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# 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 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 a powerful, reliable, and fully open-access computational package have 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 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 estimating 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](#page-33-0) [\(1954\)](#page-33-0), [Brunk](#page-32-0) [\(1955\)](#page-32-0), and [Grenan](#page-33-1)[der](#page-33-1) [\(1956\)](#page-33-1) 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](#page-34-0) [\(2008\)](#page-34-0), convex regression has attracted growing interest in econometrics, statistics, operations research, machine learning, and related fields (e.g., [Magnani and Boyd](#page-35-0) [2009;](#page-35-0) [Seijo and Sen](#page-35-1) [2011;](#page-35-1) [Lim and Glynn](#page-35-2) [2012;](#page-35-2) [Hannah and Dunson](#page-33-2) [2013;](#page-33-2) [Mazumder, Choud](#page-35-3)[hury, Iyengar, and Sen](#page-35-3) [2019;](#page-35-3) [Bertsimas and Mundru](#page-32-1) [2021\)](#page-32-1). The recent study by [Yagi, Chen,](#page-36-0) [Johnson, and Kuosmanen](#page-36-0) [\(2020\)](#page-36-0) 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 applications where the duality theory of production and consumption directly implies certain monotonicity and convexity/concavity properties for many functions of interest (e.g., [Afriat](#page-31-0) [1967,](#page-31-0) [1972;](#page-31-1) [Varian](#page-36-1) [1982,](#page-36-1) [1984\)](#page-36-2). For example, the cost function of a 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 over the entire domain 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 have increasingly been 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](#page-34-1) [2015;](#page-34-1) [Johnson and Kuosmanen](#page-34-2) [2015\)](#page-34-2). Traditionally, this field was divided into two competing paradigms: Data envelopment analysis (DEA; [Charnes, Cooper, and Rhodes](#page-32-2) [1978\)](#page-32-2) and stochastic frontier analysis (SFA; [Aigner,](#page-32-3) [Lovell, and Schmidt](#page-32-3) [1977;](#page-32-3) [Meeusen, Van, and Broeck](#page-35-4) [1977\)](#page-35-4). 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](#page-34-3) [2006;](#page-34-3) [Kuosmanen and Kortelainen](#page-34-4) [2012\)](#page-34-4) was proposed as a unified framework that combines the 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](#page-34-0) [\(2008\)](#page-34-0) is a quadratic programming (QP) problem, whereas the multiplicative logarithmic formulation first considered by [Kuosmanen and Kortelainen](#page-34-4) [\(2012\)](#page-34-4) 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](#page-33-3) [2013\)](#page-33-3) or MATLAB [\(The](#page-35-5) [Mathworks, Inc.](#page-35-5) [2021\)](#page-35-5). [Johnson and Kuosmanen](#page-34-2) [\(2015\)](#page-34-2) present detailed examples of how to calculate the basic CNLS and StoNED models in MATLAB and GAMS. Recently, the R ([R](#page-35-6) [Core Team](#page-35-6) [2024\)](#page-35-6) package Benchmarking [\(Bogetoft and Otto](#page-32-4) [2010\)](#page-32-4) provides a new function StoNED() to estimate CNLS/StoNED but limited to the additive CNLS QP formulation. Similarly, while CVXPY [\(Diamond and Boyd](#page-33-4) [2016\)](#page-33-4) and CVXOPT [\(Andersen, Dahl, and](#page-32-5) [Vandenberghe](#page-32-5) [2023\)](#page-32-5) can be applied to solve CNLS, they are also restricted to the additive model only.

<span id="page-2-0"></span>

Model	pyStoNED	GAMS MATLAB	<b>Benchmarking</b>
Convex regression			
<b>Additive CNLS</b>			
Multiplicative CNLS			
Corrected CNLS			
CQR/CER			
CNLS with z variables			
$CQR/CER$ with z variables			
CNLS with multiple outputs			
$CQR/CER$ with multiple outputs			
Isotonic CNLS			
Isotonic CQR/CER			
CNLS-G algorithm for CNLS			
$CNLS-G$ algorithm for $CQR/CER$			
Frontier estimation			
StoNED with method of moments			
StoNED with quasi-likelihood			
StoNED with kernel deconvolution			
Plotting			
One-input and one-output			
Two-input and one-output			

Table 1: Functionality comparison of different software packages.

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. To lower the barrier for applied researchers and practitioners to apply more advanced techniques that help to relax unnecessarily restrictive assumptions, the **pyStoNED** package for Python [\(Van](#page-35-7) [Rossum](#page-35-7) *et al.* [2021\)](#page-35-7) was first introduced in April 2020 to prove a freely available and userfriendly tool for the multivariate CNLS and StoNED methods.

The pyStoNED package not only translates existing codes or tools to Python, but also provides many functionalities and modules that are not available in any other package or published code (see Table [1\)](#page-2-0). Its latest edition also includes modules for convex quantile regression (CQR), convex expectile regression (CER), isotonic regression, penalized convex regression, and graphical illustration. It also facilitates efficiency measurement using the conventional DEA and free disposable hull (FDH) approaches. **pyStoNED** allows users 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 on the GitHub repository <https://github.com/ds2010/pyStoNED>.

This paper presents a tutorial of the **pyStoNED** package, briefly reviews the alternative models supported, and illustrates 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 in pyStoNED are directly applicable for semi/nonparametric regression analysis in any other contexts as well (see, e.g., traffic flow modeling by [Kriuchkov and Kuosmanen](#page-34-5) [2023\)](#page-34-5). 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 continuously.

The rest of this paper is organized as follows. Section [2](#page-3-0) describes the basic setups of the pyStoNED package, and Section [3](#page-5-0) introduces the structures of example data and the attributes of different models. Section [4](#page-8-0) describes the first step of the StoNED model (e.g., CNLS estimation) 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](#page-21-0) demonstrates the rest of the steps of the StoNED model and related codes. Section [6](#page-26-0) illustrates how to implement the CNLS-G algorithm to calculate the CNLS estimator in pyStoNED. The plot of the estimated function can be found in Section [7.](#page-28-0) Section [8](#page-30-0) concludes this paper. The list of acronyms is presented in Appendix [A.](#page-37-0) Appendices [B,](#page-37-1) [C](#page-39-0) and [D](#page-40-0) present a comparison of residuals for the same additive CNLS model solved by pyStoNED, GAMS and R/Benchmarking, respectively. Appendix [E](#page-41-0) briefly describes the variables included in the four internal datasets.

# **2. Setup**

#### <span id="page-3-0"></span>**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/](https://pypi.org/project/pystoned) [pystoned](https://pypi.org/project/pystoned). The package can be installed either from PyPI or from GitHub using:[1](#page-3-1)

```
1. pip install pystoned
```
2. pip install -U git+https://github.com/ds2010/pyStoNED

The **pyStoNED** package is built based on a few existing dependencies. It is worth highlighting that Pyomo [\(Bynum](#page-32-6) *et al.* [2021\)](#page-32-6) 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** [\(Harris](#page-33-5) *et al.*) [2020\)](#page-33-5) and pandas [\(McKinney](#page-35-8) [2010\)](#page-35-8) are used to import input-output data, manage data, and export the estimation results.  $\textbf{SciPy}$  [\(Virtanen](#page-36-3) *et al.* [2020\)](#page-36-3) provides the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm to optimize the quasi-likelihood function. Matplotlib [\(Hunter](#page-33-6) [2007\)](#page-33-6) is associated with the graphical illustration of the estimated functions.

### **2.2. Solvers**

All models supported by **pyStoNED** are either additive or multiplicative models, depending on the specification of the error term. From the optimization perspective, the additive models are usually stated as QP problems except for the CQR model, which is a linear programming (LP) problem, whereas all multiplicative models are NLP problems.

<span id="page-3-1"></span><sup>1</sup>Python *for Non-Programmers* is recommended for beginners to learn and set up their Python environment, <https://wiki.python.org/moin/BeginnersGuide/NonProgrammers>.

To solve the relevant QP or NLP problems, external off-the-shelf solvers are required. In our experience, CPLEX (CPLEX[, IBM ILOG](#page-32-7) [2009\)](#page-32-7) and MOSEK ([MOSEK](#page-35-9) ApS [2021\)](#page-35-9) provide reliable and convenient platforms for solving the QP and LP problems in the present context. The NLP problem can be efficiently solved by MINOS [\(Murtagh and Saunders](#page-35-10) [2003\)](#page-35-10) or KNITRO [\(Byrd, Nocedal, and Waltz](#page-32-8) [2006\)](#page-32-8). With the help of Pyomo, all models supported by pyStoNED are computable by these off-the-shelf solvers.

