Penalty and Augmented Lagrangian Methods for Layer-parallel Training of Residual Networks

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Abstract

Algorithms for training residual networks (ResNets) typically require forward pass of data, followed by backpropagating of loss gradient to perform parameter updates, which can take many hours or even days for networks with hundreds of layers. Inspired by the penalty and augmented Lagrangian methods, a layer-parallel training algorithm is proposed in this work to overcome the scalability barrier caused by the serial nature of forward-backward propagation in deep residual learning. Moreover, by viewing the supervised classification task as a numerical discretization of the terminal control problem, we bridge the concept of synthetic gradient for decoupling backpropagation with the parareal method for solving differential equations, which not only offers a novel perspective on the design of synthetic loss function but also performs parameter updates with reduced storage overhead. Experiments on a preliminary example demonstrate that the proposed algorithm achieves comparable or even better testing accuracy to the full serial backpropagation approach, while enabling layer-parallelism can provide speedup over the traditional layer-serial training methods.

1 Introduction

Directed neural networks with hundreds or even thousands of layers have become indispensable tools for supervised learning tasks involving large datasets [16, 17]. Training such a multi-layer network typically requires forward pass of the input data, followed by backpropagation [32] of the prediction error to execute parameter updates. However, even with the use of powerful GPUs, training modern networks remains a formidable endeavor. As such, various parallelization techniques including, but not limited to data-parallelism [19, 33], model-parallelism [6], and a combination of both [15, 30] have been proposed in the literature to reduce training runtimes. Unfortunately, none of the above methods have tackled the scalability barrier created by the inherent serial propagation of feature and error signal through the network architecture [8, 31, 4, 10].

One way of breaking the serial nature of forward-backward propagation is to apply synthetic gradients to build decoupled neural interfaces [20], where the true gradient is approximated by a learned model so that parameter of each building module can be locally updated without performing the full serial backpropagation. However, such a method may fail in training deep convolutional networks since the construction of synthetic loss function has little relation to the target objective function [28]. In another recent approach, by regarding the supervised learning task as an optimal control problem [37, 24], parareal method for solving differential equations [8, 31] is employed to replace the conventional forward and backward propagations with iterative multigrid schemes. However, in the first-state-then-

*Equal contribution. The theory is developed by Qi Sun, the experiments are implemented by Hexin Dong and Zewei Chen.

Preprint. Under review.
Figure 1: A diagram describing the construction of parallel training algorithm for residual learning.

adjoint approach, the feature map is recorded at each module and then used in a subsequent process to solve the adjoint equation, which can incur significant storage overhead \cite{7,11}.

On the other hand, the quadratic penalty method \cite{10,4} has been applied for decoupling backpropagation, although it suffers from well-known limitations such as ill-conditioning \cite{29} and poor for comparing image representations \cite{10}. Similar approaches are proposed in \cite{34,38} which loosen the exact layer-wise connections by using the alternating direction method of multipliers, however, such methods are not scalable to deep convolutional networks \cite{21} nor do adaptive to the stack of layers.

In this work, we propose a novel layer-parallel training method that breaks the intrinsically serial propagation of feature and gradient within the network itself. More specifically, the algorithm is constructed as follows (see also Figure 1)

- discrete to continuum: the deep layer limit of ResNet training procedure coincides with an ODE-constrained terminal control problem \cite{35,37}, in which the underlying network with fixed parameters is interpreted as a numerical discretization of differential equations \cite{25,3};
- relaxation with constraint violations: traditional adjoint methods \cite{36} for the solution of terminal control problem can be quite time-consuming due to the necessity of solving forward-backward differential equations, therefore, the penalty and augmented Lagrangian \cite{29}, also known as the parareal methods \cite{27,11} are employed to increase concurrency;
- continuum to discrete: a stable finite difference scheme \cite{9} is then applied to discretize the relaxed terminal control problem, which results in a decoupling of the full serial backpropagation \cite{18} after absorbing the adjoint variables into layer-wise synthetic loss functions.

The main contribution and the potential impact of our work can be summarized as follows:

- though the proposed layer-wise synthetic loss function requires no label information, its dependence on auxiliary variables allows the acceleration of training without loss of accuracy;
- by performing control updates simultaneously with the solution of adjoint equations, the storage overhead can be reduced when compared to the existing parareal approaches \cite{3};
- in contrast to the penalty method \cite{10}, the augmented Lagrangian method is applied to avoid the issue of ill-conditioning, i.e., it is not necessary to send the penalty coefficient to infinity;
- dynamical system view makes it easier to inspire ideas from mathematical sciences that do not have analogs in deep learning, e.g., stability analysis \cite{13} and adaptive stacking of layers for the decomposition of neural networks \cite{26}.

The rest of this paper is organized according to the structure depicted in Figure 1 followed by the experimental results to validate the effectiveness and efficiency of the proposed algorithms.

## 2 Supervised Learning with Residual Networks

Based on the variational analysis using \( \Gamma \)-convergence \cite{35}, the deep layer limit of ResNet training procedure (notation description is put into supplementary material due to space limitations), i.e.,

\[
\arg\min_{\{W_{\ell}\}_{\ell=0}^{L-1}, X_0 = S(y)} \left\{ \sum_{\ell=0}^{L-1} \mathbb{E}_{y \in \Omega} \left[ ||T(x_{\ell}) - h(y)|| \mid x_{\ell} = S(y) \right] \mid X_{\ell+1} = X_{\ell} + F(X_{\ell}, W_{\ell}) \right\} \tag{1}
\]

with labeled data \( \{y, h(y)\}_{y \in \Omega} \) and \( 0 \leq \ell \leq L - 1 \), takes on the form

\[
\arg\min_{\omega_{\ell}} \left\{ \mathbb{E}_{y \in \Omega} \left[ ||T(x_{\ell}) - h(y)|| \mid x_{\ell} = S(y) \right] \mid dx_{\ell} = f(x_{\ell}, w_{\ell})dt \right\} \tag{2}
\]
Figure 2: The blue/red lines describe, respectively, the forward propagation of data with true/virtual initial values and module parameters.

