QCQP-Net: Reliably Learning Feasible Alternating Current Optimal Power Flow Solutions Under Constraints

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Abstract

At the heart of power system operations, alternating current optimal power flow (ACOPF) studies the generation of electric power in the most economical way under network-wide load requirement, and can be formulated as a highly structured non-convex quadratically constrained quadratic program (QCQP). Optimization-based solutions to ACOPF (such as ADMM or interior-point method), as the classic approach, require large amount of computation and cannot meet the need to repeatedly solve the problem as load requirement frequently changes. On the other hand, learning-based methods that directly predict the ACOPF solution given the load input incur little computational cost but often generates infeasible solutions (i.e. violate the constraints of ACOPF). In this work, we combine the best of both worlds – we propose an innovated framework for learning ACOPF, where the input load is mapped to the ACOPF solution through a neural network in a computationally efficient and reliable manner. Key to our innovation is a specific-purpose "activation function" defined implicitly by a QCQP and a novel loss, which enforce constraint satisfaction. We show through numerical simulations that our proposed method achieves superior feasibility rate and generation cost in situations where the existing learning-based approaches fail.

Keywords: Alternating current optimal power flow, differentiable convex programming, non-convex quadratically constrained quadratic program

1. Introduction

As one of the most important problems in modern power system operations, the study of alternating current optimal power flow (ACOPF) focuses on finding the most economical power generation scheme under network-wide load requirement and physical transmission constraints. Mathematically, ACOPF can be formulated as non-convex quadratically constrained quadratic program (QCQP) problem with the number of decision variables and constraints scaling proportionally with nodes and transmission lines in the power grid. The most common approach for reliably solving the ACOPF problem is limited to classical nonlinear optimization algorithms, such as interior-point method, which are highly computationally expensive for modern large-scale power systems involving at least thousands of nodes. Furthermore, the constant fluctuations of the loads and conditions of

the transmission line in addition to the uncertainty of energy supplies of renewable energy resources require the ACOPF problem to be solved repeatedly online, making the current optimization-based methods limited in real life.

With the recent advances in deep learning infrastructure and the improved ability to collect and store data, learning-based approaches have been proposed to solve complex optimization problems. The first attempt to solve ACOPF with machine learning has been made in Guha et al. (2019), where the authors employ a simple feed-forward neural network to parameterize the mapping from the input to the output of the ACOPF problem. However, the special structure of the ACOPF problem presents a peculiar challenge. The constraints define a nonlinear non-convex feasibility set around the optimal solution; while the neural network can consistently generate outputs close to the optimal solution in the Euclidean distance, they are not guaranteed to lie within the constraint set. In other words, learning-based approaches often produce highly infeasible solutions that cannot be directly deployed.

To address this issue, various methods have been proposed to encourage the output of the neural network to obey ACOPF constraints (Pan et al., 2022; Donti et al., 2021). In these papers, they recognize that the solution of an ACOPF problem can be divided into 1) independent variables that control the power system operation and 2) dependent state variables that can be determined from control variables by solving the power flow equations. They propose predicting the control variables while leveraging additional loss functions to penalize constraint violation on the resulting state variables. The constraint violation loss is not readily differentiable, and different approaches such as zeroth order gradient or implicit function theorem are taken in these works to estimate/derive its gradient.

Although Pan et al. (2022); Donti et al. (2021) significantly improves the constraint satisfaction, they build on the assumption that for any given control variable produced by the neural network they can always find a feasible solution (state variables) satisfying the power flow equations. This assumption may not hold under high demand fluctuations, in which case the trained neural networks may be unreliable and cannot provide a meaningful solution. To mitigate this issue, we solve a relaxation of the power flow equations with a focus on minimizing the constraint violations of these equations, which is also desirable for a reliable and robust operation of power systems.

To achieve this, we formulate our relaxation problem as a non-convex QCQP and integrate the QCQP solver into the neural network as a differentiable activation function. We establish the differentiability of the non-convex QCQP activation function by extending the sensitivity analysis techniques in Amos and Kolter (2017), which only handles convex quadratic programs. Equipped with properly designed loss functions, our proposed framework effectively deals with the infeasibility issue observed in current learning-based approaches such as Pan et al. (2022) while showing similar competitive performance in feasible cases. Similar to ours, Singh et al. (2021) has also used sensitivity analysis results to approximate the Jacobian containing the derivatives of predictions with respect to input changes by penalizing its mismatch in the loss function in addition to prediction errors. However, their approach does not enforce constraint satisfaction while ours finds a solution with least constraint violations by using our differentiable non-convex QCQP layer in the neural network.

1.1. Main Contributions

In this work, our goal is to design an accurate and reliable end-to-end neural network architecture for predicting the solution of ACOPF while achieving high computational efficiency in both training and inference phases. As the first main contribution of our work, we propose a systematic pipeline and loss function for training a feed-forward neural network that maps the input load to the independent variables of the ACOPF solution. The state variables are then produced from the predicted independent variables by solving a relaxed variant of the power flow equations, which can be expressed as a non-convex QCQP. The relaxed power flow equations, as we discuss in details in Section 3, are an important innovation of this work and allow us to train the neural network in a much more stable way when the control variables are imperfectly predicted.