#### *Remote solver*

pyStoNED interfaces with Pyomo to access the network-enabled optimization system (NEOS) server that freely provides a large number of academic solvers for solving the additive or mul-tiplicative models remotely.<sup>[2](#page-4-0)</sup> In this case, there is no need to install solvers and corresponding licenses on local machines. Here we have a model estimated by the remote solver

```
>>> model.optimize(email = "email@address")
```
Replace the argument email@address with your email address.<sup>[3](#page-4-1)</sup> By default, the additive and multiplicative models will be solved by MOSEK and KNITRO, respectively. In addition, the users can check all the available solvers provided in NEOS via get remote solvers() and then select their preferred solver  $(e.g., \text{ solver} = "minos").$ 

```
>>> from pystoned.utils.tools import get_remote_solvers
>>> print(get_remote_solvers())
```

```
['minto', 'couenne', 'lgo', 'minos', 'filmint', 'cbc', 'sbb', 'ipopt',
'bonmin', 'lancelot', 'ooqp', 'knitro', 'miles', 'snopt', 'loqo',
'path', 'dicopt', 'l-bfgs-b', 'baron', 'cplex', 'raposa', 'pathnlp',
'octeract', 'scip', 'conopt', 'filter', 'nlpec', 'xpress', 'mosek',
 'minlp', 'gams-ampl', 'lindoglobal', 'alphaecp']
```

```
>>> model.optimize(email = "email@address", solver = 'minos')
```
The value of the option in solver could be any possible solver, which depends on the specific optimization problem and its availability. That is, there are a lot of different choices (see Table [2](#page-5-1) for the commonly used setting), but the performance of solvers varies depending on the application.

#### *Local solver*

Pyomo also provides an application programming interface for pyStoNED to import the local solvers. In the **pyStoNED** package, **MOSEK** is attached as the internal dependency to solve the additive model. Note that the academic license for **MOSEK** is required to be installed; see The tutorial of **MOSEK** license installation is available at more tutorial on this installation.<sup>[4](#page-4-2)</sup> After that, we can use the following command to calculate the additive models.

<span id="page-4-1"></span><span id="page-4-0"></span><sup>&</sup>lt;sup>2</sup>NEOS server: State-of-the-art solvers for numerical optimization, <https://neos-server.org/neos>.

<sup>3</sup>As of January 2021, the NOES server requires a valid email address in all submissions; see NEOS Server FAQ <https://neos-guide.org/content/FAQ#email>.

<span id="page-4-2"></span> $^4$ <https://pystoned.readthedocs.io/en/latest/install/index.html#solver>.

<span id="page-5-1"></span>



#### >>> model.optimize(OPT\_LOCAL)

The parameter OPT LOCAL is added in the function  $\text{optimize}(\ldots)$  to indicate that the model is computed locally. By default, the additive model is solved by **MOSEK**. Furthermore, we can check if other solvers are preinstalled in the local environment. For example, in the following case, CPLEX has been installed on the machine using an academic license, and therefore, we can utilize it to solve the additive model.

```
>>> from pystoned.utils.tools import check_local_solver
>>> print(check_local_solver("cplex"))
```
True

```
>>> model.optimize(OPT_LOCAL, solver = 'cplex')
```
Overall, the remote solver through the NEOS server is highly recommended for all light computing jobs with no more than 500 observations. The local solver for calculating the multiplicative model will be supported in **pyStoNED** when a license for an appropriate NLP solver is available.

## **3. Data structures and dataset**

#### <span id="page-5-0"></span>**3.1. Data structures**

Data pre-processing is the first step to using 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  $x_i$  and output variables  $y_i$ for observed decision making unit (DMU)  $i = 1, 2, \ldots, n$ . For a model considering operational conditions and practices, contextual variables  $z_i$  can be used. The directional distance function (DDF) based models handle the multi-dimensional inputs and outputs with given directional vectors  $g^x$  and  $g^y$ , respectively. The DDF based models also consider undesired outputs  $b_i$  and its directional vector  $g^b$ . Table [3](#page-6-0) summarizes the data structures used in all the CNLS/StoNED models.

#### **3.2. Internal data**

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

<span id="page-6-0"></span>

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

Table 3: Data structures.

1. Finnish electricity distribution firms (load\_Finnish\_electricity\_firm).

The data of Finnish electricity distribution firms are collected from [Kuosmanen](#page-34-6) [\(2012\)](#page-34-6) and [Kuosmanen, Saastamoinen, and Sipiläinen](#page-34-7) [\(2013\)](#page-34-7). The data consist of seven variables: Three different expenditures are used as inputs (i.e., OPEX, CAPEX, and TO-TEX);[5](#page-6-1) Energy, Length, and Customers are considered as outputs; Further, PerUndGr is denoted as the contextual variable. Table [5](#page-41-1) presents the description of this dataset.

2. GHG abatement cost of OECD countries (load\_GHG\_abatement\_cost).

The data on the greenhouse gas (GHG) abatement cost of OECD countries are provided by [Kuosmanen, Zhou, and Dai](#page-35-11) [\(2020\)](#page-35-11). The data contain two input variables (i.e., CPNK and HRSN), one good output variable (i.e., VALK), and one undesirable output variable  $(i.e., GHG)$  (see Table [6\)](#page-41-2).

3. Data provided with Tim Coelli's Frontier 4.1 (load\_Tim\_Coelli\_frontier).

The classic 60-firm dataset attached in Frontier 4.1 [\(Coelli](#page-32-9) [1996\)](#page-32-9) includes two input variables (i.e., capital and labour) and one output variable (i.e., output) (see Table [7\)](#page-41-3).

4. Rice Production in the Philippines (load\_Philipines\_rice\_production).

The Rice Production in the Philippines dataset collected from [Coelli, Rao, O'Donnell,](#page-32-10) [and Battese](#page-32-10) [\(2005\)](#page-32-10) consists of 17 different variables. The different variables can be organized into diversified combinations for target models (see Table [8\)](#page-42-0).

These datasets can be imported through the module dataset of pyStoNED. The variables in Tables [5–](#page-41-1)[8](#page-42-0) are used as parameters of dataset to upload the input data. The following example demonstrates how to upload the input-output data of the Finnish electricity distribution firms dataset. We first import the dataset module using the function load\_Finnish\_electricity\_firm (Line 1) and define the  $x$  and  $y$  according to the imported dataset (Line 2).<sup>[6](#page-6-2)</sup> We then check the input and output data using the function print().

<span id="page-6-1"></span> $5$ Note that TOTEX = OPEX + CAPEX. It is possible to use TOTEX as an aggregate input or model OPEX and CAPEX as two separate input variables.

<span id="page-6-2"></span><sup>&</sup>lt;sup>6</sup>In addition to the presented example, we can download other datasets using the corresponding dataset module, e.g., downloading the GHG data: from pystoned.dataset import load\_GHG\_abatement\_cost.

```
>>> from pystoned.dataset import load Finnish_electricity_firm
>>> data = load Finnish electricity firm(x select = ['Energy', 'Length',
... 'Customers'], y_select = ['TOTEX'], z_select = ['PerUndGr'])
>>> print(data.x)
[[ 75 878 4933]
      ...
 [ 105 575 9084]]
>>> print(data.y)
[[ 1612]
    ...
 [ 1776]]
>>> print(data.z)
[[][][][][][][][][][][][][][][][][][][][][][][][][][][][][][][][][][][][][...
 [0.59]]
```
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. 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 Line 2 should be

```
>>> data = load_Finnish_electricity_firm(x_select = ['Energy', 'Customers'],
\ldots y_select = ['TOTEX'])
```
#### **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 [4](#page-8-1) is the input-output data stored in an Excel file (e.g., table1.xlsx), the following code utilizes pandas to read the dataset from table1.xlsx and organize the data with NumPy. Input *x* is a matrix, and output *y* is an array.

In the following example, we first import the packages NumPy and pandas in Lines 1 and 2. Line 3 is used to read the table.xlsx file from the local disk, and the rest of the lines define the input and output variables. See more examples in Section [6.](#page-26-0)

```
>>> import numpy as np
>>> import pandas as pd
>>> df = pd.read_excel("table1.xlsx")
\Rightarrow \Rightarrow y = df['output']
```

id		$output$ input $1$ input $2$	
	120	10	55
'2	80	30	49
100	90	25	72

Table 4: An example of user's own dataset.

```
\gg \times 1 = df['input1']>>> x1 = np.asmatrix(x1) . T\Rightarrow x2 = df['input2']>>> x2 = np.asmatrix(x2).T>>> x = np.\text{concatenate}((x1, x2), axis = 1)\gg print(y)
0 120
...
99 90
\gg print(x)
[[ 10 55]
...
[ 25 72]]
```
#### **4. Shape-constrained nonparametric regression**

<span id="page-8-0"></span>In this section, we review the commonly seen shape-constrained nonparametric regression models supported by **pyStoNED** and then illustrate how they can be solved and implemented in the developed package.[7](#page-8-2)

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

<span id="page-8-3"></span>
$$
y_i = f(\boldsymbol{x}_i) + \varepsilon_i \tag{1}
$$

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  $\boldsymbol{x}_i = (x_{i1}, x_{i2}, \dots, x_{im})'$  denotes the input vector of unit *i*. 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](#page-34-8) [2010](#page-34-8) for a review). In this paper, we assume certain axiomatic properties (e.g., monotonicity, concavity) instead of

<span id="page-8-2"></span><sup>&</sup>lt;sup>7</sup>In addition, **pyStoNED** can also be used to solve other deterministic frontier models (e.g., DEA and FDH). See more DEA and FDH tutorials at <https://pystoned.readthedocs.io/>.

prespecified functional form for the function *f* and apply the following nonparametric methods to estimate the function *f*.

