GPU-Accelerated Primal Learning for Extremely Fast Large-Scale Classification

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Abstract

One of the most efficient methods to solve $L_2$-regularized primal problems, such as logistic regression and linear support vector machine (SVM) classification, is the widely used trust region Newton algorithm, $TRON$ [33]. While $TRON$ has recently been shown to enjoy substantial speedups on shared-memory multi-core systems [30, 17], exploiting graphical processing units (GPUs) to speed up the method is significantly more difficult, owing to the highly complex and heavily sequential nature of the algorithm. In this work, we show that using judicious GPU-optimization principles, $TRON$ training time for different losses and feature representations may be drastically reduced. For sparse feature sets, we show that using GPUs to train logistic regression classifiers in LIBLINEAR is up to an order-of-magnitude faster than solely using multithreading. For dense feature sets—which impose far more stringent memory constraints—we show that GPUs substantially reduce the lengthy SVM learning times required for state-of-the-art proteomics analysis, leading to dramatic improvements over recently proposed speedups. Furthermore, we show how GPU speedups may be mixed with multithreading to enable such speedups when the dataset is too large for GPU memory requirements; on a massive dense proteomics dataset of nearly a quarter-billion data instances, these mixed-architecture speedups reduce SVM analysis time from over half a week to less than a single day while using limited GPU memory.

1 Introduction

Over the past decade, GPUs have become valuable computing resources to accelerate the training of popular machine learning models, playing a key role in the widespread use of deep models and the growing ecosystem of deep learning packages [7, 9, 1, 24, 37]. When a training algorithm admits an efficient GPU implementation (such as primal methods like $L-BFGS$ [34] and variants of gradient descent), the speedups gained using GPUs, as opposed to only CPUs, are often substantial. For instance, in PyTorch [37], training a logistic regression classifier on the $rcv1$ [31] dataset with gradient descent is 14.6 times faster using a Tesla V100 GPU versus using 24 CPU threads with an Intel Xeon Gold 5118 (similarly, training with $L-BFGS$ in this example is 13.1 times faster using the V100, detailed in Appendix A).

Specialized solvers commonly provide even more speed. For the previous logistic regression example, using just a single CPU thread with scikit-learn’s [38] $TRON$ solver—the primal learning algorithm for logistic regression and SVM classification/regression adapted from LIBLINEAR [10]—is 94.7 and 10.9 times faster than GPU-accelerated gradient descent and $L-BFGS$, respectively, implemented in PyTorch. However, while significant work has been done to further accelerate $TRON$ and many other extremely fast machine learning solvers [21, 45, 29, 25, 26] using multiple CPU cores [5, 23, 22, 30, 8, 39, 46, 17], analogous GPU speedups for such efficient algorithms are typically lacking.

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This lack of GPU exploitation is due to the specialized structure and complexity of these algorithms, which naturally lend themselves to multithreaded speedups on shared memory systems, yet resist optimizations on GPU architectures.

For example, TRON relies on random access to features for SVM losses, which is naturally supported in multithreaded systems, but prevents memory coalescing (and is thus deleterious) for GPU computation. Furthermore, large memory transfers between the CPU and GPU are expensive, so that the complex, sequential dependency of variables in specialized algorithms like TRON make optimal GPU use difficult. Indeed, we show that while most of the computational bottlenecks for logistic regression in TRON are linear algebra operations [30] (for which GPUs greatly outperform CPUs), using TRON’s original variable access pattern in LIBLINEAR results in poor GPU performance—performing even worse than using only a single CPU thread on one of the presented datasets.

Herein, we show that using just a single CPU, excellent training speedups are achievable by overly CPU-specialized machine learning algorithms such as TRON. In particular, for different feature representations and loss functions, we show that TRON training times may be drastically reduced using judicious GPU-optimization principles.

Sparse Features. For sparse feature representations, we successively optimize TRON for logistic regression (referred to as TRON-LR) in LIBLINEAR using several strategies to: a) decouple the sequential dependence of variables, b) minimize the number of large-memory transfers between GPU and CPU, and c) maximize parallelism between the CPU and GPU. We show that while TRON’s original variable access pattern limits the effectiveness of GPU computation, using a single CPU thread with our GPU optimizations results in a 70.8% improvement in training time (averaged over the presented datasets) over the single-threaded version of TRON in standard LIBLINEAR. In addition, we show that mixing our GPU optimizations with multithreading provides further speedups, resulting in an average 89.2% improvement over single-thread optimized TRON and an average 65.2% improvement over TRON in the multithread-optimized version of LIBLINEAR [30].

