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## Enhancing Neurodynamic Approach with Physics-Informed Neural Networks for Solving Non-Smooth Convex Optimization Problems

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## Enhancing Neurodynamic Approach with Physics-Informed Neural Networks for Solving Non-Smooth Convex Optimization Problems

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#### Abstract

This paper proposes a deep learning approach for solving non-smooth convex optimization problems (NCOPs), which have broad applications in computer science, engineering, and physics. Our approach combines neurodynamic optimization with physics-informed neural networks (PINNs) to provide an efficient and accurate solution. We first use neurodynamic optimization to formulate an initial value problem (IVP) that involves a system of ordinary differential equations for the NCOP. We then introduce a modified PINN as an approximate state solution to the IVP. Finally, we develop a dedicated algorithm to train the model to solve the IVP and minimize the NCOP objective simultaneously. Unlike existing numerical integration methods, a key advantage of our approach is that it does not require the computation of a series of intermediate states to produce a prediction of the NCOP. Our experimental results show that this computational feature results in fewer iterations being required to produce more accurate prediction solutions. Furthermore, our approach is effective in finding feasible solutions that satisfy the NCOP constraint.

Keywords: Non-smooth convex optimization problem, Neurodynamic optimization, Physics-informed neural network, Numerical integration method, Ordinary differential equation

#### 1. Introduction

- Non-smooth convex optimization problems (NCOPs) are an important class of optimization problems
- that arise in various real-world applications. While traditional optimization methods have been successful in
- solving many smooth convex optimization problems, they are not well-suited to handle the nonsmoothness
- 5 of the objective functions in NCOPs. This has led to the development of alternative approaches, such as
- 6 neurodynamic optimization.
- Neurodynamic optimization is a promising approach for solving NCOPs (Qin & Xue, 2014). It involves
- 8 the implementation of a circuit-based neurodynamic model to solve the optimization problem in real time.
- 9 This approach has many potential applications, such as in resource allocation (Jia et al., 2021), feature
- selection (Wang et al., 2023), and coordination of multi-manipulator systems (Hou et al., 2010).
- The use of neurodynamic optimization to solve NCOPs typically involves three steps. First, a first-order

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ordinary differential equation (ODE) system is used to model the NCOP. The ODE system must be shown to have a globally convergent property, meaning that the state solution of the system converges to the optimal solution of the NCOP as time approaches infinity, regardless of the starting point. Second, classical numerical integration methods such as Runge-Kutta methods or backward differentiation formulas are used to numerically obtain the state solution of the ODE system (Burden et al., 2015). Third, the state at the end of a given time range, called the end state, is taken as to be the predicted solution of the NCOP. However, this approach has a drawback. That is, the numerical integration method has to compute all the intermediate states, from the initial state to the end state, to solve the optimization problem, which makes it inefficient.

To overcome this limitation, we propose a novel approach that combines neurodynamic optimization with physics-informed neural networks to provide an efficient and accurate solution. Unlike the traditional numerical integration method, our improved approach can directly predict the entire state solution, including the end state. This approach allows for efficient and accurate optimization of NCOPs without requiring the computation of all intermediate states.

Here we want to clarify the difference between our work and Neural ODEs. (Chen et al., 2018). Neural ODEs are a class of neural networks that interpret transformations within the model as a continuous process and use ODEs to characterize this process. Training such a model involves solving an ODE using numerical integration methods, and recent research bypasses the use of numerical integration methods to improve computational efficiency (Biloš et al., 2021). However, it is important to emphasize that the primary goal of a neural ODE is not to solve a particular ODE per se, but rather to address traditional supervised learning challenges, such as time series modeling. In our case, the task at hand is to solve an ODE system derived from an NCOP. In this context, the neural network acts as a surrogate model that is specifically trained to approximate the solution of the ODE system.

#### 1.1. Related Works

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Neuraodynamic Optimization. Neurodynamic optimization is a class of methods that model constrained optimization problems using ODE systems. This approach was first introduced by Hopfield & Tank
(1985) to solve the traveling salesman problem. Since then, neurodynamic optimization has been applied to
a wide range of optimization problems, including linear and quadratic programming problems (Xia & Wang,
2000), general convex programming problems (Kennedy & Chua, 1988; Xia et al., 2008), biconvex optimization problems (Che & Wang, 2018), global optimization problems (Che & Wang, 2019), and pseudoconvex
problems (Guo et al., 2011; Bian et al., 2018; Liu et al., 2022). These methods typically use the Lyapunov
stability theorem to prove that the constructed ODE system has a global convergence property, which means
that any state solution of the ODE system converges to an optimal solution of the target problem.

Physics-Informed Neural Networks (PINNs). Another line of research included in our work is the use of deep learning to solve differential equations. As a representative approach, PINNs (Raissi et al., 2019) are a class of neural networks that integrate physical laws described by PDEs and boundary conditions into the training losses. Thus, the neural network is trained to become the solution of the PDE. PINNs have a

wide range of successful applications, such as identifying material properties (Shukla et al., 2021a), optimizing sensor locations (Jagtap et al., 2022b), and investigating complex fluid dynamics, including supersonic and high-speed flows (Jagtap et al., 2022a; Mao et al., 2020). To facilitate the use and application of PINNs, several software packages have been developed and are available to the scientific community (Lu et al., 2021; Chen et al., 2020).

Numerous methods and theoretical explorations have been introduced to improve the computational performance of PINNs. From the theoretical side, research has been conducted to understand the error estimates associated with PINNs. Mishra & Molinaro (2022) investigates the generalization error of PINNs in approximating a class of inverse problems (Mishra & Molinaro, 2022), and De Ryck et al. (2022) provides error estimates for the PINN approximation of the Navier-Stokes equations. On the methodological side, a prominent strategy is the development of domain decomposition methods, which divide the problem domain into several subdomains, each of which is addressed by a separate PINN. This approach creates interconnected PINN solutions that allow independent treatment of each subdomain while preserving the interconnections across the partitioned domains (Jagtap et al., 2020c; Shukla et al., 2021b; Hu et al., 2022a; Penwarden et al., 2023; Hu et al., 2022b). To further improve the performance of PINNs, adaptive activation functions have been investigated, which add learnable parameters to the activation function (Jagtap et al., 2020b,a, 2022b; Jagtap & Karniadakis, 2023). These innovations in PINNs are reshaping the landscape of solution methods for solving complex scientific and engineering problems.

#### 66 1.2. Contributions

- Our paper presents several key contributions:
- We propose a novel approach for solving NCOPs that enhances neurodynamic optimization with PINNs, avoiding the use of numerical integration methods.
- We improve the PINN to adapt to the NCOP by incorporating the initial condition into the neural network and using only one neural network to predict all system states.
- We design a specialized training algorithm that leverages the structure of NCOPs to optimize the performance of our proposed approach. The neural network is trained to simultaneously satisfy the ODE system and minimize the NCOP objective function.
- Our experimental results demonstrate several advantages of our approach over classical numerical integration methods and vanilla PINNs. Our approach requires fewer iterations to produce more accurate predicted solutions, and it finds a feasible solution to the problem more quickly.

#### 8 1.3. Outline

The remaining sections are organized as follows: Section 2 provides the necessary background for understanding the paper, including an introduction to the NCOP and the neurodynamic optimization used to

model it. In Section 3, we present our proposed neural network for solving the NCOP. Section 4 details the design of the loss function and the training algorithm for the neural network. Section 5 presents the results of our experiments on solving the NCOP using the proposed approach, and compares our approach with the existing methods. Finally, Section 6 summarizes the main results of the paper and outlines possible directions for future research.

#### 2. Neurodynamic Approach for Modelling NCOP

Section 2.1 introduces the NCOP, which is the goal of this paper. In Section 2.2, we show how to model the NCOP using a neurodynamic approach. In Section 2.3, we introduce the PINN method for solving PDEs.

#### 89 2.1. NCOP

We consider the following optimization problem:

$$\begin{cases} \min_{x} f(x) \\ \text{s.t.} \end{cases}$$

$$g(x) \le \mathbf{0}$$

$$Ax = b,$$

$$(1)$$

where  $x = (x_1, x_2, ..., x_n)^T \in \mathbb{R}^n$  is the decision variables, and  $f : \mathbb{R}^n \to \mathbb{R}$  is the objective function.  $g(x) = (g_1(x), g_2(x), ..., g_m(x))^T : \mathbb{R}^n \to \mathbb{R}^m$  represents the inequality constraints, and  $u = (u_1, u_2, ..., u_m)$ represents the dual variables of the inequality constraints. Ax = b represents the equality constraints with  $A \in \mathbb{R}^{k \times n}$  and  $A \in \mathbb{R}^k$ .  $A \in$ 

In this paper, we consider the case where f(x) and g(x) are convex but not necessarily smooth, and A is of full row rank. We denote  $x^*$  and  $u^*$  as the optimal primal and dual solutions, respectively.

**Definition 1** (Subgradient and subdifferential). A vector  $l \in \mathbb{R}^n$  is a subgradient of  $f : \mathbb{R}^n \to \mathbb{R}$  at  $x \in \text{dom } f$  if the following holds

$$f(z) \ge f(x) + l^T(z - x), \quad \forall z \in \text{dom } f.$$
 (2)

The set of all subgradients of f at x is called the subdifferential of f at x and is denoted by  $\partial f(x)$ .

