Exploiting Invariance in Training Deep Neural Networks
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Abstract
Inspired by two basic mechanisms in animal visual systems, we introduce a feature transform technique that imposes invariance properties in the training of deep neural networks. The resulting algorithm requires less parameter tuning, trains well with an initial learning rate 1.0, and easily generalizes to different tasks. We enforce scale invariance with local statistics in the data to align similar samples at diverse scales. To accelerate convergence, we enforce a $GL(n)$-invariance property with global statistics extracted from a batch such that the gradient descent solution should remain invariant under basis change. Profiling analysis shows our proposed modifications takes $\sim 5\%$ of the computations of the underlying convolution layer. Tested on convolutional networks and transformer networks, our proposed technique requires fewer iterations to train, surpasses all baselines by a large margin, seamlessly works on both small and large batch size training, and applies to different computer vision and language tasks.

Introduction
The pupillary light reflex constricts the pupil in bright light and dilates the pupil in dim light (Bear, Connors, and Paradiso 2020). This mechanism controls the amount of light passing into the eye, allowing common features to be extracted from signals of different scales. In addition, retinal receptive fields use center-surround structures to filter and sharpen images (Hubel and Wiesel 1962) (Supp. Fig. 6 a, b), removing a bell-shaped autocorrelation present in real-world visual signals. Intriguingly, all other receptive field configurations discovered in Hubel and Wiesel’s seminal research (Supp. Fig. 6 c, d, e) have found artificial analogs in the first layer filters learned by modern convolutional neural networks (Zeiler and Fergus 2014) (Fig. 5 a,b).

While convolutional networks continue to push the envelope in computer vision tasks, state-of-the-art training recipes are still limited by scope and scale. Specifically, when moving from image classification to object detection, different normalization techniques need to be used. Most algorithms perform well at a specific scale, and there is usually a significant drop in accuracy when the training batch size is too large or too small (Wu and He 2018; Singh and Krishnan 2020).

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Figure 1: (a) Validation AP curves of a Mask R-CNN network when trained with network deconvolution++ (ND++), frozen batch normalization and group normalization. (b) Top-1 validation accuracy of ResNet-50 when trained on ImageNet with ND++ and SyncBN using batch size of 256, the training finishes better and faster than using batch size 256 using the same hardware. (c) mIoU curves of DeepLabv3 with a ResNet-101 backbone trained on the Cityscapes dataset using ND++ and SyncBN. ND++ consistently outperforms baselines and produces more stable mIoU curves. (d) ND++ significantly improves upon ND when training ViT-B_16 on the CIFAR datasets.
large batch training without algorithm change. By enforcing
the invariance properties at every layer of the network, we
accelerate training convergence and surpass baseline accu-

racy by a large margin on the ImageNet (Deng et al. 2009),
MS COCO (Lin et al. 2014), and Cityscapes (Cords et al.
2016) datasets for image classification, object detection,
and semantic segmentation, respectively (Fig. 1). In our sup-
plementary materials, we also show promising results for train-
ing transformers on multiple vision and language tasks.

Our main findings are the following:

• We propose a drop-in modification before the linear lay-
ers in a network to explicitly enforce these two invariance
properties, significantly reducing training iterations and
surpassing baseline accuracy by a large margin.

• Training with this modification is robust to different op-
timizer configurations: using the theoretically optimal
learning rate for the linear case of 1.0 can successfully
train a wide range of deep networks.

• Our implementation takes \(\sim 5\%\) (Supp. Table 8) of the
cost of the underlying convolution layer and incorporates
a cross-GPU synchronization which surpasses synchro-
nized batch normalization by a large margin in both small
and large batch regime.

• The benefits of the proposed modification generalize to
emerging architectures in vision and language.

Background

Backward Correction Methods

The complicated loss landscapes (Li et al. 2017) of neu-
ral networks create numerous challenges for training. Deep
neural networks are generally over-parameterized. The pres-
ence of strong correlation between features induces areas of
pathological curvature in the landscape and inhibits effec-
tive training. Small gradients are common in these pathol-
ogical regions, and the problem is exacerbated by small linear
layers and common activation functions. These issues were
traditionally addressed by correcting the gradients (Nocedal
and Wright 2006; Martens 2010; Ye et al. 2017), that is, by
modifying the backward pass. The most popular methods
ormalize the gradient scale to avoid the vanishing gradi-

ent problem and smooth the direction by using previous gra-
dients as a momentum term (Kingma and Ba 2014). More
advanced methods, such as Newton’s method, use approxi-
mate curvature information to modify the gradient direction
(Fig. 2). However, high computational costs limit these algo-
rithms to small-scale problems (Martens and Grosse 2015;
Desjardins et al. 2015). They have not been widely shown to
surpass first-order gradient descent methods.

Forward Correction Methods

Forward transforms provide an alternative approach to
address the challenges in training deep neural net-
works (Huang et al. 2020). Batch normalization (Ioffe and
Szegedy 2015) is a common and powerful example that stan-

dardizes the distribution of features in each dimension. This
stretching with a diagonal matrix works perfectly only for
uncorrelated, axis-aligned features, suggesting that the op-
timality of standardization depends on the choice of basis.

Given the inherent correlation in real-world data, the fea-
ture covariance matrix is generally ill-conditioned and not
diagonal. As a result, gradient descent training usually takes
unnecessary steps towards the solution (Fig. 2(b)). Recently,
more accurate transforms have been proposed to utilize the
covariance matrix and remove the pairwise correlation be-
tween features (Huang et al. 2018; Ye et al. 2018; Huang
et al. 2019; Pan et al. 2019; Ye et al. 2020). If the features
are transformed to be axis-aligned and have unit-variance,
the loss landscape is more isotropic. Gradient descent con-
verges more quickly and accurately (Fig. 2(c)).

Motivations

We start our investigation with a toy example of a one-
layer network (Eq. 1). Rigorous analysis of this simple setup
reveals a surprising depth of insight into the fundamental
training problem. The analysis explains the utility of vari-
ous modern techniques to facilitate training and leads us to
a more advantageous design.

