Optimization Inspired Multi-Branch Equilibrium Models

Abstract

Works have shown the strong connections between some implicit models and optimization problems. However, explorations on such relationships are limited. Most works pay attention to some common mathematical properties, such as sparsity. In this work, we propose a new type of implicit model inspired by the designing of the systems' hidden objective functions, called the Multi-branch Optimization induced Equilibrium networks (MOptEqs). The model architecture is designed based on modelling the hidden objective function for the multi-resolution recognition task. Furthermore, we also propose a new training strategy inspired by our understandings of the hidden objective function. In this manner, the proposed model can better utilize the hierarchical patterns for recognition tasks and retain the abilities for interpreting the whole structure as trying to obtain the minima of the problem's goal. Comparing with the state-of-the-art models, our MOptEqs not only enjoys better explainability but are also superior to MDEQ with less parameter consumption and better performance on practical tasks. Furthermore, we also implement various experiments to demonstrate the effectiveness of our new methods and explore the applicability of the model's hidden objective function.

1 Introduction

Whereas Deep Neural Networks (DNNs) have achieved great success in many real-world tasks such as computer vision and neural language process, the limited interpretability of DNNs greatly hinders their further development.

However, many traditional machine learning methods, e.g.,matrix recovery (Zhang et al., 2018b; 2015; Liu & Li, 2016), subspace clustering (You et al., 2016), image deblurring (Liu et al., 2014) and so on, can be interpreted into minimizing the following objective functions:

$$\min_{\mathbf{Z}, \mathbf{E}} f(\mathbf{Z}) + g(\mathbf{E}), \ s.t. \ \mathbf{X} = \mathbf{A}\mathbf{Z} + \mathbf{B}\mathbf{E}.$$

where $\mathbf{A} \in \mathbb{R}^{m \times d_1}$, $\mathbf{B} \in \mathbb{R}^{m \times d_2}$, $\mathbf{X} \in \mathbb{R}^{m \times n}$, and $f(\cdot)$ and $g(\cdot)$ are convex functions designed by the modelling of their properties. For this count, the interpretability of such methods is much better than DNNs. Furthermore, these methods can also enjoy state-of-the-art and robust performance on these tasks. We call such interpretability these methods enjoy as "mathematical interpretability", i.e., whether the whole network structure can be summarized as a compact mathematical model that can be mathematically analyzed.

Except for these methods, the Optimization Induced Equilibrium Networks (OptEqs) proposed by Xie et al. (2021) recover the whole OptEqs system for recognition to an optimization problem. The forward propagation for OptEqs and its hidden objectives can be depicted as follows, enjoying good interpretability as these traditional works.

$$\mathbf{z}^* = \mathbf{W}^\top \sigma(\mathbf{W}\mathbf{z}^* + \mathbf{U}g(\mathbf{x}) + \mathbf{b}), \ \mathbf{y} = \mathbf{W}_c\mathbf{z}^*,$$

$$\min_{\mathbf{z}} G(\mathbf{z}; g(\mathbf{x})) = \min_{\mathbf{z}} \left[\mathbf{1}^\top \ f(\mathbf{W}^{-1\top}\mathbf{z}) - \left\langle \mathbf{U}g(\mathbf{x}) + \mathbf{b}, \mathbf{W}^{-1\top}\mathbf{z} \right\rangle + \frac{1}{2}\|\mathbf{W}^{-1\top}\mathbf{z}\|^2 - \frac{1}{2}\|\mathbf{z}\|^2 \right]. \tag{1}$$

Although OptEqs proves that its forward propagation can be regarded as minimizing certain objective function and shows its strong interpretability, some weaknesses for OptEqs are

worth exploring. First, although OptEqs performs better than some implicit models, these models only consider a single view (or resolution) of the input in their implicit parts. We call these models single-view implicit models in the following. However, nearly all the state-of-the-art pattern recognition systems (Lee et al., 2009b; Wang et al., 2019a; Huang et al., 2017; He et al., 2016; Burt & Adelson, 1987) benefit from the multi-layer or multi-resolution feature extractors in domains like computer vision and audio processing. Secondly, new modules induced by the objective function they proposed are limited, which mainly consider the math properties of the output features like sparsity, but whether these properties can benefit image recognition tasks is unexplored.

MDEQ (Bai et al., 2020) is the state-of-the-art implicit model so far, which utilizes the multi-scale information from samples by multi-branch structure and branches fusion. Nevertheless, MDEQ is more likely to be a traditional neural network than OptEqs and MonDEQ (Winston & Kolter, 2020), since its whole structure is designed like other explicit DNNs (like stacking residual blocks and its traditional fusion method). Such architecture prevents it from retaining good interpretability as we desired.