#### 2.2. Neurodynamic Approach

Now, let  $x : \mathbb{R} \to \mathbb{R}^n$  and  $u : \mathbb{R} \to \mathbb{R}^m$  be some time dependent functions. The aim of a neurodynamic approach is to construct a first-order ODE system to govern x(t) and u(t), such that they will settle down to the optimal primal and dual solutions of the NCOP (1). In this paper, the two-layer neurodynamic approach

in Qin & Xue (2014) is adopted, where the ODE system is described as follows:

$$\frac{dx}{dt} \in -(I-U)\left[\partial f(x) + \partial g(x)^T (U+g(x))^+\right] - A^T \rho (Ax-b),$$

$$\frac{du}{dt} = \frac{1}{2} \left(-U + (U+g(x))^+\right),$$
(3)

where  $U = A^T (AA^T)^{-1} A$ ,  $I \in \mathbb{R}^{n \times n}$  is the identity matrix,  $\rho(s) = (\tilde{\rho}(s_1), \tilde{\rho}(s_2), \dots, \tilde{\rho}(s_k))^T$ , and for  $i = 1, 2, \dots, k$ ,

$$\tilde{\rho}(s_i) = \begin{cases} 1 & \text{if } s_i > 0, \\ [-1, 1] & \text{if } s_i = 0, \\ -1 & \text{if } s_i < 0. \end{cases}$$
(4)

To simplify the discussion, we denote  $y(t) = (x(t)^T, u(t)^T)^T$  and define:

$$\Phi(y) = \begin{bmatrix} -(I-U) \left[ \partial f(x) + \partial g(x)^T (U+g(x))^+ \right] - A^T \rho (Ax - b) \\ \frac{1}{2} \left( -U + (U+g(x))^+ \right) \end{bmatrix}.$$
 (5)

Thus, the ODE system (3) can be written as  $\frac{dy}{dt} \in \Phi(y)$ .

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Definition 2 (State solution). Consider an ODE system  $\frac{dy}{dt} \in \Phi(y)$ , where  $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ . Given  $(t_0 \in \mathbb{R}^n)$ , a vector value function  $y : \mathbb{R} \to \mathbb{R}^n$  is called a state solution, if it satisfies the ODE system  $\frac{dy}{dt} \in \Phi(y)$  and the initial condition  $y(t_0) = y_0$ .

In particular, we call y(t) the state at time t. Given a time interval  $[t_0, T]$ , we call y(T) the end state on that time interval.

**Theorem 1** (Qin & Xue (2014)). Consider a NCOP (1) and its derived ODE system (3). Given any initial condition  $y(t_0) = y_0$ , the state solution y(t) of the ODE system converges to an optimal solution  $y^*$  as time t approaches infinity, i.e.

$$\lim_{t \to \infty} y(t) = y^*,\tag{6}$$

where  $y^* = (x^{*T}, u^{*T})^T$ ,  $x^*$  and  $u^*$  are the optimal primal and dual solutions to the NCOP.

In particular, if the NCOP contains only one optimal solution  $x^*$ , then the ODE system is called globally asymptotically stable at  $y^*$ .

Initial Value Problem (IVP) Construction. In practice, in order to use the neurodynamic approach to solve the NCOP, we need to construct an IVP consisting of three components: 1) the ODE system (3), 2) an initial condition  $y(t_0) = y_0$ , and 3) a time range  $t \in [t_0, T]$ . y(t) for  $t \in [t_0, T]$  represents the state solution of this IVP problem over the time range  $[t_0, T]$ , where the end state, y(T), is considered to be the predicted solution to the NCOP. According to Theorem 1, the larger the time range  $[t_0, T]$ , the closer y(T) is to the optimal solution  $y^*$  of the NCOP.

2.3. Physics-Informed Neural Networks (PINNs)

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In this subsection, we introduce the powerful framework of PINNs for solving PDEs. For clarity and to make this subsection self-contained, please note that the mathematical notations used in this subsection are independent of those used in other sections. The mathematical notations should be interpreted only in the context of this subsection.

A typical PDE problem can be expressed in the following general form:

$$D_x(u;\lambda) = f(x), x \in \Omega \subset \mathbb{R}^d$$

$$\mathcal{B}_k(u) = g_k(x), x \in \partial\Omega \subset \mathbb{R}^d, \text{for } k = 1, 2, \dots, n_b,$$
(7)

parameters.  $\mathcal{B}_k(\cdot)$  denotes to the boundary conditions, which can be of the Dirichlet, Neumann, or mixed type. For problems involving temporal dynamics, time t is considered as part of x, and the initial conditions can be treated as a unique type of boundary condition. Let  $\{x_b^{(i)}, u_b^{(i)}\}_{i=1}^{N_b}$  and  $\{x_d^{(i)}\}_{i=1}^{N_d}$  be the sets of randomly selected training points and residual points, respectively. These points are usually drawn from an unknown distribution. Let  $u_{\Theta}$  be a surrogate function

where  $D_x(\cdot)$  is the differential operator, and  $u:\Omega\cup\partial\Omega\to\mathbb{R}$  is the solution to be found.  $\lambda$  denotes the PDE

respectively. These points are usually drawn from an unknown distribution. Let  $u_{\Theta}$  be a surrogate function based on a neural network with model parameters  $\Theta$ . The goal of the PINN approach is to learn a surrogate function  $u_{\Theta}$  to approximate the solution u for a given PDE.

The loss function for PINNs can be expressed as:

$$\mathcal{L}(\Theta) = W_b \, \text{MSE}_b \left(\Theta; \{x_b^{(i)}, u_b^{(i)}\}_{i=1}^{N_b}\right) + W_d \, \text{MSE}_d \left(\Theta; \{x_d^{(i)}\}_{i=1}^{N_d}\right), \tag{8}$$

where  $W_b$  and  $W_d$  represent the weights for the data and residual losses, respectively.  $\text{MSE}_b\left(\Theta; \{x_b^{(i)}, u_b^{(i)}\}_{i=1}^{N_b}\right) + \text{and } \text{MSE}_d\left(\Theta; \{x_d^{(i)}\}_{i=1}^{N_d}\right)$  are given by:

$$MSE_{b}\left(\Theta; \{x_{b}^{(i)}, u_{b}^{(i)}\}_{i=1}^{N_{b}}\right) = \frac{1}{N_{b}} \sum_{i=1}^{N_{b}} \left| u^{(i)} - u_{\Theta}\left(x_{u}^{(i)}\right) \right|^{2},$$

$$MSE_{d}\left(\Theta; \{x_{d}^{(i)}\}_{i=1}^{N_{d}}\right) = \frac{1}{N_{d}} \sum_{i=1}^{N_{d}} \left| D_{x}(u_{\Theta}(x_{d}^{(i)}); \lambda) - f(x_{d}^{(i)}) \right|^{2},$$

$$(9)$$

where  $MSE_b$  measures the data mismatch term, which enforces the boundary conditions as constraints.  $MSE_d$  evaluates the PDE residual at a finite set of collocation points. The neural network parameters  $\Theta$  are determined by minimizing the loss function in (8).

A distinct advantage of PINNs is their ability to integrate both experimental and synthetic training data into the loss function. One of the central mechanisms facilitating this integration is the computation of the PDE residual using automatic differentiation (Baydin et al., 2018), which provides an efficient and accurate evaluation of the PDE operator. Thus, PINNs transform the task of solving a PDE into an optimization problem, where the global minimum of the loss function signifies the solution to the PDE. This capability

- positions PINNs as a grid-free method, alleviating the often cumbersome process of mesh generation.
- Remark 1. The ODE system (3) under consideration is a particular case of the PDE problem (7). The key differences are as follows:
- The solution of the ODE system is a function with only one input, while the PDE solution is a function with multiple inputs.
- The ODE system involves multiple differential equations, each corresponding to a state dynamic, whereas
  the PDE typically involves only a single equation with multiple variables.
- Mathematically, PINNs typically aim to find a solution  $u: \mathbb{R}^d \to \mathbb{R}$ , where d is the number of variables.

  In contrast, the solution sought in the ODE system is  $u: \mathbb{R} \to \mathbb{R}^n$ , where n is the number of differential equations in the system.

#### 3. Modified PINN Model

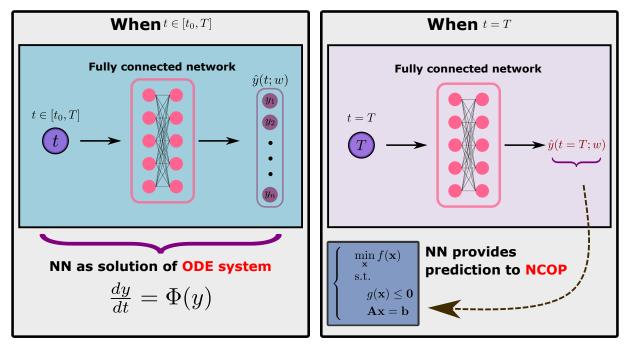


Figure 1: Neural network solution for the ODE system and the NCOP. Left: When  $t \in [t_0, T]$ , the model  $\hat{y}(t; w)$  itself is considered to be an approximate state solution of the ODE system. Right: When t = T, the model returns the prediction,  $(\hat{x}, \hat{u}) = \hat{y}(t = T; w)$ , where  $\hat{x}$  and  $\hat{u}$  represent the primal and dual predictions for the NCOP, respectively.