where the input and output layers, namely, $S$ and $T$, are assumed to be fixed [14] for the ease of illustration. By introducing the Lagrange functional with multiplier $p_t$ [12], the iterative method with step size $\eta > 0$ for finding the extremal is given by (see supplementary material for more details)

$$
\begin{align*}
\begin{aligned}
\frac{dx_t}{dt} &= f(x_t, w_t), & x_0 &= S(y), \quad \text{(state equation)} \\
\frac{dp_t}{dt} &= -p_t \frac{\partial f(x_t, w_t)}{\partial x}, & p_1 &= \frac{\partial \varphi(x_1)}{\partial x}, \quad \text{(adjoint equation)} \\
w_t &\leftarrow w_t - \eta \left( p_t \frac{\partial f(x_t, w_t)}{\partial w} \right), & 0 \leq t \leq 1, \quad \text{(control updates)}
\end{aligned}
\end{align*}
$$

which is consistent with the standard backpropagation method by taking the limit as $L \to \infty$.

Clearly, the iterative methods for solving not only the discrete problem (24) but also the continuous problem (27) result in several forms of locking [20], namely,

- forward locking: no module can process its incoming data before the previous node in the directed forward network have executed;
- backward locking: no module can capture the loss change w.r.t. its state before the previous node in the backward network have executed;
- update locking: no module parameters can be updated before all the dependent nodes have executed in both the forwards and backwards modes.

Although recent hardware developments have gradually increased the capability of data-parallelism [19, 33], model-parallelism [6], and a combination of both [30] for neural network training, none of them could overcome the scalability barrier caused by the serial forward-backward propagation through the network itself [8]. As such, breaking the aforesaid locking issues is another promising approach to speed up the training time, which can be highly desirable for practical implementations.

### 3 Penalty and Augmented Lagrangian Methods

To avoid the necessity of solving forward-backward differential equations (28-29) for control updates (31) at each iteration, constraint violations through the penalty and augmented Lagrangian methods [29] are introduced in this section in order to increase the concurrency, i.e., the second path in Figure 1 which are also known as the parareal or multiple shooting methods [27, 1].

#### 3.1 Forward Pass using Auxiliary Variables

To employ $K \in \mathbb{N}_+$ processors for the solution of forward pass equation (28), we introduce a partition of the time interval $[0, 1]$ into several disjoint intervals as shown in Figure 2, i.e.,

$$
0 = s_0 < \ldots < s_k < s_{k+1} < \ldots < s_K = 1.
$$

Now we are ready to define states $\{x_t^k\}_{k=0}^{K-1}$ such that the underlying dynamic evolves according to the initial value problem that originates from auxiliary variable $\lambda_k$ with control variable $w_t^k$, i.e.,

$$
x_{s_k}^k = \lambda_k, \quad \frac{dx_t^k}{dt} = f(x_t^k, w_t^k)dt \quad \text{on } (s_k, s_{k+1}].
$$
Here, \( x_{k}^{k} \) and \( x_{k}^{k} \) refer to the right and left limits of the possibly discontinuous function \( x_{t}^{k} \) at the interface \( t = s_{k} \). It is obvious that the solution to state equation (28) satisfies the equality \( x_{t}^{k} = x_{t}^{k} \) for any \( t \in [s_{k}, s_{k+1}] \) and \( 0 \leq k \leq K - 1 \) if and only if

\[
w_{k}^{k} = w_{k}|_{(s_{k}, s_{k+1}]} \quad \text{and} \quad \lambda_{k} = x_{k}^{s_{k}}.
\]

or, equivalently, the auxiliary variable \( \lambda_{k} = x_{k}^{s_{k}^{-1}} \) with \( x_{s_{0}}^{s_{0}} = x_{0} \) to replace the second equality.

In other words, with the notations above, the terminal control problem (27) can be rewritten as

\[
\arg \min_{\{w_{k}^{k}\}_{k=0}^{K-1}} \left\{ \varphi(x_{s_{K}}^{K-1}) \bigg| x_{s_{k}}^{k-1} = \lambda_{k} \text{ and } x_{s_{k}}^{k} = x_{k}= \lambda_{k}, \ d_{k} = f(x_{k}, w_{k})dt \text{ on } (s_{k}, s_{k+1}) \right\}
\]

(7)

### 3.2 Penalty Method for Control Updates

Note that the exact connection in (7) is loosened when incorporating external auxiliary variables, a penalty function \( \psi(\lambda, x) = \| \lambda - x \| \) (the metric will be specified later) measuring the discrepancy between \( \lambda_{k} \) and \( x_{s_{k}^{-1}} \) is often introduced in order to satisfy the equality-constraint (28) approximately, which leads to an optimal control problem with both terminal and intermediate loss functions.

\[
\arg \min_{\{w_{k}, \lambda_{k}\}_{k=0}^{K-1}} \left\{ \varphi(x_{s_{K}}^{K-1}) + \sum_{k=0}^{K-1} \beta \# \psi(\lambda_{k}, x_{s_{k}}^{k-1}) \bigg| x_{s_{k}}^{k} = \lambda_{k}, \ d_{k} = f(x_{k}, w_{k})dt \text{ on } (s_{k}, s_{k+1}) \right\}
\]

where \( \beta > 0 \) is a penalty coefficient, \# the total number of elements in the input variables of penalty function, and \( \psi(\lambda_{0}, x_{s_{0}}^{-1}) = \psi(x_{0}, x_{0}) = 0 \) by definition. Accordingly, the Lagrange functional

\[
\mathcal{L}_{p}(x_{k}, p_{k}, w_{k}, \lambda_{k}) = \varphi(x_{s_{K}}^{K-1}) + \sum_{k=0}^{K-1} \beta \# \psi(\lambda_{k}, x_{s_{k}}^{k-1}) + \int_{s_{k}}^{s_{k+1}} p_{k}^{k}(f(x_{k}, w_{k}) - x_{k})dt
\]