Dense Features. For dense feature representations, we show that GPUs substantially reduce SVM learning times for state-of-the-art analysis of dense proteomics datasets [27]. Overcoming the random access restrictions of TRON SVM learning (referred to as TRON-SVM), we show that using just a single GPU leads to an average as much as triples the performance of recently proposed speedups for this application [17]. On a large-scale dataset of over 23 million data instances, these GPU speedups reduce SVM learning time from 14.4 hours down to just 1.9 hours. Furthermore, dense feature sets impose stringent GPU memory constraints, particularly for the massive datasets regularly produced in biological experiments. Thus, we demonstrate how GPU optimizations may be mixed with multithreading to significantly reduce GPU memory constraints. On a massive proteomics dataset consisting of over 215 million data instances—which exceeds memory requirements for GPU-only speedups—these mixed-architecture speedups drastically outperform recent multithread-optimized solvers, reducing standard analysis time from 4.4 days down to just 19.7 hours.

The paper is organized as follows. In Section 2, we describe relevant previous work speeding up TRON for both sparse and dense feature sets on shared memory systems. In Section 3, we define the general TRON algorithm and computational bottlenecks encountered minimizing different loss functions. In Sections 4 and 5, we discuss how the computational bottlenecks in algorithms like TRON natively resist GPU speedups, and GPU-optimization principles to overcome these hurdles (providing the resulting GPU optimizations for the objectives and feature architectures under study). We demonstrate that the presented GPU-optimizations drastically outperform recent multithreaded speedups in Section 6, and conclude with future avenues extending the presented work to other high-performance GPU packages (such as PyTorch) in Section 7.

2 Previous Work

Serving as the primal solver in the popular package LIBLINEAR [10], TRON has been extensively tested and shown to enjoy superior speed and convergence compared to other second-order solvers, such as the widely-used quasi-Newton algorithm L-BFGS [34] and the modified Newton algorithm L2-SVM-MFN [29] (one of the fastest algorithms for large-scale primal SVM learning). TRON’s convergence speed for logistic and SVM losses in LIBLINEAR has further been theoretically improved by refining trust-region update rules [20] and applying a preconditioner matrix to help stabilize optimization [19]. In [30], multithreaded optimizations in shared-memory multi-core systems were extensively explored to speed up TRON’s computational bottlenecks (further described in Section 3)
for logistic regression. Evaluating several multithreading libraries (i.e., OpenMP, Intel’s Math Kernel Library, and the sparse matrix multiplication package librsb) over a large number of datasets, OpenMP was found to provide the best multithreaded performance and was subsequently integrated into the multi-core release of LIBLINEAR.

2.1 SVM Classification Using TRON for Fast Large-Scale Proteomics Analysis

In proteomic analysis pipelines, SVM classification using Percolator [27] is a critical step towards accurately analyzing protein data collected via tandem mass spectrometry (MS/MS). Given a collection of MS/MS spectra representing the protein subsequences (called peptides) present in a biological sample, the first stage of proteomics analysis typically consists of identifying the input spectra by searching (i.e., scoring and ranking) a database of peptides. This first stage thus results in a list of peptide-spectrum-matches (PSMs) and their respective scores. In practice, however, database-search scoring functions are often poorly calibrated, making PSMs from different spectra difficult to compare and diminishing overall identification accuracy. To correct for this, the list of PSMs, as well as dense feature vectors describing each match, are fed into Percolator for recalibration.

Percolator first estimates PSM labels (i.e., correct versus incorrect) using false discovery rate analysis [28], then trains a linear SVM to classify correct and incorrect identifications. These two steps are iterated until convergence and the input PSM scores are subsequently recalibrated using the final learned SVM parameters. Furthermore, to prevent overfitting and improve generalizability within each iteration, three-fold cross-validation is carried out over three disjoint partitions of the original dataset, followed by further nested cross-validation within each fold [13].

The accuracy improvements of Percolator recalibration have been well demonstrated for a wide variety of PSM scoring functions—e.g., linear [27, 6, 44], p-value based [12, 18, 32], and dynamic Bayesian networks [14]—and complex PSM feature sets—e.g., Fisher kernels [15, 16], subscores of linear functions [40], ensembles of scoring functions [42], and features derived using deep models [11]. However, due to the iterative training of many SVMs during cross-validation, Percolator requires substantial analysis times for large-scale datasets commonly collected in MS/MS experiments. Initial work sought to speed up Percolator runtimes by randomly sampling a small portion of the data to train over [35], but this was subsequently shown to unpredictably diminish the performance of learned parameters [17]. Thus, to combat these lengthy analysis times without affecting learned SVM parameters, recent work [17] applied extensive systems-level speedups and multithreading in both Percolator’s original primal solver, L2-SVM-MFN, and TRON (heavily optimized to utilize dense feature vectors). While both optimized solvers were shown to significantly improve Percolator training times for large-scale data, TRON displayed markedly superior performance.