**Model Description.** We propose a modified PINN model to solve the NCOP. Our model can be expressed by the following equation:

$$\hat{y}(t;w) = y_0 + \left(1 - e^{-(t - t_0)}\right) N(t;w), \quad t \in [t_0, T],$$
(10)

where N(t; w) is a fully connected neural network with trainable parameters w.  $y_0$  is a given initial point for the ODE system.  $[t_0, T]$  is a given time range. The auxiliary function  $(1 - e^{-(t-t_0)})$  ensures that the neural network always satisfies the initial condition  $\hat{y}(t = t_0; w) = y_0$  regardless of w.

Improvements to PINN. The proposed model (10) can be seen as a modified version of the PINN to adapt to the considered problem. In particular, we make three improvements. First, we use the Lagaris method to handle the initial conditions of the ODE system (Lagaris et al., 1998). Second, we use only one neural network to handle all the differential equations of the entire ODE system, whereas, in the original method, each neural network handles only one differential equation of the system. Finally, we use the exponential form for the auxiliary function, which has been shown to improve convergence, as demonstrated in previous studies (Mattheakis et al., 2020). Our experiments confirm this improvement in convergence, which is likely due to the reduced influence of the neural network as time progresses further from the initial time.

Approximate State Solution to the ODE. As shown in Figure 1 (Left), the proposed model (10) itself is an approximate state solution of the ODE system (3) on the time range  $[t_0, T]$ , i.e,

$$\hat{y}(t;w) \approx y(t), \quad t \in [t_0, T], \tag{11}$$

where y(t) is the true state solution of the ODE system. While the input time t of the model  $\hat{y}(t;w)$  can be take any real number, we specifically use  $\hat{y}(t;w)$  as the solution of the ODE over the time range  $[t_0,T]$ . As a result, we restrict the input of  $\hat{y}(t;w)$  to the time range  $t \in [t_0,T]$ .

**Predicted Solution to the NCOP.** The end state of the proposed model, i.e.,  $\hat{y}(t = T; w)$ , is used as the predicted solution to the NCOP (1), as shown in Figure 1 (Right). The following equation shows how  $\hat{y}(t = T; w)$  approximates the optimal solution  $y^*$ :

$$\hat{y}(t=T;w) \approx y(T) \approx y^*. \tag{12}$$

Here,  $\hat{y}(t=T;w) \approx y(T)$  indicates that the end state of our model approximates the true end state, and  $y(T) \approx y^*$  comes from Theorem 1, indicating that the true end state is the predicted solution of the NCOP.

#### 163 4. Model training

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#### 4.1. Training Objective

**Loss Function.** We define the loss function of the proposed model (10) as follows:

$$\mathcal{L}(t,w) = \left\| \frac{\partial \hat{y}(t;w)}{\partial t} - \Phi(\hat{y}(t;w)) \right\|, \tag{13}$$

where  $\Phi(\cdot)$  refers to the ODE system (3), which corresponds to the NCOP to be solved.  $\|\cdot\|$  is the Euclidean norm.  $\Phi(\hat{y}(t;w))$  is the expected derivative according to the ODE system.  $\frac{\partial \hat{y}(t;w)}{\partial t}$  is the actual derivative

of the model, which can be computed using automatic differentiation tools such as PyTorch or JAX (Paszke et al., 2019; Bradbury et al., 2018).  $\mathcal{L}(t, w)$  represents the difference between the two at time t and with network parameters w.

Embedding the NCOP into the Loss Function. The NCOP is integrated into the loss computation process through the ODE system rather than as a component of the neural network. A neural network is created as an empty framework without a specific goal to solve a particular NCOP. Instead, by reformulating the NCOP as an ODE system and embedding it into the loss function, the neural network is trained toward solving the NCOP.

**Objective Function.** The goal of training the proposed model is to minimize the following objective function:

$$J(w) = \int_{t_0}^{T} \mathcal{L}(t, w)dt, \tag{14}$$

which is the integral of the loss function over the time range  $[t_0, T]$ . The loss value  $\mathcal{L}(t, w)$  represents the error of the model at time t, while the objective function J(w) represents the total error of the model over the time range  $[t_0, T]$ .

**Batch Loss.** However, the objective function J(w) is computationally intractable to compute due to its integral part. Therefore, in practice, we train the model by minimizing the following batch loss:

$$\mathcal{L}(\mathbb{T}, w) = \frac{1}{|\mathbb{T}|} \sum_{t \in \mathbb{T}} \mathcal{L}(t, w), \tag{15}$$

where  $\mathbb{T}$  is a set of randomly sampled time points from the interval  $[t_0, T]$ , and  $|\mathbb{T}|$  denotes the size of this set. In this way, we can approximate the integral in the objective function J(w) by a sum of loss values over the set of sampled times. By minimizing the batch loss, we can effectively train the model to solve the NCOP.

#### 81 4.2. Algorithm Design

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<u>O</u>bjective value <u>u</u>nder <u>C</u>onstraints (OuC) Metric. We introduce an evaluation metric called OuC to measure how well a predicted solution,  $x_{\text{pred}}$ , solves the NCOP:

$$OuC(x_{pred}) = \begin{cases} f(x_{pred}) & \text{if } x_{pred} \in \Omega, \\ +\infty & \text{otherwise }, \end{cases}$$
 (16)

where  $\Omega$  is the feasible set defined as  $\Omega = \{x | x \leq g(x), Ax = b\}$ . The OuC metric evaluates a predicted solution by setting OuC to positive infinity or a very large real number when the predicted solution is not feasible, and to the objective value when it is feasible.

**Projection Mapping onto Equality Constraints.** To increase the likelihood of  $OuC(x_{pred})$  being a real value instead of infinite, we employ the following projection function to map  $x_{pred}$  to the set of equality constraints,

$$P_{eq}(x_{\text{pred}}) = x_{\text{pred}} - A^T \left( A A^T \right)^{-1} \left( A x_{\text{pred}} - b \right). \tag{17}$$

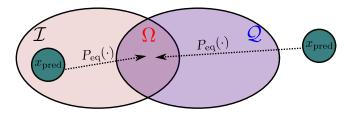


Figure 2:  $\mathcal{I}$  and  $\mathcal{Q}$  denote the feasible set of inequality constraints and equality constraints, respectively.  $\Omega = \mathcal{I} \cap \mathcal{Q}$  denotes the general feasible set of the problem.  $P_{eq}$  is a projection function that maps  $x_{\text{pred}}$  onto  $\mathcal{Q}$ .

By definition, the evaluation metric  $OuC(x_{pred})$  attains a real value only when  $x_{pred}$  lies within the feasible set  $\Omega$ . As illustrated in Figure 2, there are two circumstances when  $P_{eq}$  aids in projecting  $x_{pred}$  onto the feasible set:

- $x_{\text{pred}}$  satisfies the inequality constraints but fails to meet the equality constraints, i.e.,  $x_{\text{pred}} \in \mathcal{I} \mathcal{Q}$ .
- $x_{\text{pred}}$  does not satisfy both the inequality and equality constraints, i.e.,  $x_{\text{pred}} \notin \mathcal{I} \cup \mathcal{Q}$ .

In both of the above scenarios,  $P_{eq}$  has a reasonable chance of mapping  $x_{\text{pred}}$  onto the feasible set  $\Omega$ , resulting in the value of OuC being a real number rather than infinite.