We can regard the relaxed power flow equations from a different angle as a specific-purpose activation function tailored to the ACOPF problem. As a second main contribution, we establish the conditions under which this activation function is a differentiable mapping from the control variables to the state variables, and derive closed-form expressions of the (sub)gradient. This ensures that the downstream constraint violation loss on the state variables can be back-propagated. We name our proposed architecture QCQP-Net and show its structure in Figure 1. We numerically evaluate the performance of the proposed QCQP-Net on ACOPF problems of various scales in Section 5. The results show that in large power systems with wide load variations where the existing approaches fail to learn, QCQP-Net stably learns highly feasible solutions with low generation costs.

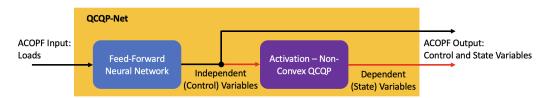


Figure 1: QCQP-Net Architecture. Computation path in red only taken in training phase.

1.2. Related Works

This paper presents a novel learning framework specifically designed for reliably and efficiently solving ACOPF problems. It closely relates to the existing works that study ACOPF from both optimization and deep learning perspectives, and is inspired by recent advances in differentiable convex programming. We discuss the relevant literature in these domains to give context to our novelty.

ACOPF: From an optimization perspective, a large volume of works seek to design provably convergent algorithms for ACOPF (Cvijic et al., 2012; Kar et al., 2017; Yuan and Hesamzadeh, 2019; Sun and Sun, 2021; Wang et al., 2022) and to numerically accelerate classic nonlinear optimization solver through massively parallelized computation (Roberge et al., 2016; Huang and Dinavahi, 2017; Araújo et al., 2019; Kim and Kim, 2022; Zhang et al., 2023). In the learning regime, two main lines of work include 1) learning an end-to-end mapping from input of the ACOPF problem to the output (Singh et al., 2021; Donti et al., 2021; Nellikkath and Chatzivasileiadis, 2022; Pan et al., 2022) and 2) learning parameters and/or sub-steps within an optimization solver (Baker, 2019; Zhang and Zhang, 2022; Zeng et al., 2022; Sadat and Sahraei-Ardakani, 2021). While the former approaches allow for much faster inference, it may suffer higher constraint violation risk than the

latter (which makes it less reliable and suitable for solving safety-critical power system problems). Our work is exactly motivated to address this issue.

Differentiable Convex Programming: Introduced in Amos and Kolter (2017) and later popularized by Agrawal et al. (2019), differentiable convex programming treats a convex optimization problem as an implicit definition of a mapping from the parameters of the optimization problem to the optimal solution. By carefully analyzing how a unit change in the parameters impacts the optimal solution through the lens of KKT conditions, Amos and Kolter (2017); Agrawal et al. (2019) devise an innovative method for computing the (sub)gradients of the mapping. Applications of differentiable convex programming span neural network layer design (Amos and Kolter, 2017; Agrawal et al., 2019; Wang et al., 2019), inverse problems (Liang et al., 2019; Mourya and Mota, 2023), computer vision (Chen et al., 2020; Yeh et al., 2022), mechanism design (Curry et al., 2022; Zeng et al., 2023), and many other domains. In this work we develop techniques to differentiable through a QCQP with quadratic equality constraints, which is much more challenging to handle due to the non-convexity. However, important pieces of our innovation are built upon Amos and Kolter (2017).

Outline of the paper. The rest of the paper is structured as follows. In Section 2, we present the formulation of ACOPF and its important structure. In Section 3, we propose a novel loss function for training an end-to-end prediction model for ACOPF by exploiting the problem structure. Evaluating the gradient of the loss function requires differentiating through a non-convex QCQP with quadratic equality constraint. We discuss how such differentiation can be performed in Section 4. Section 5 presents the numerical simulations that demonstrate the stable and effective training of our end-to-end prediction model. Finally, we conclude in Section 6.

2. ACOPF Formulation

We consider a power system represented by a connected graph with a set $(\mathcal{B}, \mathcal{L})$ of buses and connected lines, respectively. Each node $i \in \mathcal{B}$, also referred to as a bus, has a complex power demand denoted as $d_i = p_i^d + j * q_i^d$ for some $p_i^d, q_i^d \in \mathbb{R}$. The voltage of bus i is $v_i \in \mathbb{C}$, and we use e_i and f_i to denote the real and imaginary parts, i.e. $v_i = e_i + j * f_i$. A subset of buses may have a power generator attached, and we use $\mathcal{B}_{PV} \subseteq \mathcal{B}$ to denote the set of nodes with at least one generator attached. We use \mathcal{G}_i to denote the collections of generators attached to bus i and define $\mathcal{G} := \bigcup_{i \in \mathcal{B}} \mathcal{G}_i$. Each generator $g \in \mathcal{G}$ can generate complex power with a real part $p_g \in \mathbb{R}$ and imaginary part $q_g \in \mathbb{R}$.

The edge of the graph, also referred to as a branch, represents a directed transmission line between two buses. For each branch $(i,j) \in \mathcal{L}$ from bus i to j, p_{ij} and q_{ij} denote the real and imaginary power flow in the normal direction. Power may also flow in the reverse direction, and we use p_{ij} and q_{ij} to denote the reverse power flow through branch $(i,j) \in \mathcal{L}$. It is worth noting that p_{ji} and q_{ji} may not simply be the negative of p_{ij} and q_{ij} but are determined from the voltage at bus i and j by solving a system of power flow equations (1d)-(1g), where parameters B_{ij} , G_{ij} , B_{ji} , $G_{ji} \in \mathbb{R}$ are dictated by the physical properties of the power system.