implies that adjoint variable \( p_{k}^{k} \) satisfies the backward differential equations (23)

\[
dp_{k}^{k} = -p_{k}^{k} \frac{\partial f(x_{k}, w_{k})}{\partial x}dt \text{ on } (s_{k}, s_{k+1}),
\]

\[
p_{k}^{s_{k+1}} = (1 - \delta_{k,K-1}) \frac{\beta \#}{\beta \#} \frac{\partial \psi(\lambda_{k+1}, x_{s_{k+1}}^{k+1})}{\partial x} + \frac{\partial \varphi(x_{s_{k+1}}^{k+1})}{\partial x},
\]

for any \( 0 \leq k \leq K - 1 \) (detailed derivations are provided in the supplementary material). Here, the notation \( \delta_{k,K-1} \), or \( \delta \) for short, represents the Kronecker Delta function throughout this work.

On the other hand, the update rule for control variables follows from the steepest descent method

\[
w_{k}^{k} \leftarrow w_{k}^{k} - \eta \left( p_{k}^{k} \frac{\partial f(x_{k}, w_{k})}{\partial w} \right) \text{ on } (s_{k}, s_{k+1}),
\]

(10)

for \( 0 \leq k \leq K - 1 \), while various gradient-based algorithms [11, 29] can be applied for the correction of auxiliary variables at each iteration, e.g.,

\[
\lambda_{0} \equiv x_{0} \quad \text{and} \quad \lambda_{k} \leftarrow \lambda_{k} - \eta \left( \frac{\beta \#}{\beta \#} \frac{\partial \psi(\lambda_{k}, x_{s_{k}}^{k-1})}{\partial \lambda} + p_{k}^{s_{k}} \right) \quad \text{for } 1 \leq k \leq K - 1.
\]

(11)

As a result, the penalty method for solving the minimization problem (27) at each iteration consists of

- local operations (6), (33) and (10) • communicate to correct auxiliary variables (11)

which breaks the forward, backward and update locking issues mentioned before.

Note that by choosing \( \psi(\lambda, x) = \| \lambda - x \|_{L}^{2} \), it can be inferred from (11) that constraint violations of the approximate minimizer to problem (32) satisfy

\[
\lambda_{k} - x_{s_{k}}^{k-1} \approx -\frac{\beta \#}{2\beta} p_{s_{k}}^{k} \quad \text{for } 1 \leq k \leq K - 1
\]

(12)
whereas the penalty method (12) provides only one option. As a consequence, the ill-conditioning
of quadratic penalty approach can be avoided without increasing
its simplicity and intuitive appeal, it suffers from well-known limitations such as ill-conditioning
for large values of penalty coefficient [29] and poor quality for feature extraction [10]. In addition,
the best penalty coefficient setting is often different for different datasets, hence a wise strategy for
choosing penalty function and coefficient is of crucial importance to the practical performance.
Alternatively, the nonsmooth exact penalty method, e.g., \( \psi(\lambda, x) = \| \lambda - x \|_2 \), can often find a solution by performing a single unconstrained minimization, but the non-smoothness
may create complications [29].

3.3 Augmented Lagrangian Method for Control Updates

To make the approximate solution nearly satisfy the equality-constraint (28) even for moderate values
of \( \beta \), a different kind of exact penalty approach is the augmented Lagrangian method [29], that is,

\[
\mathcal{L}_{AL}(x^k_t, p^k_t, w^k_t, \lambda_k, \kappa_k) = \mathcal{L}_P(x^k_t, p^k_t, w^k_t, \lambda_k) - \sum_{k=0}^{K-1} \kappa_k(\lambda_k - x^{k-1}_{s^k})
\]

where \( \kappa_k \) represents an explicit Lagrange multiplier corresponding to the \( k \)-th constraint in (7).

By calculus of variations [23], the adjoint variable \( p^k_t \) satisfies the backward differential equations

\[
dp^k_t = -p^k_t \frac{\partial f(x^k_t, w^k_t)}{\partial x} dt \quad \text{on } [s_k, s_{k+1}],
\]

\[
p^k_{s_{k+1}} = (1 - \delta_{k,K-1}) \left( \beta \frac{\partial \psi(\lambda_{k+1}, x^{k}_{s_{k+1}})}{\partial x} + \kappa_{k+1} \right) + \delta_{k,K-1} \frac{\partial \psi(x^{k}_{s_{k+1}})}{\partial x},
\]

for \( 0 \leq k \leq K - 1 \), while the update rule for control variables is defined for \( 0 \leq k \leq K - 1 \) that

\[
w^k_t \leftarrow w^k_t - \eta \left( p^k_t \frac{\partial f(x^k_t, w^k_t)}{\partial w} \right) \quad \text{on } [s_k, s_{k+1}].
\]

In contrast to the penalty method [11], the correction of auxiliary variables now takes on the form

\[
\lambda_0 = x_0 \quad \text{and} \quad \lambda_k \leftarrow \lambda_k - \eta \left( \beta \frac{\partial \psi(\lambda_k, x^{k-1}_{s_k})}{\partial \lambda} + p^k_{s_k} - \kappa_k \right) \quad \text{for } 1 \leq k \leq K - 1.
\]

Similar in spirit, by choosing \( \psi(\lambda, x) = \| \lambda - x \|_2^2 \), formula (15) indicates that constraint violations
of the augmented Lagrangian method satisfy

\[
\lambda_k - x^{k-1}_{s_k} \approx \frac{\#}{2\beta} (\kappa_k - p^k_{s_k}) \quad \text{for } 1 \leq k \leq K - 1
\]

which offers two ways of improving the consistency constraint: increasing \( \beta \) or sending \( \kappa_k \to p^k_{s_k} \),
whereas the penalty method [12] provides only one option. As a consequence, the ill-conditioning
of quadratic penalty approach can be avoided without increasing \( \beta \) indefinitely. Under such circumstances, the update rule for Lagrange multiplier can be deduced from (16), namely,

\[
\kappa_0 = 0 \quad \text{and} \quad \kappa_k \leftarrow \kappa_k - \eta \frac{\#}{2\beta} \left( \lambda_k - x^{k-1}_{s_k} \right) \quad \text{for } 1 \leq k \leq K - 1.
\]

