Batch-Expansion Training: An Efficient Optimization Framework

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Abstract

We propose Batch-Expansion Training (BET), a framework for running a batch optimizer on a gradually expanding dataset. As opposed to stochastic approaches, batches do not need to be resampled i.i.d. at every iteration, thus making BET more resource efficient in a distributed setting, and when disk-access is constrained. Moreover, BET can be easily paired with most batch optimizers, does not require any parameter-tuning, and compares favorably to existing stochastic and batch methods. We show that when the batch size grows exponentially with the number of outer iterations, BET achieves optimal $\tilde{O}(1/\epsilon)$ data-access convergence rate for strongly convex objectives. Experiments in parallel and distributed settings show that BET performs better than standard batch and stochastic approaches.

1 Introduction

State-of-the-art optimization algorithms used in machine learning broadly tend to fall into two main categories: batch methods, which visit the entire dataset once before performing an expensive parameter update, and stochastic methods, which rely on a small subset of training data, to apply quick parameter updates at a much greater frequency. Both approaches present different trade-offs. Stochastic updates often provide very good early performance, since they can update the parameters a considerable number of times before even a single batch update finishes. On the other hand, by accessing the full dataset at each step, batch algorithms can better utilize second-order information about the loss function, while taking advantage of parallel and distributed computing architectures. Finding approaches that provide the best of both worlds is an important area of research. In this paper, we propose a new framework which—while closer to batch in spirit—enjoys the benefits of stochastic methods. In addition, our framework addresses a practical issue observed in real-world industrial settings, which we now describe.

In industrial server farms, compute resources for large jobs become available only in a phased manner. When running a batch optimizer, which requires loading the entire dataset, one has to wait until all the machines become available before beginning the computation. Moreover, the training data, which typically consists of user logs, is distributed across multiple locations. This data needs to be normalized, often by communicating summary statistics or subsets of the data across the network. Since stochastic optimization algorithms only deal with a subset of the data at a time, one can largely avoid the bottleneck of data normalization by preparing mini-batches at a time. However, now each data point needs to be visited multiple times randomly, and this requires performing many random accesses from a hard-disk or network attached storage (NAS), which is inherently slow. Moreover, extending stochastic optimization to the distributed setting is still an active area of research. This raises the question of whether the compute and data-availability delays could be avoided in batch methods, and how that would affect the training time.

We propose Batch-Expansion Training (BET), an adaptive, parameter-free meta-algorithm, which can be paired with most batch optimization methods to accelerate their performance in sequential, parallel, as well as distributed settings, addressing the issues discussed above. Our approach
hinges on the following observation: initially, when only a subset of the data is available, the statistical error (the error that arises because one is observing a sample from the true underlying data distribution) is large. Therefore, we can tolerate a large optimization error (the error that arises because of the iterative nature of the batch optimizer). However, as the sample size increases, the statistical error decreases and the corresponding optimization error that we can tolerate also decreases. BET exploits this by initially training models with large optimization error on smaller subsets of the data, and iteratively loading more training data, and driving down the optimization error.

Relying on classical results in statistical learning theory, we show that any optimizer exhibiting linear convergence rate can be effectively accelerated by periodically doubling the data size after a certain number of iterations. We propose a simple parameter-free algorithm, which dynamically decides the optimal number of iterations between each data expansion, adapting to the performance of a batch optimizer provided as a black box method. Experiments using Nonlinear Conjugate Gradient (CG), as well as the L-BFGS method, demonstrate the versatility of our framework. We show that for strongly convex losses BET achieves the same asymptotic $\tilde{O}(1/e)$ convergence rate as SGD in terms of data accesses (and is strictly faster than regular batch updates). However, unlike stochastic methods, BET reuses all of the data that has already been loaded, which helps it scale very well in parallel and distributed settings, as confirmed by the experimental results.

2 Related Work

There has been a recent explosion of interest in optimization methods for machine learning, both in the batch and stochastic paradigms. Algorithms like Stochastic Variance Reduced Gradient method [15] and related approaches [22][10] mix SGD-like steps with some batch computations to control the stochastic noise. Others have proposed to parallelize stochastic training through large mini-batches [16][17]. However, these methods do not address the issues of compute and data-availability delays that we discussed above. Additionally, two-stage approaches have been proposed [1][24], which employ SGD at the beginning followed by a batch optimizer (e.g., L-BFGS). These methods are much more limited than BET, which allows for multiple stages of optimization, with clear practical benefits. Interleaving computation with data loading was shown to have significant practical benefits by [18]. However, that work is confined to training on a single machine and did not provide any theoretical convergence guarantees. In contrast, we largely focus on the distributed setting and provide convergence guarantees.