Assume we are given a linear regression problem with a
mean squared error loss (Eq. 1). \(\hat{y}\) is the continuous or
discrete response data to be regressed. This formulation can be
used for prediction or classification. In the typical setting,
the output \(y = Xw\) is given by multiplying the inputs \(X\)
with an unknown weight vector \(w\) for which we are solving.
Let \(N\) be the number of samples, \(d\) the feature dimension,
and \(X\) either the \(N \times d\) or augmented \(N \times (d + 1)\) data
matrix \((X|1)\), if we include a bias.

\[
\text{Loss}_\text{MSE} = \frac{1}{2} E[|y - \hat{y}|^2] = \frac{1}{2N} \|Xw - \hat{y}\|^2. \tag{1}
\]

Local Statistics vs Global Statistics

Given a \(N \times d\) data matrix \(X\), we refer to the column statis-
tics as the global statistics and the row statistics as local
statistics. Mini-batch statistics represent an approximation

\[\text{Figure 2: A toy picture of loss landscapes and gradient steps.} \]

\[\text{Figure 2(a): Highly correlated, non-standardized data.} \]

\[\text{Figure 2(b): Correlated but standardized data.} \]

\[\text{Figure 2(c): With standardized and uncorrelated data, vanilla gradient descent coincides with} \]

\[\text{Newton’s method (Proposition 1).} \]

\[\text{Motivations} \]

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to the global statistics of the whole dataset. Batch normalization (Ioffe and Szegedy 2015) standardizes the $d$ column vectors. This can be visualized as a coordinate transform that stretches the data along each axis based on global statistics (Fig. 2 (a) to (b)). Training then solves for a new set of weights $w_{RN}$ in this transformed space.

On the other hand, sample-based normalization (Ba, Kiros, and Hinton 2016; Wu and He 2018; Singh and Krishnan 2020) stretches each sample by removing the scale and bias in each row of $X$ according to the local statistics. Viewed from the original space, training corresponds to finding $N$ sets of sample-variant weights $\{w_i\}$ that both stretch the samples and fit the model.

$GL(n)$-invariance

One may ask whether the solution of Eq. 1 found using a given algorithm changes under a change of basis. That is, if we use any invertible linear transform, i.e., a member of the general linear group $GL(n)$ (Artin 2011), to transform the features, will we simply reach an equivalent solution in a different coordinate system? If the solution is invariant under the operation of $GL(n)$, we will call the training algorithm $GL(n)$-invariant.

Assuming $X^tX$ is invertible for our toy problem, the unique solution can be found by setting the gradient to 0, \[
\frac{\partial Loss}{\partial w} = \frac{1}{N}X^t(Xw - \hat{y}) = 0,
\]

\[w = (X^tX)^{-1}X^t\hat{y}. \tag{2}\]

Let us consider the impact of different correction methods on the ability of gradient descent-based algorithms to find this solution.

**Case 1 (backward correction/Newton’s method):** For simplicity, suppose we start from $w_0 = 0$, then \[
\frac{\partial Loss}{\partial w}|_{w_0} = -\frac{1}{N}X^t\hat{y}. \]

Letting $H = \frac{1}{N}X^tX = \nabla^2 w$, we see from Eq. 2 that $w = -H^{-1}\frac{\partial Loss}{\partial w}$. This derivation shows us how the gradients can be manipulated in the backward fashion to accelerate convergence (Martens and Grosse 2015; Desjardins et al. 2015; Ye et al. 2017): (1) approximate the curvature with $H$ and apply an inverse correction to decorrelate the gradient, $H^{-1}\frac{\partial Loss}{\partial w}$, then (2) take a descent step using a learning rate of 1.0: $w = w_0 - 1.0 \cdot H^{-1}\frac{\partial Loss}{\partial w}$. This process demonstrates that forward correction can achieve the power of Newton’s method if we (1) decorrelate the feature columns with global statistics and (2) use a learning rate 1.0.

**Proposition 1.** The optimal solution can be found in one step with the forward correction if and only if the feature columns are standardized and uncorrelated.

**Proof.** With these features we have $\frac{1}{N}X^tX = I$, and the optimal explicit solution (Eq. 2) simplifies to $w = \frac{1}{N}X^t\hat{y}$. After one iteration of gradient descent, $w_{new} = w_{old} - \eta \frac{1}{N}X^t(Xw_{old} - X^t\hat{y})$. By substituting $\frac{1}{N}X^tX = I$, we find that $\eta = 1.0$ is optimal and yields convergence in a single iteration.

Scale Invariance

In our toy problem, the output scales linearly with the input, $(aw)w = a(Xw)$. In fact, this property generalizes to common networks with linear layers and ReLU-like activation functions. If we consider a task like bounding box prediction, this suggests that we can scale the box size by simply changing the input brightness, which should clearly be avoided. Through the pupillary light reflex, animal visual systems introduce a scale invariance property so that differently scaled inputs generate similarly scaled features. Although transforming using global statistics can guarantee $GL(n)$-invariance as discussed above, it does not result in scale invariance. Since scale invariance is a concern in some tasks, we utilize both global and local statistics (where samples are transformed individually) in the algorithm. We defer the explanation of details to the next section.

Optimizing the Formulation

Influenced by the batch normalization, most normalization algorithms (Ba, Kiros, and Hinton 2016; Wu and He 2018; Singh and Krishnan 2020; Huang et al. 2018, 2019; Pan et al. 2019) adopt a post-normalization design, normalizing $y = Xw$ after the linear transform rather than normalizing $X$. Since post-normalization restricts the representation power of $y$, two extra parameters are introduced to remove this limitation: $Loss_{MSE} = \frac{1}{n_N}||Xw - \mu\Sigma^{-1}\gamma + \beta - \hat{y}||^2$. As a result, the toy problem contains more than necessary parameters $\{w, \gamma, \beta\}$ instead of $w$ to be optimized. However, the optimal convergence property that we find on the toy problem no longer holds with the introduction of the redundancy. This motivates us to optimize our design to remove the redundancy while maintaining full representation power.