Therefore, the main challenge for us is to design a class of implicit models that can perform better than MDEQ and retain the ability for recovering the whole structure as an optimization problem. The contributions for our work are listed below:

- We propose a multi-branch implicit model, called Multi-branch OptEqs (MOptEqs), which efficiently utilizes different scales inputs with better performance and smaller model size. Furthermore, our model still retains its connection to an optimization problem.
- We propose some properties modelled as new terms for the model's hidden objective function from our analysis on the relationships between branches and their hierarchical dependencies. With such a problem's formulation, we obtain the fusion module in our MOptEqs, called Hierarchical Heritage and Diversity Module (HH&D Module).
- Apart from the new module design, we also propose the Perturbation Enhanced training strategy (PE) for our MOptEqs from our analysis on the model's hidden objective function. The new strategy cannot only enhance the performance of our MOptEqs, but also improve the robustness of our models.

1.1 Related Works

Implicit Models. Nearly all modern deep learning approaches use *explicit* models, which provide an explicit computation graph for the forward propagation. In contrast, the computation graphs for *implicit* models are "flexible" or can be assumed as having "infinite" depth. For example, Neural ODEs (Chen et al., 2018; Massaroli et al., 2020) encode their neural architectures by a differential system with learnable parameters. Then the implicit ODE solvers they used is equivalent to a continuous ResNet taking infinitesimal steps. Furthermore, the training process of Neural ODEs can be depicted as finding a differential system of a certain type (like heat equations) by updating its learnable parameters which demonstrate that Neural ODE also enjoy interpretability to a certain extent.

Moreover, the computation of the forward propagation of DEQ (Bai et al., 2019; Winston & Kolter, 2020) can be depicted as solving the following equilibrium state:

$$\mathbf{z}^* = \sigma(\mathbf{W}\mathbf{z}^* + \mathbf{U}g(\mathbf{x}) + \mathbf{b}), \ \mathbf{y} = \mathbf{W}_c\mathbf{z}^*,$$

where $\mathbf{x} \in \mathbb{R}^{d_{in}}$, $\mathbf{z}^* \in \mathbb{R}^d$ are the inputs and equilibrium points of DEQ, $\mathbf{W}, \mathbf{U}, \mathbf{W}_c$ are learnable weights, $\mathbf{y}$ are final outputs and g is a small explicit model to project the input $\mathbf{x}$ from real-world domain to the feature space, which is widely used in neural architectures. $g(\cdot)$ usually consists of one or two convolution layers. Satisfying some analytical conditions such as norm constraints for weights or outputs, the computation graphs for solving $\mathbf{z}^*$ can also be viewed as forwarding a proper neural network with infinite depth. But unlike DNNs, implicit models can use shallower computation graphs computed by some accelerated root-finding problems for their forward and backward propagation. Due to the above reasons, such simple models can achieve comparable results with more efficient parameters and memory costs.

Because of the flexibility and interpretability for implicit models, the design of implicit models draws much attention these days (Ghaoui et al., 2019; Gould et al., 2019). Apart from the models illustrated above, many kinds of other implicit models have been proposed, including differentiable physics engines (Qiao et al., 2020; de Avila Belbute-Peres et al., 2018), logical structure learning (Wang et al., 2019b) and implicit neural blocks (Li et al., 2020).

Model Interpretaiblity. Many researchers nowadays are trying to make their proposed method more interpretable. Although there are many kinds of approaches to achieve this goal, we marginally divide them into two parts: "Empirical" and "Mathematical" interpretability. Many works, such as (Zhang et al., 2018a; Zhang & Zhu, 2018; Bau et al., 2018), attempt to empirically disassemble the black box by characterizing some statistical or structural information like the outputs and gradients of neural networks' middle layers. Apart from that, researchers (Djolonga & Krause, 2017; Amos & Kolter, 2017; Xie et al., 2019; Chan et al., 2020) also managed to understand the neural architecture by linking it to a mathematical problem. In this way, researchers can analyze the black box by its corresponding mathematical problem. Furthermore, new components can be proposed due to the analysis of these problems. Our model aims to design a new DEQ architecture with proper mathematical interpretability. Compared with the former works, our model can deal with the classification tasks with better performances with novel components.

2 Multi-Branch Optimized Induced Equilirium Models

2.1 The proposed architecture for the Multi-Branch OptEqs

Although OptEqs can maintain its ability to reformulate the whole architecture as a solution of minimizing an objective function they designed (i.e. the mathematical interpretability), its performance is still weak. Motivated by the huge improvement gained from processing multi-scale inputs in MDEQ, we'd like to design a multi-scale OptEqs architecture with state-of-the-art performance and preserve mathematical interpretability.

To achieve this goal, we first parallel several OptEqs like MOptEqs (Details can be found in Appendix.A.1). The most important problem is how to design the fusion method of each branch that suits our purpose. However, the existing fusion method can not satisfy our target. Simply using non-parametric operators (like addition) can ensure the interpretability, but the performance is poor. Utilizing convolutional blocks like those used in MDEQ and other works (Ronneberger et al., 2015; Wang et al., 2019a) can improve the performance. Nevertheless, they cannot be reformulated as optimization problems, which means their mathematical interpretability is poor. For this account, we'd like to design our fusion method by modelling the architecture's hidden problems and convert them to novel fusion components.