For any bus i, we use $\mathcal{N}_i^{\text{from}}$ and $\mathcal{N}_i^{\text{to}}$ to denote its (directed) neighbors, i.e. $\mathcal{N}_i^{\text{from}} = \{j: (i,j) \in \mathcal{L}\}$ and $\mathcal{N}_i^{\text{to}} = \{j: (j,i) \in \mathcal{L}\}$.

The objective of the ACOPF problem, formulated in (1), is to find the most economic set points of generators that satisfy the power demand p_i^d, q_i^d at every node i under capacity limits and physical transmission laws. The generation cost function is quadratic in the real power output, where $c_{1,g}, c_{2,g} \in \mathbb{R}_+$ are non-negative constant parameters for all $g \in \mathcal{G}$. Eqs. (1b)-(1c) are known

as power balance equations and encode the power transmission laws along with Eqs. (1d)-(1g). Eqs. (1h) state that the power flow magnitude between bus i and j cannot exceed the limit \bar{s}_{ij} . Eq. (1i) restricts the voltage at a bus to lie within a tolerable range. Eqs. (1j) represent the capacity of the power generators. The optimization problem can be expressed in a matrix form as a QCQP, but is obviously non-convex due to the quadratic equality constraints in Eqs. (1b)-(1g).

$$\min_{p_g, q_g, f_i, e_i, p_{ij}, q_{ij}, p_{ji}, q_{ji}} \sum_{g \in \mathcal{G}} (c_{2,g} p_g^2 + c_{1,g} p_g)$$
(1a)

s.t.
$$G_{ii}(e_i^2 + f_i^2) + \sum_{j \in \mathcal{N}_i^{\text{fr}}} p_{ij} + \sum_{j \in \mathcal{N}_i^{\text{to}}} p_{ji} - \sum_{g \in \mathcal{G}_i} p_g + p_i^d = 0, \quad \forall i \in \mathcal{B}$$
 (1b)

$$-B_{ii}(e_i^2 + f_i^2) + \sum_{j \in \mathcal{N}_i^{\text{fr}}} q_{ij} + \sum_{j \in \mathcal{N}_i^{\text{to}}} q_{ji} - \sum_{g \in \mathcal{G}_i} q_g + q_i^d = 0, \quad \forall i \in \mathcal{B}$$
 (1c)

$$p_{ij} = -G_{ij} \left(e_i^2 + f_i^2 - e_i e_j - f_i f_j \right) - B_{ij} \left(e_i f_j - e_j f_i \right), \quad \forall (i, j) \in \mathcal{L}$$
 (1d)

$$p_{ji} = -G_{ji} \left(e_j^2 + f_j^2 - e_j e_i - f_j f_i \right) - B_{ji} \left(e_j f_i - e_i f_j \right), \quad \forall (i, j) \in \mathcal{L}$$
 (1e)

$$q_{ij} = B_{ij} \left(e_i^2 + f_i^2 - e_i e_j - f_i f_j \right) - G_{ij} \left(e_i f_j - e_j f_i \right), \quad \forall (i,j) \in \mathcal{L}$$
 (1f)

$$q_{ji} = B_{ji} \left(e_j^2 + f_j^2 - e_j e_i - f_j f_i \right) - G_{ji} \left(e_j f_i - e_i f_j \right), \quad \forall (i, j) \in \mathcal{L}$$
 (1g)

$$p_{ij}^2 + q_{ij}^2 \le \bar{s}_{ij}^2, \quad p_{ji}^2 + q_{ji}^2 \le \bar{s}_{ij}^2, \quad \forall (i,j) \in \mathcal{L},$$
 (1h)

$$\underline{v}_i^2 \le e_i^2 + f_i^2 \le \bar{v}_i^2, \quad \forall i \in \mathcal{B} \tag{1i}$$

$$\underline{p}_{q} \le p_{g} \le \overline{p}_{g}, \quad \underline{q}_{q} \le q_{g} \le \overline{q}_{g}, \quad \forall g \in \mathcal{G}, \tag{1j}$$

The input to the optimization program is the power demands $x = \{p_i^d, q_i^d : i \in \mathcal{B}\} \in \mathbb{R}^{2|\mathcal{B}|}$. The output is the decision variables p_g, q_g, e_i, f_i , which are heavily coupled. When real power p_g and voltage magnitude v_i are given for all $g \in \mathcal{G}, i \in \mathcal{B}_{PV}$, the rest of the decision variables can be determined by the following system of power flow equations (if a solution exists):

(1b)
$$- (1g), \quad e_i^2 + f_i^2 = v_i^2, \quad \forall i \in \mathcal{B}_{PV}.$$
 (2)