Enforcing Invariance in Training Neural Networks

We demonstrate how the problems in the previous section can be naturally resolved. Some complementary information can be found in recent works (Ye et al. 2020).
To improve the network training, we enhance the linear transform in neural networks by applying the principles derived from the toy problem. We discuss how to enhance three common linear transform layers, starting from analyzing the data matrix \( X \) in the network.

Case 1. The data matrix \( X \) of a fully-connected layer is constructed straightforwardly by stacking \( N \) rows of \( d \) or \( d + 1 \) dimensional feature vectors. We put our emphasis on the data matrix construction of convolution and (cross-)correlation layers.

Case 2. A convolution operation can be expressed in multiple ways in the spatial domain. We can expand the kernel of size \( k \) into a \((n - k + 1) \times n\) convolution matrix \( W \), or unroll the overlapping windows of \( x \) into a \((n - k + 1) \times k\) data matrix \( X \): 
\[
y = x * w = X w_{flipped}.
\]

We provide a 1d convolution example using \( k = 3 \) (in the ‘valid’ mode according to Matlab terminology):
\[
\begin{pmatrix}
  y_1 \\
  y_2 \\
  \vdots \\
  y_{n-k+1}
\end{pmatrix} =
\begin{pmatrix}
  w_1 & w_2 & w_3 \\
  w_2 & w_3 & w_1 \\
  \vdots & \vdots & \vdots \\
  w_{n-k} & w_{n-k+1} & w_{n-k+2}
\end{pmatrix}
\begin{pmatrix}
  x_1 \\
  x_2 \\
  \vdots \\
  x_n
\end{pmatrix}
\]

Case 3. The correlation operation (also called transposed convolution, or sometimes misnamed as deconvolution) is the adjoint operation of the convolution, and involves padding the data by \( k - 1 \) on each side (corresponding to the ‘full’ mode in Matlab terminology) and using the unflipped kernel. The data matrix of correlation only differs from that in the convolution by the zero padding and is omitted here.

By closely looking at the different columns in the convolution/correlation data matrix \( X \) (case 2), one can find a rarely discussed problem in the training of networks. Since real-world data exhibits strong autocorrelation, and the neighboring columns of the data matrix correspond to shifting the signal by one pixel, the feature dimensions in the convolution/correlation data matrices are heavily correlated. Therefore gradient descent training cannot converge efficiently with existing standardization techniques (Fig. 2 (b)) or just by decorrelating the feature channels in a layer.

Connection with Frequency Domain Normalization

In signal processing, removing such pixel-wise autocorrelation has a long history and can be achieved through a process called whitening deconvolution (Gonzalez and Woods 2006). This correlation removal process can be generalized to every layer of a convolution neural network and we call this procedure network deconvolution. Usually this is achieved in the frequency domain through spectral whitening, i.e. a normalization in the frequency domain:
\[
\mathcal{F}(x) = \frac{\mathcal{F}(x)}{\sqrt{\mathcal{F}^*(x) \cdot \mathcal{F}(x)}}.
\]

This elegant normalization shows a profound insight: the optimal standardization for the convolution operation should in fact be carried out in the frequency domain. Note that frequency multiplication corresponds to a spatial domain convolution, and the frequency division corresponds to a spatial domain deconvolution. Moreover, the deconvolution kernel \( \mathcal{F}^{-1}(\frac{1}{\mathcal{F}(x)}) \) has been found to resemble the center-surround structures in animal visual systems (Supp. Fig. 6(a,b)) (Hubel and Wiesel 1962; Hyvärinen, Hurri, and Hoyer 2009; Ye et al. 2020). Four lines of Matlab code are provided here for a quick verification (Fig. 3).

**Spatial Domain Implementation**

Algorithm 1: Proposed Computation for a Convolution Layer

1. **Input:** Feature tensor \( X_{N \times C \times H \times W} \)
2. Scale features along first dimension \( X_{scaled} = SX \)
3. Convert feature channels to data matrices along second dimension
4. for \( i \in \{1, \ldots, C\} \) do
   5. \( X_i = im2col(X_{scaled}[:,i,:,:]) \)
   6. end for
7. \( X = [X_1, \ldots, X_C] \) Horizontally Concatenate
8. \( Cov = \frac{1}{N} X^T X \) %Cross GPU Sync
9. \( D \approx (Cov + \epsilon \cdot I)^{-\frac{1}{2}} \) %via Inverse Newton Iterations
10. **Output:** \( Y = Conv(SX, DW) \)

For a practical implementation for convolutional networks, it is better to carry out the deconvolution computation in the spatial domain using the data matrix \( X \) to match the small kernels that are used in practice. Specifically we calculate the covariance matrix \( Cov = \frac{1}{N} X^T X \), find its unique principal inverse square root \( D = Cov^{-\frac{1}{2}} \), and then use this matrix to transform the data matrix: \( X_0 = X \cdot D \). Note that \( \frac{1}{N} X_0^T X_0 = Cov^{-\frac{1}{2}} \cdot Cov \cdot Cov^{-\frac{1}{2}} = I \). As the transformed features are uncorrelated and standardized, faster convergence is achieved in this corrected space (Fig. 2(c)). We
track the correction $D$ during training and use the running average during testing.

For a convolution/correlation layer with $C$ channels, we construct the data matrix for each channel then horizontally concatenate the $C$ data matrices into a wider matrix (with $Ck^2/k$ columns for $1d/2d$). Deconvolution with this wider matrix removes the correlation of $k$-by-$k^2$ nearby pixels and $C$ feature channels at once (see Algorithm 1).