3 Trust Region Newton Methods for Primal Classification

Consider feature vectors \( x_i \in \mathbb{R}^n, i = 1, \ldots, l \) and label vector \( y \in \{-1, 1\}^l \), and let \( X = [x_1 \ldots x_l]^T \) be the feature matrix. For vectors, index-set subscripts denote subvectors and for matrices, pairs of index-set subscripts denote submatrices. The general objective, which we wish to minimize w.r.t. \( w \), is

\[
f(w) = \frac{1}{2} \| w \|_2^2 + C \sum_{i=1}^{l} \ell(w; x_i, y_i),
\]

where \( \frac{1}{2} \| w \|_2^2 \) is the regularization term, \( C > 0 \) is a regularization hyperparameter, and \( \ell(w; x_i, y_i) \) is a loss function.

When \( \ell(w; x_i, y_i) = \log(1 + e^{-y_i w^T x_i}) \), commonly referred to as the logistic loss, minimizing Equation 3 corresponds to learning a classifier using logistic regression. Similarly, minimizing Equation 3 when \( \ell(w; x_i, y_i) = (\max(0, 1 - y_i w^T x_i))^2 \), commonly referred to as the quadratic SVM or L2-SVM loss, corresponds to learning a linear SVM classifier. We denote Equation 3 under the logistic loss as \( f_{L2}(w) \) and, under the L2-SVM loss, as \( f_{L2}(w) \).

TRON is detailed in Algorithm 2. At each iteration, given the current parameters \( w \) and trust region interval \( \Delta \), TRON considers the following quadratic approximation between function parameters,

\[
f(w + d) - f(w) \approx q(d) = \nabla f(w)^T d + \frac{1}{2} d^T \nabla^2 f(w) d.
\]
Algorithm 1 The TRON algorithm

1: Given \( w, \Delta, \) and \( \sigma_0 \)
2: Calculate \( f(w) \) \quad // Critically depends on \( z = X^T w \)
3: while Not converged do
4: \hspace{1em} Find \( d = \text{argmin}_v q(v) \) s.t. \( ||v||_2 \leq \Delta \). \quad // Critically depends on \( \nabla f(w), \nabla^2 f(w)v \)
5: \hspace{1em} Calculate \( f(w + d), \sigma = \frac{f(w + d) - f(w)}{q(d)} \) \quad // Critically depends on \( z = X^T(w + d) \)
6: \hspace{1em} if \( \sigma > \sigma_0 \) then
7: \hspace{2em} \( w \leftarrow w + d, \) increase trust region \( \Delta \).
8: \hspace{1em} else
9: \hspace{2em} Shrink \( \Delta \).
10: \hspace{1em} end if
11: end while

A truncated Newton step \( (d \) on line 4 in Algorithm 2), confined in the trust region, is then found using a conjugate gradient procedure. If \( q(d) \) is close to \( f(w + d) - f(w) \), \( w \) is updated to \( w + d \) and the trust region interval is increased for the subsequent iteration. Otherwise, \( w \) remains unchanged and the trust region interval is shrunk.

Note that the function evaluation \( f(w) \)–which critically depends on computing \( z = X^T w \) for both losses–must be computed for each new iteration, as well as the gradient and Hessian for Equation 4. However, computing only the Hessian-vector product in Equation 4 avoids loading the entire Hessian into memory (which would be intractable for large datasets). Thus, the most intensive portions of TRON are the computations of \( z = X^T w, \nabla f(w), \) and \( \nabla^2 f(w)v \) (where \( v \) is the optimization variable in line 4 of Algorithm 2), summarized for both losses in Table 1. Further derivation of these quantities is available in Appendix B.