Hierarchical Heritage Modeling. State-of-the-art explicit models for image tasks are explicitly structured into sequential stages and process different resolutions hierarchically (He et al., 2016; Shelhamer et al., 2017; Lee et al., 2009a), which implies that features should be extracted hierarchically. In other words, the posterior branches should inherit from their prior ones, which we call such property hierarchical heritage. In our work, we are going to formulate such correlation of neighbouring branches in the hidden objective function by adding the following inner-product term into its origin:

$$\mathcal{H}(\mathbf{z}_i, \mathbf{z}_j) = \mathbf{z}_i^\top \mathbf{P}_{i:j} \mathbf{z}_j \qquad (2)$$

where $\mathbf{z}_i \in \mathbb{R}^{d_i}, \mathbf{z}_j \in \mathbb{R}^{d_j}, \mathbf{P}_{i:j} \in \mathbb{R}^{s_i \times s_j}$ denotes the Average Downsample (its transpose can be regarded as a weighted nearest upsample) or Identity matrix suited to the shape of $\mathbf{z}_i$ and $\mathbf{z}_j$ ($i < j$ or $j = 1, i = L$). This term only estimate the summation for the similarity of i-th and j-th branch's channels with the same channel index, which we call them *corresponding channels*, as shown in the above equation.

When $\mathbf{z}_i$ and $\mathbf{z}_j$ are similar, the inner product will be large. Otherwise, the result will become small, which implies that the relationship of corresponding channels is weak. In this way, we can ensure the similarity of corresponding channels of the near branches. Except for the relations between different branches' corresponding channels, the relationships between dis-corresponding channels are explored in the following section.

Diversity Modeling. In addition to the hierarchical relations for corresponding channels, works (Pang et al., 2019; Amada et al., 2021) have shown enhancing the diversities between branches can also improve the model's improvements. For this account, we also consider making different branches extract various features to improve the representation abilities of different branches. To achieve such a goal, we add a diversity term in the objective function Eqn.(3) if we assume that $i < j$,

$$\mathcal{D}(\mathbf{z}_i, \mathbf{z}_j) = \sum_{k_1=1}^{C} \sum_{\substack{k_2=1 \\ k_2 \neq k_1}}^{C} |\mathbf{vec}^{-1}(\mathbf{z}_i)^{(k_1)\top} \mathbf{vec}^{-1}(\mathbf{P}_{i:j}\mathbf{z}_j)^{(k_2)}|, \tag{3}$$

where $\mathbf{vec}^{-1}$ is the inverse vectorization operator convert the vectorized feature $\mathbf{z}_i \in \mathbb{R}^{d_i \times 1}$ to a matrix in $\mathbb{R}^{\frac{d_i}{C} \times C}$ with C channels and $\mathbf{vec}^{-1}(\mathbf{z}_i)^{(k)} \in \mathbb{R}^{\frac{d_i}{C} \times 1}$ denotes the k-th channel of i-th branch in practice. Since we have already considered the relationships between the corresponding channels in the hierarchical term, we only tries to estimate the diversities of dis-corresponding channels of the i-th and j-th branches in this term. As the diversity term goes small, the diversities between the branches become stronger.

The architecture of MOptEqs and its hidden problem. With the two terms we proposed, we can reformulate the hidden objective for our problem by replacing the L_2 norm with our new modelling as follows:

$$\min_{\mathbf{z}_1,...,\mathbf{z}_L} G(\mathbf{z}_1, ..., \mathbf{z}_L; g(\mathbf{x})) = \min_{\mathbf{z}_1,...,\mathbf{z}_L} \sum_{i=1}^{L} \left[\mathbf{1}^\top f(\mathbf{W}_i^{-1\top}\mathbf{z}_i) - \left\langle \mathbf{U}_i g(\mathbf{x}) + \mathbf{b}_i, \mathbf{W}_i^{-1\top}\mathbf{z} \right\rangle \right.$$
$$\left. + \frac{1}{2}(\lambda \mathcal{D}(\mathbf{z}_i, \mathbf{z}_{i+1}) + \|\mathbf{W}^{-1\top}\mathbf{z}_i\|^2 - \mathcal{H}(\mathbf{z}_i, \mathbf{z}_{i+1})) \right]. \tag{4}$$

where $g(\mathbf{x})$ is the input feature with raw input $\mathbf{x}$, hyperparamter λ is a positive constant, $\mathbf{z}_i \in \mathbb{R}^{d_i \times 1}$ and f is the positive orthant $f(x) = \mathbb{I}\{x \geq 0\}$ and $(I + \partial f)^{-1}$ is the ReLU activation function. We set $\mathcal{D}(\mathbf{z}_L, \mathbf{z}_{L+1}) = \mathcal{D}(\mathbf{z}_L, \mathbf{z}_1)$ and $\mathcal{H}(\mathbf{z}_L, \mathbf{z}_{L+1}) = \mathcal{H}(\mathbf{z}_L, \mathbf{z}_1)$ when $i = L$ to complete the loop of relationship. The two terms we added tries to make the corresponding channels of different branches correlated by maximizing the $\mathcal{H}$ term and enhancing the diversities of different branches by minimizing $\mathcal{D}$ term. We note that $\mathcal{H}$ and $\mathcal{D}$ are not conflict since they are handling different pairs of channels for branches.