Consequently, the augmented Lagrangian approach for solving problem (27) at each iteration includes

- local operations [9], [15] and (14)
- correction of auxiliary variables (15) and multipliers (17)

which not only breaks the forward, backward and update locking issues mentioned before but also lessen the ill-conditioning of quadratic penalty method and the tuning of penalty coefficient.
4 Parallel Training of Residual Networks

After employing a stable finite difference scheme [9] for the discretization of the dynamical system established in section 3, a non-intrusive layer-wise parallel training algorithm is proposed in this section to speed up the ResNet training procedure. In particular, by letting \( \kappa_k = 0 \) for any \( 0 \leq k \leq K - 1 \), the augmented Lagrangian method degenerates to the proposed penalty approach and hence the latter is omitted in what follows.

4.1 Parallel Backpropagation using Synthetic Gradients

Recall the partitioning of \([0, 1]\) associated with the original deep ResNet (24)

\[
0 = t_0 < t_1 < \ldots < t_L = t \Delta t < t_{L+1} < \ldots < t_{L+nK} = 1,
\]

its shallow ResNet counterpart is built by choosing a coarsening factor \( n > 1 \) and extracting every \( n \)-th module as shown in Figure 2 or, to put it differently, state equation (28) with a coarser partition

\[
t_0 = s_0 < \ldots < s_k < s_{k+1} < \ldots < s_K = t_L,
\]

that can be trained with low accuracy at a correspondingly low cost. By replicating the trained blocks [2], we obtain an effective initial guess for auxiliary and control variables in (32).

Furthermore, \([s_k, s_{k+1}]\) is uniformly divided into \( n \) sub-intervals, i.e.,

\[
s_k = t_{kn} < t_{kn+1} < \ldots < t_{kn+n-1} < t_{kn+n} = s_{k+1}
\]

for \( 0 \leq k \leq K - 1 \), we have by (6) that feature flow of the \( k \)-th sub-network evolves according to

\[
X^k_{kn} = \lambda_k,
\]

\[
X^k_{kn+1} = X^k_{kn} + F(X^k_{kn+m}, W^k_{kn+m})
\]

(18)

where \( 0 \leq m \leq n - 1 \). Then by using the stable numerical scheme that naturally arises from the discrete-to-continuum transition in section 2 the discretization of (13) satisfies backward dynamic

\[
P^k_{kn+m+1} = P^k_{kn+m+1} + P^k_{kn+m+1} \frac{\partial F(X^k_{kn+m}, W^k_{kn+m})}{\partial X} = \frac{\partial X^k_{kn+m+1}}{\partial W} P^k_{kn+m+1} + \frac{\partial \lambda_k}{\partial X} P^k_{kn+m+1},
\]

(19)

\[
P^k_{kn+n} = (1 - \delta_{k,K-1}) \left( \beta \frac{\partial \psi(\lambda_{k+1}, X^k_{kn+n})}{\partial X} + \kappa_{k+1} \right) + \frac{\partial \lambda_k}{\partial X} P^k_{kn+m+1}
\]

(20)

In other words, for any \( k \)-th interval and arbitrary \( 0 \leq m \leq n \), the adjoint variable in (19) equals to

\[
P^k_{kn+m} = (1 - \delta_{k,K-1}) \left( \beta \frac{\partial \psi(\lambda_{k+1}, X^k_{kn+n})}{\partial X} + \kappa_{k+1} \frac{\partial X^k_{kn+m}}{\partial X^k_{kn+n}} \right) + \frac{\partial \lambda_k}{\partial X} P^k_{kn+m+1}
\]

(21)

which captures the terminal and layer-wise synthetic loss changes, i.e., the second and the first term on the right-hand-side of (20), w.r.t. hidden layers for \( k = K - 1 \) and \( 0 \leq k \leq K - 2 \), respectively. In contrast to the straightforward approach [27, 8] where the iterations are performed by first solving state equation (9), then adjoint equation (33) afterwards, and finally control updates (10), we propose to conduct control updates simultaneously with the solution of adjoint equation after solving the state equation. Then for any \( 0 \leq k \leq K - 1 \) and \( 0 \leq m \leq n \), parameter updates associated with the \( k \)-th sub-ResNet can be deduced from (18) and (20), that is,

\[
W^k_{kn+m} \leftarrow W^k_{kn+m} - \eta \left( \frac{\partial F(X^k_{kn+m}, W^k_{kn+m})}{\partial W} P^k_{kn+m+1} \right)
\]

\[
W^k_{kn+m} = W^k_{kn+m} - \eta \left( 1 - \delta \left( \beta \frac{\partial \psi(\lambda_{k+1}, X^k_{kn+n})}{\partial X} + \kappa_{k+1} \frac{\partial X^k_{kn+m}}{\partial X^k_{kn+n}} \right) + \left( \delta \right) \frac{\partial \lambda_k}{\partial X} P^k_{kn+m+1} \right)
\]

(21)

where the stable discretization scheme is applied to guarantee the accurate gradient information [9]. Next, we have by (15) and (20) that the correction of auxiliary variables satisfies \( \lambda_k \rightleftharpoons x_0 \) and

\[
\lambda_k \leftarrow \lambda_k - \eta \left( \beta \frac{\partial \psi(\lambda_k, X^k_{kn-1})}{\partial \lambda} + (1 - \delta) \left( \beta \frac{\partial \psi(\lambda_{k+1}, X^k_{kn+n})}{\partial X^k_{kn+n}} + \kappa_{k+1} \frac{\partial X^k_{kn+m}}{\partial X^k_{kn+n}} \right) + \frac{\partial \psi(X^k_{kn+n})}{\partial X^k_{kn+n}} \right)
\]

(22)
for $1 \leq k \leq K - 1$, while the update rule for Lagrangian multiplier $\kappa_k$ is given by

$$
\kappa_0 = 0 \quad \text{and} \quad \kappa_k \leftarrow \kappa_k - \eta \frac{\delta}{2\beta} \left( \lambda_k - X_k^{k-1} \right) \quad \text{for} \quad 1 \leq k \leq K - 1.
$$

Clearly, correction operations (22) and (23) require communication between adjacent layers which can impede the performance of parallel computations.