#### **4.1. Convex nonparametric least squares**

### *Additive CNLS model*

[Hildreth](#page-33-0) [\(1954\)](#page-33-0) was the first to consider the nonparametric regression subject to monotonicity and concavity constraints in the case of a single input variable *x*. [Afriat](#page-31-1) [\(1972\)](#page-31-1) also proposes methods to impose convexity on estimating a production function. [Kuosmanen](#page-34-0) [\(2008\)](#page-34-0) extends Hildreth's approach to the multivariate setting with the multidimensional inputs *x*, and refers to it as the CNLS. CNLS builds upon the assumption that the production function *f* belongs to a family of continuous, monotonic increasing, and globally concave (convex) functions, imposing the same production axioms as standard DEA (see further discussion in [Kuosmanen](#page-34-8) [and Johnson](#page-34-8) [2010\)](#page-34-8). The two additive multivariate CNLS formulations are defined as

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

<span id="page-9-0"></span>
$$
\min_{\alpha,\beta,\varepsilon} \sum_{i=1}^{n} \varepsilon_i^2
$$
\n
$$
s.t. \quad y_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' \mathbf{x}_i \le \alpha_j + \beta_j' \mathbf{x}_i \quad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\beta_i \ge 0 \qquad \forall i
$$
\n(2)

• Cost function (i.e., regression function *f* is convex and increasing).

<span id="page-9-1"></span>
$$
\min_{\alpha,\beta,\varepsilon} \sum_{i=1}^{n} \varepsilon_i^2
$$
\n
$$
s.t. \quad y_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' \mathbf{x}_i \ge \alpha_j + \beta_j' \mathbf{x}_i \quad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\beta_i \ge 0 \qquad \forall i
$$
\n(3)

where  $\alpha_i$  and  $\beta_i$  define the intercept and slope parameters of tangent hyperplanes that characterize the estimated piecewise linear frontier, respectively. The first constraint can be interpreted as a multivariate regression equation, the second constraint imposes convexity (concavity), and the third constraint imposes monotonicity. Problems [\(2\)](#page-9-0) and [\(3\)](#page-9-1) allow for variable returns to scale (VRS), and other specifications of returns to scale can be imposed by an additional constraint on the intercept term  $\alpha_i$ . If  $\alpha_i = 0$ , problems [\(2\)](#page-9-0) and [\(3\)](#page-9-1) impose constant returns to scale (CRS). Note that both [\(2\)](#page-9-0) and [\(3\)](#page-9-1) are QP problems and hence can be solved by MOSEK or CPLEX.

The basic additive CNLS model can be estimated by **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 estimated coefficients (e.g.,  $\hat{\alpha}_i$ ) can be displayed on the screen directly using .display alpha() or stored in the memory using .get\_alpha().

We first present an example to solve the VRS production model.

```
>>> 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'],
\ldots y_select = ['Energy'])
>>> model = CNLS(y = data.y, x = data.x, z = None,\ldots cet = CET_ADDI, fun = FUN_PROD, rts = RTS_VRS)
>>> model.optimize(OPT_LOCAL)
>>> 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 : in the state : Upper : Fixed : Stale : Domain
   0 : None : -22.93587954013432 : None : False : False : Reals
    ...
   88 : None : -22.8603341852995 : None : False : False : Reals
beta : beta
  Size=178, Index=beta_index
  Key : Lower : Value : 1999 : Upper : Fixed : Stale : Domain
   (0, 0) : 0.0 : 0.13585804486689262: None : False : False : Reals
   ...
  (88, 1) : 0.0 : 0.011417186366215866: None : False : False : Reals
epsilon : residual
  Size=89, Index=I
  Key : Lower : Value : 000 : Upper : Fixed : Stale : Domain
   0 : None : -2.802404436894662 : None : False : False : Reals
    ...
   88 : None : -0.8851559509243998 : 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 MOSEK solver. Lines 7–9 directly display the estimated coefficients (i.e.,  $\hat{\alpha}_i$ ,  $\hat{\beta}_i$ , and  $\hat{\varepsilon}_i$ ) on screen, and Lines 10–12 store the estimates in memory with a special variable name (e.g., alpha). See the online supplementary zip file for all the replicated scripts and results.

Appendix [B](#page-37-1) presents the full estimated CNLS residuals that are equivalent to those in GAMS (cf. Appendix [C\)](#page-39-0). Note that the estimated alpha and beta coefficients in pyStoNED may be slightly different from those in GAMS because the optimal solution is generally not unique in terms of those coefficients, and hence there exist alternate optima [\(Kuosmanen](#page-34-0) [2008;](#page-34-0) [Dai](#page-32-11)  $2021$ .<sup>[8](#page-11-0)</sup> The estimated residuals by **Benchmarking** are reported in Appendix [D.](#page-40-0) The scatter plot in Figure [3](#page-40-1) shows that the estimated residuals by pyStoNED and Benchmarking are similar, but not exactly the same. Further, the sum of squared residuals of **Benchmarking** is 0.17% higher than that of pyStoNED and GAMS, suggesting that Benchmarking fails to converge to the global optimum.

#### *Multiplicative CNLS model*

The Cobb-Douglas and translog functions are commonly used functional forms for the function *f*, where the error term  $\varepsilon$  affects output *y* in a multiplicative fashion. Thus, we next consider a multiplicative specification in the present nonparametric setting. Under the multiplicative error structure, model [\(1\)](#page-8-3) is rephrased as

<span id="page-11-2"></span><span id="page-11-1"></span>
$$
y_i = f(\boldsymbol{x}_i) \exp\left(\varepsilon_i\right) \tag{4}
$$

Applying the log-transformation to [\(4\)](#page-11-1), we have

<span id="page-11-3"></span>
$$
\ln y_i = \ln f(\boldsymbol{x}_i) + \varepsilon_i \tag{5}
$$

To estimate [\(5\)](#page-11-2), we reformulate the additive production model [\(2\)](#page-9-0) and obtain the following log-transformed CNLS formulation.

$$
\min_{\alpha,\beta,\phi,\varepsilon} \sum_{i=1}^{n} \varepsilon_i^2
$$
\n*s.t.* 
$$
\ln y_i = \ln(\phi_i + 1) + \varepsilon_i \quad \forall i
$$
\n
$$
\phi_i = \alpha_i + \beta_i' \mathbf{x}_i - 1 \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' \mathbf{x}_i \le \alpha_j + \beta_j' \mathbf{x}_i \quad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\beta_i \ge 0 \qquad \forall i
$$
\n(6)

where  $\phi_i + 1$  is the CNLS estimator of  $\mathsf{E}[y_i \mid \mathbf{x}_i]$ . The value of one is added here to ensure 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(·)). The rest of the constraints are the same as those of the additive models. The use of  $\phi_i$ 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

<span id="page-11-0"></span><sup>&</sup>lt;sup>8</sup>The additive CNLS model can also be solved using other convex optimization tools such as **CVXPY** or CVXOPT. To apply these tools, a user must create QP matrices manually and then plug them into an off-theshelf solver. For the interesting readers, see an additional example where the additive CNLS model is solved by CVXOPT, <https://github.com/ds2010/CNLS-Python>.

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  $(6)$  includes nonlinear constraints, we need to use NLP solvers such as MINOS and KNITRO.

We next demonstrate the estimation of multiplicative cost function under VRS and CRS. Let the type of model cet parameter be CET\_MULT (multiplicative model). Note that the following NLP models are remotely solved by KNITRO 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',
\ldots 'Customers'], y select = ['TOTEX'])
>>> model1 = CNLS(CWLS(y = data.y, x = data.x, z = None,\ldots cet = CET_MULT, fun = FUN_COST, rts = RTS_VRS)
>>> model1.optimize('email@address')
>>> model2 = CNLS(CWLS(y = data.y, x = data.x, z = None,... cet = CET MULT, fun = FUN COST, rts = RTSCRS)>>> model2.optimize('email@address')
>>> model1.display_residual()
>>> model2.display_residual()
```
#### **4.2. Convex quantile and expectile regression**

Quantile regression estimates the conditional median or other quantiles of the response variable [\(Koenker and Bassett](#page-34-9) [1978;](#page-34-9) [Koenker](#page-34-10) [2005\)](#page-34-10), whereas the CNLS estimator focuses on the conditional mean  $E[y_i | x_i]$ . In this section, we extend CNLS to CQR [\(Wang, Wang, Dang,](#page-36-4) [and Ge](#page-36-4) [2014\)](#page-36-4) and CER [\(Kuosmanen](#page-34-1) *et al.* [2015\)](#page-34-1), see [Kuosmanen and Zhou](#page-35-12) [2021](#page-35-12) and [Dai,](#page-32-12) [Kuosmanen, and Zhou](#page-32-12) [2023a](#page-32-12) for further elaboration of both CQR and CER. Note that both quantile and expectile estimators are generally more robust to outliers and heteroscedasticity than the conditional mean.