Several works explore the idea of batch expansion in various forms. [7][14] propose using stochastic mini-batches of gradually increasing size paired with optimizers like gradient descent or Newton-CG. The algorithms proposed there strongly rely on stochastic sampling, which makes them less resource-efficient than BET, and not applicable to certain distributed settings. The convergence guarantees offered in [7] are limited to using gradient descent as the inner optimizer, and heavily rely on the independence conditions present in stochastic sampling. Recently, [19][9] proposed variants of the Newton’s method and of the SAGA [10] algorithm which run on increasing batch sizes. However, both of those methods pose challenges in large-scale distributed settings (expensive hessian computation required for Newton’s method and sequential stochastic updates in SAGA). The crucial advantage of our meta-algorithm is that it can be used with any inner batch optimizer as a black box, including quasi-Newton methods like L-BFGS, making this approach more broadly applicable and scalable. Similarly, our time complexity analysis is more general in that it applies to a wide range of inner optimizers.

3 Batch-Expansion Training

We consider a standard composite convex optimization problem arising in regularized linear prediction. Given a dataset $Z = \{(x_i, y_i)\}_{i=1}^N$, we aim to approximately minimize the average regularized loss

$$\hat{f} \triangleq \frac{1}{N} \sum_{i=1}^N \ell(z_i(w)) + \frac{\lambda}{2} \|w\|^2,$$

where $z_i = (x_i, y_i)$ and $\ell(z_i(w)) \triangleq f((w, \phi(x_i)), y_i)$ is the loss of predicting with a linear model $(w, \phi(x_i))$ against a target label $y_i$. Any iterative optimization algorithm in this setting will produce a sequence of models $\{w_t\}_{t=1}^T$ with the goal that $w_T$ has small optimization error $\hat{g}(w_T)$ with respect to the exact optimum $w^*$, where

$$\hat{g}(w) \triangleq \hat{f}(w) - \hat{f}(\hat{w}^*), \quad \hat{w}^* \triangleq \arg \min_w \hat{f}(w).$$

Note that our true goal is to predict well on an unseen example $z = (x, y)$ coming from an underlying distribution. The right regularization $\lambda$ for this task can be determined experimentally or from the statistical guarantees of loss function $\ell$, as discussed in [25][24]. In this paper, however, we will assume that an acceptable $\lambda$ was chosen and concentrate on the problem of minimizing $\hat{f}$.

3.1 Linear convergence of the batch optimizer

Adding $\ell_2$-norm regularization in function $\hat{f}$ makes it $\lambda$-strongly convex. In this setting, many popular batch optimization algorithms enjoy linear convergence rate $[21]$. Namely, given arbitrary model $w$ and any $c > 1$, after at most $O(\log(c))$ iterations - where a single iteration can look at the entire dataset - we can reduce its optimization...
The general task of an optimization algorithm is to return a model with small optimization error $\hat{g}(w) \leq \epsilon$. For selecting an effective optimization error tolerance $\epsilon$ in a machine learning problem, we often look at the estimation error by a multiplicative factor of $c$, obtaining $w'$ such that $\hat{g}(w') \leq c^{-1} \cdot \hat{g}(w)$.

Consider the scenario where data is abundant, but we have a limited time budget for training the model. In this case, the practitioner would select the data size so that we can reach the smallest effective optimization error tolerance (dashed curve in Figure 1b) within the allotted training time. Vertical line in Figure 1b shows the reduction in optimization error that the algorithm has to achieve to obtain the desired tolerance. If we use a batch optimizer for this task, the training time is determined by two factors. First, as the dataset grows, each iteration takes longer (e.g. for linear optimizers the iteration time is proportional to the data size, as discussed in Section 5.1). Second, the algorithm has to perform larger number of iterations, the smaller the effective optimization error tolerance. Combined, those two effects result in training time, which, for linear optimizers, grows faster than linearly with the data size (see Figure 1i).

In this paper, we propose that instead of finding the optimal dataset size at the beginning, we first load a small subset of the data, train the model until we reach the corresponding effective optimization error tolerance, then we load more data, and optimize further, etc. Vertical lines in Figure 1b illustrate how the optimization error is reduced in the multiple stages working with increasing dataset sizes. This procedure benefits from inexpensive iterations in the early stages, as shown in Figure 1c, with vertical lines corresponding to the training time for each data size, and the horizontal line showing the time budget (note that the budget shown for this method is the same as the one used in Figure 1b). Thus, our approach is able to reach smaller effective optimization error tolerance within the same time budget compared to fixing the dataset size at the beginning, as seen by comparing Figures 1b and 1i.