Consequently, parallel training of ResNet for supervised classification task (24) can be formulated as

- layer-wise forward pass (18)
- layer-wise backpropagation (35)
- communicate to correct (22-23)

at each iteration, which not only breaks the forward, backward and update locking effects but also reduces the storage overhead compared with the parareal approach proposed in [8].

4.2 Non-intrusive Implementation Details

The stage-wise parallel training approach is summarized in algorithm 1 for deep residual learning, which can be applied in a non-intrusive way w.r.t. the existing network architectures. Besides, we denote by $K = 1$ the traditional method using the full serial forward-backward propagation.

Figure 3: Two-stage penalty method: learning curves of constraint violation, training loss through the full serial forward pass and testing accuracy w.r.t. different settings of the penalty coefficient.

Figure 4: Two-stage augmented Lagrangian method: learning curves of constraint violation, training loss through the full serial forward pass and testing accuracy w.r.t. different penalty coefficients.

Figure 5: Comparison of penalty and augmented Lagrangian methods using $K = 2, 3$ and $4$ stages.

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*Trainable parameters in the input and output layers, i.e., $S$ and $T$, can be automatically learned by coupling into the first and last sub-ResNets respectively.

†Since the uniform decomposition of deep networks is adopted in our experiments, noise injection to $\lambda_{K-1}$ can help the last shallow sub-ResNet to prevent overfitting.
Algorithm 1: Layer-parallel training method for deep residual learning

// Initialization.
[1] divide the ResNet containing $L = Kn$ building modules into $K$ stages (see Figure 2);
[2] generate initial values for network parameters and auxiliary variables (using the ResNet trained with few epochs or the multilevel training strategy proposed in [2]);
[3] set multipliers to zero; // switch to penalty method if $\kappa_k = 0$ hereafter
[4] pick a suitable metric, e.g., squared $\ell_2$-norm, $\ell_1$-norm or $\ell_\infty$-norm, for penalty function;
[5] choose positive sequences of increasing coefficients $\{\beta_j\}_{j=1}^J$ and decreasing tolerances $\{\tau_j\}_{j=1}^J$;
[6] schedule proper learning rates for network parameters, auxiliary variables and multipliers;

// Training Procedure.

for $j \leftarrow 1$ to $J$ \textbf{(number of epochs)} do

foreach mini-batch input data do

parfor $k \leftarrow 0$ to $K - 1$ do

// stage-wise forward pass using auxiliary variable

for $m \leftarrow 0$ to $n - 1$ do

$X_{kn+m}^k = \lambda_{kn+m}^mb \cdot X_{kn+m+1}^k = X_{kn+m}^k + F(X_{kn+m}^k, W_{kn+m})$

// stage-wise backpropagation using synthetic loss

for $m \leftarrow 0$ to $n - 1$ do

if $k \neq K - 1$ then

$W_{kn+m}^k \leftarrow W_{kn+m}^k - \eta \left( \frac{\beta_j \partial \psi(\lambda_{kn+m}^{mb}, X_{kn+m}^k)}{\#} + \kappa_{k+1}^mb \frac{\partial X_{kn+m}^k}{\partial W_{kn+m}^k} \right)$

else

$W_{kn+m}^k \leftarrow W_{kn+m}^k - \eta \frac{\partial \phi_{mb}(X_{kn+m}^k)}{\partial W_{kn+m}^k}$

// communicate to correct

for $k \leftarrow 1$ to $K - 1$ do

while $\psi(\lambda_{kn+m}^{mb}, X_{kn+m}^{k-1}) > \tau_j$ do

if $k \neq K - 1$ then

$\lambda_k^{mb} \leftarrow \lambda_k^{mb} - \eta \left( \frac{\beta_j \partial \psi(\lambda_k^{mb}, X_{kn}^k)}{\#} + \kappa_{k+1}^mb \frac{\partial X_k^k}{\partial \lambda_k^{mb}} \right)$

else

$\lambda_k^{mb} \leftarrow \lambda_k^{mb} - \eta \left( \frac{\partial \phi_{mb}(X_{kn}^k)}{\partial X_k^k} - \kappa_k^{mb} \right)$

$\kappa_k^{mb} \leftarrow \kappa_k^{mb} - \eta \frac{\#}{2\beta_j}(\lambda_k^{mb} - X_k^{k-1})$ \textbf{// quadratic penalty function}


5 Experiments

To validate our method against the full serial backpropagation, the proposed Algorithm 1 is applied to decouple and train a ResNet with 122 layers on small scale datasets. As a preliminary example, we consider a supervised classification problem that groups grid points into three-level sets, (detailed descriptions of the dataset and network architecture are put into supplementary material).