We name $y_c = ((p_g)_{g \in \mathcal{G}_i}, v_i)_{i \in \mathcal{B}_{PV}}$ the control variables, as the specification of y_c is sufficient for controlling the operation of the power system. We denote by y_s the other decision variables of Eq. (1) and refer to them as state variables. Letting $\mathcal{Y} \subseteq \mathbb{R}^{|\mathcal{G}| + |\mathcal{B}_{PV}|}$ and $\mathcal{S} \subseteq \mathbb{R}^{|\mathcal{G}| + 2|\mathcal{B}| + 4|\mathcal{L}|}$ denote the space of control and state variables, we define $PF : \mathcal{Y} \times \mathbb{R}^{2|\mathcal{B}|} \to \mathcal{S}$ as the mapping from control variables and input demands to the state variables as the solution of Eq. (2). Under this notation, we can rewrite the ACOPF objective in Eq. (1) as

$$\min_{y_c \in \mathcal{C}_c, y_s \in \mathcal{C}_s} \sum_{g \in \mathcal{G}} (c_{2,g} p_g^2 + c_{1,g} p_g) \quad \text{subject to} \quad y_s \in PF(y_c, x)$$
(3)

where $C_c \subseteq \mathcal{Y}$ and $C_s \subseteq \mathcal{S}$ represent the (convex) feasibility sets of control and state variables, respectively, as follows:

$$\mathcal{C}_{c} = \left\{ ((p_{g})_{\mathcal{G}_{i}}, v_{i})_{i \in \mathcal{B}_{PV}} : \underline{p}_{g} \leq p_{g} \leq \overline{p}_{g}, \ \forall g \in \mathcal{G}, \quad \underline{v}_{i} \leq v_{i} \leq \overline{v}_{i}, \ \forall i \in \mathcal{B}_{PV} \right\}, \\
\mathcal{C}_{s} = \left\{ ((q_{i}^{g})_{i \in \mathcal{G}_{i}}, e_{i}, f_{i}, p_{ij}, q_{ij}, p_{ji}, q_{ji})_{i \in \mathcal{B}} : \underline{v}_{i}^{2} \leq e_{i}^{2} + f_{i}^{2} \leq \overline{v}_{i}^{2}, \ \forall i \in \mathcal{B} \setminus \mathcal{B}_{PV}, \\
\underline{q}_{g} \leq q_{g} \leq \overline{q}_{g}, \ \forall g \in \mathcal{G}, \quad p_{ij}^{2} + q_{ij}^{2} \leq \overline{s}_{ij}^{2}, \ p_{ji}^{2} + q_{ji}^{2} \leq \overline{s}_{ij}^{2}, \ \forall (i, j) \in \mathcal{L} \right\}.$$

Note that $PF(y_c, x)$ many have a unique solution, multiple solutions, or no solution for arbitrary control variable y_c and load x.

3. A Constrained Machine Learning Approach to ACOPF

The (non-convex) QCQP in (3) can be stably solved by various existing algorithms including the interior-point method. However, as the size of power system scales up, the amount of computation required by an optimization solver becomes enormous. Considering the fact that the ACOPF problem needs to be repeatedly solved in real-life power systems as the power demand constantly changes, we are motivated to investigate alternative approaches that trade-off slight sub-optimality of the solution for computational efficiency.

3.1. ML Approach for Control Prediction

Given a fixed power system, our aim is to design a data-driven learning-based method that leverages samples of paired input and output of the ACOPF problem solved for the specific system under varying loads. Suppose we have N sample pairs $\{(x^n,y^n):n=1,\ldots,N\}$ where x^n denotes the power demands from the n_{th} sample and y^n denotes the optimal solution of (1) under input x^n , which we can split into control and state variables $y^n=(y^n_c,y^n_s)$. A straightforward supervised learning framework for predicting the control variables y^n_c from x^n looks for a mapping $g:\mathbb{R}^{2|\mathcal{B}|}\to\mathcal{Y}$ that minimizes the data mismatch as follows: $\min_g\sum_{n=1}^N\|g(x^n)-y^n_c\|^2$, where we parameterize the mapping g by a feed-forward neural network.

Despite its simplicity, this objective does not enforce constraint satisfaction, especially on the state variable. Specifically, $PF(g(x^n), x^n)$, the state variable resulting from the predicted control, may not lie within the constraint set C_s . Such infeasible solutions require post-processing before they can be deployed; even after post-processing, the solutions are not guaranteed to be feasible and may degrade in generation cost.

To explicitly enforce the constraints to be satisfied, our work proposes a more sophisticated loss function that penalizes both data mismatch and constraint violation. Our initial proposal is to solve

$$\min_{g} \sum_{n=1}^{N} \left(\|g(x^{n}) - y_{c}^{n}\|^{2} + w \cdot r_{\mathcal{C}_{s}} \left(PF(g(x^{n}), x^{n}) \right) \right)$$
(4)

where w is a given weight value (e.g. 0.1 and 1.0 for our numerical experiment), and $r_{\mathcal{C}_s}$ is the following penalty associated with the violation of constraint set \mathcal{C}_s

$$\begin{split} r_{\mathcal{C}_s}\!\!\left((q_g)_{g\in\mathcal{G}},(e_i,f_i)_{i\in\mathcal{B}},(p_{ij},q_{ij})_{ij\in\mathcal{L}},(p_{ji},q_{ji})_{ij\in\mathcal{L}}\right) \! = \! \sum_{g\in\mathcal{G}}\!\!\left(\max\{0,\underline{q}_g - q_g\} + \max\{0,q_g - \overline{q}_g\}\right) \\ + \sum_{(i,j)\in\mathcal{L}}\!\!\left(\max\{0,p_{ij}^2 + q_{ij}^2 - \overline{s}_{ij}^2\} + \max\{0,p_{ji}^2 + q_{ji}^2 - \overline{s}_{ij}^2\}\right). \end{split}$$