In the following proposition, we conclude that the calculation of our MOptEqs is equivalent to solving the stationary points $\nabla_{\mathbf{z}_i} G = 0$.

Proposition 1 *The proposed multi-branch structure induced by Eqn(4) can be depicted as solving the equilibrium points $\widetilde{\mathbf{z}}^* := [\mathbf{z}_1^{\top *}, ..., \mathbf{z}_L^{\top *}]^\top \in \mathbb{R}^{\sum_{i=1}^{L} d_i}$ for the following equations:*

$$\widetilde{\mathbf{z}} = \widetilde{\mathbf{W}}^\top \sigma(\widetilde{\mathbf{W}} h(\tilde{\mathbf{z}}) + \widetilde{\mathbf{U}} g(\mathbf{x}) + \widetilde{\mathbf{b}})$$

$$\textit{where } \widetilde{\mathbf{W}} = \begin{bmatrix} \mathbf{W}_1 & & \\ & \ddots & \\ & & \mathbf{W}_L \end{bmatrix}, \widetilde{\mathbf{U}} = [\mathbf{U}_1^\top, ..., \mathbf{U}_L^\top]^\top, \widetilde{\mathbf{b}} = [\mathbf{b}_1^\top, ..., \mathbf{b}_L^\top]^\top. \tag{5}$$

And $h(\tilde{\mathbf{z}}) = [h_1(\mathbf{z}_1, \mathbf{z}_L, \mathbf{z}_2)^\top, .., h_i(\mathbf{z}_i, \mathbf{z}_{i-1}, \mathbf{z}_{i+1})^\top, .., h_L(\mathbf{z}_L, \mathbf{z}_{L-1}, \mathbf{z}_1)^\top]^\top$ and each h_i is defined as the mapping from $\mathbb{R}^{d_i} \times \mathbb{R}^{d_{i+1}} \times \mathbb{R}^{d_{i-1}}$ to $\mathbb{R}^{d_i}$,

$$h(\mathbf{z}_i, \mathbf{z}_{i-1}, \mathbf{z}_{i+1}) = \frac{1}{2}(\mathbf{P}_{i:i+1}\mathbf{z}_{i+1} + \mathbf{P}_{i-1:i}^\top \mathbf{z}_{i-1})$$

$$- \frac{\lambda}{2}\mathbf{vec}(\mathbf{vec}^{-1}(\mathbf{P}_{i:i+1}\mathbf{z}_{i+1})\mathbf{sign}[\mathbf{M}_{i:i+1} - \mathbf{diag}(\mathbf{M}_{i:i+1})])$$

$$- \frac{\lambda}{2}\mathbf{vec}(\mathbf{vec}^{-1}(\mathbf{P}_{i-1:i}^\top \mathbf{z}_{i-1})\mathbf{sign}[\mathbf{M}_{i-1:i}^\top - \mathbf{diag}(\mathbf{M}_{i-1:i})]),$$

$$\mathbf{M}_{i:i+1} = \mathbf{vec}^{-1}(\mathbf{P}_{i:i+1}\mathbf{z}_{i+1})^\top \mathbf{vec}^{-1}(\mathbf{z}_i),$$

$$\mathbf{M}_{i-1:i} = \mathbf{vec}^{-1}(\mathbf{z}_i)^\top \mathbf{vec}^{-1}(\mathbf{P}_{i-1:i}^\top \mathbf{z}_{i-1}).$$

The equilibrium points for the above formula are also the first-order stationary points for the optimization problem Eqn(4).

(a) MOptEqs' structure.

(b) HH&D's structure ($\mathbf{z}_{pi} = h_i(\mathbf{z}_i, \mathbf{z}_{i-1}, \mathbf{z}_{i+1})$).

Figure 1: The structure of the MOptEqs and HH&D Module. Dotted lines in the figure denotes the upsampling, downsampling or identity operators to suit the size of each branch, $\otimes$ denotes multiplication operator, $\oplus$ denotes addition operator, **RD** operator processes a matrix by removing its diagonal, **SIGN** operator convert each element of a matrix to its sign and the $d_i = CH_iW_i$ with C is the channel number and H_i, W_i are the height and width of the feature map.

The proof of the proposition is listed in Appendix.A.3. In this manner, we obtain the proposed architecture MOptEqs, its forward propagation is equivalent to find the equilibrium points of Eqn(5), and such process can also be regarded as solving the stationary points of the optimization problem (4). The whole structure is also shown in Figure.1 (a) and we also draw figures to illustrate the practical process of h_i (HH&D) on its right (Figure.1 (b)). We also evaluate the effectiveness of such modelling in Section. 3.2's experiments.