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Algorithm 1: Deep learning solver for convex optimization problems
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Input: A COP; A time range [t_0, T]; An initial condition (t_0, y_0)
    Output: Predicted primal and dual solutions \hat{x}_{\text{best}} and \hat{u}_{\text{best}}.
 1 Function Main:
          ODE system \Phi(\cdot) \leftarrow the COP
 2
          Construct a NN model \hat{y}(t; w).
 3
          (\hat{x}_{\text{best}}, \hat{u}_{\text{best}}) \leftarrow \hat{y}(t = T; w)
  4
          \epsilon_{\text{best}} = \text{Evaluate}(\hat{x}_{\text{best}})
 5
          while iter \leq \max iter do
 6
               \mathbb{T} \sim U(t_0,T);
                                                                                                         \triangleright Sample a batch of times, \mathbb{T}.
  7
               \mathcal{L}(\mathbb{T},w);
  8
                                                                                                                      ▷ Forward propagation.
 9
               w = w - \nabla_w \mathcal{L}(\mathbb{T}, w) ;
                                                                                     \triangleright Update w through backward propagation.
               (\hat{x}_{\text{curr}}, \hat{u}_{\text{curr}}) = \hat{y}(t = T; w) ;
                                                                      ▷ Extract the predicted solution from the model.
10
               \hat{x}_{\text{curr}} = P_{eq}(\hat{x}_{\text{curr}}) ;
                                                                                   \triangleright Project \hat{x}_{\mathtt{curr}} onto equality constraints.
11
                OuC_{curr} = OuC(\hat{x}_{curr});
                                                                                                	riangleright Calculate the OuC value of \hat{x}_{	exttt{curr}} .
12
               if OuC_{curr} < OuC_{best} then
13
                    OuC_{best} = OuC_{curr};
                                                                                                           ▷ Update the best OuC value.
14
                     (\hat{x}_{\text{best}}, \hat{u}_{\text{best}}) = (\hat{x}_{\text{curr}}, \hat{u}_{\text{curr}}) ;
                                                                                                         ▷ Update the best prediction.
15
16
         return (\hat{x}_{\text{best}}, \hat{u}_{\text{best}})
18 end
```

**Pipeline.** Algorithm 1 summarizes how to use our proposed method to solve the NCOP. First, we need to specify an initial condition  $y(t_0) = y_0$  and a time range  $[t_0, T]$  to construct the IVP. Then, we instantiate the proposed model (10), which serves as an approximate state solution for this IVP. The model is trained by performing gradient descent on the batch loss (15) to improve the approximation. Note that our solver is completely based on the deep learning infrastructure and does not require any standard optimization solver or numerical integration solver.

Optimal Result Retention (ORR) Mechanism. A key to Algorithm 1 is that we use an ORR 198 mechanism based on the OuC metric (16). Specifically, at each iteration, the algorithm compares the OuC 199 value at the current iteration, denoted as OuC<sub>curr</sub>, with the best OuC value found so far, denoted as OuC<sub>best</sub>. 200  $(\hat{x}_{\text{curr}}, \hat{u}_{\text{curr}})$  and  $(\hat{x}_{\text{best}}, \hat{u}_{\text{best}})$  represent the current prediction and the best prediction found so far, respec-201 tively. If OuC<sub>curr</sub> is less than OuC<sub>best</sub>, it means that the model found a better prediction in this iteration. The 202 algorithm updates  $OuC_{best}$  to equal  $OuC_{curr}$  and stores the best prediction as  $(\hat{x}_{best}, \hat{u}_{best}) = (\hat{x}_{curr}, \hat{u}_{curr})$ . 203 This mechanism ensures that the best prediction obtained by the model is maintained throughout the training 204 process, improving the overall performance of the algorithm. 205

Neural Network Solution Procedure. Our approach employs gradient descent on the batch loss (15) to improve the neural network prediction at each iteration. Assume that the maximum number of training iterations is M. The evolution of the neural network is represented by  $\hat{y}(t; w_1), \hat{y}(t; w_2), \dots, \hat{y}(t; w_M)$ , where  $w_i$  and  $\hat{y}(t; w_i)$  denote the network parameters and the approximate state solution at the i-th iteration, respectively. The predicted end states are  $\hat{y}(t = T; w_1), \hat{y}(t = T; w_2), \dots, \hat{y}(t = T; w_M)$ , where  $\hat{y}(t = T; w_i)$  represents the prediction to the NCOP at the i-th iteration.

#### 5. Experiments

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Neural Network Setup. To implement our proposed model and the ODE system, we used PyTorch 1.12.1 with CUDA 11.2 (Paszke et al., 2019) and JAX 0.4.1 (Bradbury et al., 2018). Our neural network architecture consisted of a single layer fully connected network with 100 neurons and a Tanh activation function. For training, we used the Adam optimizer (Kingma & Ba, 2014) with a learning rate of 0.001, and a batch size of 128.

**Evaluation metrics.** We used two metrics to measure the performance of the model: 1) The OuC metric, as defined in equation (16). 2) Computational time, which measures the time required to achieve a desired accuracy.

#### 5.1. Comparisons with Numerical Integration Methods

In this subsection, we compare our proposed method with six classical numerical integration methods:
Runge-Kutta 45 (RK45), Runge-Kutta 23 (RK23), Dormand-Prince 853 (DOP853), Backward Differentiation
Formula (BDF), Radau, and LSODA. All of these methods are available in the Scipy library (Virtanen et al.,
2020). The RK45, RK23, and DOP853 are explicit Runge-Kutta methods, while the BDF and Radau are
implicit methods. LSODA is an adaptive method that automatically switches between explicit and implicit
methods depending on the stiffness of the ODE system.

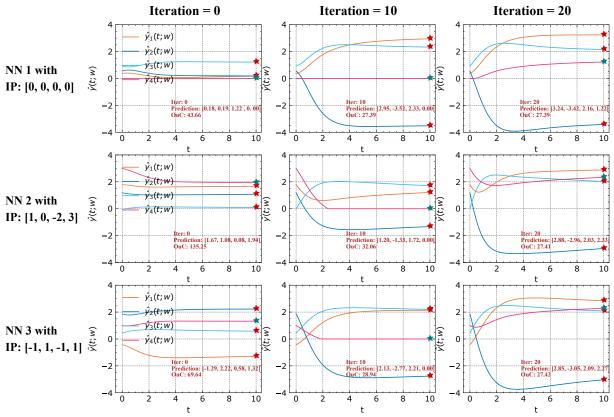
#### **Example 1:** We aim to solve the following NCOP:

$$\min_{x} f(x) = 10(x_1 + x_2)^2 + (x_1 - 2)^2 + 20|x_3 - 3| + e^{x_3}$$
s.t.
$$g(x) = (x_1 + 3)^2 + x_2 - 36 \le 0$$

$$h(x) = 2x_1 + 3x_2 + 5x_3 - 7 = 0.$$
(18)

The feasible set of this problem is convex, and the objective function is convex but non-smooth due to its inclusion of absolute values.

Construction of IVPs. We model the problem (18) by the ODE system (3) and set the time range as  $[t_0, T] = [0, 10]$ . We choose three initial points to study, namely [0, 0, 0, 0], [1, 0, -2, 3], and [-1, 1, -1, 1], which result in three IVPs. Based on these three initial points, we construct each of the three proposed neural networks (10) as approximate state solutions to the IVPs.



**★** Primal prediction

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★ Dual prediction

Figure 3: Neural network solutions to problem (18). The three neural networks are initialized with three different initial points (IPs). Each row shows a neural network as a function at selected training iterations.

**Neural Network Solution.** Figure 3 shows the solution process of our approach. Each horizontal row represents the evolution of a neural network trained by Algorithm 1. Each sub-figure shows  $\hat{y}(t; w)$ 

for  $t \in [0, 10]$ , which represents the approximate state solution of the IVP at a given training iteration. Here, we must emphasize that  $\hat{y}(t; w)$  is implemented by one neural network with four output units, and  $\hat{y}(t; w) = (\hat{y}_1(t; w), \hat{y}_2(t; w), \hat{y}_3(t; w), \hat{y}_4(t; w))$ . In particular, the end state has

$$\hat{y}(t=10;w) = \left(\underbrace{\hat{y}_1(t=10;w), \hat{y}_2(t=10;w), \hat{y}_3(t=10;w)}_{=\hat{x}}, \underbrace{\hat{y}_4(t=10;w)}_{=\hat{u}}\right), \tag{19}$$

where  $\hat{x}$  and  $\hat{u}$  represent the predicted primal and dual solutions, respectively, of the problem (18).