3.2. Infeasible Power Flow System

Training under the loss function in (4), however, may be unstable. The challenge comes from the fact that we may not always find a feasible solution $PF(g(x^n), x^n)$. This happens either because $PF(g(x^n), x^n) = \emptyset$ under control prediction $g(x^n)$ and/or load sample x^n , or because a numerical

method (e.g. Newton-Raphson) cannot find a solution due to the lack of convergence guarantee. Training stagnates when this issue arises and the entire learning pipeline can be broken. To address the issue and stabilize training, we introduce slack variables $\sigma \in \mathbb{E}^{2|\mathcal{B}|}$ that captures the the minimum gap in power demand satisfaction for the power flow equations to have a solution. Under the control prediction $g(x^n)$ and demand load x^n , we find approximate state variables by solving the following optimization program (which can be written as a non-convex QCQP after a simple reformulation of the objective):

$$(\widehat{y}_s^n, \widehat{\sigma}^n) \in \operatorname{argmin}_{y_s \in \mathcal{S}, \sigma \in \mathbb{R}^{2|\mathcal{B}|}} \|\sigma\|_1 \quad \text{subject to} \quad y_s \in PF(g(x^n), x^n + \sigma),$$
 (5)

where $||sigma||_1$ is reformulated and linearized with two nonnegative slack variables. To stably learn a constrained ACOPF solution, we ultimately solve the bi-level optimization problem

$$\min_{g} L(g) \triangleq \sum_{n=1}^{N} (\|g(x^n) - y_c^n\|^2 + w \cdot r_{\mathcal{C}_s}(\widehat{y}_s^n))$$
 (6)

where \widehat{y}_s^n is defined in the lower-level optimization problem (5). The loss function is tailored to the learning of ACOPF solutions leveraging the structure of the problem and is novel in the literature to the best of our knowledge. From a computational perspective, this loss, nevertheless, introduces significant challenges. Since \widehat{y}_s^n is a function of $g(x^n)$ only defined implicitly through (5), it is unclear how the gradient of $r_{\mathcal{C}_s}(\widehat{y}_s^n)$ can be computed with respect to g, or even more fundamentally, whether $r_{\mathcal{C}_s}(\widehat{y}_s^n)$ is differentiable. In the next section, we provide an affirmative answer to the question and present a systematic method for deriving the (sub)gradient of L with respect to $g(x^n)$ by adapting and extending techniques from differentiable convex programming. Being able to evaluate this (sub)gradient means that we can compute the $\nabla_g L(g)$ through the chain rule, which allows us to optimize L(g) using first-order algorithms.

4. Differentiable QCQP

In this section, we show that under the second-order sufficient condition any QCQP of the form

$$z^* = \arg\min_{z \in \mathbb{R}^k} \quad \frac{1}{2} z^\top P_0 z + q_0^\top z \tag{7a}$$

s.t.
$$\frac{1}{2}z^{\top}P_{i}z + q_{i}^{\top}z + r_{i} \le 0 \quad \forall i = 1, \dots, m_{I},$$
 (7b)

$$\frac{1}{2}z^{\top}D_{i}z + h_{i}^{\top}z + g_{i} = 0 \quad \forall i = 1, \dots, m_{E}$$
 (7c)

defines a differentiable mapping from the parameters $P_0 \in \mathbb{R}^{k \times k}, q_0 \in \mathbb{R}^k, \{P_i \in \mathbb{R}^{k \times k}\}, \{q_i \in \mathbb{R}^k : i = 1, \cdots, m_I\}, \{r_i : \in \mathbb{R} : i = 1, \cdots, m_I\}, \{D_i \in \mathbb{R}^{k \times k}\}, \{h_i \in \mathbb{R}^k : i = 1, \cdots, m_E\}, \{g_i : \in \mathbb{R} : i = 1, \cdots, m_E\}$ to the optimal solution z^* . We derive the gradient of $\ell(z^*)$ with respect to these parameters, where $\ell : \mathbb{R}^k \to \mathbb{R}$ can be any downstream loss function on z^* . When the second-order sufficient condition does not hold, we derive the subgradients within the subdifferentials $\partial_{P_0} \ell$, $\partial_{q_0} \ell$, etc, which allows subgradient descent/ascent to be performed on the downstream loss function. We note that (7) is a more general problem that covers (5) as a special case.