2.2 The proposed Training Strategy for MOptEqs

Researches (Kong et al., 2020; Xie et al., 2020; Tang et al., 2021) have discovered that small perturbations can enhance the generalization abilities of neural architectures in various tasks and models. Most efficient works use adversarial perturbations based on gradients (Xie & Yuille, 2020) for such a trick. However, such a strategy will slow the training process since they need at least one more back-propagation in each training step for perturbations, which is time-consuming. Unlike these methods, we can acquire more computation efficient perturbations because our models can be formulated as minimizing an objective function we designed. Then we can replace the maximum problem (details in Appendix.A.2) for adversarial perturbation with maximizing our architecture's hidden objective function G, since we assume MOptEq's performance will go worse if $G(\mathbf{z}; g(\mathbf{x}))$ changes a lot at $g(\mathbf{x})$'s neighborhoods since the forward propagation of MOptEqs is minimization $G(\mathbf{z}; g(\mathbf{x}))$.

Assumption 1 *For a well trained OptEqs with its objective function denoted as $G(\mathbf{z}; g(\mathbf{x}))$ and a natural sample $\mathbf{x}$ which can be correctly classified. If an input perturbation $\|\delta\|_\infty \leq \epsilon$ can cause one of the following changes:*

$$|G(\mathbf{z}'^*; g(\mathbf{x}) - \delta) - G(\mathbf{z}^*; g(\mathbf{x}))| \geq L_1\epsilon,$$
$$\|\mathbf{z}'^* - \mathbf{z}^*\|_2 \geq L_2\epsilon.$$

with $L_1, L_2 > 1$, it may lead the OptEqs to the wrong results with high probability.

For the second part of the assumption, it's common sense and widely used in the analysis of adversarial robustness (Zhang et al., 2021; Li et al., 2020). With the above assumption, we can generate the perturbations by maximizing the objective function $G(\mathbf{z}; g(\mathbf{x}))$ for our MOptEqs. Since our MOptEqs can be regarded as a kind of "implicit" ensembling that parallels several equilibrium models, we decide to inject the perturbations acquired for the prior branch to the posterior one, like boosting to enhance the performance.

Then the hidden objective function of MOptEqs with $G(\mathbf{z}; g(\mathbf{x}))$ is shown as follows,

$$\min_{\mathbf{z}_1,...,\mathbf{z}_L} G(\mathbf{z}_1,...,\mathbf{z}_L; g(\mathbf{x})) = \min_{\mathbf{z}_1,...,\mathbf{z}_L} \sum_{i=1}^{L} \left[\mathbf{1}^\top f(\mathbf{W}_i^{-1\top}\mathbf{z}_i) - \left\langle \mathbf{U}_i(g(\mathbf{x}) - \delta_{i-1}) + \mathbf{b}_i, \mathbf{W}_i^{-1\top}\mathbf{z} \right\rangle \right.$$
$$\left. + \frac{1}{2}\left(\lambda \mathcal{D}(\mathbf{z}_i, \mathbf{z}_{i+1}) + \|\mathbf{W}^{-1\top}\mathbf{z}_i\|^2 - \mathcal{H}(\mathbf{z}_i, \mathbf{z}_{i+1}) \right) \right],$$
$$s.t. \quad \delta_i = \underset{\|\delta_i\|_\infty \leq \epsilon}{\mathrm{argmax}}\, \mathbf{1}^\top f(\mathbf{W}_i^{-1\top}\mathbf{z}_i) - \left\langle \mathbf{U}_i(g(\mathbf{x}) - \delta_i) + \mathbf{b}_i, \mathbf{W}_i^{-1\top}\mathbf{z}_i \right\rangle \text{ for i} \in [1, \mathrm{L}].$$

where $\delta_0 = 0$. And the problem becomes a bilevel optimization problem. The solution to the lower-level problem is $\delta_i = \epsilon\,\mathbf{sign}(\mathbf{U}_i^\top \mathbf{W}_i^{-1\top}\mathbf{z}_i)$. Since the perturbation can be obtained by feeding the output of the activation layer $\sigma(\mathbf{W}\mathbf{z} + \mathbf{U}g(\mathbf{x}) + \mathbf{b})$ to the transposed convolution layer with weight $\mathbf{U}_i$, we call it reconstructed perturbation. Compared with the adversarial perturbations based on gradients, our perturbations can be acquired directly by matrix-vector multiplication instead of iteratively built by gradients. For this account, such a process does not require much computation cost. Following the above steps, we obtain a harmful perturbed direction for the prior branches and then added them to their posterior branches. We note that our perturbation is added to the input feature $g(\mathbf{x})$ instead of the raw input.

Proposition 2 *For a natural sample* $\mathbf{x}$ *and a well trained OptEqs*

$$\mathbf{z}^* = \mathbf{W}^\top \sigma(\mathbf{W}\mathbf{z}^* + \mathbf{U}g(\mathbf{x}) + \mathbf{b})$$

with its hidden objective function denoted as $G(\mathbf{z}; g(\mathbf{x}))$, *for* $g'(\mathbf{x}) = g(\mathbf{x}) - \delta$ *and* $\delta = \epsilon\,\mathbf{sign}(\mathbf{U}_i^\top \mathbf{W}_i^{-1\top}\mathbf{z}_i)$, *which obeys the constraint* $\|\delta\|_\infty \leq \epsilon$. $\mathbf{z}'^*$ *and* $\mathbf{z}^*$ *are defined as follows:*

$$\mathbf{z}'^* = \underset{\mathbf{z}}{\mathrm{argmin}}\, G(\mathbf{z}; g'(\mathbf{x})),$$
$$\mathbf{z}^* = \underset{\mathbf{z}}{\mathrm{argmin}}\, G(\mathbf{z}; g(\mathbf{x})).$$