#### *Convex quantile regression*

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

<span id="page-12-0"></span>
$$
\min_{\alpha,\beta,\varepsilon^+, \varepsilon^-} \tau \sum_{i=1}^n \varepsilon_i^+ + (1 - \tau) \sum_{i=1}^n \varepsilon_i^-
$$
\n
$$
s.t. \quad y_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i^+ - \varepsilon_i^- \quad \forall i
$$
\n
$$
\alpha_i + \beta_i' \mathbf{x}_i \le \alpha_j + \beta_j' \mathbf{x}_i \qquad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\beta_i \ge \mathbf{0} \qquad \forall i
$$
\n
$$
\varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0 \qquad \forall i
$$
\n(7)

where the quantile  $\tau$  splits the observations  $100 \cdot \tau\%$  above and  $100 \cdot (1 - \tau)\%$  below, and  $\varepsilon_i^+$  and  $\varepsilon_i^-$  denote the two non-negative components. The objective function in [\(7\)](#page-12-0) 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 [\(2\)](#page-9-0). See [Dai](#page-32-11) [\(2021\)](#page-32-11), Dai *[et al.](#page-32-12)* [\(2023a\)](#page-32-12), and [Dai, Kuosmanen, and Zhou](#page-33-7) [\(2023b\)](#page-33-7) for more recent developments on CQR models.

#### *Convex expectile regression*

Convex quantile regression [\(7\)](#page-12-0) may suffer from non-uniqueness due to that problem [\(7\)](#page-12-0) is an LP problem [\(Kuosmanen](#page-34-1) *et al.* [2015\)](#page-34-1). To address this problem, [Kuosmanen](#page-34-1) *et al.* [\(2015\)](#page-34-1) propose a CER approach, where a quadratic objective function is used to ensure unique estimates of the quantile functions. Consider the following QP problem

<span id="page-13-0"></span>
$$
\min_{\alpha,\beta,\varepsilon^+, \varepsilon^-} \tilde{\tau} \sum_{i=1}^n (\varepsilon_i^+)^2 + (1 - \tilde{\tau}) \sum_{i=1}^n (\varepsilon_i^-)^2
$$
\n
$$
s.t. \quad y_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i^+ - \varepsilon_i^- \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' \mathbf{x}_i \le \alpha_j + \beta_j' \mathbf{x}_i \qquad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\beta_i \ge 0 \qquad \forall i
$$
\n
$$
\varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0 \qquad \forall i
$$
\n(8)

where the expectile  $\tilde{\tau} \in (0,1)$  is not the same as the quantile  $\tau$ , but it can be converted from/to the quantile *τ* (Dai *[et al.](#page-32-12)* [2023a\)](#page-32-12). See [Dai, Zhou, and Kuosmanen](#page-33-8) [\(2020\)](#page-33-8), [Kuosmanen](#page-35-11) *et al.* [\(2020\)](#page-35-11), and [Kuosmanen and Zhou](#page-35-12) [\(2021\)](#page-35-12) for the empirical applications of CER.

The alternative module CQER includes the function  $CQR(y, x, \ldots)$  that is designed to solve the CQR problem and the function  $CER(y, x, \ldots)$  to solve the CER problem. Therefore, we use the CQER.CQR() and CQER.CER() to define the CQR problem (see, e.g., Line 5 in the following example) and the CER problem, respectively. The other parameters' settings are similar to those in module CNLS(). To display the estimated  $\varepsilon_i^+$  and  $\varepsilon_i^-$ , the functions .display positive residual() and .display negative residual() are designed in the new module CQER. 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
>>> from pystoned import dataset as dataset
>>> data = dataset.load GHG abatement cost(x_select = ['HRSN', 'CPNK',
\ldots '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()
```
#### **4.3. Contextual variables**

A firm's productive performance to operate efficiently typically depends on operational conditions and practices, such as the production environment and firm-specific characteristics (i.e., technology selection and managerial practices). [Johnson and Kuosmanen](#page-33-9) [\(2011,](#page-33-9) [2012\)](#page-33-10) refer to both variables that characterize operational conditions and practices as contextual variables.

- Contextual variables are often, though not always, external factors that are beyond the control of firms.
	- **–** Examples: Competition, regulation, weather, location;
	- **–** Policymakers may influence the operating environment.
- Contextual variables can also be internal factors.
	- **–** Examples: Management practices, ownership;
	- **–** A better understanding of the internal factors can help the firm improve performance.

By introducing the contextual variables  $z_i = (z_{i1}, z_{i2}, \ldots, z_{ir})'$ , the multiplicative model [\(5\)](#page-11-2) is reformulated as a partial log-linear model to take the operational conditions and practices into account.

<span id="page-14-0"></span>
$$
\ln y_i = \ln f(\boldsymbol{x_i}) + \boldsymbol{\lambda}' \boldsymbol{z}_i + \varepsilon_i
$$

where parameter vector  $\lambda = (\lambda_1, \ldots, \lambda_r)$  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 section, we consider the multiplicative production model as our starting point.

#### *CNLS with z variables*

Following [Johnson and Kuosmanen](#page-33-9) [\(2011\)](#page-33-9), we incorporate the contextual variables in the multiplicative CNLS model and redefine it as follows

$$
\min_{\alpha,\beta,\lambda,\varepsilon} \sum_{i=1}^{n} \varepsilon_i^2
$$
\n
$$
s.t. \quad \ln y_i = \ln(\phi_i + 1) + \lambda' z_i + \varepsilon_i \quad \forall i
$$
\n
$$
\phi_i = \alpha_i + \beta_i' x_i - 1 \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' x_i \le \alpha_j + \beta_j' x_i \qquad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\beta_i \ge 0 \qquad \forall i
$$
\n(9)

Denote by  $\hat{\lambda}$  the coefficients of the contextual variables obtained as the optimal solution to the above nonlinear problem. [Johnson and Kuosmanen](#page-33-9) [\(2011\)](#page-33-9) 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 .display\_lamda() is used to display the marginal effect of contextual variables. In the following example, we estimate a log-transformed cost function model with *z* variable. Note that the model specification is assumed to be CRS in this example.

```
>>> from pystoned import CNLS
>>> 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 = CNLS(y = data.y, x = data.x, z = data.z,... cet = CET_MULT, fun = FUN_COST, rts = RTS_CRS)
>>> model.optimize('email@address')
>>> model.display_lamda()
```
#### *CER with z variables*

Following [Kuosmanen, Tan, and Dai](#page-35-13) [\(2023\)](#page-35-13), we can incorporate contextual variables in the multiplicative CER estimation. The reformulation of the CER model is

<span id="page-15-0"></span>
$$
\min_{\alpha,\beta,\lambda,\varepsilon^+,\varepsilon^-} \tilde{\tau} \sum_{i=1}^n (\varepsilon_i^+)^2 + (1-\tilde{\tau}) \sum_{i=1}^n (\varepsilon_i^-)^2
$$
\n
$$
s.t. \quad \ln y_i = \ln(\phi_i + 1) + \lambda' z_i + \varepsilon_i^+ - \varepsilon_i^- \quad \forall i
$$
\n
$$
\phi_i = \alpha_i + \beta_i' x_i - 1 \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' x_i \le \alpha_j + \beta_j' x_i \qquad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\beta_i \ge 0 \qquad \forall i
$$
\n
$$
\varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0 \qquad \forall i
$$
\n(10)

The following code is prepared to solve the CER model with z-variable. We now use the function CQER.CER(y, x, ...) to model CER with z-variable and assume expectile  $\tilde{\tau} = 0.5$ . 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,\ldots cet = CET_MULT, fun = FUN_COST, rts = RTS_CRS)
>>> model.optimize('email@address')
>>> model.display_lamda()
```
#### **4.4. Multiple outputs**

#### *CNLS with multiple outputs*

The convex regression approaches reviewed above have been presented within the single output, multiple input framework. This section describes the CNLS/CQR/CER approaches that use the directional distance function (DDF) to model multiple-input multiple-output data.

The DDF is a functional representation of the technology, defined as [\(Chambers, Chung, and](#page-32-13) [Färe](#page-32-13) [1996,](#page-32-13) [1998\)](#page-32-14)

$$
\vec{D}_T(\boldsymbol{x},\boldsymbol{y},\boldsymbol{g}^{\boldsymbol{x}},\boldsymbol{g}^{\boldsymbol{y}}) = \sup \{ \theta \mid (\boldsymbol{x} - \theta \boldsymbol{g}^{\boldsymbol{x}},\boldsymbol{y} + \theta \boldsymbol{g}^{\boldsymbol{y}}) \in T \},
$$

where  $(g^x, g^y)$  is a direction vector, and  $T = \{(x, y) \mid x \text{ can produce } y\}$  is the production possibility set. The DDF must always satisfy translation property and homogeneity of degree −1 in the direction vector, and it inherits the monotonicity and convexity properties of *T*.