Table 1: Training loss through the full serial forward pass, testing accuracy, runtime and speedup ratio w.r.t. fine-tuned penalty coefficients and different stage numbers on the preliminary example.

|     | Quadratic Penalty Method | Augmented Lagrangian Method |
|-----|--------------------------|----------------------------|
|     | train loss | test acc. | runtime | speedup | train loss | test acc. | runtime | speedup |
| $K = 1$ | 1.8e-3 | 92.5% | 23.52s | - | - | - | - | - |
| $K = 2$ | 5.0e-5 | 95.0% | 16.25s | 1.45 | 5.6e-4 | 95.0% | 16.47s | 1.43 |
| $K = 3$ | 6.6e-2 | 93.5% | 13.68s | 1.72 | 1.2e-2 | 93.5% | 14.83s | 1.58 |
| $K = 4$ | 9.2e-2 | 92.5% | 12.32s | 1.91 | 3.0e-2 | 92.0% | 12.85s | 1.83 |
We first report the experimental results of penalty method, \( \text{i.e.} \), multipliers \( \{\kappa_k\}_{k=0}^{K-1} \) are identically zero throughout the algorithm 1. After fixing the penalty coefficient and solving the relaxed problem (32) for few epochs, the value of followed-up penalty coefficients is chosen to be modestly larger than the previous one for another few epochs (hyperparameter configuration is provided in supplementary material). By fixing the number of stages \( K = 2 \) and correcting the auxiliary variable (11) only one time at each iteration, we observe from Figure 3 (left) that increasing \( \beta \) along iterations can significantly reduce the constraint violation (12). However, finding the approximate minimizer of (32) may become difficult when \( \beta \) grows too rapidly (the center and right figures in Figure 3).

Next, we increase the number of stages and the results are reported in Table 1. Furthermore, the learning curves of testing accuracy are displayed in Figure 5, which implies that the penalty method can achieve comparable or even better testing accuracy to the full serial backpropagation, while enabling multi-stage layer-parallelism can provide speedup over the layer-serial training method.

Similar in spirit, experimental results of the augmented Lagrangian method are reported in Figure 4 and Table 1. By fixing the number of stages \( K = 2 \), Figure 5 (left) compares the learning curves of testing accuracy between the penalty and augmented Lagrangian methods, which demonstrates that the introduction of multipliers \( \{\kappa_k\}_{k=0}^{K-1} \) can not only reduce the constraint violations (the first figure in Figure 3 and Figure 4) but also accelerate the training with an acceptable loss of accuracy.

**Broader Impact**

In this paper, the authors introduce penalty and augmented Lagrangian methods for layer-parallel training of residual networks (ResNets), which can speed up the training runtime over the traditional layer-serial training methods.

Directed neural networks with hundreds of layers have become indispensable tools in many machine learning tasks including, but not limited to, computer vision \[16, 17\], natural language processing \[5\], etc. However, even with the use of modern GPUs, compute time for training deep ResNets remains a formidable endeavor. While there exists various parallelization techniques such as data-parallelism \[19, 33\], model-parallelism \[6\] or a combination of both \[15, 30\], our research could be applied to overcome the scalability barrier created by the inherent serial forward-backward propagation within the network itself, and therefore accelerates the overall training process with comparable or even better testing accuracy.

There is a broad range of implications for using the proposed algorithms:

- though the proposed layer-wise synthetic loss function requires no label information as in the standard cases \[20\], its dependence on auxiliary variables allows the synthetic gradient to tackle the task-independent drawback \[28\];
- in contrast to the first-state-then adjoint approach \[8\], the storage overhead of our methods can be reduced by performing control updates simultaneously with the solution of adjoint equations;
- to overcome the issue of ill-conditioning for decoupling backpropagation via the quadratic penalty method \[10\], the augmented Lagrangian method is employed in our work so that there is no necessary to send the penalty coefficient to infinity.

We also encourage researchers to adopt the dynamical system viewpoint and inspire ideas from mathematical sciences that do not yet have analogs in deep learning, \textit{e.g.}, stability analysis \[13\] and adaptive stacking of layers for the decomposition of neural networks \[26\].

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Supplementary Material for “Penalty and Augmented Lagrangian Methods for Layer-parallel Training of Residual Networks”

Supervised Learning with Residual Networks

In this section, we first briefly review the benchmark residual learning framework [16] that assigns pixels in the raw input image to categories of interest as shown in Figure 6. Its deep layer limit is then introduced to bridge the supervised classification task with an ODE-constrained terminal control problem [35].

\[ y \in \Omega \]

| input layer | \( X_0 = S(y) \) | \( \cdots \) | \( X_\ell \) | \( \text{BN} \) | \( \text{ReLU} \) | \( \text{conv} \) | \( \text{BN} \) | \( \text{ReLU} \) | \( \cdot \) | \( X_{\ell+1} \) | \( \cdots \) | \( X_L \) |
|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| identity mapping | | | | | | | | | | | | | |
| cross entropy | | | | | | | | | | | | | |
| \( h(y) \) | | | | | | | | | | | | | |
| \( T(X_L) \) | | | | | | | | | | | | | |

Figure 6: A diagram describing the serial training process of a pre-activation residual network.

Specifically, given the human-labeled images, i.e., \( \{y, h(y)\}_{y \in \Omega} \), the classification task using ResNets can be formulated as the minimization problem

\[
\arg\min_{\{W_\ell\}_{\ell=0}^{L-1}} \left\{ \mathbb{E}_{y \in \Omega} \left[ \| T(X_L) - h(y) \| \mid X_0 = S(y) \right] \middle| X_{\ell+1} = X_\ell + F(X_\ell, W_\ell) \right\} \tag{24}
\]

where \( X_\ell \) denotes the input feature map of the \( \ell \)-th building block for \( 0 \leq \ell \leq L - 1 \), \( L \in \mathbb{N}_+ \) the total number of blocks, \( F \) a composition of linear and nonlinear functions as depicted in Figure 6, \( W_\ell \) the network parameters to be learned and \( \| \cdot \| \) a given metric measuring the prediction error. Here, the input and output layers, i.e., \( S \) and \( T \), are assumed to be fixed [14] for the ease of illustration.

When the backpropagation method is applied for solving problem (24), we have for \( 0 \leq \ell \leq L - 1 \),

\[
W_\ell \leftarrow W_\ell - \eta \frac{\partial \phi(X_L)}{\partial W_\ell} = W_\ell - \eta \frac{\partial \phi(X_L)}{\partial X_{\ell+1}} \frac{\partial X_{\ell+1}}{\partial W_\ell} = W_\ell - \eta \left( P_{\ell+1} \frac{\partial F(X_\ell, W_\ell)}{\partial W_\ell} \right) \tag{25}
\]

where \( \eta \) is the step size \( \phi(X_L) = \mathbb{E}_{y \in \Omega} \left[ \| T(X_L) - h(y) \| \right] \) and \( P_{\ell+1} = \frac{\partial \phi(X_L)}{\partial X_{\ell+1}} \) for simplicity.