Experiments show that the above formulation works well for simple classification tasks that do not require scale invariance (see results in Sec. 5). However, it may not work well for some other tasks such as object detection and instance segmentation where scale invariance plays an important role. To generalize to these tasks, we incorporate local statistics to remove the scale in each individual sample. This simple strategy is inspired by the biological observation that animal visual systems also use two sets of statistics for visual analysis (Hubel and Wiesel 1962; Bear, Connors, and Paradiso 2020). The retinal light reflex (Bear, Connors, and Paradiso 2020) suggests local statistics is used to adjust the scale of the signal. For a fully-connected layer, local statistics are calculated from each row of the data matrix $X$. For a convolution/correlation layer, local statistics can be calculated for one or more rows of the data matrix or even the full feature tensor at each layer. We have found empirically that the last option works well and does not introduce an excessive computational cost. At each layer we standardize each sample tensor interchangeably with $\mu, \sigma$ (Ba, Kiros, and Hinton 2016), or with mean $l_1$ norm $E(|x|)$ if we just consider the scale. Combined with the linear transform weights, our proposed feature transform is:

$$ y = S \cdot X \cdot D \cdot w. \quad (3) $$

Here $S$ is the standardization operating on the rows of $X$, a diagonal matrix ($\frac{1}{\sigma}$) if we only consider the scaling or augmented with an extra column ($\frac{1}{\mu}$) if we also consider the bias, and $D$ is the decorrelation operating on the columns of $S \cdot X$. The weights are trained in the transformed space based on the uncorrelated features $S \cdot X \cdot D$.

Our formulation transforms both the rows and columns of $X$ without introducing redundancy. Normalization using local statistics enforces scale invariance, aligning features of different scales. Normalization with global statistics enforces $GL(n)$-invariance, leading to faster convergence.

**Implementation Details**

**Cross-GPU Synchronization**

To leverage the latest advancements in hardware development, we implement cross-GPU synchronization to improve the quality of the estimates (see (Pan et al. 2019) for another independent implementation). At each layer, the covariance matrix is computed on each GPU and synchronized across all the GPUs. On an 8-GPU machine, the synchronization cost is negligible. This implementation allows us to collect reliable statistics throughout the training for all practical batch sizes. In our development, we have consistently achieved satisfactory results using per-GPU batch sizes ranging from from 2 to 1024 in an 8-GPU training environment.

**Acceleration Techniques**

We use various techniques to simplify computation and reduce the complexity of the proposed algorithm to a small fraction ($\sim 5\%$) of the cost of a convolution layer (Supp. Table 8). The memory accessing time of extracting the data matrix from a convolution/correlation layer in existing packages takes significantly more time than the underlying convolution operation. We adopt a $3\times$-subsampling for ImageNet scaled images and $5\times$-subsampling for MS COCO scaled images. The data and covariance matrices are computed using tensor patches sampled at the strided locations, reducing the construction cost by $9\times$ and $25\times$ respectively. Since the involved number of pixels is usually more than enough, this strategy maintains accuracy while keeping the computational footprint low. When the covariance matrix becomes too large, we divide the columns into blocks and decorrelate between the blocks (Ye et al. 2017; Huang et al. 2018). In our experiments, we set the number of blocks $B = 256$ for fully-connected layers and $B = 64 \times k^2$ for convolution/correlation layers.

There are multiple ways (Huang et al. 2018; Ye et al. 2018; Huang et al. 2019; Ye et al. 2020) to calculate the principal inverse square root of a matrix but algorithms that are both efficient and stable are scarce. Since explicit eigenvalue decomposition is slow, Newton-Schultz iteration becomes a faster alternative. However, the vanilla Newton-Schultz method is unstable under finite arithmetic (Ye et al. 2020)(Fig. 7), so we adopt a coupled inverse Newton iteration method that is numerically stable and works well under finite precision arithmetic (Guo and Higham 2006). Starting with $X_0 = I$, $M_0 = \text{Cov}$, the coupled inverse Newton iteration calculates $X_{k+1} = X_k \left(\frac{3I - M_k}{2}\right)$, $M_{k+1} = \left(\frac{3I - M_k}{2}\right)^2 M_k$ and produces $X_k \rightarrow \text{Cov}^{-\frac{1}{2}}$. Empirically, using 5 iterations yields good results. We also add a small diagonal matrix $cI$ to the covariance matrix to avoid rank-deficiency.

Note that for a large data matrix $X$, decorrelating columns of $X$ can require excessive computation. Previous applications are usually restricted to a small number of layers (Huang et al. 2018, 2019; Pan et al. 2019), which adds to the network design complexity. We adopt a universal design and avoid excessive computation by reordering the computation by transforming the model weights instead, $y = (S \cdot X) \cdot (D \cdot w)$ (see Algorithm 1).

**Experiments**

We refer to our improved implementation as Network Deconvolution++ (ND++), ND++ introduces scale invariance, generalizes the $GL(n)$-invariance to all three common linear transform layers (convolution/correlation/linear) in modern architectures, and uses cross-GPU synchronization to allow reliable training at different scales. In the following experiments, all linear transform layers are enhanced with ND++. In fine-tuning experiments, the pretrained backbone network is replaced with a backbone pretrained with ND++.
comparison, we have also experimented with training from scratch to verify the gain is not only from the improved backbone. Standard stochastic gradient descent is used for all experiments. We continue to use learning rate decay in the face of inherent non-linearity and mini-batch training.

### Image Classification

We demonstrate improved training on three popular CNN architectures (VGG, ResNet, DenseNet) at three scales (10/50/100 layers). With ND++, we have seamlessly increased the training to batch size 2048, eight times larger than the model zoo default setting of 256. We train in one-eighth the number of iterations but produce superior models (Table 1). All three network architectures, VGG-11/ResNet-50/ResNet-101/DenseNet-121, surpass their deeper counterparts in the model zoo after standard 90-epoch training with cosine learning rate decay. Using the official PyTorch recipe, it takes less than one day to train on a machine with 8 Nvidia A100 GPUs. On the popular ResNet-50/101 backbones and test the performance on the Cityscapes dataset (Cordts et al. 2016). We use a base resolution of 1024/2048/1280. All three network architectures, VGG-11/ResNet-50/ResNet-101/DenseNet-121, surpass their deeper counterparts in the model zoo after standard 90-epoch training with cosine learning rate decay. Using the official PyTorch recipe, it takes less than one day to train on a machine with 8 Nvidia A100 GPUs. On the popular ResNet-50/101 backbones and test the performance on the Cityscapes dataset (Cordts et al. 2016). We use a base resolution of 1024/2048/1280.