In the stochastic setting, the data generating process satisfies the assumptions introduced by [Kuosmanen and Johnson](#page-34-11) [\(2017\)](#page-34-11), then the value of the DDF is equal to the random error term

<span id="page-16-0"></span>
$$
\vec{D}_T(\bm{x},\bm{y},\bm{g}^{\bm{x}},\bm{g}^{\bm{y}}) = \varepsilon_i, \forall i.
$$

To estimate DDF empirically, we solve the following QP problem

$$
\min_{\alpha,\beta,\gamma,\varepsilon} \sum_{i=1}^{n} \varepsilon_i^2
$$
\n
$$
s.t. \quad \gamma_i' y_i = \alpha_i + \beta_i' x_i - \varepsilon_i \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' x_i - \gamma_i' y_i \le \alpha_j + \beta_j' x_i - \gamma_j' y_i \quad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\gamma_i' g^y + \beta_i' g^x = 1 \qquad \forall i
$$
\n
$$
\beta_i \ge 0, \gamma_i \ge 0 \qquad \forall i
$$
\n(11)

In addition to the same notations as the CNLS estimator, we also introduce firm-specific coefficients  $\gamma_i$  that represent marginal effects of outputs to the DDF.

The first constraint defines the distance to the boundary of *T* as a linear function of inputs and outputs. The linear approximation is based on the supporting hyperplanes of *T* analogous to CNLS [\(2\)](#page-9-0). 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.

To perform the DDF models, pyStoNED includes the module CNLSDDF(), which also allows one to include undesirable outputs denoted by *b*. We present the CNLS-DDF models in the following two examples with and without undesirable outputs. To apply the module  $CNLSDDF(y,$  $x, \ldots$ , we have to pre-define the directional vector for the parameters  $gx, gb$  (None; default), and gy (see Line 5). The module 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()
```
When considering undesirable outputs  $b$ , CNLS-DDF  $(11)$  can be reformulated as

$$
\min_{\alpha,\beta,\gamma,\delta,\varepsilon} \sum_{i=1}^{n} \varepsilon_i^2
$$
\n
$$
s.t. \quad \gamma_i' \mathbf{y}_i - \delta_i' \mathbf{b}_i = \alpha_i + \beta_i' \mathbf{x}_i - \varepsilon_i \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' \mathbf{x}_i + \delta_i' \mathbf{b}_i - \gamma_i' \mathbf{y}_i \leq \alpha_j + \beta_j' \mathbf{x}_i + \delta_j' \mathbf{b}_i - \gamma_j' \mathbf{y}_i \quad \forall i, j, \text{ and } i \neq j
$$
\n
$$
\gamma_i' g^y + \beta_i' g^x + \delta_i' g^b = 1 \qquad \forall i
$$
\n
$$
\beta_i \geq \mathbf{0}, \gamma_i \geq \mathbf{0} \qquad \forall i
$$

where the coefficients  $\delta_i$  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(y, x, b, ...) (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()
```
#### *CQR and CER with multiple outputs*

Similar to CNLS with DDF, we present another two approaches integrating DDF to convex quantile/expectile regression by using the  $CQERDDF$  () module.<sup>[9](#page-17-0)</sup>

• CQR-DDF model.

$$
\min_{\alpha,\beta,\gamma,\varepsilon^+,\varepsilon^-} \tau \sum_{i=1}^n \varepsilon_i^+ + (1-\tau) \sum_{i=1}^n \varepsilon_i^-
$$
\n
$$
s.t. \quad \gamma_i' y_i = \alpha_i + \beta_i' x_i + \varepsilon_i^+ - \varepsilon_i^- \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' x_i - \gamma_i' y_i \le \alpha_j + \beta_j' x_i - \gamma_j' y_i \quad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\gamma_i' g^y + \beta_i' g^x = 1 \qquad \forall i
$$
\n
$$
\beta_i \ge \mathbf{0}, \gamma_i \ge \mathbf{0} \qquad \forall i
$$
\n
$$
\varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0 \qquad \forall i
$$

<span id="page-17-0"></span><sup>&</sup>lt;sup>9</sup>The undesirable outputs  $b$  can also be included, similar to the CNLSDDF() module, but are omitted here to keep the discussion and notations more concise.

• CER-DDF model.

$$
\min_{\alpha,\beta,\gamma,\varepsilon^+,\varepsilon^-} \tilde{\tau} \sum_{i=1}^n (\varepsilon_i^+)^2 + (1-\tilde{\tau}) \sum_{i=1}^n (\varepsilon_i^-)^2
$$
\n
$$
s.t. \quad \gamma_i' \mathbf{y}_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i^+ - \varepsilon_i^- \qquad \forall i
$$
\n
$$
\alpha_i + \beta_i' \mathbf{x}_i - \gamma_i' \mathbf{y}_i \le \alpha_j + \beta_j' \mathbf{x}_i - \gamma_j' \mathbf{y}_i \quad \forall i, j, \text{ and } i \ne j
$$
\n
$$
\gamma_i' g^y + \beta_i' g^x = 1 \qquad \forall i
$$
\n
$$
\beta_i \ge \mathbf{0}, \gamma_i \ge \mathbf{0} \qquad \forall i
$$
\n
$$
\varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0 \qquad \forall i
$$

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  $CQER.CQR()$ . CER(). For instance, the functions .display positive residual() and .display negative residual() are used to display the estimated residuals, respectively (Lines 7 and 8).

```
>>> 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()
```
#### **4.5. Relaxing convexity**

*Isotonic CNLS*

This section introduces a variant of the CNLS estimator, isotonic CNLS that only imposes monotonicity. To relax the concavity assumption in CNLS estimation (i.e., estimating a production function), we rephrase the Afriat inequality constraint in problem [\(2\)](#page-9-0).

Define the following binary matrix  $P = [p_{ij}]_{n \times n}$  to represent isotonicity [\(Keshvari and Ku](#page-34-12)[osmanen](#page-34-12) [2013\)](#page-34-12).

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

We apply a simple enumeration method to define the elements of matrix *P* and then solve

the following QP problem

$$
\min_{\alpha,\beta,\varepsilon} \sum_{i=1}^{n} \varepsilon_i^2
$$
\n
$$
s.t. \quad y_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i \qquad \forall i
$$
\n
$$
p_{ij}(\alpha_i + \beta_i' \mathbf{x}_i) \le p_{ij}(\alpha_j + \beta_j' \mathbf{x}_i) \quad \forall i, j, \text{ and } i \neq j
$$
\n
$$
\beta_i \ge 0 \qquad \forall i
$$

Note that the concavity constraints between units *i* and *j* are relaxed whenever  $p_{ij} = 0$ . If the  $p_{ij} = 1$  for all *i* and *j*, then the above isotonic CNLS problem reduces to the CNLS problem.

To calculate the monotonic models, the pyStoNED package provides the modules ICNLS(y,  $x, \ldots$ ) and ICQER.ICQR(y,  $x, \ldots$ )/ICQER.ICER(y,  $x, \ldots$ ), of which inherit the parameter settings from the modules CNLS() and CQER(). Therefore, the implementations of ICNLS() and ICQER() are similar to those of CNLS() and CQER(). Note that the matrix *P* is enumerated as an internal function in this module.

```
>>> 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'],
\ldots y_select = ['Energy'])
>>> model = 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()
```
#### *Isotonic CQR and CER*

Similar to isotonic CNLS, the isotonic CQR and CER approaches are defined as follows [\(Dai](#page-32-12) *[et al.](#page-32-12)* [2023a\)](#page-32-12)

• Isotonic CQR.

$$
\min_{\alpha,\beta,\varepsilon^+,\varepsilon^-} \tau \sum_{i=1}^n \varepsilon_i^+ + (1-\tau) \sum_{i=1}^n \varepsilon_i^-
$$
\n*s.t.*  $y_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i^+ - \varepsilon_i^- \qquad \forall i$   
\n $p_{ij}(\alpha_i + \beta_i' \mathbf{x}_i) \le p_{ij}(\alpha_j + \beta_j' \mathbf{x}_i) \quad \forall i, j, \text{ and } i \ne j$   
\n $\beta_i \ge \mathbf{0} \qquad \forall i$   
\n $\varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0 \qquad \forall i$ 

• Isotonic CER.

$$
\min_{\alpha,\beta,\varepsilon^+,\varepsilon^-} \tilde{\tau} \sum_{i=1}^n (\varepsilon_i^+)^2 + (1-\tilde{\tau}) \sum_{i=1}^n (\varepsilon_i^-)^2
$$
\n*s.t.*  $y_i = \alpha_i + \beta_i' \mathbf{x}_i + \varepsilon_i^+ - \varepsilon_i^- \qquad \forall i$   
\n $p_{ij}(\alpha_i + \beta_i' \mathbf{x}_i) \le p_{ij}(\alpha_j + \beta_j' \mathbf{x}_i) \quad \forall i, j, \text{ and } i \ne j$   
\n $\beta_i \ge \mathbf{0} \qquad \forall i$   
\n $\varepsilon_i^+ \ge 0, \ \varepsilon_i^- \ge 0 \qquad \forall i$ 

These two isotonic CQR/CER models can be computed by using the function  $ICQR(y, x, ...)$ tau, ...) or ICER(y, x, tau, ...) embedded in pyStoNED. The following example shows an isotonic CER model solved by the developed package.

```
>>> 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'],
\ldots y select = ['Energy'])
>>> model = ICQER.ICER(y = data.y, x = data.x, tau = 0.9, z = None,\ldots cet = CET_ADDI, fun = FUN_PROD, rts = RTS_VRS)
>>> model.optimize(OPT_LOCAL)
>>> model.display residual()
```
#### **4.6. Corrected CNLS**

To pave the way to the stochastic nonparametric frontier estimation to be examined in Section [5,](#page-21-0) we complete this section with a simple deterministic approach to frontier estimation.