Evolution of the Predictions. As discussed in Section 4.2, the end state prediction  $\hat{y}(t=10;w)$  is improved by training on the entire approximate state solution. At training iteration 0, the approximate state solution is far from the true state solution, resulting in a high OuC value of the endpoint prediction. After 20 training iterations, the approximate state solution gets closer to the true state solution, and the endpoint prediction improves significantly. Notably, as these networks are constructed with different initial conditions, they have varying initial OuC values. Nonetheless, our proposed algorithm ensures that all networks converge to a prediction with an OuC value of less than 28 after 20 training iterations.

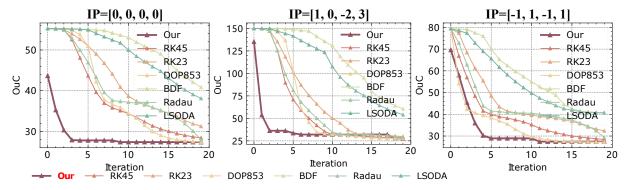


Figure 4: Comparison of our proposed method with the numerical integration methods on the OuC metric. The OuC metric is defined in Equation (16).

**OuC Performance.** Figure 4 presents a comparative analysis of the OuC drop rates for our proposed method and six traditional numerical integration methods over three different initial points. The following observations can be made:

- Our method outperforms traditional numerical integration methods in terms of OuC reduction, as evidenced by the lower OuC values achieved in fewer iterations. For example, for the initial point (IP) [0,0,0,0], our method reduces OuC from 43.66 to 28 in just five iterations, whereas the best-performing numerical integration methods, namely RK45, DOP853, and Radau, require 20 iterations to achieve comparable results. Similar results are observed for the other two initial points.
- The speed of convergence varies for different initial points, with our method showing greater robustness to different initial settings compared to numerical integration methods. While most numerical integration methods converge faster for the IP [1,0,-2,3] and slower for [0,0,0,0], our method converges at

approximately the same rate for both.

• The starting OuC values differ for various initial points, with the IP [1,0,-2,3] having the highest starting OuC value of around 135, and [0,0,0,0] having the lowest starting OuC of approximately 43. However, the results demonstrate that the OuC values do not significantly affect the speed of convergence.

Why Our Approach has Better OuC than RK45. It is important to emphasize that our approach has no advantage over classical numerical integrators such as RK45 when it comes to solving for the full solution on the IVP, i.e. the function y. As shown in Figure 4, our method outperforms these numerical integrators in the OuC metric because our approach focuses on improving the end point  $\hat{y}(t=T;w)$ , rather than the entirety of the function  $\hat{y}$ . It is also worth noting that the OuC performance metric only considers the endpoint  $\hat{y}(t=T;w)$ , not the entire function  $\hat{y}$ . The methodology we propose, described in sections 3 and 4, is deliberately designed with this specific goal in mind.

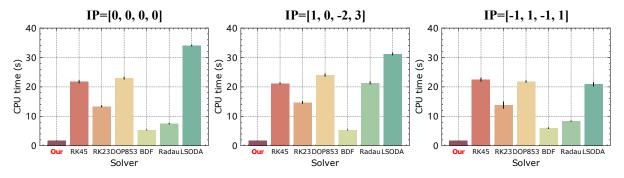


Figure 5: Comparison of our method with the numerical integration methods in terms of computational efficiency. Time is measured in seconds.

Computational Time Performance. Figure 5 shows the time needed by different solution methods to obtain an acceptable solution (i.e.,  $OuC \le 28$ ) to Problem (18). Our proposed method outperforms all considered numerical integration methods in terms of computational efficiency. The most efficient numerical integration method, BDF, still requires 10 times more computational time than our method to obtain a satisfactory solution. Moreover, the computational time of our method is less affected by different IP settings, requiring about 1.78 seconds for all three initial points. In contrast, some numerical integration methods, such as Radau and LSODA, show significant variations in computation time at different initial points.

#### 5.2. Comparisons with PINN

In this subsection, we perform an ablation study comparing the proposed method with PINN (Raissi et al., 2019) and Lagaris method (Lagaris et al., 1998) to validate the effectiveness of our method.

### Example 2:

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$$\min_{x} f(x) = |2.3x_1 + x_3 - 3.5| + |x_2 + 2x_3 - 1.8| + |1.3x_1 + x_2 + x_3 + 3|$$
s.t.
$$g(x) = x_1^2 - x_2 + x_3 + 3 \le 0$$

$$h_1(x) = x_1 + x_2 + x_3 = 0,$$

$$h_2(x) = 2x_2 + x_3 = 0.$$
(20)

We aim to solve the NCOP (20). The problem has a convex feasible set and a convex but non-smooth objective function due to its inclusion of absolute values.

Construction of IVPs. We model problem (20) as an ODE system (3) and set the time range as  $[t_0, T] = [0, 10]$ . To construct three IVPs, we choose three initial points, namely [1, -1, 0, 3], [2, 3, -2, 1], and [2, -2, 1, -2]. Based on these initial points, we instantiate three proposed neural networks (10) as approximate state solutions.

**Experimental Setup.** We compare our proposed approach with two methods: vanilla PINN and PINN with Lagaris construction method (PINN+Lagaris). Our approach can be regarded as the PINN+Lagaris method enhanced by the ORR mechanism (PINN+Lagaris+ORR). The hyperparameters and training details are the same as those in Section 5.1.

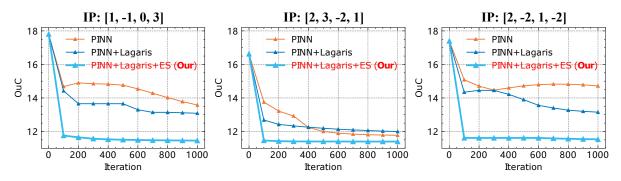


Figure 6: Comparison of our proposed method with PINN and the PINN+Lagaris method on the OuC metric. The experiment is conducted on Problem (20)

Table 1 shows the performance of the three methods over the first one hundred iterations, while Figure 6 shows their convergence behavior over the first one thousand iterations. The results reveal the following key observations:

- Our proposed approach yields an excellent predicted solution within the first 20 training iterations, consistent with the results presented in Section 5.1. In contrast, even after 1000 iterations, neither the PINN nor the PINN+Lagaris methods achieves a predicted solution that compares favorably to that of our approach.
- Our method has a higher probability of obtaining feasible solutions. As shown in Table 1, the PINN

		]	Initial point: $[1, -1, 0, 3]$				
Iteration	PINN		PINN+Lagaris		PINN+Lagaris+EC		
1001401011	Predicted solution OuC		Predicted solution	OuC	Predicted solution OuC		
0	[-0.64 1.36 -0.71 0.47] inf		[-1.00 1.00 -0.00 3.09]	inf	[-1.00 1.00 -0.00 3.09]	inf	
5	[-0.40 1.60 -1.19 1.10]	$\inf$	[-1.42 0.58 0.84 7.02]	$\inf$	$[0.05 \ 2.05 \ -2.09 \ 4.85]$	12.44	
10	$[-0.31 \ 1.69 \ -1.37 \ 2.17]$	$\inf$	$[0.16 \ 2.16 \ -2.31 \ 9.50]$ $12.77$		[-0.18 1.82 -1.64 9.25]	11.76	
20	$[0.81\ 2.81\ -3.63\ 3.53]$	14.74	[ 1.43 3.43 -4.86 6.63]	16.60	[-0.18 1.82 -1.64 9.25]	11.76	
40	$[0.72\ 2.72\ -3.44\ 5.03]$	14.45	$[0.29\ 2.29\ -2.58\ 1.91]$	13.17	[-0.18 1.82 -1.64 9.25]	11.76	
60	$[0.74\ 2.74\ -3.48\ 4.80]$	14.52	[ 1.12 3.12 -4.25 2.18] 15		[-0.18 1.82 -1.64 9.25]	11.76	
80	$[0.84\ 2.84\ -3.68\ 4.35]$	14.82	$[0.45\ 2.45\ -2.90\ 1.48]$	13.65	[-0.18 1.82 -1.64 9.25]	11.76	
100	$[0.82\ 2.82\ -3.64\ 3.96]$	14.76	$[0.19 \ 2.19 \ -2.39 \ 0.72]$	12.88	[-0.18 1.82 -1.64 9.25]	11.76	
	[ 0.02 2.02 0.01 0.00]			12.00	[-0.10 1.02 -1.04 3.20]		
	PINN		[nitial point: [2, 3, -2, 1] PINN+Lagaris	12.00	PINN+Lagaris+EC		
Iteration			Initial point: [2, 3, -2, 1]	OuC		OuC	
	PINN	]	Initial point: [2, 3, -2, 1] PINN+Lagaris Predicted solution		PINN+Lagaris+EC Predicted solution	OuC	
Iteration	PINN Predicted solution	OuC	Initial point: [2, 3, -2, 1] PINN+Lagaris	OuC	PINN+Lagaris+EC	OuC 13.54	
Iteration 0	PINN  Predicted solution  [-1.00 1.00 0.00 0.00]	OuC inf	Initial point: [2, 3, -2, 1]  PINN+Lagaris  Predicted solution  [ 0.41 2.41 -2.82 0.23]	OuC 13.54	PINN+Lagaris+EC Predicted solution [ 0.41 2.41 -2.82 0.23]	OuC 13.54 11.42	
Iteration 0 5	PINN  Predicted solution  [-1.00 1.00 0.00 0.00]  [-1.07 0.93 0.13 0.64]	OuC inf inf	Initial point: [2, 3, -2, 1]  PINN+Lagaris  Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.77 1.23 -0.46 1.52]	OuC 13.54 inf	PINN+Lagaris+EC Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.29 1.71 -1.41 1.77]		
Iteration 0 5 10	PINN  Predicted solution  [-1.00 1.00 0.00 0.00]  [-1.07 0.93 0.13 0.64]  [-1.42 0.58 0.85 2.04]	OuC inf inf inf	Initial point: [2, 3, -2, 1]  PINN+Lagaris  Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.77 1.23 -0.46 1.52] [ 0.04 2.04 -2.08 1.39]	OuC 13.54 inf 12.42	PINN+Lagaris+EC  Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.29 1.71 -1.41 1.77] [-0.29 1.71 -1.41 1.77]	OuC 13.54 11.42 11.42	