#### Table 1: Top-1 Validation Accuracy on the ImageNet Dataset. ND++ also surpasses the top-1 accuracy rates of the deeper networks in the model zoo:

| Network      | SyncBN | ND++ |
|--------------|--------|------|
| VGG-11       | 71.11  | 72.24|
| ResNet-50    | 76.25  | 77.95|
| ResNet-101   | 77.37  | 79.40|
| DenseNet-121 | 74.65  | 76.11|

#### Table 2: Bounding box AP of three Faster R-CNN implementations on the COCO 2017 dataset.

|        | MB      | MLPerf  | Detectron2 |
|--------|---------|---------|------------|
| ND++   | 37.36   | 37.37   | 39.01      |
| BN     | 36.78   | 36.35   | 37.9       |
| GN     | 36.04   | 35.9    | 38.54      |

#### Table 3: Bounding box and mask AP of three Mask R-CNN implementations on the COCO 2017 dataset.

|        | APbbox | APmask |
|--------|--------|--------|
| ND++   | 38.62  | 35.65  |
| BN     | 37.67  | 34.28  |
| GN     | 37.82  | 34.75  |

#### Table 4: Mask R-CNN trained from scratch on the COCO 2017 dataset.

|        | LR | APbbox | APmask |
|--------|----|--------|--------|
| ND++   | 0.02 | 37.81  | 34.87  |
| GN     | 0.02 | 37.76  | 34.8   |

#### Table 5: Large-scale training performance of Mask R-CNN using ND++. Our reported numbers are based on the NVIDIA implementation. ND++ significantly surpasses MegDet (Peng et al. 2017) and LAMB (Wang et al. 2020) that utilize SyncBN, warmup and optimizer change.

|        | LAMB | MegDet | ND++ |
|--------|------|--------|------|
| Batch  | APbbox | APbbox | APbbox |
| 128    | 36.7  | 37.7   | 38.61 |
| 256    | 36.7  | 37.7   | 38.40 |
| 512    | 36.5  | -      | 37.45 |

### Object Detection

We test ND++ on Faster R-CNN and Mask R-CNN, milestone object detectors from three major benchmarks, maskrcnn-benchmark(MB), MLPerf, and Detectron2. We use ResNet-50 with FPN as backbones and two fully-connected layers in the box heads. In Mask R-CNN, the mask head contains convolution and correlation layers. ND++ is used to enhance all layers. We report our numbers and evaluation curves on the COCO 2017 dataset (Tables 2, 3, Fig. 1(a,b)). Results with ResNet-101 can be found in Supp. Sec. , Supp. Tab. 9.

On all three benchmarks and with both Faster R-CNN (Table 2) and Mask R-CNN (Table 3), ND++ consistently outperforms baselines with frozen batch normalization and group normalization (Wu and He 2018) in terms of Average Precision(AP) (Fig. 1(a,b)). When training from scratch, ND++ benefits from increase the learning rate to 0.1 while group normalization ends up with worse results (Table 4, Supp. Fig. 8).

Though researchers have encountered severe challenges in scaling up the training of Mask R-CNN (Peng et al. 2017; Wang et al. 2020), we have been able to seamlessly increase the batch size and achieve good results without ad hoc techniques. Here we take the MLPerf implementation, remove the warmup stage, and fix the learning rate to 0.1 with a momentum of 0.9. We notice that frozen/synchronized batch normalization explodes at all scales without warmup while ND++ produces superior results. ND++ significantly surpasses the MLPerf accuracy goal$^2$ within the standard 12-epoch fine-tuning with batch sizes up to 256, an order of magnitude larger than most existing baseline settings (Table 5, Supp. Fig. 9).

### Semantic Segmentation

To demonstrate the usefulness of ND++ for semantic segmentation, we add ND++ layers to the DeepLabv3 architecture (Chen et al. 2017) with both ResNet-50 and ResNet-101 backbones and test the performance on the Cityscapes dataset (Cordts et al. 2016). We use a base resolution of 1024 for the images. We train for 200 epochs for all experiments unless stated otherwise. We perform fine-tuning experiments

$^2$37.7 for bounding box AP and 33.9 for mask AP.
with a ResNet-50 backbone pretrained on ImageNet an initial learning rates of 0.01 and 0.1 and momentum 0.9 for both ND++ and the SyncBN baseline, and we report the results with learning rate 0.01 for SyncBN and 0.1 for ND++ in Table 6 since these produced the best results for each network configuration. Our ResNet-50 model with ND++ achieves an mIoU of 77.50 on Cityscapes, comparable to the ResNet-101 model from the original paper with 77.82 mIoU for single-scale evaluation (Chen et al. 2017).

ND++ substantially improves over the synchronized batch norm baseline, and the acceleration is especially apparent early in training. For example, it takes less than 50 epochs for a network equipped with ND++ to beat the performance of a network trained using SyncBN for 500 epochs (Supp. Fig. 11 and Table 6) if we fine-tune using a pretrained ResNet-50 backbone.

Table 7: Experiments with an initial learning rate 1.0 and no momentum.

| Network                  | SyncBN   | ND++   |
|--------------------------|----------|--------|
| DLv3-RN-50 (scratch, 200 ep.) | 69.30    | 72.69  |
| DLv3-RN-50 (finetune, 200 ep.) | 75.70    | 77.50  |
| DLv3-RN-101 (finetune, 200 ep.) | 77.28    | 79.23  |
| DLv3-RN-50 (finetune, 50 ep.) | -        | 76.47  |
| DLv3-RN-50 (finetune, 500 ep.) | 75.71    | -      |

Table 6: Validation mIoU when fine-tuning and training from scratch on the Cityscapes dataset. DLv3 stands for DeepLabv3 and RN stands for ResNet.

Table 7: Experiments with an initial learning rate 1.0.

ResNet-50 | Mask R-CNN (MLPerf) | DeepLabv3-RN-50
|-----------|---------------------|---------------|
| top-1     | AP bbox             | mIoU (Scratch)|
| 77.66     | 38.26               | 71.64         |

Discussion

The transform we propose has simple and intuitive geometric meanings. To achieve scale invariance, each sample is stretched individually using local statistics. The global geometry of the loss landscape, however, depends on the full collection of data. We therefore utilize the global distribution of data to find a unique optimal feature transform and achieve $GL(n)$-invariance. The unique gradient direction in this space corresponds to the optimal direction in the linear case and leads to significantly accelerated training of deep neural networks.