Corrected convex nonparametric least squares  $(C<sup>2</sup>NLS)$  [\(Kuosmanen and Johnson](#page-34-8) [2010\)](#page-34-8) is a nonparametric extension of the corrected ordinary least squares (COLS), in which nonparametric least squares subject to monotonicity and concavity constraints replace the first-stage parametric ordinary least squares (OLS) regression. To estimate the frontier production function  $f$  using the C<sup>2</sup>NLS estimator, we assume that  $f$  is a monotonic increasing and globally concave production function. The key difference to model [\(1\)](#page-8-3) is that we now assume  $\varepsilon_i \leq 0$ represent technical inefficiency. Otherwise, we maintain the assumption that the inefficiencies *ε* are uncorrelated with inputs *x*.

Similar to COLS,  $C^2NLS$  includes two steps stated as follows:

- Estimate the residuals  $\varepsilon_i^{\text{CNLS}}$  by solving the additive CNLS model [\(2\)](#page-9-0).
- Obtain the shifted residuals  $\hat{\varepsilon}_i^{\text{C2NLS}} = \varepsilon_i^{\text{CNLS}} \max_j \varepsilon_j^{\text{CNLS}}$ such that  $\hat{\varepsilon}_i^{\text{C2NLS}}$  satisfy  $\hat{\varepsilon} \leq 0$  with 0 indicating efficient performance. Subsequently, we adjust the CNLS intercepts  $\alpha_i$  as

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

where  $\alpha_i^{\text{CNLS}}$  is the optimal intercept for firm *i* in the above CNLS problem and  $\hat{\alpha}_i^{\text{C2NLS}}$ is the estimated intercept term in the C<sup>2</sup>NLS problem. Slope coefficients  $\beta_i$  for C<sup>2</sup>NLS are obtained directly as the optimal solution to the CNLS problem.

To solve the  $C^2NLS$  model in **pyStoNED**, we introduce two new functions: .get adjusted re sidual() 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'],
\ldots y_select = ['Energy'])
>>> model = CNLS(CW_S(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())
```
# **5. Stochastic nonparametric envelopment of data**

<span id="page-21-0"></span>Consider now the production model with a composite error structure

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

In contrast to model [\(1\)](#page-8-3), the error term  $\varepsilon_i$  here consists of the inefficiency term  $u_i > 0$  and the stochastic noise term  $v_i$  ( $\varepsilon_i = v_i - u_i$ ). For the cost function model, the error term  $\varepsilon_i = v_i + u_i$ . Combining virtues of SFA and DEA in a unified framework, [Kuosmanen](#page-34-3) [\(2006\)](#page-34-3) and [Kuosma](#page-34-4)[nen and Kortelainen](#page-34-4) [\(2012\)](#page-34-4) propose the StoNED estimator to estimate the production/cost frontier and inefficiency. Specifically,

- Step 1: Estimating the conditional mean  $E[y_i | x_i]$  using the CNLS estimator;
- Step 2: Estimating the expected inefficiency  $\mu$  based on the residual  $\varepsilon_i^{\text{CNLS}}$ ;
- Step 3: Estimating the StoNED frontier  $\hat{f}^{\text{StoNED}}$  based on the  $\hat{\mu}$ ;
- Step 4: Estimating firm-specific inefficiencies  $E[u_i | \varepsilon_i^{\text{CNLS}}]$ .

Besides the CNLS estimator, we can apply other convex regression approaches such as isotonic CNLS and CNLS-DDF to estimate the conditional mean in the first step (see [Keshvari and](#page-34-12) [Kuosmanen](#page-34-12) [2013;](#page-34-12) [Kuosmanen and Johnson](#page-34-11) [2017\)](#page-34-11).

#### <span id="page-21-1"></span>**5.1. Estimating the expected inefficiency**

After obtaining the residuals (e.g.,  $\hat{\varepsilon}_i^{\text{CNLS}}$ ) 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  $\mu$ : Method of moments [\(Aigner](#page-32-3) *[et al.](#page-32-3)* [1977\)](#page-32-3), quasi-likelihood estimation [\(Fan, Li, and Weersink](#page-33-11) [1996\)](#page-33-11), and kernel deconvolution estimation [\(Hall and Simar](#page-33-12) [2002\)](#page-33-12). We next briefly review these three approaches and demonstrate the application of pyStoNED; see [Kuosmanen](#page-34-1) *et al.* [\(2015\)](#page-34-1) for a more detailed theoretical introduction.

#### *Method of moments*

The method of moments requires some additional parametric distributional assumptions. Under the assumptions of half-normal inefficiency,  $u_i \sim N^+(0, \sigma_u^2)$ , and normal noise,  $v_i \sim$  $N(0, \sigma_v^2)$ , the second and third central moments of the residual distribution are

$$
M_2 = \left[\frac{\pi - 2}{\pi}\right] \sigma_u^2 + \sigma_v^2
$$

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

The second and third central moments can be estimated based on the CNLS residuals as

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

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

Note that the third moment *M*<sup>3</sup> (which measures the skewness of the distribution) only depends on the standard deviation parameter  $\sigma_u$  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  $\sigma_u$  and  $\sigma_v$  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 expected inefficiency  $(\hat{\mu} = \hat{\sigma}_u \sqrt{2/\pi})$ , we provide a module StoNED() that inherits the parameter setting from the module CNLS(). We estimate the conditional expected inefficiency through the example presented below. Following the stepwise procedure outlined above, we first utilize the module CNLS() to estimate the conditional mean  $\mathsf{E}[y_i \mid x_i]$  (i.e., Lines 5–6), then apply the module StoNED(model), where the parameter model is defined as the name of the CNLS model, to decompose the estimated residuals (Line 7). We develop and import the parameter RED\_MOM (Line 3) to decompose the residuals using the moment method. We finally resort to the function .get\_unconditional\_expected\_inefficiency(RED\_MOM) included in the module StoNED() to retrieve the expected inefficiency  $\hat{\mu}$ .

```
>>> 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'])
```

```
\gg model = CNLS. CNLS(data.y, data.x, z = None,
\ldots cet = CET_MULT, fun = FUN_COST, rts = RTS_VRS)
>>> model.optimize('email@address')
>>> rd = StoNED.StoNED(model)
>>> print(rd.get_unconditional_expected_inefficiency(RED_MOM))
```
#### *Quasi-likelihood estimation*

Quasi-likelihood estimation is an alternative approach to decomposing  $\sigma_u$  and  $\sigma_v$  suggested by Fan *[et al.](#page-33-11)* [\(1996\)](#page-33-11). Given the shape of the CNLS curve, we apply the standard maximum likelihood method to estimate the parameters  $\sigma_u$  and  $\sigma_v$ . 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

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

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

Note that the quasi-likelihood function only consists of a single parameter  $\lambda$  (i.e., the signalto-noise ratio  $\lambda = \sigma_u/\sigma_v$ .<sup>[10](#page-23-0)</sup> The symbol  $\Phi$  represents the cumulative distribution function of the standard normal distribution. In the pyStoNED package, we use the BFGS algorithm provided by SciPy to estimate the maximum likelihood function.

Since we apply the quasi-likelihood estimation to decompose the residuals, we need to import the parameter RED\_QLE to the module StoNED().

```
>>> from pystoned import CNLS, StoNED
>>> from pystoned.dataset import load_Finnish_electricity_firm
>>> from pystoned.constant import CET_MULT, FUN_COST, RTS_VRS, RED_QLE
>>> data = load Finnish electricity firm(x_select = ['Energy', 'Length',\ldots 'Customers'], y_select = ['TOTEX'])
\gg 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_unconditional_expected_inefficiency(RED_QLE))
```
#### *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  $\mu$  is available by applying nonparametric kernel deconvolution,

<span id="page-23-0"></span><sup>&</sup>lt;sup>10</sup>Note the notation difference between signal-to-noise ratio  $\lambda$  and the marginal effect of contextual variable  $\lambda$  in problems [\(9\)](#page-14-0) and [\(10\)](#page-15-0).

as proposed by [Hall and Simar](#page-33-12) [\(2002\)](#page-33-12). Note that the residual  $\hat{\varepsilon}^{\text{CNLS}}_i$  is a consistent estimator of  $e^o = \varepsilon_i + \mu$  (for production model). 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](#page-33-12) [\(2002\)](#page-33-12) show that the first derivative of the density function of the composite error term  $(f'_\varepsilon)$  is proportional to that of the inefficiency term  $(f'_u)$  in the neighborhood of  $\mu$ . Therefore, a nonparametric estimator of expected inefficiency  $\mu$  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  $f_e$ .

We then import the parameter RED\_KDE to decompose the estimated CNLS residuals.