If the $\|\mathbf{W}\|_2, \|\mathbf{U}\|_2 \leq 1$ *and* $\frac{1}{N}\|\mathbf{U}^\top \mathbf{W}^{-1\top}\mathbf{z}^*\|_1 \gg \epsilon$, *where* N *is the element number of* $g(\mathbf{x})$, *then*

$$\max\left\{ G(\mathbf{z}'^*; g(\mathbf{x}) - \delta) - G(\mathbf{z}^*; g(\mathbf{x})), \sqrt{N}\epsilon\|\mathbf{z}'^* - \mathbf{z}^*\|_2 \right\} \geq \frac{1}{2}\left\{ \epsilon\|\mathbf{U}^\top \mathbf{W}^{-1\top}\mathbf{z}^*\|_1 - N\epsilon^2 \right\}.$$

The proposition demonstrates if we choose the perturbed direction to be $\epsilon\,\mathbf{sign}(\mathbf{U}^\top \mathbf{W}^{-1\top}\mathbf{z})$, at least one of the changes for the G or $\mathbf{z}^*$ will be around $\epsilon\|\mathbf{U}^\top \mathbf{W}^{-1\top}\mathbf{z}^*\|_1$ and implies each branch may perform bad on the perturbed data according to our assumptions. With the experiments in Section.3.2, we can conclude that our reconstructed perturbation is useful and our assumption is reasonable. Like boosting strategy, we can feed the perturbed data for the prior branch to its posterior branch during training to enhance the performance; we call such method as the **Perturbation Enhanced training strategy** (PE). Following experiments also show that PE can indeed enhance the performance of our MOptEqs.

2.3 Model Optimization and Forward Convergence

Forward Propagation and Implicit Differentiation. We can run root-finding algorithms to solve the roots $\tilde{\mathbf{z}}^* = [\mathbf{z}_1^*,...\mathbf{z}_L^*]$ of the following problem to reach the equilibrium states for the forward propagation (shown in Appendix.A.5):

$$\nabla_{\tilde{\mathbf{z}}} G(\mathbf{z}_1,...,\mathbf{z}_L; g(\mathbf{x})) = 0. \tag{6}$$

As for the backward propagation, we also adopt the implicit differentiation method widely used in (Bai et al., 2020; 2019; Chen et al., 2018). Instead of tracing the gradients during the forward propagation, the implicit differentiation method directly backpropagates through the equilibrium state using the Jacobian of $\mathcal{T}_\theta = \nabla_{\tilde{\mathbf{z}}} G + \tilde{\mathbf{z}}$ at $\tilde{\mathbf{z}}^*$. For a given loss $l = \mathcal{L}(\tilde{\mathbf{z}}^*, \mathbf{y})$ (where $\mathbf{y}$ is the target) and the gradients can be written as

$$\frac{\partial l}{\partial(\cdot)} = \frac{\partial l}{\partial \tilde{\mathbf{z}}^*}(\mathbf{I} - \mathbf{J}_{\mathcal{T}_\theta}|_{\tilde{\mathbf{z}}^*})^{-1}\frac{\partial \mathcal{T}_\theta}{\partial(\cdot)}. \tag{7}$$

Model	Model Size	Accuracy
Neural ODEs	172K	53.7%
Aug. Neural ODEs	172K	60.6%
Single-tire MonDEQ	854K	82.5%
Deep OptEqs[1]	199K	87.4%
Parallel-OptEqs	193K	87.4%
POptEqs(sum)	193K	88.4%
POptEqs(conv)	276K	88.9%
MOptEqs (w/o PE)	193K	89.1%
MOptEqs	193K	**89.5**%

(a) Comparison of the models with single-scales.

Model	Model Size	Accuracy
ResNet-18	10M	$92.9 \pm 0.2\%$
MonDEQ	1M	89.7%
MDEQ	2.53M	$92.6 \pm 0.2\%$
MDEQ	10M	$93.8 \pm 0.3\%$
MOptEqs	0.48M	$\mathbf{92.9 \pm 0.2}\%$
MOptEqs	1.9M	$\mathbf{94.0 \pm 0.1}\%$

(b) Comparison of the models with multiple-scales. MonDEQ here is the multi-tire monotone DEQ.

Table 1: Evaluation on CIFAR-10 for different models. "Parallel-OptEqs"(POptEqs) means our model is built without utilizing HH&D fusion (Stated in Appendix.A.1), which is formed by paralleling several OptEqs with the method stated in the brackets for fusion. "w/o PE" means MOptEqs is trained without our PE training strategy.