Note that, by chain rule, the temporary variables \( \{P_{\ell+1}\}_{\ell=0}^{L-1} \) satisfy backward dynamic

\[
P_\ell = P_{\ell+1} \frac{\partial X_{\ell+1}}{\partial X_\ell} = P_{\ell+1} + P_{\ell+1} \frac{\partial F(X_\ell, W_\ell)}{\partial X}, \quad P_L = \frac{\partial \phi(X_L)}{\partial X_L}, \tag{26}
\]

which capture the loss changes with respect to (w.r.t.) hidden layers. As a consequence, the serial backpropagation algorithm is handled by equations (26) and (25) [22], and hence the ResNet training procedure at each iteration can be regarded as the following sequential operations

- forward pass to predict (24)
- backward gradient propagation (25)
- weights update (25)

which requires hours or even days as the state-of-the-art networks may involve hundreds of layers.

Deep Layer Limit

Based on the variational analysis via discrete-to-continuum \( \Gamma \)-convergence [35], the deep layer limit of residual learning model (24) is given as

\[
\arg\min_{\omega} \left\{ \mathbb{E}_{y \in \Omega} \left[ \| T(x_1) - h(y) \| \mid x_0 = S(y) \right] \middle| dx_t = f(x_t, w_t) dt \right\}. \tag{27}
\]

1Throughout this work, \( \eta \) represents a universal constant whose value may change with context.
By introducing the Lagrange functional with multiplier $p_t$, solving the constrained optimization problem is equivalent to finding saddle points of the following Lagrange functional without constraints:

$$\mathcal{L}(x_t, w_t, p_t) = \varphi(x_1) + \int_0^1 p_t (f(x_t, w_t) - \dot{x}_t) \, dt$$

$$= \varphi(x_1) - p_1x_1 + p_0x_0 + \int_0^1 p_t f(x_t, w_t) + \dot{p}_t x_t \, dt,$$

and the variation in $\mathcal{L}(x_t, w_t, p_t)$ corresponding to a variation $\delta w$ in control $w$ takes on the form

$$\delta \mathcal{L} = \left[ \frac{\partial \varphi(x_1)}{\partial x} - p_t \right] \delta x + \int_0^1 p_t \left( \frac{\partial f(x_t, w_t)}{\partial x} + \dot{p}_t \right) \delta x + \left( \frac{\partial f(x_t, w_t)}{\delta w} \right) \delta w \, dt,$$

which leads to the necessary conditions for $w_t = w^*_t$ to be the extremal of $\mathcal{L}(x_t, w_t, p_t)$, that is,

$$\begin{align*}
dx_t &= f(x_t, w_t) dt, & x_0 &= S(y), & \text{(state equation)} \\
 dp_t &= -p_t \frac{\partial f(x_t, w_t)}{\partial x} dt, & p_1 &= \frac{\partial \varphi(x_1)}{\partial x}, & \text{(adjoint equation)} \\
 \frac{\partial f(x_t, w_t)}{\partial w} &= 0, & 0 \leq t \leq 1. & \text{(optimality condition)}
\end{align*}$$

However, directly solving this optimality system is computationally infeasible due to the curse of dimensionality, an iterative algorithm with step size $\eta > 0$ is typically used, e.g.,

$$w_t \leftarrow w_t - \eta \left( p_t \frac{\partial f(x_t, w_t)}{\partial w} \right), \quad 0 \leq t \leq 1,$$

which is consistent with the standard backpropagation method by taking the limit as $L \rightarrow \infty$.

## Calculus of Variations for Relaxed Optimization Problem

---supplementary to section 3.2 and 3.3---

Note that by forcing $\kappa_k \equiv 0$ for arbitrary $0 \leq k \leq K - 1$, the augmented Lagrangian method degenerates to the penalty method discussed in section 3.2. As such, we only consider the augmented Lagrangian approach for solving the minimization problem

$$\arg \min_{\{w_t\}_{k=0}^K} \left\{ \varphi(x_k^{K-1}) \left| \begin{array}{c}
x_k^{k-1} = \lambda_k \\
x_k^k = \lambda_k, \ dx_t^k = f(x_t^k, w_t^k) dt \end{array} \right. \right\}_{k=0}^K$$

where the Lagrangian functional is expressed as

$$\mathcal{L}(x_t^k, p_t^k, w_t^k, \lambda_k, \kappa_k) = \varphi(x_k^{K-1}) + \sum_{k=0}^{K-1} \beta \# \left\{ (\lambda_k, x_k^{k-1}, s_k) \mid \lambda_k - x_k^{k-1} - p_k^{k-1} x_k^{k-1} + p_k^k \lambda_k + \int_{s_k}^{s_{k+1}} p_k f(x_t^k, w_t^k) + \dot{p}_k x_t^k \, dt \right\}$$

which can be decomposed as parts involving $x_t^{k-1}$ and $\{x_t^k\}_{k=0}^{K-2}$ respectively:

$$I = \varphi(x_k^{K-1}) - p_k^{K-1} x_k^{K-1} + p_k^{K-1} \lambda_k - x_k^{K-1} + \int_{s_{K-1}}^{s_K} p_k^{K-1} f(x_t^{K-1}, w_t^{K-1}) + \dot{p}_k^{K-1} x_t^{K-1} \, dt,$$

$$II = \sum_{k=0}^{K-2} \beta \# \left\{ (\lambda_{k+1}, x_{k+1}^k, s_{k+1}) \mid (\lambda_{k+1} - p_{k+1}^{k+1} x_{k+1}^k + p_{k+1}^k \lambda_k + \int_{s_k}^{s_{k+1}} p_{k+1} f(x_t^k, w_t^k) + \dot{p}_k x_t^k \, dt - \kappa_{k+1} \lambda_{k+1} \right\}.$$