### 3.3 Exponentially increasing batches

We now precisely formulate the idea of training with gradually increasing data size. Suppose our goal is to return a model $\tilde{w}$ with optimization error $\hat{g}(\tilde{w}) \leq \epsilon$. In the procedure described above, we seek to obtain a sequence of gradually improving models $w_1, \ldots, w_{T-1}$ before we reach $w_T = \tilde{w}$. Any of the intermediate models (say, model $w_t$ for $t < T$) has a large optimization error relative to $\tilde{w}$, so to compute $w_t$, we can minimize an objective function with

\[ f(w_t) = \hat{g}(w_t) + \lambda_t \cdot \text{Reg}(w_t), \]

where $\text{Reg}(w_t)$ is some regularization term.
correspondingly large estimation error. Thus, we will first obtain \( w_1 \) with optimization error \( \epsilon_1 \), using \( n_1 \) data points, next we pick a smaller error tolerance \( \epsilon_2 < \epsilon_1 \) and bigger data size \( n_2 > n_1 \), computing a better model \( w_2 \), etc. so that in the end we reach \( \epsilon_T = \epsilon \). Algorithm 1 demonstrates a simple instantiation of this strategy, where at each stage we double the data size:

**Algorithm 1 Batch-Expansion Training**

1. Pick initial model \( w_0 \)
2. Load first \( n_1 \) data points
3. for \( t = 1..T \) do
4. \( w_t \leftarrow \text{run } \kappa_t \text{ iterations on } n_t \text{ data points} \)
5. \( n_{t+1} \leftarrow b_t n_t \) (increase data size)
6. Load \( n_{t+1} - n_t \) data points
7. end for
8. return \( w_T \)

The basis for the number of inner iterations \( \kappa_t \) will be explained below. Note that at stage \( t \) of the process we are working with an estimate of the loss function

\[
\hat{f}_t(w) \triangleq \frac{1}{n_t} \sum_{i=1}^{n_t} \ell_z_i(w) + \frac{\lambda}{2} \|w\|^2,
\]

which tends to \( \hat{f} \) with increasing \( t \). At this stage, the optimizer is in fact converging to an approximate optimum

\[
\hat{w}_t^* \triangleq \arg \min_w \hat{f}_t(w),
\]

rather than to the minimizer of \( \hat{f}, \hat{w}^* \). To decide how much data is needed at each stage we will describe the relationship between data size \( n_t \) and the desired optimization error \( \epsilon_t \). Note that model \( w_t \) obtained at stage \( t \) is assumed to satisfy \( \hat{g}_t(w_t) \leq \epsilon_t \), where \( \hat{g}_t \) represents optimization error for the given data subset, i.e. \( \hat{g}_t(w) = \hat{f}_t(w) - \hat{f}_t(\hat{w}_t^*) \).

When going to the next stage, the data size increases, and thus we can use optimization error function \( \hat{g}_{t+1} \), which is a better estimate of \( \hat{g} \) than \( \hat{g}_t \). In Appendix B.1 we show that function \( \hat{g}_{t+1} \) can be uniformly bounded by \( \hat{g}_t \), plus an additional term which can be interpreted as the estimation error (of \( \hat{g}_t \) with respect to \( \hat{g}_{t+1} \)):

\[
\hat{g}_{t+1}(w) \leq 2 \cdot \hat{g}_t(w) + O\left(1/\lambda n_t\right). \tag{2}
\]

As discussed earlier, the effective optimization error for data size \( n_t \) is proportional to the estimation error suffered by \( \hat{g}_t \), hence it is sufficient to demand that

\[
\hat{g}_t(w_t) \leq \epsilon_t \triangleq O\left(1/\lambda n_t\right). \tag{3}
\]

Note that this makes the optimization error tolerance \( \epsilon_t \) inversely proportional to the subset size \( n_t \), confirming our intuition that for \( t < T \), since \( \epsilon_t > \epsilon \), we can work with a batch of size \( n_t \) that is smaller than \( N \).

To establish the correct rate of growth for the data size \( n_t \), we combine (3) with the observations made in Section 3.1. First, note that the rate of decay of sequence \( \{\epsilon_t\} \) should match the convergence rate of the optimization algorithm, so that inequality \( \hat{g}_t(w_t) \leq \epsilon_t \) can be satisfied for all \( t \). Recall from Section 3.1, that a linear optimizer takes only a constant number of iterations to reduce the optimization error by a constant factor. Suppose that improvement by a factor of \( 6 \) takes \( \kappa \) iterations (going from \( w_t \) to \( w_{t+1} \)). Then, using (2) and (3) we have

\[
\hat{g}_{t+1}(w_{t+1}) \leq \frac{\hat{g}_{t+1}(w_t)}{6} \leq \frac{2 \cdot \hat{g}_t(w_t) + \epsilon_t}{6} \leq \frac{\epsilon_t}{2}.
\]

This suggests the following simple strategy: at each stage perform \( \kappa \) iterations of the optimizer, then divide the tolerance level by \( 2 \) (matching the convergence rate). Note that based on Equation (3), this corresponds to doubling the data size \( n_t \). Thus, we obtain the following simple scheme for data expansion, which maintains the desired relationship between \( n_t \) and \( \epsilon_t \):

\[
\epsilon_{t+1} = \epsilon_t / 2, \quad n_{t+1} = 2 \cdot n_t.
\]