Iteration	PINN  Predicted solution  [-1.00 1.00 0.00 0.00]  [-1.07 0.93 0.13 0.64]  [-1.42 0.58 0.85 2.04]  [-1.44 0.56 0.87 4.04]	OuC inf inf inf inf	Initial point: [2, 3, -2, 1]  PINN+Lagaris  Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.77 1.23 -0.46 1.52] [ 0.04 2.04 -2.08 1.39] [ 0.85 2.85 -3.69 2.26]	OuC 13.54 inf 12.42 14.84	PINN+Lagaris+EC  Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.29 1.71 -1.41 1.77] [-0.29 1.71 -1.41 1.77] [-0.29 1.71 -1.41 1.77]	OuC 13.54 11.42 11.42 11.42	
Iteration 0 5 10 20 40	PINN  Predicted solution  [-1.00 1.00 0.00 0.00] [-1.07 0.93 0.13 0.64] [-1.42 0.58 0.85 2.04] [-1.44 0.56 0.87 4.04] [ 0.89 2.89 -3.77 3.24]	OuC inf inf inf 14.96	Initial point: [2, 3, -2, 1]  PINN+Lagaris  Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.77 1.23 -0.46 1.52] [ 0.04 2.04 -2.08 1.39] [ 0.85 2.85 -3.69 2.26] [ 0.26 2.26 -2.53 1.21]	OuC 13.54 inf 12.42 14.84 13.09	PINN+Lagaris+EC  Predicted solution  [ 0.41 2.41 -2.82 0.23] [-0.29 1.71 -1.41 1.77] [-0.29 1.71 -1.41 1.77] [-0.29 1.71 -1.41 1.77] [-0.29 1.71 -1.41 1.77]	OuC 13.54 11.42 11.42 11.42	

Initial point: [2, -2, 1, -2]									
Iteration	PINN		PINN+Lagaris		PINN+Lagaris+EC				
	Predicted solution	OuC	Predicted solution	OuC	Predicted solution	OuC			
0	[-0.65 1.35 -0.7 0. ]	inf	[-1.05 0.95 0.1 0. ]	inf	[-1.05 0.95 0.1 0. ]	inf			
5	[-0.68 1.32 -0.65 0.44]	$\inf$	[-2.78 -0.78 3.56 1.67]	$\inf$	[-0.10 1.90 -1.80 6.38]	12.01			
10	[-1.53 0.47 1.05 2.08]	$\inf$	[-1.21 0.79 0.41 5.23]	$\inf$	[-0.10 1.90 -1.80 6.38]	12.01			
20	[-1.66 0.34 1.32 5.54]	$\inf$	$[2.03\ 4.03\ -6.06\ 9.]$	18.39	[-0.23 1.77 -1.54 6.37]	11.62			
40	[ 0.42 2.42 -2.84 6.84]	13.56	[ 0.53 2.53 -3.05 3.46]	13.88	[-0.23 1.77 -1.54 6.37]	11.62			
60	[ 1.24 3.24 -4.47 6.27]	16.01	$[0.67\ 2.67\ -3.34\ 5.02]$	14.31	[-0.23 1.77 -1.54 6.37]	11.62			
80	[ 1.3 3.3 -4.6 5.42]	16.2	0.63 2.63 -3.25 3.59	14.18	[-0.23 1.77 -1.54 6.37]	11.62			
100	[ 1.27 3.27 -4.54 4.92]	16.11	[ 0.59 2.59 -3.19 3.69]	14.08	[-0.23 1.77 -1.54 6.37]	11.62			

Table 1: Comparison of PINN, PINN+Lagaris, and PINN+Lagaris+EC (Our approach) for three different initial points with predicted solutions and corresponding OuC values. inf indicates that the predicted solution is not in the feasible set.

method returns 'inf' 11 times for the three IP configurations, while the Lagaris method reduces this occurrence to 7. In contrast, our method returns 'inf' only twice, both times in the first round, indicating that it can reach a feasible solution more quickly.

- Neither the PINN method nor the PINN+Lagaris method maintains an optimal solution during the optimization process. As shown in Table 1, the PINN method and the PINN+Lagaris method achieve good OuC values of 12.33 and 12.04, respectively, for the IP [2, 3, -2, 1] at the 100th iteration. However, neither method maintains this level of performance, and their OuC values increase in subsequent iterations.
- The Lagaris method can improve the performance of vanilla PINN, as shown in Figure 6. However, this improvement is not substantial and varies depending on the IP configuration. For example, the improvement is significant for the first and third initial points but negligible for the second IP.

#### 304 5.3. Hyperparameter Study

In this subsection, we perform a hyperparameter study on the following NCOP.

#### Example 3:

$$\min_{x} f(x) = ||Cx - d||_{1}$$
s.t.
$$g_{1}(x) = x_{1}^{2} - x_{2} + x_{3} + x_{5} - x_{8} - 10 \le 0,$$

$$g_{2}(x) = |x_{1} - x_{3} + x_{4} + x_{7}| - 4.8 \le 0,$$

$$h(x) = x_{1} + x_{3} + x_{5} + x_{7} - 1 = 0,$$
(21)

where  $\|\cdot\|_1$  denotes the  $L^1$  norm, and

$$C = \begin{pmatrix} 1 & 4 & 2 & 2 & 1.3 & 4 & 2 & 1 \\ 2.8 & 2 & 1.6 & 3.2 & 0 & 2 & 1 & 1 \\ 1 & 4 & 2.3 & 2 & 2.5 & 0 & 5 & 1 \\ 1 & 1 & 1 & 3.1 & 2.3 & 0 & 0.8 & 1 \end{pmatrix}, \quad d = \begin{pmatrix} 1.5 \\ -3.8 \\ 6.2 \\ 7.5 \end{pmatrix}.$$
(22)

Example 3 involves a nonsmooth objective function and a nonsmooth inequality constraint  $g_2(x)$ .

To set up the algorithm, we choose the IP as an all-ones vector and the time range as [0, 10]. In the following, we discuss the computational performance for different neural network sizes and different learning rates.

Model Size. In Figures 7 (A) and (B), we investigate the computational performance of neural networks with various widths and depths, and the optimal result is obtained with a 700-neuron-wide, single-layer structure. In (A), with a maximum of 1000 training iterations, networks with fewer neurons (such as 100, 300, and 500) underperform due to their model capacity, limiting further improvements in OuC even with

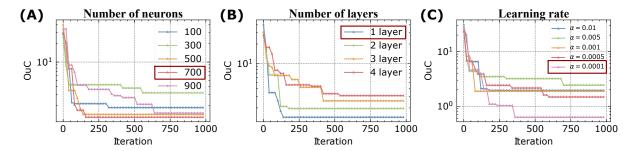


Figure 7: Hyperparameter study. (A): OuC performance on different numbers of neurons in a single layer neural network with a learning rate of 0.01. (B): OuC performance of different layers in a multilayer neural network with 500 neurons per layer and a learning rate of 0.01. (C): OuC performance at different learning rates in a two-layer neural network with 500 neurons per layer.

more training. Conversely, a network with more neurons (such as 900) shows underperformance, likely due to insufficient model training, and its OuC would potentially improve with additional training. In (B), a single layer neural network is shown to outperform other configurations. Taken together, these results underscore the need to find the most appropriate network structure for a given NCOP problem. An overly complex network would require an excessive amount of computing resources for optimization that may not be necessary. Conversely, a network that is too simple would not find the appropriate solution, regardless of the amount of training. Thus, the size of the neural network should be determined by factors related to the NCOP being solved. These include the number of decision variables, the constraints, and the complexity of both the objective and constraint functions.

Learning Rate. Figure 7(C) shows the performance of neural networks trained with different learning rates. At iteration 1000, the optimal performance is observed at the learning rate of  $\alpha = 0.0001$ . It is important to note that if we zoom into the first 100 iterations, a larger learning rate  $\alpha = 0.001$  is more effective. This suggests that the choice of learning rate should depend on the actual preferences of the user. The advantage of a large learning rate is that it can find a better prediction for the NCOP in a short time, while the disadvantage is that it performs poorly in the long run. In contrast, a small learning rate finds better solutions in the long run. Overall, the choice of learning rate should be determined by the user's specific requirements for speed and accuracy.

 $5.4. L^1$  Norm Minimization Problem

Consider the following NCOP problem:

## Example 4:

$$\min_{x} f(x) = ||x||_{1}$$
s.t.
$$g_{i}(x) = x_{10*(i-1)+1}^{2} + x_{10*(i-1)+2}^{2} + \dots + x_{10*(i-1)+10}^{2} - 20 \le 0, \quad i = 1, 2, \dots, 300$$

$$h(x) = Ax - b = 0.$$
(23)

	Description	Initial $f(x)$	Initial $\max_{i=1,2,\dots,300}(g_i(x))$	Initial $h(x)$	Initial OuC	OuC at iteration 100	OuC at iteration 1000	OuC at iteration 3000	OuC at iteration 10000
IP1	All-ones vector: $(1, 1, \dots, 1)$	3000.0	-10.0	5984.	inf	133.92	7.08	6.31	5.81
IP2	All-threes vector: $(3,3,\ldots,3)$	9000.0	70	17984	inf	202	118	25	6.00
IP3	All-negative ones vector: $(-1, -1, \dots, -1)$	3000.0	-10.0	-6016	inf	166.10	8.65	6.23	6.23
IP4	Alternating sequence of 2 and -2: $(2, -2, \dots, 2, -2)$	6000.0	20	-16	inf	643	16.62	16.62	16.62
IP5	First half entries are 1 and the rest are 3: $(1,1,\ldots,3)$	5700.0	70	14084	inf	946	380	344	95

Table 2: Description of IPs and their OuC performance at different algorithm iterations. Columns 2 to 6 describe the IPs and the their initial information, and columns 7 to 10 describe their OuC values at different training iterations.

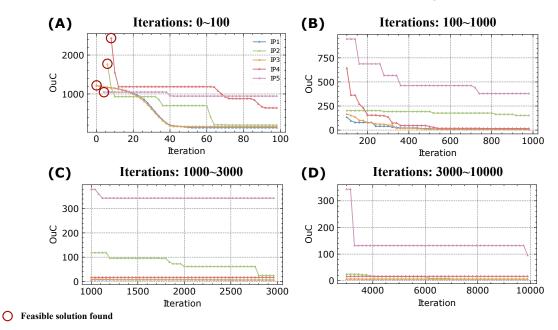


Figure 8: OuC performance with various IP configurations. The detailed descriptions for the five IPs are given in Table 2. In (A), the red circle indicates the first time a feasible solution is found. (A), (B), (C), and (D) show the results of the algorithm iterations  $0\sim100$ ,  $100\sim1000$ ,  $1000\sim3000$ , and  $3000\sim10000$ , respectively.