```
>>> from pystoned import CNLS, StoNED
>>> from pystoned.dataset import load_Finnish_electricity_firm
>>> from pystoned.constant import CET_MULT, FUN_COST, RTS_VRS, RED_KDE
>>> data = load Finnish electricity firm(x select = ['Energy', 'Length',
... 'Customers'], y_select = ['TOTEX'])
\gg> 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 unconditional expected inefficiency(RED_KDE))
```
#### **5.2. Estimating the StoNED frontier**

Having estimated the expected inefficiency  $\hat{\mu}$  in Section [5.1,](#page-21-1) we can estimate the efficient frontier by adjusting the conditional mean function estimated by CNLS. In this subsection we briefly discuss the cases of the additive and multiplicative models under VRS and CRS. Given the fact that the function estimated by CNLS is only unique for the observed data points  $(x_i, y_i)$ , we then follow [Kuosmanen and Kortelainen](#page-34-4) [\(2012\)](#page-34-4) to estimate the unique conditional mean function  $\hat{g}_{\min}^{\text{CNLS}}(\boldsymbol{x})$  under VRS. Note that CRS is imposed by setting  $\alpha = 0$ .

$$
\hat{g}_{\min}^{\mathrm{CNLS}}(\boldsymbol{x}) = \min_{\alpha,\beta}\{\alpha + \boldsymbol{\beta}'\boldsymbol{x} \mid \alpha + \boldsymbol{\beta}'\boldsymbol{x}_i \geq \hat{g}^{\mathrm{CNLS}}(\boldsymbol{x}_i),\forall i\}
$$

where  $\hat{g}^{\text{CNLS}}(\boldsymbol{x}_i)$  is the conditional mean function estimated by the CNLS estimator. We subsequently shift the conditional mean function  $\hat{g}_{\min}^{\text{CNLS}}(\boldsymbol{x})$  to the frontier using

- Production function.
	- $-$  Additive model:  $\hat{f}^{\textrm{StoNED}}(\boldsymbol{x}) = \hat{g}^{\textrm{CNLS}}_{\textrm{min}}(\boldsymbol{x}) + \hat{\mu};$
	- $-$  Multiplicative model:  $\hat{f}^{\text{StoNED}}(\boldsymbol{x}) = \hat{g}^{\text{CNLS}}_{\text{min}}(\boldsymbol{x}) \cdot \exp(\hat{\mu}).$
- Cost function.

 $-$  Additive model:  $\hat{f}^{\textrm{StoNED}}(\boldsymbol{x}) = \hat{g}^{\textrm{CNLS}}_{\textrm{min}}(\boldsymbol{x}) - \hat{\mu};$ 

 $-$  Multiplicative model:  $\hat{f}^{\text{StoNED}}(\boldsymbol{x}) = \hat{g}^{\text{CNLS}}_{\text{min}}(\boldsymbol{x}) \cdot \exp(-\hat{\mu}).$ 

In the following example, we demonstrate how to obtain the StoNED frontier via the package. The method of moments is utilized to decompose the CNLS residuals and calculate  $\hat{\mu}$ , and we then use .get\_stoned() to obtain the StoNED frontier (the last line).

```
>>> 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_stoned(RED_MOM))
```
#### **5.3. Estimating firm-specific inefficiencies**

If the efficient production or cost frontier is the object of interest, there is no need to proceed further to Step 4. [Kuosmanen](#page-34-1) *et al.* [\(2015\)](#page-34-1) emphasize that unbiased and consistent estimators of the frontier are available, however, there is no consistent method for estimating firm-specific efficiencies in the cross-sectional setting under noise. In essence, in this subsection we engage in the daunting task of trying to predict a realization of a random variable based on a single observation that is subject to noise. A reader should be duly warned that this is a highly speculative exercise.

Prediction of firm-specific inefficiency relies heavily on the parametric distributional assumptions. After estimating the expected inefficiency  $\mu$  using the methods of the moment (MOM) or quasi-likelihood estimation (QLE), we can employ the JLMS estimator proposed by [Jondrow, Lovell, Materov, and Schmidt](#page-34-13) [\(1982\)](#page-34-13) to estimate the firm-specific inefficiencies [\(Johnson and Kuosmanen](#page-34-2) [2015\)](#page-34-2). Under the assumption of a normally distributed error term and a half-normally distributed inefficiency term, [Jondrow](#page-34-13) *et al.* [\(1982\)](#page-34-13) formulate the conditional distribution of inefficiency  $u_i$ , given  $\hat{\varepsilon}_i$ , and proposes the inefficiency estimator as the conditional mean  $E[u_i \mid \hat{\varepsilon}_i].$ 

The conditional expected inefficiency  $E[u_i \mid \hat{\varepsilon}_i]$  for production function and cost function are

• Production function.

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

where  $\mu_{*i} = -\hat{\varepsilon}_i \sigma_u^2/\sigma^2$ ,  $\sigma_*^2 = \sigma_u^2 \sigma_v^2/\sigma^2$ ,  $\lambda = \sigma_u/\sigma_v$ , and  $\sigma^2 = \sigma_u^2 + \sigma_v^2$ . The symbol  $\phi$  is the standard normal density function, and the symbol  $\Phi$  denotes the cumulative distribution function of the standard normal distribution.

• Cost function.

 $w<sup>₁</sup>$ 

$$
\mathsf{E}[u_i \mid \hat{\varepsilon}_i] = \mu_{*i} + \sigma_* \left[ \frac{\phi(-\mu_{*i}/\sigma_*)}{1 - \Phi(-\mu_{*i}/\sigma_*)} \right] = \sigma_* \left[ \frac{\phi(\varepsilon_i \lambda/\sigma)}{1 - \Phi(-\varepsilon_i \lambda/\sigma)} + \frac{\varepsilon_i \lambda}{\sigma} \right]
$$
  
ere  $\mu_* = \varepsilon \sigma_u^2/\sigma^2$ ,  $\sigma_*^2 = \sigma_u^2 \sigma_v^2/\sigma^2$ ,  $\lambda = \sigma_u/\sigma_v$ , and  $\sigma^2 = \sigma_u^2 + \sigma_v^2$ .

The firm-level technical efficiency (TE) can be expressed based on the estimated conditional mean as

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

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 8) or to RED\_QLE (i.e., using the quasi-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,
\ldots cet = CET_MULT, fun = FUN_COST, rts = RTS_VRS)
>>> model.optimize('email@address')
>>> rd = StoNED.StoNED(model)
>>> print(rd.get_technical_inefficiency(RED_MOM))
```
# **6. CNLS-G algorithm**

<span id="page-26-0"></span>Since convex regression approaches impose the convexity (concavity) of the regression function using the Afriat inequality, the computation can become 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 computation, [Lee, Johnson,](#page-35-14) [Moreno-Centeno, and Kuosmanen](#page-35-14) [\(2013\)](#page-35-14) 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.](#page-35-14)* [\(2013\)](#page-35-14).

To illustrate the CNLS-G algorithm, we follow Lee *[et al.](#page-35-14)* [\(2013\)](#page-35-14) to generate the input and output variables. In this section, we assume an additive production function with two-input and one-output,  $y = x_1^{0.4} \times x_2^{0.4} + \varepsilon$ . We randomly draw the inputs  $x_1$  and  $x_2$  from a uniform distribution,  $x \sim U[1, 10]$ , and the error term  $\varepsilon$  from a normal distribution,  $\varepsilon \sim N(0, 0.7^2)$ . We generate 500 artificial observations, estimate the CNLS problem [\(2\)](#page-9-0) and the CER problem [\(8\)](#page-13-0), and calculate the firm-level technical efficiency using the CNLS-G algorithm.

#### <span id="page-27-0"></span>**6.1. Solving CNLS model**

We first compare the running time of the 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(). Note that the module CNLSG() has the same parameters as the module CNLS(). Line 3 imports NumPy to provide multidimensional arrays and functions for linear algebra. We use time to count the running time for CNLS estimation (see Lines 4, 9, and 12) and employ the function .get runningtime() to directly obtain the running time for CNLS-G algorithm (Line 15). To replicate the experiment, we set a random seed using  $np.random.seted(0)$ . Lines 6-8 generate the variables  $x, \varepsilon$ , and  $y$ . model1 and model2 are the 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 .get\_totalconstr() (Line 17).

```
>>> 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))
\gg epsilon = np.random.normal(loc = 0, scale = 0.7, size = 500)
>>> y = x[:, 0]**0.4 * x[:, 1]**0.4 + epsilon
\gg t1 = time.time()
\gg>> model1 = CNLS.CNLS(y, x, z = None, cet = CET_ADDI, fun = FUN_PROD,
\ldots rts = RTS_VRS)
>>> model1.optimize(OPT_LOCAL)
\gg> CNLS_time = time.time() - t1
\Rightarrow \Rightarrow model2 = CNLSG.CNLSG(y, x, z = None, cet = CET ADDI, fun = FUN_PROD,
\ldots 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())
```
#### **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.](#page-27-0) Note that the CNLS-G algorithm can also solve the CQR model via the function CQERG.CQRG(y,  $x, \ldots$ ).

```
>>> 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))>>> epsilon = np.random.normal(loc = 0, scale = 0.7, size = 500)
>>> y = x[:, 0] **0.4 * x[:, 1] **0.4 + epsilon\gg tau = 0.5
\gg t1 = time.time()
>>> model1 = CQER.CER(y, x, tau, z = None, cet = CET_ADDI, fun = FUN_PROD,\ldots rts = RTS_VRS)
>>> model1.optimize(OPT_LOCAL)
\gg \geq CER_time = time.time() - t1>>> model2 = CQERG.CERG(y, x, tau, z = None, cet = CET_ADDI, fun = FUN_PROD,\ldots 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())
```
#### **6.3. Calculating the expected inefficiency**