It is important that \( n_t \) grows exponentially with \( t \). This allows for a considerable improvement in runtime. Let us say that \( \epsilon_0 = O(1) \) and \( T \) stages are needed to reach the final desired tolerance \( \epsilon \), i.e. \( T = \log(\epsilon_0/\epsilon) = O(\log(1/\epsilon)) \). Moreover, using (3) the suitable size of the full dataset is \( N = O(1/\lambda \epsilon) \). If we assume that one iteration of the linear optimizer takes time proportional to the data size, then the time complexity of the optimization when using batch-expansion is given by

\[
\sum_{t=1}^{T} \kappa n_t = \kappa n_0 \sum_{t=1}^{T} 2^t = O(\kappa N) = O\left(\frac{K}{\lambda \epsilon}\right).
\]

On the other hand, when running the same optimizer on full dataset from the beginning, the time complexity becomes

\[
O(\kappa N \cdot T) = O\left(\frac{K}{\lambda \epsilon} \cdot \log(1/\epsilon)\right).
\]

Note that to establish convergence of the proposed algorithm, it is only required that the dataset is randomly permuted, i.e. that each subset \( \{z_i\}_{i=1}^{n_t} \) represents a random portion of the data. However, the batches used in different stages do not need to be independent of each other, which is why we can reuse data from previous stages. Section 3.4 precisely formulates the ideas discussed above, and a careful analysis of the time complexity is given in Theorem 4.1.

### 3.4 Two-track algorithm

How many iterations of the proposed expansion procedure should be performed at each stage? From our high-level analysis, we concluded that a roughly constant number of updates should be sufficient for any stage (using a linear optimizer), since each time we aim to make the same multiplicative improvement to the optimization error suffered.
by our model. However, that constant may depend on the type of loss function, the dataset, as well as the optimizer used, and moreover, in practice the right number of iterations may in fact vary to some extent between the stages. Therefore, we need a practical method of deciding the right time to double the data. Consider the following experiment: we run two optimization tracks in parallel, first one for the batch of size $n_1$, the other for half of that batch. One update on the bigger batch takes longer than an update on the smaller one. Which track will make better progress towards the optimum of the bigger batch in the same amount of time? If the starting model is far enough from the optimum $\bar{w}_t$, then the faster updates will initially have an advantage. However, as the convergence proceeds, only the slower track can get arbitrarily close, so at some point it will move ahead of the fast one (in terms of the loss $\hat{f}_t(w)$). Denote the starting model as $w_{t,0}$. The secondary track (running on half of the batch) also starts at the same point, denoted as $w_{t-1,0} = w_{t,0}$, and they are both updated:

$$w_{t,s+1} \leftarrow \text{Update}(w_{t,s}, n_t),$$

$$w_{t-1,s+1} \leftarrow \text{Update}(w_{t-1,s}, n_{t-1}),$$

where $\text{Update}(w, n)$ is one step of the optimizer, with respect to model $w$, on the batch $\{z_i\}_{i=1}^n$. Let $c_s$ and $c'_s$ be the total runtimes of the first and second track after $s$ iterations, respectively, and let $s_1(s) = \max\{c_0, c_0 \leq c'_s\}$ be the number of iterations that the slower track completes in the time it took the faster track to do $s$. To compare the performance of the two tracks we will use the condition:

$$\hat{f}_t(w_{t,s_1(s)}) < \hat{f}_t(w_{t-1,s}).$$ (4)

**Algorithm 2 Two-Track Optimizer**

Initialize $w_{1,0} = w_{0,0}$ arbitrarily, $s \leftarrow 0$, $t \leftarrow 1$

Pick any $2 \leq n_1 = 2n_0 < N$

while $n_t < N$ do

$$w_{t+1} \leftarrow \text{Update}(w_{t,s}, n_t),$$

$$w_{t-1,s+1} \leftarrow \text{Update}(w_{t-1,s}, n_{t-1}),$$

$$s \leftarrow s + 1,$$

$$s_1 \leftarrow \max\{s_0 : c_0 \leq c'_s\},$$

if $\hat{f}_t(w_{t,s_1}) < \hat{f}_t(w_{t-1,s})$ then

$$n_{t+1} \leftarrow 2n_t,$$

$$w_{t,0}, w_{t+1,0} \leftarrow w_{t,s},$$

$$t \leftarrow t + 1,$$

$$s \leftarrow 0.$$ 

end if

end while

while stopping condition not met do

$$w_{t,s+1} \leftarrow \text{Update}(w_{t,s}, N),$$

$$s \leftarrow s + 1.$$ 

end while

return $w_{t,s}$

Algorithm 2 describes Batch-Expansion Training implemented using the Two-Track strategy. Note that in this algorithm we run the two tracks sequentially, in an alternating order, however running them in parallel would further improve the overall performance.