where  $x \in \mathbb{R}^{3000}$ ,  $A \in \mathbb{R}^{1 \times 3000}$ , with the first half entries of A being 1 and the rest 3, and b = 16.

**IPs Description.** We examine five different IPs, which are listed in Table 2. The IPs are used to configure Algorithm 1 to solve problem (23). As shown in the table, all the five IPs have large initial objective values, with IP2, IP4, and IP5 failing to satisfy the inequality constraint, i.e.,  $\max_{i=1,2,\ldots,300} (g_i(x)) \geq 0$ , and all IPs failing to meet the equality constraint, i.e.,  $h(x) \neq 0$ . These observations indicate that the IPs initially do not solve Example 4 well and are far from the optimal solution.

Based on the five IPs, the OuC values at different algorithm iterations are shown in Table 2 and Figure 8. We observe that:

As shown in Figure 8-(A), our algorithm quickly finds a feasible solution that satisfies both the inequality
and equality constraints. Moreover, once the first feasible solution is found, the subsequent solutions
given by the algorithm are all within the feasible set.

- The final solutions given by the algorithm are acceptable. After going through the entire solution process, the OuC values associated with the IPs decrease significantly. For IP1, the OuC decreases from 3000 to 5.81 (100% → 0.2%), and similar results can be found for other IPs. Given the fact that problem (23) has a known lower bound 0 for the objective value. This indicates that the final solutions produced by the proposed algorithm are already very close to the optimal solution.
- The OuC decreasing speed or convergence rate varies under different IP configuration. The convergence rate and final result of IP1~IP4 are significantly better than those of IP5. This may be because IP5 is the farthest from the optimal solution, and thus requires a larger time range and more model training. Nevertheless, the proposed algorithm still significantly improves the OuC performance of IP5 (100% → 1.6%) with the given experimental setup.
- Most of the decrease in OuC values occurs in the first 1000 iterations. In particular, IP1, IP2, and IP4 reduce the OuC values to about 10 within only 1000 iterations, which is already very close to the final result, demonstrating the efficiency of the algorithm.

#### 5.5. NCOP Problem Set

**Problem Set Description.** We construct a set of NCOPs based on Example 4 (23), where each NCOP problem takes the following form:

$$\min_{x} f(x) = ||x||_{1}$$
s.t.
$$g_{i}(x) = x_{10*(i-1)+1}^{2} + x_{10*(i-1)+2}^{2} + \dots + x_{10*(i-1)+10}^{2} - c^{(k)} \le 0, \quad i = 1, 2, \dots, 100$$

$$h(x) = A^{(k)}x - b^{(k)} = 0.$$
(24)

where  $x \in \mathbb{R}^{1000}$ ,  $A^{(k)} \in \mathbb{R}^{1000}$ ,  $b^{(k)} \in \mathbb{R}$ , and  $c^{(k)} \in \mathbb{R}$ .  $A^{(k)}$ ,  $b^{(k)}$ ,  $c^{(k)}$  are sampled from uniform distributions U(1,5), U(10,20), U(20,30), respectively. We randomly generate 100 different problem data  $\{(A^{(k)},b^{(k)},c^{(k)})\}$  to form 100 different NCOPs. These problem datasets  $\{(A^{(k)},b^{(k)},c^{(k)})\}_{k=1}^{100}$  can be accessed from the link<sup>1</sup>. Consistent with previous experimental subsections, we set the time range for all NCOPs to [0,10] and the IP  $y_0$  as an all-one vector.

Figure 9 shows the resolution of these 100 NCOPs using our neural network approach, and Table 3 shows the statistical information for these OuC results at different iterations. A clear trend can be seen is that all the OuC values decrease as training progresses. Starting from a mean of 372.79, the OuC value drops to 24.00 after 1000 iterations (a reduction from 100% to 6.4%). This trend of decreasing OuC values is not only observed at the mean, but also consistently observed at the 25%, 50%, 75%, and 90% quantiles. Of particular note is the impressive magnitude of this reduction. The significant reduction in OuC values

<sup>1</sup>https://drive.google.com/drive/folders/1D\_3HP-fBp9tew4IgDroIQtgVb8vU-vG0?usp=drive\_link

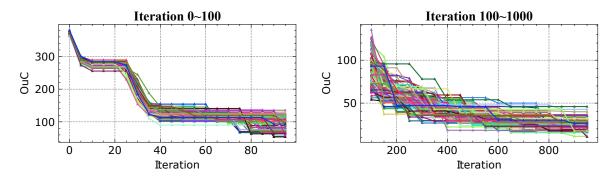


Figure 9: OuC values of the 100 NCOPs at different training iterations. Left and right show the results of iterations  $0\sim100$  and  $100\sim1000$ , respectively.

Iteration	Mean	STD	25% quantile	50% quantile	75% quantile	90% quantile
0	372.79	3.93	370.11	372.46	375.05	378.15
20	277.87	6.21	274.28	278.69	282.21	284.90
40	130.84	14.12	121.48	130.32	142.55	148.95
60	120.27	9.91	114.34	120.55	126.57	129.90
80	108.60	18.59	102.61	113.15	121.67	127.45
100	89.10	18.81	72.78	88.25	101.73	117.89
300	49.08	9.55	43.14	48.21	53.61	61.63
500	37.23	7.61	32.01	36.37	42.91	46.19
700	30.13	6.95	25.86	29.85	34.31	39.05
999	24.00	6.17	20.73	23.64	27.64	30.35

Table 3: Statistical data of OuC values for 100 NCOPs at different training iterations. The table shows the mean, standard deviation (STD), and values at the 25%, 50% (median), 75%, and 90% quantiles of the OuC distribution at each iteration.

indicates that our method efficiently navigates the solution space, making steady progress towards optimality.

This highlights the potential of our approach for tackling a wide variety of NCOPs. In summary, these results

provide a strong indication of the effectiveness of our proposed method for solving NCOPs, demonstrating

its robustness and efficiency over a wide range of problem datasets.

#### 373 6. Conclusion

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In this study, we present a deep learning-based methodology for solving NCOPs. The proposed methodology is a fruitful fusion of neurodynamic optimization and PINNs. Methodologically, we have extended the PINN approach to accommodate neurodynamic optimization. In addition, we have developed a novel training algorithm that increases computational efficiency by exploiting the problem structure of NCOPs. Experimental results have demonstrated the effectiveness of the proposed method on a number of NCOPs. The computational performance can be further improved by tuning the hyperparameters and refining the training details.

In addition, our results have identified several avenues for future research. Specifically, we recommend investigating better methods for selecting initial points and time ranges, exploring different network architectures and advanced neurodynamic optimization techniques. Further development in these areas will undoubtedly improve the effectiveness and robustness of our approach, making it an important tool for

385 addressing NCOPs in diverse applications.

#### 386 Bibliography

- Baydin, A. G., Pearlmutter, B. A., Radul, A. A., & Siskind, J. M. (2018). Automatic differentiation in machine learning: a survey. *Journal of machine learning research*, 18.
- Bian, W., Ma, L., Qin, S., & Xue, X. (2018). Neural network for nonsmooth pseudoconvex optimization with general convex constraints. *Neural Networks*, 101, 1–14.
- Biloš, M., Sommer, J., Rangapuram, S. S., Januschowski, T., & Günnemann, S. (2021). Neural flows: Efficient alternative to neural odes. *Advances in Neural Information Processing Systems*, 34, 21325–21337.
- Bradbury, J., Frostig, R., Hawkins, P., Johnson, M. J., Leary, C., Maclaurin, D., Necula, G., Paszke,
- <sup>394</sup> A., VanderPlas, J., Wanderman-Milne, S., & Zhang, Q. (2018). JAX: composable transformations of
- Python+NumPy programs. URL: http://github.com/google/jax.
- Burden, R. L., Faires, J. D., & Burden, A. M. (2015). Numerical analysis. Cengage learning.
- Che, H., & Wang, J. (2018). A two-timescale duplex neurodynamic approach to biconvex optimization. *IEEE Transactions on Neural Networks and Learning Systems*, 30, 2503–2514.
- Che, H., & Wang, J. (2019). A collaborative neurodynamic approach to global and combinatorial optimization. Neural Networks, 114, 15–27.
- Chen, F., Sondak, D., Protopapas, P., Mattheakis, M., Liu, S., Agarwal, D., & Giovanni, M. D. (2020).
- 402 NeuroDiffEq: A Python package for solving differential equations with neural networks. Journal of Open
- Source Software, 5, 1931. URL: https://doi.org/10.21105/joss.01931. doi:10.21105/joss.01931.
- Chen, R. T., Rubanova, Y., Bettencourt, J., & Duvenaud, D. K. (2018). Neural ordinary differential equations. Advances in neural information processing systems, 31.
