily applicable to nonparametric regression analysis in any other context as well. We hope that the convex regression and related techniques could also prove useful in other application areas where shape constraints play an essential role. For example, optimization behavior also implies specific convexity constraints in the context of consumer demand analysis (see, e.g., Afriat, 1967; Varian, 1982).

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A. List of Acronyms

COLS : Corrected Ordinary Least Squares

C²NLS : Corrected Convex Nonparametric Least Squares

CER : Convex Expectile Regression

CNLS : Convex Nonparametric Least Squares

CNLS-G : Convex Nonparametric Least Squares Generic Algorithm

CQR : Convex Quantile Regression
CRS : Constant Returns to Scale
DDF : Directional Distance Function
DEA : Data Envelopment Analysis

DMU : Decision-Making UnitFDH : Free Disposal HullMOM : Method of Moments

QLE : Quasi-likelihood Estimation

ICNLS : Isotonic Convex Nonparametric Least Square

ICER : Isotonic Convex Quantile Regression ICQR : Isotonic Convex Expectile Regression

SFA : Stochastic Frontier Analysis

StoNED : Stochastic Nonparametric Envelopment of Data

StoNEZD: Stochastic Semi-nonparametric Envelopment of Z Variables Data

KDE : Kernel Density EstimationVRS : Variable Returns to Scale

B. Estimated CNLS residuals: an additive VRS model (GAMS)

```
160 VARIABLE e.L
                             error terms
1
     -2.802,
                  2
                         1.414,
                                     3
                                         -22.224
                                                           -350.911,
                                                                          5
                                                                              -13.700
6
    101.015,
                  7
                       -28.872,
                                     8
                                         -14.040,
                                                       9
                                                             -0.847,
                                                                          10
                                                                               56.894
                                         -20.230,
                                                            -70.008,
11
    285.507,
                  12
                       679.384,
                                     13
                                                       14
                                                                          15
                                                                                10.507
16
     74.597,
                  17
                        -6.539,
                                     18
                                         -30.076,
                                                       19
                                                            -40.135,
                                                                          20
                                                                              -27.778
                                     23
                                                             23.951,
21
     48.760,
                  22
                        87.008,
                                          22.481,
                                                       24
                                                                          25
                                                                               -2.142
26
    -22.837,
                  27
                       -37.861,
                                     28 -351.071,
                                                       29
                                                             66.858,
                                                                          30
                                                                              -21.703
31
     -8.951,
                  32
                       216.006,
                                          37.597,
                                                       34
                                                            -31.811,
                                                                          35
                                                                              -23.785
                                     33
36
                                                                          40
  -201.341,
                  37
                       -69.290,
                                            6.269,
                                                       39
                                                              3.756,
                                                                              -74.607
                                     38
41
     -1.975,
                  42
                       -11.971,
                                     43 -236.746,
                                                       44
                                                              6.575,
                                                                          45
                                                                               11.657
46
    -20.004,
                  47
                       -67.215,
                                     48
                                          -5.239,
                                                       49
                                                            -55.947,
                                                                          50
                                                                              265.514
                       -17.651,
                                                       54
                                                             38.854,
51
       1.924,
                  52
                                     53
                                           4.656,
                                                                          55
                                                                                -2.903
                                                       59
                                                             28.393,
56
    349.528,
                  57
                       163.991,
                                     58
                                          35.001,
                                                                          60
                                                                              -99.132
61
     32.789,
                  62 -604.040,
                                     63
                                         197.101,
                                                       64
                                                             21.411,
                                                                          65
                                                                              -26.755
66
    -15.130,
                  67
                        29.384,
                                     68
                                        -128.271,
                                                       69
                                                            -16.445,
                                                                          70
                                                                              -13.386
71 -293.862,
                                                             -9.804,
                  72
                        -2.551,
                                     73
                                         476.620,
                                                       74
                                                                          75
                                                                               32.090
76
    -17.241,
                  77
                       114.768,
                                     78
                                           -3.852,
                                                       79
                                                             35.396,
                                                                          80
                                                                              -62.937
81
      8.919,
                  82
                       349.397,
                                     83
                                         -80.700,
                                                       84
                                                          -604.758,
                                                                          85
                                                                              -59.840
                                          -6.061,
                                                             -0.885
86
      6.718,
                  87
                         6.174,
                                     88
                                                       89
```

C. Estimated CNLS residuals: an additive VRS model (pyStoNED)

```
epsilon : residual
   Size=89, Index=I
                                      : Upper : Fixed : Stale : Domain
   Key: Lower: Value
          None : -2.8024040090178914 :
                                         None : False : False :
                                                                 Reals
                                         None : False : False :
                   1.4140528128759229 :
                                                                 Reals
     2:
          None: -22.223744892648355:
                                         None : False : False
                                                                 Reals
     3
          None
                     -350.91097508901 :
                                         None : False : False
                                                                 Reals
     4:
           None: -13.699899937048826:
                                         None : False : False :
                                                                 Reals
     5
          None :
                   101.01484316190096 :
                                         None : False : False :
                                                                 Reals
           None: -28.872348336757398:
                                         None : False : False :
                                                                 Reals
     7 :
                                         None : False : False :
          None : -14.039749134653078 :
                                                                 Reals
     8
          None: -0.8474521090027167:
                                         None : False : False :
                                                                 Reals
     9:
                                         None : False : False :
          None:
                    56.89430545783776 :
                                                                 Reals
     10:
          None:
                    285.5068982735597 :
                                         None : False : False :
                                                                 Reals
     11:
          None:
                    679.3838738157001 :
                                         None : False : False :
                                                                 Reals
     12:
          None : -20.230026149875016 :
                                         None : False : False :
                                                                 Reals
     13:
                   -70.00793999792549 :
                                         None : False : False
          None :
                                                                 Reals
     14:
          None:
                   10.506530291158015 :
                                         None : False : False :
                                                                 Reals
                    74.59733583012911:
                                         None : False : False :
     15:
          None:
                                                                 Reals
     16:
           None:
                   -6.538916384385139 :
                                         None : False : False
                                                                 Reals
     17:
                                         None : False : False :
          None: -30.076412673918952:
                                                                 Reals
     18:
                   -40.13473761433872 :
                                         None : False : False :
          None :
                                                                 Reals
          None : -27.777867439090812 :
     19:
                                         None : False : False :
                                                                 Reals
                                         None : False : False :
     20:
          None:
                    48.75945800794108:
                                                                 Reals
     21:
           None:
                    87.00800578768963:
                                         None : False : False
                                                                 Reals
    22:
          None:
                   22.480756177157602 :
                                         None : False : False :
                                                                 Reals
    23:
          None:
                     23.9507283965699 :
                                         None : False : False :
                                                                 Reals
                                         None : False : False :
    24:
          None : -2.1416654007527427 :
                                                                 Reals
    25 :
          None: -22.836604777669237:
                                         None : False : False :
                                                                 Reals
     26:
          None: -37.861048214358334:
                                         None: False: False
                                                                 Reals
    27
          None :
                   -351.0709400239564 :
                                         None : False : False :
                                                                 Reals
          None :
                                         None : False : False :
    28:
                     66.8575905653208 :
                                                                 Reals
    29:
          None: -21.702814864843447:
                                         None : False : False :
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```

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