### 3.5 Discussion

We found that the choice to increase data size by a factor of 2 at each stage (rather than by a different factor) is not crucial for the optimization performance (both theoretically and in practice), therefore this parameter does not require tuning. The initial subset size $n_0$ also does not affect performance significantly - generally, the larger $n_0$ we select, the more updates will be performed before first data expansion, but as long as the initial subset is small enough, total optimization time will remain close to optimal. Thus, Algorithm 2 does not require any tuning to achieve good performance. Moreover, our method can be paired with many popular batch optimizers, and it will automatically adapt its behavior to the selected inner optimizer, as shown in Section 5.1.

It is important to note that the fraction of data accessed by the algorithm is only gradually expanded as optimization proceeds. Moreover, BET iterates multiple times over the data points that have already been loaded. Thus, it is very resource efficient in a way that can be beneficial with:

**Slow disk-access.** Loading data from disk to memory can be a significant bottleneck [18]. Performing multiple iterations over the data points while extra data is being loaded in parallel provides speed-up.

**Resource ramp-up.** In distributed computing, often not all resources are made available immediately at the beginning of the optimization [20], which similarly leads to gradual data availability.

### 4 Complexity Analysis

In this section, we provide theoretical guarantees for the time complexity of Batch-Expansion Training and compare them to other approaches. For the remainder of this section, we assume that the inner optimizer for some $\kappa > 1$ and for every $t$, $w$ exhibits linear convergence:

$$\hat{g}_t(\text{Update}(w, n_t)) \leq (1 - (1/\kappa)) \hat{g}_t(w).$$

For the sake of complexity analysis, we discuss a parameterized variant of our approach, described in Algorithm 3 and establish complexity results for it. Here, the number of updates needed at each stage is a fixed parameter $\hat{k}$.

**Assumptions.** We assume that the feature mapping $\phi(\cdot)$ (see 1 and the discussion below it) is $B$-bounded, i.e. it satisfies $\|\phi(x_i)\| \leq B$, and that the loss function $\ell(z_i, w) = \ell(z_i, w)$ is $L$-Lipschitz in $z_i$ for all $w$. Moreover, we will use the fact that $f$ is $\lambda$-strongly convex, due to the use of $\ell_2$-norm regularization. The result below holds with high
Algorithm 3 Optimal BET

**Input:** Target tolerance $\epsilon$
- Pick $\epsilon_0$, $n_0$
- Initialize $w_0 \leftarrow 0$, $t \leftarrow 0$ and $\hat{\kappa} = \lceil \log(6) \rceil$

**while** $3 \cdot \epsilon_t > \epsilon$ **do**
- $n_{t+1} \leftarrow 2n_t$
- $w_{t,0} \leftarrow w_t$
- **for** $s = 1..\hat{\kappa}$
  - $w_{t,s} \leftarrow \text{Update}(w_{t,s-1}, n_{t+1})$
- **end for**
- $w_{t+1} \leftarrow w_{t,\hat{\kappa}}$
- $\epsilon_{t+1} \leftarrow \epsilon_t / 2$
- $t \leftarrow t + 1$
**end while**

**return** $w_T$

Suppose that $\epsilon_0$ satisfies Lemma 1. We can show by induction that (with probability $1 - \delta$) for all $t \leq T$, model $w_t$ is an $\epsilon_t$-approximate solution for $\hat{f}_t$, i.e. that $\hat{g}_t(w_t) \leq \epsilon_t$. Base case is given by (5). The inductive step follows from:

$$
\hat{g}_{t+1}(w_{t+1}) \leq \frac{2 \cdot \hat{g}_t(w_t) + \epsilon_t}{6} \leq \epsilon_{t+1}.
$$

Next, we verify that $w_T$ is an $\epsilon$-approximate solution for $\hat{f}$:

$$
\hat{g}(w_T) \leq 2 \cdot \hat{g}_T(w_T) + \epsilon_T \leq 3 \cdot \epsilon_T \leq \epsilon.
$$

Finally, we move on to complexity analysis. The number of iterations in the algorithm is $T = O(\log(\epsilon_0/\epsilon))$, since:

$$
2^T \geq \frac{2 \cdot \epsilon_0}{\epsilon_{T-1}} < 6 \cdot \frac{\epsilon_0}{\epsilon}.
$$

Assuming that one update of the inner optimizer requires $C$ passes over the data, we obtain the data-access complexity:

$$
\sum_{t=1}^{T} \hat{\kappa} C n_t = C \hat{\kappa} n_0 \sum_{t=1}^{T} 2^t \leq 2C \hat{\kappa} n_0 \cdot 2^T = O \left( n_0 \epsilon_0 \cdot \frac{\kappa}{\epsilon} \right).
$$

See Section B.2 for details regarding the log terms.