And the calculation of $\frac{\partial l}{\partial \tilde{\mathbf{z}}^*}(\mathbf{I} - \mathbf{J}_{\mathcal{T}_\theta}|\tilde{\mathbf{z}}^*)^{-1}$ is equivalent to solve root $\mathbf{m}$ for the following equation:

$$\mathbf{m}(\mathbf{I} - \mathbf{J}_{\mathcal{T}_\theta}|\tilde{\mathbf{z}}^*) + \frac{\partial l}{\partial \tilde{\mathbf{z}}^*} = 0. \tag{8}$$

As for the root-finding algorithm, we can use Broyden method (Broyden, 1965), Anderson Method (Anderson, 1965; Bai et al., 2021) or other root-finding methods to solve Eqn(6) for the equilibrium state and Eqn(8) for the backward gradient.

Forward Convergence. Like other implicit models, we need to make some constraints on parameters in order to make the whole MOptEqs $\mathcal{T}_\Theta(\tilde{\mathbf{z}}; \mathbf{x})$ ($\tilde{\mathbf{z}}$ here is $\{\mathbf{z}_i\}_{i=1}^L$) be a contractive mapping. For the MOptEqs without considering HH&D (Eqn.9), the models can easily converge with $\|\mathbf{W}_i\|_2 \leq \zeta < 1$. But since we use the HH&D module, we need to choose proper λ to ensure the convergence, around or less than $\frac{1}{C}$ will be appropriate, which does not need ζ to be too small. We also conduct experiments to verify the convergence in Fig.4 in Appendix. A.7.

3 Experimental Results

In this section, we conduct experiments for the image classification tasks on CIFAR-10,CIFAR-100 Krizhevsky et al. (2009) and ImageNette implemented on the PyTorch (Paszke et al., 2017) platform to demonstrate the effectiveness of our model. Details are listed in Appendix..A.6.

3.1 Comparison of Prior Implicit Models

In this part, we decide to verify the superiority of MOptEqs in two aspects. First, we build the single-scale MOptEqs and compare the empirical results with other single-scale implicit models. And then we compare the experimental results with prior implicit models that utilize the multi-scale inputs like MDEQs, the state-of-the-art implicit model with multi-resolution.

Implicit Models with Single View. In this part, we compare our MOptEqs with other single-view implicit models with comparable model sizes. Like OptEqs who uses three blocks for their experiment, we first construct our small MOptEqs with three branches whose outputs share the same size and the channel number $C = 32$. Results in Table.1 (a) demonstrates that our MOptEqs structure can even enhance the performance for recognition tasks under the single-view cases. Compared to the multi-branch model without fusion (POptEqs), our MOptEqs' HH&D can efficiently utilize the relationships between different branches and lead the model to better performance. Our superiority also holds compared with former multi branches fusion methods: "sum" (non-parametric module) and "conv" (parametric module). Meanwhile, we can also conclude the effectiveness of our perturbation enhanced training strategy from the table since its performance is the best.

Model	Model Size	Accuracy
MDEQ	2.6M	$70.8 \pm 0.2\%$
	11M	$72.4 \pm 0.2\%$
MOptEqs	1.9M	$\mathbf{73.4 \pm 0.2}\%$

(a) Evaluation on CIFAR-100 for models.

Model	Model Size	Accuracy
MDEQ	2.5M	$90.5 \pm 0.2\%$
	10M	$91.3 \pm 0.3\%$
MOptEqs	1.9M	$\mathbf{92.1 \pm 0.2}\%$

(b) Evaluation on Imagenette for models.

Table 2: Evaluation on CIFAR-100 and ImageNette for MDEQ and MOptEqs.

Implicit Models with Multiple Scales. Moreover, we conduct experiments compared with other models which handling multi-scale inputs. Like MDEQ, we construct our MOptEqs with four branches with resolution size equals to 32,16,8,4. Other details can be found in Appendix.A.6. From Table.1 (b) and as shown in Table.2 (a), one can see that our MOptEqs not only outperforms the widely used explicit model ResNet-18 (He et al., 2016), but also shows better performance compared with MDEQ with fewer parameters on CIFAR, which is one of the best models. The empirical results for the multi-scale models further verify the superiority of MOptEqs and its training strategy.

Apart from experiments on small images, we also conduct experiments on ImageNette, which is a subset of 10 classes from ImageNet. Compared with MDEQ, our MOptEqs consistently perform better shown in Table.2 (b). Nevertheless, as one can see from the results, the difference between MDEQ and our model becomes much bigger in the CIFAR-100 and Imagenette with the same training hyper-parameters. Such a phenomenon demonstrates that the performance of our model is much more stable than MDEQ. Apart from these experiments, we also conducted ablation studies for our models in the following section.

3.2 The comprehensive understanding of MOptEqs

(a) MOptEqs.   (b) POptEqs.   (c) MOptEqs.   (d) POptEqs.

Figure 2: Visualization of the channels correlations for the MOptEqs and POptEqs.

Visualization of the impact for the HH&D module. In this section, we try to estimate the effect of our HH&D module. We finish experiments in this part using three-branch MOptEqs with 16 channels for each branch to make the visualization more clear.