Given auxiliary variables $\{\lambda_k\}_{k=0}^{K-1}$ associated with multipliers $\{\kappa_k\}_{k=0}^{K-1}$, the variation in Lagrangian functional $\mathcal{L}(x_t^k, p_t^k, w_t^k, \lambda_k, \kappa_k)$ corresponding to a variation $\Delta w_t^k$ in control $w_t^k$ takes on the form

$$\delta \mathcal{L} = \left( \frac{\partial \varphi(x_k^{K-1})}{\partial x} - p_k^{K-1} \right) \delta x_k^{K-1} + \int_{s_{K-1}}^{s_K} \left( p_k^{K-1} \frac{\partial f(x_t^{K-1}, w_t^{K-1})}{\partial x} + \dot{p}_k^{K-1} \right) \delta x_t^{K-1} \, dt$$

$$+ \sum_{k=0}^{K-2} \beta \# \left\{ (\lambda_{k+1}, x_{k+1}^k, s_{k+1}) + \kappa_{k+1} x_{k+1}^k + p_{k+1}^k \lambda_k + \int_{s_k}^{s_{k+1}} p_{k+1} f(x_t^k, w_t^k) + \dot{p}_k x_t^k \, dt \right\} \delta x_t^k \, dt,$$

For notational simplicity, $\frac{dx_t}{dt}$ and $\dot{x}_t$ are used to denote the time derivative of $x_t$ throughout this work.
which implies that adjoint variable $p_k^k$ satisfies the backward differential equations:

$$
 dp_k^k = -p_k^k \frac{\partial f(x_k^k, w_k^k)}{\partial x} dt \text{ on } [s_k, s_{k+1}],
$$

$$
 p_{k+1}^k = (1 - \delta_k, K - 1) \left( \beta \frac{\partial \psi(\lambda_{k+1}, X_k^{k+1})}{\partial x} + \kappa_{k+1} \right) + \delta_{k, K-1} \frac{\partial \varphi(x_k^{k-1})}{\partial x},
$$

for any $0 \leq k \leq K - 1$. Here and in what follows $\delta_{k, K-1}$ represents the Kronecker Delta function.

**Parallel Backpropagation using Synthetic Gradients**

--- supplementary to section 4.1

To discretize the update rule for control variables for any $0 \leq k \leq K - 1$

$$
 w_k^i \leftarrow w_k^i - \eta \left( p_k \frac{\partial f(x_k^i, w_k^i)}{\partial w} \right) \text{ on } [s_k, s_{k+1}],
$$

the specific scheme arising from the discrete-to-continuum transition (see section 3) is used, that is,

$$
 W_{kn+m}^k \leftarrow W_{kn+m}^k - \eta \left( (1 - \delta_k, K-1) \left( \beta \frac{\partial \psi(\lambda_{k+1}, X_k^{k+n})}{\partial X} + \kappa_{k+1} \right) \frac{\partial X_k^{kn+n}}{\partial W_{kn+m}} + \delta_{k, K-1} \frac{\partial \varphi(X_k^{k+n})}{\partial W_{kn+m}} \right)
$$

where the equality holds by substituting the reformulation of $p_k^k$ and $X_k^k$ in section 4.1. Therefore, the update of network parameters satisfies the layer-wise backpropagation

$$
 W_{kn+m}^k \leftarrow W_{kn+m}^k - \eta \left( (1 - \delta_k, K-1) \left( \beta \frac{\partial \psi(\lambda_{k+1}, X_k^{k+n})}{\partial X} + \kappa_{k+1} \frac{\partial X_k^{kn+n}}{\partial W_{kn+m}} \right) + \delta_{k, K-1} \frac{\partial \varphi(X_k^{k+n})}{\partial W_{kn+m}} \right)
$$

for any $0 \leq k \leq K - 1$ and arbitrary $0 \leq m \leq n$. In other words, the synthetic loss function defined for the $k$-th stage takes on the form

$$
 (1 - \delta_k, K-1) \left( \beta \frac{\partial \psi(\lambda_{k+1}, X_k^{k+n})}{\partial X} + \kappa_{k+1} \frac{\partial X_k^{kn+n}}{\partial W_{kn+m}} \right) + \delta_{k, K-1} \frac{\partial \varphi(X_k^{k+n})}{\partial W_{kn+m}}
$$

which can be applied for the parameter updates of the $k$-th stage via the standard backpropagation approach.

**Experiments**

--- supplementary to section 5

As a preliminary example, we consider a supervised classification problem that groups grid points into three level sets, where the training dataset contains 200 points drawn uniformly at random from $\Omega = [-1, 1]^2$ (see Figure 7) and the test dataset consists of another 200 different points.

Besides the input and output layers using fully connected operations, the network used for training consists of 60 building modules where the construction of each block is shown in Figure 8.

We adopt the squared $\ell_2$-norm for the penalty approach. The initial value of penalty coefficient is set to be $\beta = 1$, and is multiplied by $\beta$-rise= 0.1 at 100 and 250 epochs. The penalty coefficient for augmented Lagrangian method is initially set to be $\beta = 0.1$, and is multiplied by $\beta$-rise= 0.1 at 100 and 250 epochs. The learning rate for the multiplier is chosen to be $10^{-9}$. All models are trained with the full-batch gradient descent algorithm, where the training starts with a learning rate of 0.1 for each stage, and is divided by 10 at 70 and 150 epochs.

To supplement our experimental results, Figure 9 depicts the testing performance of penalty and augmented Lagrangian methods w.r.t. different numbers of stages, which implies that increasing the number of stages can further accelerate the training procedure.
Figure 7: Classes of the preliminary example in which the level sets are characterized by ring-shaped regions bounded, respectively, by three concentric circles of radius 0.5, 0.75 and 1.

Figure 8: Building module of the ResNet adopted for our experiments.

Figure 9: Learning curves of testing accuracy w.r.t. different numbers of stages for penalty and augmented Lagrangian methods.