### 5 Experiments

In this section we present experimental results showing the benefits of applying BET acceleration to batch optimizers and demonstrating scalability of the method in parallel and distributed settings. As the optimization problem we use logistic loss with $\ell_2$-norm regularization trained on several standard LIBSVM datasets (see Table 1). All algorithms start with the initial model vector $w$ set to all zeros. BET was implemented as shown in Algorithm 2 without any parameters that required tuning. The results are presented using test set accuracy and training objective, the latter being shown in terms of the log Relative Functional Value Difference

$$
\log \text{RFVD}: \log \left( \frac{\hat{f}(w) - \hat{f}(\hat{w}^*)}{\hat{f}(w^*)} \right).
$$

All algorithms were implemented in the PETSc [2] [3] [4] framework, with the data split between multiple computing
cores to achieve parallelization speed-up (we used 16 cores in most experiments). For splice-site dataset, data was additionally divided between multiple machines.

| Dataset, size | Train/Test | Dim. | λ  |
|--------------|------------|------|----|
| url, 1GB     | 1.8M/0.5M  | 3.2M | 1e-8 |
| covtype, 19GB| 0.5M/69k   | 170k | 1e-6 |
| webspam, 30GB| 250k/100k  | 16.6M| 1e-6 |
| splice-site, 1.5TB | 25M/4.6M  | 11.7M| 2e-10 |

Table 1: A list of datasets and regularization used for the experiments. For covtype, features were expanded to all monomials of degree 3.

5.1 Adapting to inner optimizers

To demonstrate the flexibility of our framework, in this section we use two different inner optimizers with BET:

1. Nonlinear Conjugate Gradient method (CG), using Fletcher-Reeves [13] formula, with exact line-search;

2. Limited-memory BFGS (L-BFGS) [8].

Both of those methods are linear optimizers that employ strategies for enhancing the basic gradient descent direction. Note, that CG uses a memory vector updated at each iteration. When the loss function changes from $\hat{f}_t$ to $\hat{f}_{t+1}$, one might expect that memory vector to become invalid, rendering CG ineffective. However, we observe that BET is still very effective at accelerating memory-based algorithms.

Figure 2 shows the performance comparison of using BET with the two inner optimizers on webspam dataset, contrasted with both of them ran in regular batch mode. First, we can see that L-BFGS is a much more effective optimizer than Nonlinear CG, thus in all of the following experiments we used L-BFGS as the inner optimizer. However, both methods significantly benefit from BET. In fact, in the early phase of the optimization, performance of BET is similar with either of the optimizers. However, once batch expansion reaches close to the full dataset, quality of the underlying optimizer starts to play an important role. Circular dots on the BET plots in Figure 2 mark the points when batch size is doubled during the optimization. We observed that the average number of iterations per stage of BET is larger when the inner optimizer is CG. This matches our expectation, since the theory suggests that the number of iterations per stage should be inversely proportional to the convergence rate of the inner optimizer.

5.2 Combining the benefits of batch and stochastic

In this experiment, we examine the trade-offs between batch and stochastic methods, showing how BET fits into this comparison. A batch optimizer typically starts off slower than a stochastic one, but once it gets closer to the optimum, we expect to see a fast convergence behavior. Thus, depending on which tolerance level we select, we would choose the appropriate optimizer. This is shown on a sample plot for the covtype dataset in Figure 3, where we...
use Parallel SGD [27] as the stochastic algorithm and L-BFGS as the Batch method, with all algorithms running on a 16 core machine (for the sake of clarity, only a portion of the full convergence time is shown). We also tested mini-batch SVRG as an alternative stochastic approach. However, due to the high communication cost, this method exhibited much slower per iteration time, and for this reason we did not include the results in the paper. To obtain the reported performance for Parallel SGD we had to tune the step size on a chunk of data, which adds to the overall optimization time, whereas BET is a parameter-free method. Our algorithm gets the best of both worlds, since it behaves like a stochastic method at the beginning, and then like a batch method towards the end. More plots are presented in Appendix A showing datasets which favor either batch or stochastic methods. In summary, BET performs as well as the best method for each dataset, with no tuning necessary.

5.3 Parallelization speed-up

The goal of this experiment is to analyze the parallelization speed-up of BET and compare it with the speed-up of Batch. We set this up as follows: we run to convergence and find the final accuracy, then for each method, we vary the number of cores and measure the time it takes to reach within 0.25% of optimum accuracy. For this experiment we selected the url dataset to demonstrate a stark contrast with Parallel SGD. The method achieves close to linear speed-up only for up to 4 cores, after which its performance flattens. This behavior can be attributed to the fact that as we increase the number of cores, a single iteration of Parallel SGD becomes less and less effective, which in some cases may negate the parallelization speed-up altogether. Batch methods, on the other hand, behave much more reliably with parallelization, because their iterations produce the same effect regardless of the number of cores. Figure 4 shows the speed-up factors for BET, Batch and Parallel SGD. BET achieves similar speed-up as Batch, due to the fact that parallelization happens in the inner optimizer, which is the same for both methods.