We can apply the CNLS-G algorithm to calculate the unconditional expected inefficiency  $\hat{\mu}$ more efficiently. In the first step of the StoNED() estimator, we use the module CNLSG( $y, x$ ,  $\ldots$ ) as a substitute for the module CNLS(y, x,  $\ldots$ ).

```
>>> from pystoned import CNLSG, 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',
\ldots 'Customers'], y select = ['TOTEX'])
\gg> model = CNLSG.CNLSG(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_unconditional_expected_inefficiency(RED_MOM))
```
# **7. Graphical illustration of estimated functions**

<span id="page-28-0"></span>To illustrate how the estimated regression function looks like, the pyStoNED package provides the functions plot.plot2d() and plot.plot3d() to plot two- and three-dimensional (2D and 3D) functions. As with the usage of the module  $StoNED(y, x, \ldots)$ , we first estimate the nonparametric regression such as CNLS, CQR, and isotonic CNLS and then apply the plot

<span id="page-29-0"></span>

Figure 1: CNLS and CQR estimates.

function to draw the figures. In this section, we use the internal data provided with Tim Coelli's Frontier 4.1 to demonstrate the 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 9 and 10 define and solve the CNLS and CQR models, respectively. Lines 8 and 11 are used to plot the estimated functions. There are four parameters in the module  $plot2d(...):$  The first is the model's name, the second parameter x\_select defines which the selected input x is, the third and last are the given names of the legend and generated picture, respectively. Figure [1](#page-29-0) depicts the functions estimated by the CNLS and CQR model.

```
>>> 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'],
\ldots y_select = ['output'])
>>> CNLS_model = CNLS.CNLS(y = data.y, x = data.x, z = None,\ldots cet = CET_ADDI, fun = FUN_PROD, rts = RTS_VRS)
>>> CNLS_model.optimize(OPT_LOCAL)
>>> plot2d(CNLS_model, x_select = 0, label_name = "CNLS estimated function",
      fig\_name = "CNLS_2d")>>> CQR_{\text{model}} = CQER_{\text{C}}QR(y = data.y, x = data.x, tau = 0.5, z = None,... cet = CET_ADDI, fun = FUN_PROD, rts = RTS_VRS)
>>> CQR_model.optimize(OPT_LOCAL)
>>> plot2d(CQR_model, x_select = 0, label_name = "CQR estimated function",
      fig_name = "CQR_2d")
```
<span id="page-30-1"></span>

Figure 2: 3D plot of the piece-wise linear function estimated with CNLS.

#### **7.2. Two-input and one-output**

We first use the linear interpolation technique to obtain the 3D surface because CNLS estimates hyperplanes at the observed data points. 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 the 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](#page-30-1) presents the estimated 3D function.

```
>>> from pystoned import CNLS
>>> from pystoned.plot import plot3d
>>> 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 = ['capital', 'labour'],
\dots y_select = ['output'])
>>> CNLS model = CNLS.CNLS(y = data.y, x = data.x, z = None,
\ldots 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")
```
### **8. Conclusions**

<span id="page-30-0"></span>Convex regression and related methods provide an appealing way to impose shape constraints without making restrictive assumptions about the functional form. As these techniques are becoming increasingly popular, there is a great demand for a powerful, reliable, and fully open-access computational package. Several existing tools or packages have been developed and can be utilized in certain special cases. For example, R/Benchmarking only supports additive CNLS/StoNED models, not CQR/CER or other more recent models. CVXOPT and **CVXPY** require that the user is able to manually construct the necessary QP matrices, which can be challenging for applied researchers and practitioners with limited experience in mathematical programming. Therefore, the developed pyStoNED package aims to fully address this need, providing a comprehensive set of functions for estimating CNLS, StoNED, and their numerous variants.

This paper has reviewed the models and specifications currently supported by pyStoNED and demonstrated its use with empirical examples taken from the literature on 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](#page-35-15) [2020\)](#page-35-15). More efficient computational algorithms such as the CNLS-A proposed by [Dai](#page-32-11) [\(2021\)](#page-32-11) are under active development and will be included in future editions of pyStoNED.

We hope that the **pyStoNED** package could contribute to raising the standards of empirical applications in productivity and efficiency analysis, and facilitate more meaningful and relevant empirical evidence that influence managerial and policy decisions. The basic idea of the StoNED approach is to enable applied researchers and practitioners of efficiency analysis to integrate existing tools and techniques from different domains such as econometrics, statistics, operational research, and machine learning into a logically consistent unified framework, and 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 cost and production functions, 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](#page-31-0) [1967;](#page-31-0) [Varian](#page-36-1) [1982\)](#page-36-1).

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# **A. List of acronyms**

<span id="page-37-0"></span>COLS: Corrected ordinary least squares

C <sup>2</sup>NLS: 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 unit

FDH: Free disposal hull

MOM: Method of moments

QLE: Quasi-likelihood estimation

ICNLS: Isotonic convex nonparametric least squares

SFA: Stochastic frontier analysis

StoNED: Stochastic nonparametric envelopment of data

StoNEZD: Stochastic semi-nonparametric envelopment of *Z* variables data

KDE: Kernel density estimation

<span id="page-37-1"></span>VRS: Variable returns to scale

# **B. CNLS residuals according to** pyStoNED



![](_page_38_Picture_148.jpeg)

![](_page_39_Picture_143.jpeg)

# **C. CNLS residuals according to GAMS**

<span id="page-39-0"></span>![](_page_39_Picture_144.jpeg)

![](_page_40_Picture_142.jpeg)

# <span id="page-40-1"></span><span id="page-40-0"></span>**D. CNLS residuals according to R/**Benchmarking

![](_page_40_Figure_3.jpeg)

Estimated residuals by R/Benchmarking

Figure 3: Scatterplot of residuals by pyStoNED and Benchmarking.

	$[1,] -7.8886697$		$[2,]$ -4.2032470	$[3,] -26.3619713$	$[4,]$ -340.7346628
	$[5,] -20.4750870$	[6, 1]	99.8192026	$[7,]$ -34.9414506	$[8,] -16.0153732$
	$[9,] -6.6921578$		[10, 354.4126408]	$[11, ]$ 292.9020295	[12,] 674.1823463
	$[13,] -24.5033276$		$[14,] -73.0074133$ $[15,] -9.0744802$		[16,] 76.2853110
	$[17,] -13.4107689$		$[18,] -36.5828830 [19,] -46.0007323$		$[20,] -27.7717236$
	$[21,]$ 47.7153749		$[22,]$ 84.6132198 [23,] 12.8106176		$[24,]$ 25.9149204
	$[25,]$ -8.9327371		$[26, ] -27.3697694 [27, ] -41.8614644$		$[28,] -341.8454225$
[29,]	59.6833391		$[30, ] -24.1589554 [31, ] -14.9332809$		[32,] 211.3275027
[33.]	36.0900266		$[34,]$ -34.4012906 $[35,]$ -26.2801031		$[36,] -200.4334730$
[37,]	$-68.8716540$		$[38,]$ 0.7430369 $[39,]$ -3.5393839		$[40,] -70.1454171$
[41,]	2.0062502			$[42,] -19.2397146$ $[43,] -227.9417288$	$[44,]$ 1.3279244
[45,]	6.5195718		$[46, ] -26.4450121 [47, ] -60.1349080$		$[48,] -13.4667633$
[49.]	$-53.8479333$		$[50,]$ 276.5003033 $[51,]$ -5.0199937		$[52,]$ -18.2306460
[53,]	$-0.1603049$		$[54,]$ 41.6619683 [55,] -8.9830611		$[56,]$ 360.9327664
[57,]	165.2316377		$[58,]$ 29.7256506 [59,] 25.8260238		$[60,] -100.9986163$

![](_page_41_Picture_121.jpeg)

# <span id="page-41-1"></span><span id="page-41-0"></span>**E. Description of variables in the four internal datasets**

![](_page_41_Picture_122.jpeg)

Table 5: Finnish electricity distribution firms.

<span id="page-41-2"></span>![](_page_41_Picture_123.jpeg)

<span id="page-41-3"></span>Table 6: GHG abatement cost of OECD countries.

![](_page_41_Picture_124.jpeg)

Table 7: Data provided with Tim Coelli's Frontier 4.1.

<span id="page-42-0"></span>![](_page_42_Picture_154.jpeg)

Table 8: Rice production in the Philippines.

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![](_page_42_Picture_155.jpeg)