- De Ryck, T., Jagtap, A. D., & Mishra, S. (2022). Error estimates for physics informed neural networks approximating the navier-stokes equations. arXiv preprint arXiv:2203.09346, .
- Guo, Z., Liu, Q., & Wang, J. (2011). A one-layer recurrent neural network for pseudoconvex optimization
   subject to linear equality constraints. *IEEE Transactions on Neural Networks*, 22, 1892–1900.
- Hopfield, J. J., & Tank, D. W. (1985). "Neural" computation of decisions in optimization problems. Biological
   cybernetics, 52, 141–152.
- Hou, Z.-G., Cheng, L., Tan, M., & Wang, X. (2010). Distributed adaptive coordinated control of multi-
- manipulator systems using neural networks. Robot intelligence: An advanced knowledge processing ap-
- proach, (pp. 49–69).

- 415 Hu, Z., Jagtap, A. D., Karniadakis, G. E., & Kawaguchi, K. (2022a). Augmented physics-informed neu-
- ral networks (apinns): A gating network-based soft domain decomposition methodology. arXiv preprint
- arXiv:2211.08939, .
- <sup>418</sup> Hu, Z., Jagtap, A. D., Karniadakis, G. E., & Kawaguchi, K. (2022b). When do extended physics-informed
- neural networks (xpinns) improve generalization? SIAM Journal on Scientific Computing, 44, A3158-
- 420 A3182.
- 421 Jagtap, A. D., & Karniadakis, G. E. (2023). How important are activation functions in regression and
- classification? a survey, performance comparison, and future directions. Journal of Machine Learning for
- Modeling and Computing, 4.
- Jagtap, A. D., Kawaguchi, K., & Em Karniadakis, G. (2020a). Locally adaptive activation functions with
- slope recovery for deep and physics-informed neural networks. Proceedings of the Royal Society A, 476,
- 426 20200334.
- Jagtap, A. D., Kawaguchi, K., & Karniadakis, G. E. (2020b). Adaptive activation functions accelerate
- convergence in deep and physics-informed neural networks. Journal of Computational Physics, 404, 109136.
- <sup>429</sup> Jagtap, A. D., Kharazmi, E., & Karniadakis, G. E. (2020c). Conservative physics-informed neural networks on
- discrete domains for conservation laws: Applications to forward and inverse problems. Computer Methods
- in Applied Mechanics and Engineering, 365, 113028.
- <sup>432</sup> Jagtap, A. D., Mao, Z., Adams, N., & Karniadakis, G. E. (2022a). Physics-informed neural networks for
- inverse problems in supersonic flows. Journal of Computational Physics, 466, 111402.
- Jagtap, A. D., Shin, Y., Kawaguchi, K., & Karniadakis, G. E. (2022b). Deep kronecker neural networks: A
- general framework for neural networks with adaptive activation functions. Neurocomputing, 468, 165–180.
- <sup>436</sup> Jia, W., Liu, N., & Qin, S. (2021). An adaptive continuous-time algorithm for nonsmooth convex resource
- allocation optimization. IEEE Transactions on Automatic Control, 67, 6038–6044.
- 438 Kennedy, M. P., & Chua, L. O. (1988). Neural Networks for Nonlinear Programming. IEEE Transactions
- on Circuits and Systems, 35, 554-562. doi:10.1109/31.1783.
- 440 Kingma, D. P., & Ba, J. (2014). Adam: A method for stochastic optimization. arXiv preprint
- arXiv:1412.6980,.
- 442 Lagaris, I. E., Likas, A., & Fotiadis, D. I. (1998). Artificial neural networks for solving ordinary and partial
- differential equations. IEEE Transactions on Neural Networks, 9, 987–1000. doi:10.1109/72.712178.
- 444 Liu, N., Wang, J., & Qin, S. (2022). A one-layer recurrent neural network for nonsmooth pseudoconvex
- optimization with quasiconvex inequality and affine equality constraints. Neural Networks, 147, 1–9.

- 446 Lu, L., Meng, X., Mao, Z., & Karniadakis, G. E. (2021). DeepXDE: A Deep Learning Library for Solving
- Differential Equations. SIAM Review, 63, 208-228. URL: http://dx.doi.org/10.1137/19M1274067.
- doi:10.1137/19m1274067.
- 449 Mao, Z., Jagtap, A. D., & Karniadakis, G. E. (2020). Physics-informed neural networks for high-speed flows.
- 450 Computer Methods in Applied Mechanics and Engineering, 360, 112789.
- <sup>451</sup> Mattheakis, M., Sondak, D., Dogra, A. S., & Protopapas, P. (2020). Hamiltonian neural networks for solving
- equations of motion. arXiv preprint arXiv:2001.11107, .
- 453 Mishra, S., & Molinaro, R. (2022). Estimates on the generalization error of physics-informed neural networks
- for approximating a class of inverse problems for pdes. IMA Journal of Numerical Analysis, 42, 981–1022.
- Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein,
- N., Antiga, L., Desmaison, A., Köpf, A., Yang, E., DeVito, Z., Raison, M., Tejani, A., Chil-
- amkurthy, S., Steiner, B., Fang, L., Bai, J., & Chintala, S. (2019). PyTorch: An impera-
- tive style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer,
- 459 F. d Alché-Buc, E. Fox, & R. Garnett (Eds.), Advances in Neural Information Processing Sys-
- tems. Curran Associates, Inc. volume 32. URL: https://proceedings.neurips.cc/paper/2019/file/
- bdbca288fee7f92f2bfa9f7012727740-Paper.pdf.arXiv:1912.01703.
- <sup>462</sup> Penwarden, M., Jagtap, A. D., Zhe, S., Karniadakis, G. E., & Kirby, R. M. (2023). A unified scalable
- framework for causal sweeping strategies for physics-informed neural networks (pinns) and their temporal
- decompositions. arXiv preprint arXiv:2302.14227, .
- Qin, S., & Xue, X. (2014). A two-layer recurrent neural network for nonsmooth convex optimization problems.
- 466 IEEE transactions on neural networks and learning systems, 26, 1149–1160.
- 467 Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning
- framework for solving forward and inverse problems involving nonlinear partial differential equations. Jour-
- nal of Computational Physics, 378, 686-707. URL: https://www.sciencedirect.com/science/article/
- 470 pii/S0021999118307125. doi:https://doi.org/10.1016/j.jcp.2018.10.045.
- Shukla, K., Jagtap, A. D., Blackshire, J. L., Sparkman, D., & Karniadakis, G. E. (2021a). A physics-informed
- neural network for quantifying the microstructural properties of polycrystalline nickel using ultrasound
- data: A promising approach for solving inverse problems. IEEE Signal Processing Magazine, 39, 68–77.
- 474 Shukla, K., Jagtap, A. D., & Karniadakis, G. E. (2021b). Parallel physics-informed neural networks via
- domain decomposition. Journal of Computational Physics, 447, 110683.
- <sup>476</sup> Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E.,
- Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J.,

- Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., Carey, C. J., Polat, Feng, Y., Moore,
- E. W., VanderPlas, J., Laxalde, D., Perktold, J., Cimrman, R., Henriksen, I., Quintero, E. A., Harris,
- 480 C. R., Archibald, A. M., Ribeiro, A. H., Pedregosa, F., van Mulbregt, P., Vijaykumar, A., Bardelli, A. P.,
- Rothberg, A., Hilboll, A., Kloeckner, A., Scopatz, A., Lee, A., Rokem, A., Woods, C. N., Fulton, C.,
- Masson, C., Häggström, C., Fitzgerald, C., Nicholson, D. A., Hagen, D. R., Pasechnik, D. V., Olivetti, E.,
- Martin, E., Wieser, E., Silva, F., Lenders, F., Wilhelm, F., Young, G., Price, G. A., Ingold, G.-L., Allen,
- G. E., Lee, G. R., Audren, H., Probst, I., Dietrich, J. P., Silterra, J., Webber, J. T., Slavič, J., Nothman,
- J., Buchner, J., Kulick, J., Schönberger, J. L., de Miranda Cardoso, J. V., Reimer, J., Harrington, J.,
- Rodríguez, J. L. C., Nunez-Iglesias, J., Kuczynski, J., Tritz, K., Thoma, M., Newville, M., Kümmerer, M.,
- Bolingbroke, M., Tartre, M., Pak, M., Smith, N. J., Nowaczyk, N., Shebanov, N., Pavlyk, O., Brodtkorb,
- P. A., Lee, P., McGibbon, R. T., Feldbauer, R., Lewis, S., Tygier, S., Sievert, S., Vigna, S., Peterson,
- S., More, S., Pudlik, T. et al. (2020). SciPy 1.0: fundamental algorithms for scientific computing in
- Python. Nature Methods, 17, 261-272. URL: http://www.nature.com/articles/s41592-019-0686-2.
- doi:10.1038/s41592-019-0686-2.
- Wang, Y., Wang, J., & Tao, D. (2023). Neurodynamics-driven supervised feature selection. Pattern Recognition, 136, 109254.
- <sup>494</sup> Xia, Y., Feng, G., & Wang, J. (2008). A novel recurrent neural network for solving nonlinear optimization problems with inequality constraints. *IEEE Transactions on neural networks*, 19, 1340–1353.
- <sup>496</sup> Xia, Y., & Wang, J. (2000). A recurrent neural network for solving linear projection equations. Neural

  Networks, 13, 337–350.