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# PyTorch-like forward implementation for a linear layer

def forward_impl(X, weight, bias, eps=1e-5):
    # 1. Scale-invariance
    X_norm = X.abs().mean(dim=-1, keepdim=True)
    X = X / (X_norm + eps)
    # 2. Calculate mu, cov, cov_isqrt
    X_mean = X.mean(0)
    XX_mean = X.t() @ X / X.shape[0]
    Id = torch.eye(X.shape[-1])
    X_cov = XX_mean - X_mean.unsqueeze(1) @ X_mean.unsqueeze(0) + eps * Id
    X_cov_isqrt = isqrt_newton_schulz_autograd(X_cov)
    # 3. S * X * D * W = (S * X) * (D * W)
    w = weight @ X_cov_isqrt
    b = bias - (w @ (X_mean.view(-1, 1))).view(-1)
    return F.linear(input, w, b)

---

**Source Code**

We present a PyTorch-like code snippet showing our modifications to a linear layer.

The full source code can be accessed from: https://github.com/amazon-research/network-deconvolution-pp

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**Cat Receptive Fields**

![Receptive fields in the cat retina. Reproduced from (Hubel and Wiesel 1962), Fig. 2.](image)

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**Further Discussion**

We can compute the covariance matrix \( \text{Cov}_1 = X'_1 X_1 \) from the data matrix \( X_1 \) of feature channel 1 to remove the correlation in nearby pixels. For multiple channels we construct \( X = [X_1, ..., X_C] \) and compute a larger covariance matrix \( \text{Cov} = X'X \). The diagonal blocks \( X'_i X_i \) of this matrix measure the correlation of nearby pixels in each channel. The off-diagonal blocks \( X'_i X_j \) measures the (pixel-wise) correlation across different channels \( i \) and \( j \). The transform we propose has a simple form for each sample: \( z(x) = \Sigma^{-0.5}(s(x) - \mu) \), where \( s(x) \) is a simple scaling for each sample. \( \mu, \Sigma \) are computed from a batch.

Our formulation in Sec. is based on the mathematical convolution. In most deep learning packages, the ‘convolution’ is implemented without flipping the kernel and is therefore in fact the ‘correlation’ operation. This misnaming does not affect the properties that we discuss throughout the paper.

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**Scale Invariance**

We present our argument on scale invariance based on linear transforms without the bias term. Though the bias term can potentially mitigate the problem, it cannot introduce scale invariance. In classification problems, the softmax function introduces scale invariance to the logits. This is why we see smaller improvement from scale invariance compared to object detection.

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**GL(n)-Invariance**

![During the training, every minibatch has an individual loss landscape (visualized in green and blue). These loss landscapes are used during the training. During the testing, the global loss landscape (visualized in red) is used. This picture gives us intuition about the training/testing inconsistency and how issue should be properly addressed, as discussed in the text.](image)

Here we present a global picture of \( GL(n) \)-invariance. The ideal solution is to generate the global loss landscape with the whole dataset (Fig. 7(red)). Due to hardware limitations, training is conducted in minibatches. During training, different batches of data give rise to different loss landscapes (Fig. 7(green and blue)). These landscapes from sampled data generate noisy gradient directions that do not lead to the optimal solution for the whole dataset (Fig. 7(red)). Gradient descent follows these noisy gradients in an online fashion to update weights. Due to this approximation, it is beneficial to use learning rate decay or increase the batch size (Smith, Kindermans, and Le 2018) towards the end of the training. However, using the running average covariance matrix to transform a batch of data yields poor performance. This incorrect transform can result in a heavily curved loss landscape. Therefore, the covariance needs to be calculated from the same batch of data to avoid divergence. The evaluation, however, is based on the global loss landscape over the whole dataset (Fig. 7(red)). The global transform can be achieved through the use of running average statistics. Methods that use global statistics such as the batch normalization are known to have this inconsistency in training and testing. The inconsistency can be alleviated by reducing the learning rate towards the end of the training or calculating the global statistics more accurately. One can also transform...
back to the original space (with the help of \( \text{Cov}^{-\frac{1}{2}} \)) to eliminate the inconsistency. The methods that only utilize local statistics (Ba, Kiros, and Hinton 2016; Wu and He 2018; Singh and Krishnan 2020) to achieve consistency in training and testing in fact use a suboptimal geometry in the training and therefore have slower convergence.

**Complexity Analysis**

We derive the complexity of our proposed transform in a matrix multiplication layer \( Y = (S \cdot X) \cdot (\text{Cov}^{-\frac{1}{2}} \cdot W) \). The complexity analysis can be easily generalized to convolution and correlation layers (Ye et al. 2020). \( W \) is the weight matrix and has dimensions \( C_{h_{in}} \times C_{h_{out}} \). \( S \cdot X \) introduces scale invariance. Note that \( S \) is either diagonal or augmented with an extra column if we include bias. The complexity is \( O(N \times C_{h_{in}}) \), which is linear to the scale of \( X \). We put the emphasis on the computation of \( \text{Cov}^{-\frac{1}{2}} \cdot W \). We first assume \( X \) has been reshaped to \( N \cdot C_{h_{in}} \times B \). The covariance matrix is calculated based on the reshaped \( X \) and has a size of \( B \times B \). The computation of the covariance matrix has complexity \( O(B \cdot \frac{N \cdot C_{h_{in}}}{B} \cdot B) = O(N \cdot C_{h_{in}} \cdot B) \). Coupled inverse Newton-Schulz iterations (5-iterations) are therefore conducted on matrices of size \( B \times B \). Solving for the inverse square root takes \( O(B^{3}) \). Next we assume \( W \) has been reshaped from \( C_{h_{in}} \times C_{h_{out}} \) to \( B \times (\frac{C_{h_{in}}}{B} \cdot C_{h_{out}}) \), weight transform \( \text{Cov}^{-\frac{1}{2}} \cdot W \) is a simple matrix multiplication with complexity \( O(B^{2} \cdot \frac{C_{h_{in}}}{B} \cdot C_{h_{out}}) = O(B \cdot C_{h_{in}} \cdot C_{h_{out}}) \). The overall complexity is \( O(N \cdot C_{h_{in}} \cdot B + B^{3} + B \cdot C_{h_{in}} \cdot C_{h_{out}}) = O((N \cdot C_{h_{in}} + B^{2} + C_{h_{in}} \cdot C_{h_{out}}) \cdot B) \). This can be a small fraction of the cost of the matrix multiplication operation that has a complexity of \( O(N \times C_{h_{in}} \times C_{h_{out}}) \) if we use a small \( B \). The simple derivation above can be easily generalize to the case of convolution and correlation layers. Note that \( N \) is approximately equal to the number of pixels at each layer.