5.4 Distributed optimization

Batch optimization shows the most benefits when dealing with large-scale datasets, which do not fit into the memory of a single machine. BET easily scales up to this setting as seen in Figure 5 running on the splice-site data, with 20 machines, and 50 cores per machine, compared against Batch and Parallel SGD in the same setup. Since the dataset is highly skewed, the results are shown in terms of area under Precision-Recall curve (auPRC).

Note that BET reaches close to optimum test auPRC much more quickly than Batch or Parallel SGD. Moreover, until that point batch-expansion has not reached the full training data, which means that if the data were loaded in parallel with the optimization, the optimization time would be partially absorbed into the loading time. In our experiments, each one of the 1000 processes independently reads a separate chunk of data, however this procedure still takes at least 1500 seconds even on a high-performance cluster. Thus, a portion of BET’s optimization time can be absorbed into data loading.

6 Conclusions

We proposed Batch-Expansion Training, a simple parameter-free method of accelerating batch optimizers in a way that is both theoretically and experimentally efficient. BET does not require tuning and can be paired with any optimizer, offering advantages in parallel and distributed settings.
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A Additional Experiments

| Dataset, size | Train/Test | Dim. | λ |
|---------------|------------|------|---|
| HIGGS, 8GB    | 10.5M/0.5M | 28   | 1e-10 |
| url, 1GB      | 1.8M/0.5M  | 3.2M | 1e-8  |

Table 2: A list of additional datasets and regularization used for the experiments.

In this section we look at two datasets with very different properties. First one, HIGGS, is large, but extremely low dimensional. In this case, given an overabundance of data, if we look at the accuracy plot (see Figure 6), the Batch algorithm takes much longer to converge than Parallel SGD. For url, the batch expansion happens relatively early on in the optimization, and from that point on the algorithm is simply running full L-BFGS. Those two extreme cases show the versatility and robustness of our proposed meta-algorithm.

B Proof Details for Theorem 4.1

B.1 Proof of Lemma 1

First, we formulate a uniform-convergence bound, which closely resembles Theorem 1 from [25]. The only difference is that they consider PAC setting: sampling an i.i.d. dataset \( Z \) from a fixed distribution, and comparing the finite-sample objective \( \hat{f} \) computed using \( Z \) with the true objective \( f \), which is an expectation over the distribution. On the other hand, we consider an increasing sequence of datasets \( Z_t = \{z_i\}_{i=1}^{n_t} \), selected by a uniformly random permutation of the full dataset \( Z \). Note, that we assume the algorithm never observes the full dataset, only loading as much data as needed. Taking the limit of \( N \to \infty \), the relationship between any subset \( Z_t \) and the full dataset \( Z \) becomes statistically equivalent to i.i.d. sampling from any fixed underlying distribution. Given that our goal is generalization to predicting on new data, that simplification is reasonable, although the analysis does go through in the strict optimization setting, where \( N \) is finite. However, even with this assumption, we still need to describe the relationship between two consecutive subsets in the sequence, which does not fit the i.i.d. sampling model. To that end, we can view \( Z_t \) as a fraction of elements from \( Z_{t+1} \), selected uniformly at random without replacement. We now describe the relationship between the two consecutive loss estimates in this sequence. Note, that in this section the big-O notation hides only fixed numeric constants.

Lemma 2 With probability \( 1 - \delta \), for all \( w \) and all \( 0 \leq t \leq T \) we have

\[
\hat{g}_{t+1}(w) \leq 2 \hat{g}_t(w) + O\left(\frac{L^2B^2\log(T/\delta)}{\lambda n_t}\right). \tag{9}
\]

Proof The proof is very similar to [25], except we replace standard Rademacher Complexity with Permutational Rademacher Complexity (PRC), proposed in [26]. Let us fix \( t \), and consider a specific set of instances \( Z_{t+1} \), from which a random subset \( Z_t \) is sampled (without replacement). Following [25], for any \( r > 0 \) we define

\[
\mathcal{H}_{t,r} \triangleq \left\{ \hat{h}_w^r = \frac{h_w^r}{4k_{t,r}(w)} : w \in W \right\},
\]

where

\[
k_{t,r}(w) \triangleq \min\{k' \in \mathbb{Z}^+ : \hat{f}_{t+1}(w) \leq r^{k'}\}
\]

and

\[
h_w^r(z) \triangleq \ell_z(w) - \ell_z(\bar{w}_{t+1}^*).
\]