Inspired by the literature on differentiable quadratic programming (Amos and Kolter, 2017) and convex programming (Agrawal et al., 2019), we exploit a key structure to drive the innovation – the

KKT equations of (7) are preserved at the optimal solution (z^*, ν^*, λ^*) under differential changes in the parameters, where $\nu^* \in \mathbb{R}^{m_I}$ and $\lambda^* \in \mathbb{R}^{m_E}$ are the optimal dual variables associated the inequality and equality constraints, respectively. More specifically, under differential changes $\{dP_i\}, \{dq_i\}, \{dr_i\}, \{dD_i\}, \{dh_i\}, \{dg_i\}$, we can find how dz^* will change accordingly by solving a linear system of equations of the form

$$M\left[(dz^*)^\top, (d\nu^*)^\top, (d\lambda^*)^\top \right]^\top = b\Big(\{dP_i\}, \{dq_i\}, \{dr_i\}, \{dD_i\}, \{dh_i\}, \{dg_i\} \Big), \tag{8}$$

where we define in the appendix the matrix $M \in \mathbb{R}^{(k+m_I+m_E)\times(k+m_I+m_E)}$, which only depends on the parameters and optimal solution of (7), and the vector $b(\{dP_i\},\{dq_i\},\{dr_i\},\{dD_i\},\{dh_i\},\{dg_i\}) \in \mathbb{R}^{k+m_I+m_E}$, which is a function of the differentials of parameters. Setting the differentials of the parameters to appropriate identity matrices/tensors and solving this system of equations give the partial derivatives $\frac{\partial z^*}{\partial P_i}, \frac{\partial z^*}{\partial q_i}$, etc., by definition.

When z^* is used to compute a differentiable downstream loss $\ell(z^*)$, we design a computationally efficient method for propagating the gradient of the loss through the QCQP to all parameters. We state the main results below and defer the detailed derivation to the appendix.

Theorem 1 Suppose that strict complementary slackness, linear constraint qualification and second-order sufficient conditions hold at (x^*, ν^*, λ^*) . Then, the matrix M is invertible and ℓ is a differentiable function of the QCQP parameters. Given $\frac{\partial \ell}{\partial z^*}$, we have

$$\nabla_{P_0} \ell = z^* d_z^{\top}, \quad \nabla_{q_0} \ell = d_z, \quad \nabla_{P_i} \ell = \nu_i^* z^* d_z^{\top} + \frac{1}{2} \nu_i^* z^* (z^*)^{\top} d_{\nu_i}, \quad \nabla_{q_i} \ell = \nu_i^* d_z + z^* d_{\nu_i}$$

$$\nabla_{r_i} \ell = d_{\nu_i}, \quad \nabla_{D_i} \ell = \lambda_i^* z^* d_z^{\top} + \frac{1}{2} d_{\lambda_i} z^* (z^*)^{\top}, \quad \nabla_{h_i} \ell = \lambda_i^* d_z + z^* d_{\lambda_i}, \quad \nabla_{g_i} \ell = d_{\lambda_i},$$
(9)

where $d_z \in \mathbb{R}^k, d_\nu \in \mathbb{R}^{m_I}, d_\lambda \in \mathbb{R}^{m_E}$ are the solutions to

$$\left[d_z^\top,\ d_\nu^\top,\ d_\lambda^\top\right]^\top = -M^{-\top} \left[\left(\frac{\partial \ell}{\partial z^*}\right)^\top,\ \cdots\ 0\ \cdots,\ \cdots\ 0\ \cdots \right]^\top.$$

In the theorem, we state a sufficient condition on the differentiability of the QCQP and provide a systematic way of computing the gradients of the downstream loss on z^* with respect to the QCQP parameters. We note that when the assumptions of Theorem 1 do not hold, M may not be invertible, and the QCQP in general is not differentiable. In that case, the expressions in (9) are the subgradients where d_z , d_ν , d_λ are any solutions of the the under-determined system

$$-M^{\top} \left[d_z^{\top}, \ d_{\nu}^{\top}, \ d_{\lambda}^{\top} \right]^{\top} = \left[\left(\frac{\partial \ell}{\partial z^*} \right)^{\top}, \ \cdots \ 0 \ \cdots, \ \cdots \ 0 \ \cdots \right]^{\top}. \tag{10}$$

In our work, we take the solution with the smallest ℓ_2 norm.

5. Numerical Experiments

In this section, we demonstrate the performance of the proposed approach for ACOPF. We do not assume that power flow has a solution. If no solution exists for the power flow, we find a solution that minimizes the violation of the power balance constraints, as proposed in (5). We highlight that our approach is capable of training the neural network model even with control prediction that can

cause no solution of the power flow system (i.e., $PF(g(x^n), x^n) = \emptyset$). Note that Newton-Rhapson method fails to converge for such cases.

Our numerical experiments aim to demonstrate that the model can be successfully trained even with a number of training and testing epochs with the samples of infeasible power flow system (i.e., no solution and thus positive slack values).

5.1. Experiment Settings

We generate the training and testing data sets by solving the problem with perturbation of the active and reactive loads by random numbers uniformly generated from (-1,1). We consider three IEEE test instances, each of which has 30, 118, and 300 buses, taken from PGLib-OPF v21.07. Because some problems can be infeasible with the random perturbations, we use the problem formulation that penalizes the violation of the power balance constraints. Each sample s of the data set consists of p_s^d , q_s^d , p_g^* , q_g^* , e_i^* , f_j^* , where p_g^* , q_g^* , e_i^* , f_j^* are local optimal solution obtained by Ipopt v3.14.12. The training data set has 10,000 samples, and the testing data set has 2,500 samples.

We have implemented the proposed approach by using PyTorch v2.0.1, where the optimization problem is modeled with Pyomo v6.7.0 and solved by Ipopt v3.14.12. The trainings were parallelized with Horovod v0.28.1. All the experiments were run on a Linux workstation with 144 CPUs of Intel(R) Xeon(R) Gold 6140 CPU @ 2.30GHz.