We note that arbitrary loss functions (and combinations thereof) may be used in Equation 3, thus allowing future work utilizing the highly efficient TRON in popular automatic differentiation [4] packages [37, 1, 41, 36]. However, these packages rely on GPUs for optimal performance, the use of which TRON natively resists (as we’ll see, and rectify, for the two loss functions considered).

| Logistic Loss | L2-SVM Loss |
|---------------|-------------|
| \( z = X^T w, \) to compute \( f_{LR}(w) \) | \( z = X^T w, \) to compute \( f_{L2}(w) \) |
| \( \nabla f_{LR}(w) = w + C \sum_{i=1}^{l} (h(y_i, z_i) - 1) y_i x_i, \) where \( h(y_i, z_i) = (1 + e^{y_i z_i})^{-1} \) | \( \nabla f_{L2}(w) = w + 2C X (I - y x^T), \) where \( I \equiv \{i | 1 - y_i z_i > 0 \} \) is an index set and the operator : denotes all elements along the corresponding dimension (i.e., all columns in this case) |
| \( \nabla^2 f_{LR}(w)v = v + C X (D(Xv)), \) where \( D \) is a diagonal matrix with elements \( D_{i,i} = h(y_i, z_i)(1 - h(y_i, z_i)) \) | \( \nabla^2 f_{L2}(w)v = v + 2C X^T (I - y x^T) \) |

Table 1: TRON major bottleneck computations for logistic and L2-SVM losses.

4 Accelerating TRON-LR training using GPUs

Assume a shared-memory multi-core system and a single GPU with sufficient memory for the variables in Table 1 (this is later relaxed in Section 5). Herein, the CPU is referred to as the host and the GPU is referred to as the device.

TRON-LR runtime is dominated by three major matrix-vector multiplications in the bottleneck computations listed in Table 1: \( z = X^T w, \nabla^2 f_{LR}(w)v, \) and \( \nabla f_{LR}(w) = w + C X \hat{z}, \) where \( \hat{z} = (h(y_i, z_i) - 1)y_i. \) For instance, profiling TRON-LR in LIBLINEAR training on the large-scale SUSY [3] dataset, these three matrix-vector multiplications account for 82.3% of total training time. We thus first attempt to accelerate TRON-LR by computing these quantities quickly on the device (as was similarly done in [30] using multithreading).

In LIBLINEAR, this first attempt at GPU acceleration (called TRON-LR-GPU0) is implemented using cuSPARSE to perform sparse linear algebra operations as efficiently as possible for LIBLINEAR’s
sparse feature representation. Compared to the standard single-threaded implementation of \textsc{Liblinear} on the \textsc{Susu} dataset, \textsc{Tron-LR-GPU}\textsuperscript{0} achieves a speedup of 0.65–\textsc{Tron-LR-GPU}\textsuperscript{0} is actually slower than the single-threaded \textsc{Liblinear}! \textsc{Tron-LR-GPU}\textsuperscript{0} fares better on other presented datasets, but performs poorly overall (displayed in Figure 1).

4.1 Sequentially Dependent Variables

The critical issue encountered by \textsc{Tron-LR-GPU}\textsuperscript{0} is \textsc{Tron}'s overly sequential dependency of variables; once variable vectors are computed on the GPU, they are immediately needed on the host CPU to proceed with the next step of the algorithm. For instance, computing the bottleneck \( z = X^T(w + d) \) using \textsc{CuSparse} is fast, but \( z \) must immediately be transferred back to the host to compute \( f_{\text{LR}}(w + d) \) (in line 5 of Algorithm 2). However, large-memory transfers between the host and device are expensive, especially when either the host or device are waiting idle for the transaction to complete (steps to conceal transfer latency are discussed in Appendix C).

Furthermore, all other major operations in Algorithm 2 are locked in the same manner as the previous bottleneck example: the trust region update (lines 6–10) can not proceed without the value of \( f_{\text{LR}}(w + d) \), and, without either the updated \( w \) or trust region, operations for the next iteration's truncated Newton step (line 4) are unable to run concurrently in an attempt to conceal transfer latency. Clearly, this pattern of variable access is suboptimal for GPU use (best evidenced by \textsc{Tron-LR-GPU}\textsuperscript{0}'s performance in Section 6).

4.2 Decoupling Dependencies to Maximize Host and Device Parallelism

To optimally use the GPU, we must first decouple the sequential dependency of variables discussed in Section 4.1. Recall that, for \( \nabla f_{\text{LR}}(w) \), the vector \( \hat{z} \) is such that \( \hat{z}_i = (h(y_i z_i) - 1)y_i \). To decrease sequential dependencies on the computational bottleneck \( z = X^T(w + d) \), we first note that calculation of \( f_{\text{LR}}(w + d) \) always precedes \( \nabla f_{\text{LR}}(w + d) \). Thus, to decouple gradient variables, once \( z \) is calculated on the device, we prepare all device-side variables needed to compute \( X^T \hat{z} \) in the event that \( \sigma > \sigma_0 \). Specifically, after computing \( z = X^T(w + d) \) on the device, we use a custom \textsc{CUDA} kernel to compute both \( \hat{z} \) and the reduction \( f_{\text{LR}}(w + d) = \frac{1}{2}||w + d||_2^2 + C \sum_{i=1}^l \log(1 + e^{-y_i z_i}) \) (note that the scalar output of the reduction, i.e. \( f_{\text{LR}}(w + d) \), is immediately available to the host).