Our aim is to analyze the empirical average of the function values from \( \mathcal{H}_{t,r} \) evaluated on a given instance set \( Z \):

\[
\bar{h}_{t,r}^r(Z) = \frac{1}{|Z|} \sum_{z \in Z} h_w^r(z).
\]

We can translate the task of comparing \( \hat{g}_{t+1} \) and \( \hat{g}_t \) to describe it in terms of the function class \( \mathcal{H}_{t,r} \):

\[
\hat{g}_{t+1}(w) - \hat{g}_t(w) = \hat{g}_{t+1}(w) - (\hat{f}_t(w) - \hat{f}_t(\bar{w}_{t+1}^*))
\]

\[
\leq \hat{g}_{t+1}(w) - (\hat{f}_t(w) - \hat{f}_t(\bar{w}_{t+1}^*))
\]

\[
= 4k_{t,r}(w) \left[ \bar{h}_{t,r}^r(Z_t) - \bar{h}_{t,r}^r(Z_{t+1}) \right].
\]

To compare \( \bar{h}_{t,r}^r(Z_t) \) with \( \bar{h}_{t,r}^r(Z_{t+1}) \), we use Theorem 5 [25], which provides transductive risk bounds through expected PRC of function class \( \mathcal{H}_{t,r} \), conditioned on set \( Z_{t+1} \):

\[
\mathbb{Q}(\mathcal{H}_{t,r}, Z_{t+1}) \triangleq \mathbb{E}\left[ Q_{n_t,n_t/2}(\mathcal{H}_{t,r}, Z_t) \mid Z_{t+1} \right].
\]

Here, the randomness only comes from selecting \( Z_t \) as a subset of \( Z_{t+1} \). For any \( \delta > 0 \), with probability at least \( 1 - \delta \),

\[
\sup_w \left| \bar{h}_{t,r}^r(Z_t) - \bar{h}_{t,r}^r(Z_{t+1}) \right|
\]

\[
\leq \mathbb{Q}(\mathcal{H}_{t,r}, Z_{t+1}) + \sup_{w} \sup_{z} h_w^r(z) \cdot O\left( \sqrt{\frac{\log(1/\delta)}{n_t}} \right).
\]

Note, that \( \mathbb{Q}(\mathcal{H}_{t,r}, Z_{t+1}) = O(R_{n_t}(\mathcal{H}_{t,r})) \) (see [26]), where \( R_{n_t} \) is the standard Rademacher Complexity. The remainder of the proof proceeds identically as in [23] (up to numerical constants), i.e. by bounding both terms \( Y_1 \) and...
Figure 6: Comparing BET, Batch and Parallel SGD for HIGGS (left) and url (right) datasets, running on 16 cores. BET is as good as the best method in each case.

We return to the proof of Lemma 1. Using Lipschitz and boundedness assumptions for the loss $\ell$ and mapping $\phi$, as well as strong convexity of the regularized objective, we obtain initial tolerance of the loss estimate:

$$\hat{g}_0(w_0) = \tilde{f}_0(w_0) - \tilde{f}_0(\hat{w}_0^*) \leq \frac{1}{n_0} \sum_{i=1}^{n_0} (\ell_z(w_0) - \ell_z(\hat{w}_0^*)) \leq LB \|\hat{w}_0^*\| \leq LB \sqrt{\frac{2 \hat{g}_0(w_0)}{\lambda}},$$

where $\hat{g}_0(w_0) \leq \frac{2L^2B^2}{\lambda}$. We used the fact that $w_0$ is set to zero only for applying inequality $\|w_0\| \leq \|\hat{w}_0^*\|$ to drop the regularization terms (any initialization satisfying that requirement is acceptable).

Finally, Condition (7) regards the relationship between approximation error estimate $\hat{g}_T$ and full approximation error $\hat{g}$. This bound can be obtained by repeating the same argument as in Lemma 2. We can either assume $N \to \infty$ and use standard Rademacher complexity, as in Theorem 1, [25], or stay with the finite optimization model and apply PRC. Thus, we can set $\epsilon_0$ to satisfy the conditions of Lemma 1.

\[ \epsilon_0 \geq K \log \left( \frac{\log(\epsilon_0/\delta)}{\delta} \right), \]

with $K = O(L^2B^2/\lambda)$. It is easy to show that for small enough $\epsilon$ it suffices to set

$$\epsilon_0 \leq 2K \log \left( \frac{\log(1/\epsilon)}{\delta} \right) = O \left( \frac{L^2B^2}{\lambda} \cdot \left( \log \log(1/\epsilon) + \log(1/\delta) \right) \right).$$

Thus, setting $n_0 = 1$, we obtain the final complexity bound in Theorem 4.1 as

$$O \left( \frac{\kappa}{\lambda \epsilon} \cdot L^2B^2 \cdot \left( \log \log(1/\epsilon) + \log(1/\delta) \right) \right).$$