We use the feed-forward neural network with two layers and the sigmoid function as output. We use the same architectures proposed in (Pan et al., 2022). Detailed experiment settings are given in Table 1. Recall that the input and output dimensions are $|\mathcal{B}_{PV}| + |\mathcal{G}|$ and $2|\mathcal{B}|$, respectively. All the models were trained by Adam optimizer with the learning rates given in the table.

IEEE Test System	${\cal B}$	$\mathcal{B}_{ ext{PV}}$	${\cal G}$	${\cal L}$	# parameter per layer	w	learning rate
30-bus	30	5	6	41	64, 32	1.0	10^{-4}
118-bus	118	53	54	231	256, 128	1.0	10^{-4}
300-bus	300	68	69	411	1024, 512	0.1	10^{-6}

Table 1: Experiment setting for each IEEE test system

5.2. Small Test Cases

Figure 2 presents the training and testing performances of the proposed approach for the small test networks: IEEE 30- and 118-bus network systems. The prediction loss and penalty loss values in the figure measure the first and second terms of (6). The total loss measures L(g). The 100% test accuracy (i.e., feasibility ratio) has been obtained within 10 epochs for both small systems; that is, the control predictions $g(x^n)$ made from the trained models result in feasible state solutions with respect to the power flow equations (2) for all 2,500 test samples. Our results are consistent to that presented in Pan et al. (2022), where the power flow equations of (2) are solved as compared to the optimization (5) in our approach.

5.3. Large Test Case with Infeasible Power Flow

We demonstrate that the neural network model can be successfully trained even when some control prediction leads to infeasible power flow equations. In Figure 3 we report the training loss, the number of infeasible power flow solves, and the accuracy of the model over the training epochs for the IEEE 300-bus network data. Recall that (2) has no solution if the values of the slack variable σ

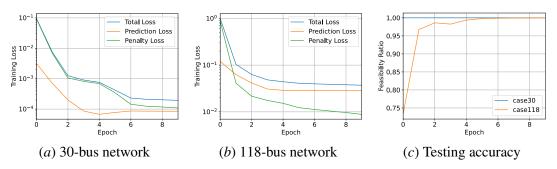


Figure 2: Performances on small grid networks (IEEE 30- and 118-bus systems)

in (5) are positive. The model trained on IEEE 300-bus network system achieves a test accuracy of 92% after 200 epochs. In a number of training and testing epochs (Figure 3b), we observe that the neural network predicts control variables that result in the infeasible state variables. While reducing over the epochs as the neural network learns more accurate controls, a positive number of infeasible power flow cases still appear in many of the later epochs. We observe that the training epochs with such infeasible cases experience the spikes in the penalty loss value. We highlight that our approach with the QCQP activation function (with slack variables) allows the neural network to still learn and improve when such infeasible cases arise, while existing approaches relying on the power flow equation solver (e.g. Pan et al. (2022)) do not.

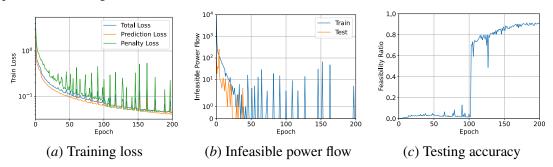


Figure 3: Training and testing performances on the IEEE 300-bus network

6. Concluding Remarks

Our work proposes a learning-based framework for solving the notoriously challenging ACOPF problem with the aim of achieving computational efficiency and reliably generating high-quality feasible solutions. We identify that a common issue of the existing approaches in this domain Pan et al. (2022); Donti et al. (2021) lies in the assumption that the power flow equation admits a solution for any neural-network-predicted control variables, which does not always hold. Training gets disrupted when the power flow solver fails to produce a feasible solution. We address this issue by modeling the power flow as a non-convex QCQP problem that minimizes the constraint violation. By leveraging and generalizing techniques from differentiable convex programming, we derive (sub)gradient of the state variables with respect to the control variables, which allows the loss function on state variables to be properly back-propagated. We show through numerical simulations that our proposed framework stably learns solutions with high feasibility rate and low generation in large systems with wide load variations, in which existing approaches fail to train. Future work may include the incorporation of minimizing the power flow violation into the training loss function, which will train the model to predict a control solution while avoiding the power flow violation.

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References

- Akshay Agrawal, Brandon Amos, Shane Barratt, Stephen Boyd, Steven Diamond, and J Zico Kolter. Differentiable convex optimization layers. *Advances in neural information processing systems*, 32, 2019.
- Brandon Amos and J Zico Kolter. OptNet: Differentiable optimization as a layer in neural networks. In *International Conference on Machine Learning*, pages 136–145. PMLR, 2017.
- Igor Araújo, Vincent Tadaiesky, Diego Cardoso, Yoshikazu Fukuyama, and Ádamo Santana. Simultaneous parallel power flow calculations using hybrid CPU-GPU approach. *International Journal of Electrical Power & Energy Systems*, 105:229–236, 2019.
- Kyri Baker. Learning warm-start points for AC optimal power flow. In 2019 IEEE 29th International Workshop on Machine Learning for Signal Processing (MLSP), pages 1–6. IEEE, 2019.
- Bo Chen, Alvaro Parra, Jiewei Cao, Nan Li, and Tat-Jun Chin. End-to-end learnable geometric vision by backpropagating pnp optimization. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 8100–8109, 2020.
- Michael J Curry, Uro Lyi, Tom Goldstein, and John P Dickerson. Learning revenue-maximizing auctions with differentiable matching. In *International Conference on Artificial Intelligence and Statistics*, pages 6062–6073. PMLR, 2022.
- Sanja Cvijic, Peter Feldmann, and Marija Hie. Applications of homotopy for solving AC power flow and AC optimal power flow. In 2012 IEEE Power and Energy Society General Meeting, pages 1–8. IEEE, 2012.