**Runtime Analysis**

Here we report the CPU time for a few representative layers in a Mask R-CNN network to verify the claim about the complexity of our proposed algorithm (Table 8). The batch size is set to 16, the subsampling stride is set to 5 to compute the covariance matrix, and timing is averaged over 10 batches. Note that the overall computation required for introducing the \( GL(n) \)-invariance is comparable to introducing scale invariance and is usually a small fraction of the time taken by the convolution layer. Moreover, extracting the data matrix, which takes the most time, shares the same computation as the underlying convolution, and therefore would not be required with proper optimization. However, this sharing mechanism is not currently supported in common software packages. This lack of low-level optimization leads to extended wall time in our experiments.

**Experiment Details**

**Image Classification**

For the ImageNet classification experiments, we tested three weight decay levels (1e-4/5e-4/1e-3) and report the highest accuracy for both the synchronized batch normalization baseline and ND++. We have also tested batch normalization without synchronization and find the synchronized version usually gives a better result; we therefore use it as the baseline. The baseline model achieves the reported accuracy with weight decay factors 1e-4/5e-4/5e-4 respectively for VGG-11/Resnet-50/DenseNet-121. Correlated features create pathological regions that prevents the usage of large weight decay (Fig 2). With ND++, larger weight decay factors can be used and the optimal factors are 5e-4/1e-3/1e-3. For DenseNet, the baseline model takes more GPU RAM than the machine can hold and the result with batch size 1024 is reported here to compare with our batch size 2048 result. Due to the latency of the customized implementation, the wall time of ND++ is longer but still acceptable. By using the large batch size, the number of calls to the slow functions is reduced, and we finish the training in a shorter time compared to the original batch size of 256. With batch size 256, the baseline with SyncBN took 29 hours to train the ResNet-50. With batch size 2048, the complete version of ND++ finishes in the same time with superior accuracy. If remove scale invariance, ND++ finishes in 24 hours with a negligible drop in accuracy. At batch size 2048, ND++ without scale invariance takes 23/24/36 hours for VGG-11/ResNet-50/DenseNet-121 while the SyncBN baselines take 18/19/21 hours. Enforcing scale invariance slows training by 20% with little change in performance. The experiments are conducted on an AWS EC2 P3dn.24x instance. Note that the reported timing allows plenty of room for future improvements: besides sharing the extraction of the data matrix, layerwise standardization can be accelerated with sampling techniques.

For ImageNet training, we see a tiny improvement by enforcing scale invariance, while synchronization does not seem to give us a significant gain due to the per GPU batch

| Kernel | 7 | 3 | 3 | 1 | 1 |
|--------|---|---|---|---|---|
| Stride | 2 | 1 | 1 | 1 | 2 |
| \( C_{h_{in}} \) | 64 | 64 | 256 | 128 | 1024 |
| \( H \) | 800 | 200 | 200 | 100 | 50 |
| \( W \) | 1333 | 333 | 333 | 166 | 83 |
| \( \frac{\mu}{\sigma} \) | 0.75 | 0.99 | 3.84 | 1.94 | 1.95 |
| \( \frac{2^{-\sigma}}{2-\mu} \) | 1.81 | 2.39 | 9.38 | 4.74 | 4.73 |
| Get \( X \) | 0.72 | 0.93 | 6.22 | 2.81 | 2.93 |
| \( \text{Cov} = \frac{1}{N}X^T X \) | 1.43 | 0.7 | 2.75 | 1.36 | 1.4 |
| \( D = \text{Cov}^{-\frac{1}{2}} \) | 0 | 0.14 | 0.13 | 0.13 | 0.13 |
| \( D \cdot W \) | 0 | 0 | 0.02 | 0.02 | 0.84 |
| \( \text{Conv} \) | 30.16 | 3.4 | 30.56 | 7.31 | 46.6 |

Table 8: CPU runtime (in seconds) for a few representative settings in a Mask R-CNN network. The top rows in the first block show the layout in the network, the rows in the second block shows the runtime for two local normalization methods, the rows in the third block show the runtime for the \( GL(n) \)-invariance. The last row shows the runtime of the convolution layer.
size of 256. If we remove both synchronization and scale invariance, the top-1 accuracy of ResNet-50 drops slightly to 77.80%.

### Object Detection

![Figure 8: Bounding box and mask AP curves during validation when training the Mask R-CNN network from scratch. Note that with the more standard learning rate of 0.1, ND++ produces superior results compared to the GN baseline.](image)

![Figure 9: Bounding box and mask AP curves during validation when using large batch sizes to fine-tune the Mask R-CNN network.](image)

For object detection, we report additionally results of training Mask R-CNN on Detectron2. We attach figures of training from scratch with different learning rates (Supp. Fig. 8) and fine-tuning with large batch sizes (Supp. Fig. 9). In most experiments we achieve impressive performance with ND++ while using a learning rate of 0.1 and a momentum of 0.9. This combination has an effective learning rate of 1.0 (Li et al. 2020). Our transformation can make better use of this optimal learning rate compared to existing methods. The partially corrected gradients with standardization have less optimal direction and less useful scale. Smaller learning rates need to be used to avoid divergence.

| Batch size (epochs) | Frozen BN | GN | ND++ |
|---------------------|-----------|----|------|
| 128                 | NaN       | 33.46 | 31.09 |
| 256                 | NaN       | 35.6  | 35.09 |
| 512                 | NaN       | 35.6  | 35.09 |

Table 10: Results of using an initial starting learning rate 1.0 to train a Mask R-CNN network.