We tries to verify our HH&D module's effect in two aspects. First, we plot scatter figures for the values of $\frac{\sum_{i=1}^{L} \sum_{j \in \mathcal{N}(i)} \mathcal{D}(\mathbf{z}_i, \mathbf{z}_j)}{L(C^2 - C)}$ (denoted as *Average D*) and $\frac{\sum_{i=1}^{L} \sum_{j \in \mathcal{N}(i)} \mathcal{H}(\mathbf{z}_i, \mathbf{z}_j)}{LC}$ (denoted as *Average H*) for 100 randomly chosen samples ($\mathcal{N}(i)$ denotes neighboring branch of the i-th branch). Since the hidden optimization problem is to maximizing $\mathcal{H}$ while minimizing $\mathcal{D}$, we find that our MOptEqs (Figure.2(a)) can induce the output features to reach such goal compared with POptEqs (MOptEqs without HH&D) (Figure.2(b)).

Furthermore, we also plot heatmaps of the first two branches' correlation score ($|\mathbf{vec}^{-1}(\mathbf{z}_2)\mathbf{vec}^{-1}(\mathbf{z}_1)^{\top}| \in \mathbb{R}^{16 \times 16}$) for a randomly chosen sample shown in Figure.2(c)(d). One can see that MOptEqs' heatmap (Fig.2(c)) is more likely to be a diagonal matrix while heatmap Fig.2(d) for POptEqs looks random. The heatmap shows that our HH&D can induce the model to perform as our demand, which means corresponding channels for adjacent branches can be more correlated, while the dis-corresponding channels are unrelated due to our architecture design. The visualizations and former results on different datasets verify the effectiveness of our modelling and our HH&D modules' design.

Figure 3: (a) Test accuracy changes with respect to the perturbation size for different perturbed directions. (b) Test Accuracy for small MOptEqs (w. and w/o. PE) under PGD attack with different inner iterations. (c) Plot of the accuracies for the small MOptEqs without HH&D trained by the extended loss with respect to various γ.

Evaluation of the reconstructed perturbation. We compare our perturbation with randomly generated ones in a one-branch well-trained MOptEqs to validate its effectiveness. We first feed a natural sample $\mathbf{x}$ to the model and acquire output $\mathbf{z}$ for $\mathbf{x}$ and generate our reconstructed perturbation using such output and then feed it to the model. Furthermore, we add the perturbations generated by Binomial distribution ($\mathbb{P}(\delta_i = \epsilon) = \mathbb{P}(\delta_i = -\epsilon) = 0.5$) and Uniform distribution $\mathcal{U}[-\epsilon, \epsilon]$ to input features $g(\mathbf{x})$ for comparison. The result of each distribution is averaged for five trials. Figure.3(a) shows our perturbation generated by maximizing G is much more effective, which validates the effectiveness of our reconstructed perturbations and the rationality of our assumptions and analysis in Section.2.2.

Robustness of our MOptEqs trained by PE strategy. In addition to improving the generalization abilities for models as shown in Sec.3.1, perturbations with proper size may also enhance the robustness of our MOptEqs, shown in Figure.3(b). We conduct experiments on small MOptEqs (the same setting as Sec.3.1's single-view model). Our perturbation enhanced training strategy goes stronger as ϵ increases. The figure shows that accuracy for the model trained naturally drops quicker than trained by PE strategy. Overall, trained with appropriate reconstructed perturbation can partly improve the robustness of our MOptEqs.

MOptEqs vs. adding Regularizers in training loss. Apart from our HH&D modules, adding $\mathcal{D}$ and $\mathcal{H}$ to the training loss is one of the most popular methods for obtaining outputs with certain properties. In order to demonstrate the superiority of our module empirically, we conduct experiments for our MOptEqs trained by cross-entropy and POptEqs (MOptEqs (w/o. HH&D)) trained by the cross-entropy loss adding $\gamma \sum_{i=1}^{L} (\mathcal{H}(\mathbf{z}_i, \mathbf{z}_{i+1}) - \lambda \mathcal{D}(\mathbf{z}_i, \mathbf{z}_{i+1}))$ as regularizers (we call it augmented loss). Then we drew its test accuracy for different γ trained by the augmented loss (λ is the same as ours) shown in Figure.3(c).

With proper γ, POptEqs trained by additional loss can perform better than $\gamma = 0$. Such phenomenon demonstrates the effectiveness of our HH&D Modelling. Furthermore, the figure demonstrates the superiority of our model since the traditional method is consistently worse than ours. We left some other explorations for our model in the Appendix due to the space limit.

4 CONCLUSION

We introduce the multi-branch optimization induced equilibrium models (MOptEqs), a new extension of OptEqs that can utilize multiscale information for recognition tasks and retain its ability to recover to an optimization problem whose solution is equivalent to the equilibrium states of our model. The model architecture is designed based on modelling the hidden objective function for the multi-resolution recognition task. Furthermore, we also propose a new training strategy inspired by our understandings of the hidden optimization problem. The empirical results show the advantages of our proposed methods. The success of our HH&D module and PE training strategy demonstrates the deep link between the optimization problem and neural architecture and may motivate further explorations.

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