- Priya L Donti, David Rolnick, and J Zico Kolter. DC3: A learning method for optimization with hard constraints. In *International Conference on Learning Representations*, 2021.
- Neel Guha, Zhecheng Wang, Matt Wytock, and Arun Majumdar. Machine learning for AC optimal power flow. *arXiv preprint arXiv:1910.08842*, 2019.
- Shengjun Huang and Venkata Dinavahi. Performance analysis of GPU-accelerated fast decoupled power flow using direct linear solver. In 2017 IEEE Electrical Power and Energy Conference (EPEC), pages 1–6. IEEE, 2017.
- Rabi Shankar Kar, Zhixin Miao, Miao Zhang, and Lingling Fan. Admm for nonconvex AC optimal power flow. In 2017 North American power symposium (NAPS), pages 1–6. IEEE, 2017.
- Youngdae Kim and Kibaek Kim. Accelerated computation and tracking of AC optimal power flow solutions using gpus. In *Workshop Proceedings of the 51st International Conference on Parallel Processing*, pages 1–8, 2022.
- Junbang Liang, Ming Lin, and Vladlen Koltun. Differentiable cloth simulation for inverse problems. *Advances in Neural Information Processing Systems*, 32, 2019.
- Rahul Mourya and João FC Mota. MCNeT: Measurement-consistent networks via a deep implicit layer for solving inverse problems. In *ICASSP 2023-2023 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 1–5. IEEE, 2023.
- Rahul Nellikkath and Spyros Chatzivasileiadis. Physics-informed neural networks for AC optimal power flow. *Electric Power Systems Research*, 212:108412, 2022.
- Xiang Pan, Minghua Chen, Tianyu Zhao, and Steven H Low. DeepOPF: A feasibility-optimized deep neural network approach for AC optimal power flow problems. *IEEE Systems Journal*, 17 (1):673–683, 2022.
- Vincent Roberge, Mohammed Tarbouchi, and Francis Okou. Optimal power flow based on parallel metaheuristics for graphics processing units. *Electric Power Systems Research*, 140:344–353, 2016.
- Sayed Abdullah Sadat and Mostafa Sahraei-Ardakani. Initializing successive linear programming solver for ACOPF using machine learning. In 2020 52nd North American Power Symposium (NAPS), pages 1–6. IEEE, 2021.
- Manish K Singh, Vassilis Kekatos, and Georgios B Giannakis. Learning to solve the AC-OPF using sensitivity-informed deep neural networks. *IEEE Transactions on Power Systems*, 37(4): 2833–2846, 2021.
- Kaizhao Sun and Xu Andy Sun. A two-level ADMM algorithm for AC OPF with global convergence guarantees. *IEEE Transactions on Power Systems*, 36(6):5271–5281, 2021.
- Po-Wei Wang, Priya Donti, Bryan Wilder, and Zico Kolter. Satnet: Bridging deep learning and logical reasoning using a differentiable satisfiability solver. In *International Conference on Machine Learning*, pages 6545–6554. PMLR, 2019.

- Qi Wang, Chenhui Lin, Wenchuan Wu, Bin Wang, Guannan Wang, Haitao Liu, Hongyu Zhang, and Jun Zhang. A nested decomposition method for the AC optimal power flow of hierarchical electrical power grids. *IEEE Transactions on Power Systems*, 2022.
- Raymond A Yeh, Yuan-Ting Hu, Zhongzheng Ren, and Alexander G Schwing. Total variation optimization layers for computer vision. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 711–721, 2022.
- Zhao Yuan and Mohammad Reza Hesamzadeh. Second-order cone AC optimal power flow: convex relaxations and feasible solutions. *Journal of Modern Power Systems and Clean Energy*, 7(2): 268–280, 2019.
- Sihan Zeng, Alyssa Kody, Youngdae Kim, Kibaek Kim, and Daniel K Molzahn. A reinforcement learning approach to parameter selection for distributed optimal power flow. *Electric Power Systems Research*, 212:108546, 2022.
- Sihan Zeng, Sujay Bhatt, Eleonora Kreacic, Parisa Hassanzadeh, Alec Koppel, and Sumitra Ganesh. Near-optimal fair resource allocation for strategic agents without money: A data-driven approach. *arXiv preprint arXiv:2311.10927*, 2023.
- Ling Zhang and Baosen Zhang. Learning to solve the AC optimal power flow via a lagrangian approach. In 2022 North American Power Symposium (NAPS), pages 1–6. IEEE, 2022.
- Weiqi Zhang, Youngdae Kim, and Kibaek Kim. On solving unit commitment with alternating current optimal power flow on gpu. *arXiv preprint arXiv:2310.13145*, 2023.