In this task, the lack of support to our customized implementation becomes more apparent due to the small training batch and layerwise standardization. In the MLOp implementation, training and validating Mask R-CNN for 12 epochs takes 5 hours for the frozen batch normalization baseline, 6 hours for the group normalization baseline, can take more than 10 hours for ND++ using on an AWS EC2 P4d.24x instance with 8 GPUs. We notice that the seemingly simple layerwise standardization takes a significant amount of time. The runtime is 14 hours if we remove both scale and bias (Box AP 38.4), 11 hours if we remove just the scale (Box AP 38.3), and 9 hours if we do not apply scale invariance at all (Box AP 37.5). The wall time can be significantly reduced if we increase the batch size and reduce the number of function calls. At batch size 64, our slowest run takes 11 hours (3 hours faster), reaching Box AP 38.7 and Mask AP 35.6, superior to a recent method that trains with twice as many steps (Yan et al. 2020). Besides optimizing these operations through low-level changes to the software package, we can also use standardization layers in only a subset of the network. Our experimentation during development indicates that applying standardization only in the RPN can maintain high-quality results. Here we report the numbers for the slow but universal design. For large batch experiments, we remove the warmup iterations and increase the weight decay factor for large batch sizes. For batch sizes of 128/256/512, the weight decay factors we use are 2.5e-4/5e-4/1e-3. We distribute the computation over 2/4/8 machines. For these experiments, slow inter-machine communication is the major bottleneck. We use the AWS Elastic Fiber Adaptor to speed up the inter-node communication without changing the code. These multi-machine experiments (including training and evaluation) finish in 7/5/4 hours respectively.

We also tested using an initial learning rate of 1.0 to train the Mask R-CNN network under different normalization techniques. We notice the training with Frozen Batch Normalization explodes early in the training. Group Normalization finishes with significantly worse results. ND++ ends up with competitive results (Supp. Table 10).

### Semantic Segmentation

For semantic segmentation, we use the 2975 images with fine annotations and report results on the validation split with 500 images on the Cityscapes dataset. In all experiments, we perform standard data augmentation. We perform distributed training on 8-GPU machines for 200 epochs with a minibatch size of 3. We reduce the learning rate on a default polynomial schedule with exponent 0.9 and use a weight decay of 0.0001.

We see accelerated training and improved final perfor-
Table 11: Ablation studies for DeepLabv3 with a ResNet-50 backbone on the Cityscapes dataset. We train from scratch for each condition for 200 epochs.

|               | Validation mIoU |
|---------------|-----------------|
| ND++          | 72.71           |
| ND++ w/o scale inv. | 72.69           |
| ND++ w/o sync  | 69.82           |
| BN            | 69.30           |

performance on the validation set both when training from scratch and when fine-tuning with a pretrained backbone (Supp. Fig. 12 (a)). While the model equipped with ND++ layers takes approximately 30% longer per epoch to train, the accelerated training convergence more than makes up for the increased time per epoch (Fig. 12 (b)).

Similar to object detection, we find cross-GPU synchronization markedly improves performance (from 69.82% to 72.69%) for semantic segmentation (Supp. Table 11). However, unlike for object detection, enforcing scale invariance has very little effect. Given this fact, we report results without enforcing scale invariance in Table 6 and Fig. 1.

**Training Transformer Models for Language Tasks**

We also find promising results when training two Transformer models (Vaswani et al. 2017) for language tasks using the code from Fairseq. We remove the Layer Normalization layers in the baseline Transformer model and insert our modifications in the linear transform layers. The original transformer models require warmup iterations for successful training. After modification with ND++, we can start with a large learning rate and remove the warmup iterations.

For the German to English translation task on the IWSLT14 dataset, the BLEU score of ND++ after 20k iterations is 35.9 vs 35.2 of the baseline. For the language model training on WikiText-103, the Perplexity is reduced from 31.48 of the baseline model to 29.54. For these experiments the max token size is 4096 per GPU and we train on 8 Nvidia A100 GPUs. The baseline models are trained with the inverse square root learning decay after 4k warmup iterations. After modifying with ND++, we notice using a simple cosine learning rate decay as in vision tasks significantly accelerates convergence.

**Relation to Other Decorrelation Methods**

We highlight a few differences between our work and recent whitening techniques (Huang et al. 2018; Pan et al. 2019). Our deconvolution is a normalization in the frequency domain. This is the optimal feature transform for convolution operation, while recent works are developed for non-convolutional operations. We follow the simple yet important mathematical justification to insert it before the weights, removing the redundancy and avoiding
Figure 13: Top-1 validation accuracy curves of ResNet-50 when trained on ImageNet with ND++, Switchable Whitening(SW), IterNorm using batch size of 2048.

potential problems related to extra parameters as in BatchNorm. Moreover, we avoid the computational cost of explicit decorrelation by fusing the decorrelation matrix with the weight matrix in the linear transform. Without this, per-sample whitening could incur high computational cost. Due to this limitation, most recent works (Huang et al. 2018, 2019; Pan et al. 2019) have restricted the use of whitening to only a few layers of the network. Additionally, the coupled inverse newton iteration method we adopt, along with the Denman-Beavers iteration in (Ye et al. 2018), are stable to finite arithmetic while the vanilla Newton-Schulz method diverges under certain conditions (Ye et al. 2020)(Fig. 7).

We compare our results with IterNorm and Switchable Whitening(SW) in various settings according to their code availability. In all settings ND++ achieves faster and better convergence than IterNorm and SW(Fig. 13). Interestingly, we found our simple design performs slightly better than the ensemble design of SW that incorporates multiple normalization/whitening techniques while using less computational space. This suggests that the ensemble design has potential for further improvement by including ND++ as a module (Table. 12). When training the ResNet-50 with a learning rate of 1.0 and no momentum on the ImageNet, ND++ achieves a top accuracy of 77.66 versus 76.85 for SW and 76.57 for IterNorm. We tried to compare the results of training ResNet-101 but SW ran out of GPU RAM. Nevertheless, our number of 79.4 with 90 epochs of training is higher than the 78.6 reported in their paper with 100 epochs of training.