Thus, if \( \sigma > \sigma_0 \), the variable \( \hat{z} \) is already in device memory and the gradient is quickly calculated using \textsc{CuSparse} on the device as \( \nabla f_{\text{LR}}(w + d) = w + d + X^T \hat{z} \). Finally, \( \nabla f_{\text{LR}}(w + d) \) is transferred from device to host, which is notably efficient when \( l \gg n \) (i.e., the optimal setting for primal learning).

This set of operations accomplishes several optimizations simultaneously:

- **Decoupling dependencies, avoiding large transfers:** \( z \) and \( \hat{z} \) are completely decoupled of any dependency for host-side computation, thanks to the custom reduction and kernel. This saves several large transfers of \( z, \hat{z} \) from (and to) the device, and avoids the need to conceal transfer latency.
- **Coalesced memory:** the device performs optimally as all operations allow memory coalescing.
- **Device saturation:** an uninterrupted series of intensive computation is performed on the device (i.e., no device-side stalls due to host dependencies).
- **Host and device parallelism:** the complete decoupling of \( z, \hat{z} \) allows more independent operations to be run on the host while the device runs concurrently.

We complete the total GPU-optimization of \textsc{Tron-LR} by considering the remaining bottleneck, the Hessian-vector product \( \nabla^2 f_{\text{LR}}(w) v = I + C X^T (D X v) \). As with the previous optimizations, device variables are maximally decoupled from host-side dependencies, while using device-side functions which allow peak performance. In particular, we compute the diagonal matrix \( D \) in the same custom \textsc{CUDA} kernel used to compute \( \hat{z} \) (where \( D_{i,i} = h(y_i z_i)(1 - h(y_i z_i)) \)). \( D \) is also used in later host computations (for preconditioning [19]), so \( D \) is immediately transferred from device to host on an asynchronous device stream (the stream is synchronized just prior to host-variable use).

The candidate Newton step \( v \) (which is only of dimension \( n \)) is transferred from device to host on an asynchronous stream, and the following decompositions of \( \nabla^2 f_{\text{LR}}(w) v \) are added to this same stream: \( a_0 = X v, a_1 = D a_0, a_2 = C X^T a_1 \). \( a_0 \) and \( a_2 \) are computed using \textsc{CuSparse},
while \(a_i\) is computed using a custom kernel for element-wise multiplication along \(D\)’s diagonal. \(\nabla^2f_{\text{LR}}(w)v\) is then transferred from host to device. However, the rest of the conjugate procedure is sequentially dependent on the dot-product \(v^T \nabla^2f_{\text{LR}}(w)v\). In order to relieve this dependence while the \(\nabla^2f_{\text{LR}}(w)v\) transfers from device to host, \(v^T \nabla^2f_{\text{LR}}(w)v\) is computed on the device and the resulting scalar is available immediately to the host.

### Decreasing runtimes via mixed-architecture speedups.

While computations remain which may be accelerated using the same GPU-optimization principles, allocating additional device vectors becomes problematic for large-scale datasets and current GPU memory ranges. Thus, in addition to the previously described GPU optimizations, we accelerate remaining bottleneck areas using multithreading. In particular, multithreading using OpenMP is used to accelerate vector-matrix-vector multiplications in the conjugate gradient procedure (previously optimized using loop unrolling) and application of the preconditioner matrix [19] (which is jointly sped up using existing device-side computation during the Hessian-vector product optimizations).

### 5 Accelerating TRON-SVM training using GPUs

Focusing on speeding up SVM learning in the state-of-the-art software Percolator [27]—which uses dense feature vectors to analyze large-scale proteomics datasets—the GPU-optimization principles from Section 4.2 are applied to TRON-SVM: device-side variables are decoupled from dependent host-side computations, necessary transfers are run asynchronously in parallel with the maximum number of host/device operations, and linear algebra operations are extensively and efficiently carried out using cuBLAS. However, speed ups in TRON-SVM possess a key difficulty for GPU computation; for \(z = X^Tw\), the active set \(I \equiv \{i: y_i z_i > 0\}\) is recomputed every iteration. Thus, computation of both \(\nabla f_{\text{LR}}(w)\) and \(\nabla^2f_{\text{LR}}(w)\) requires the submatrix \(X_I\). (as seen in Table 1).

While accessing \(X_I\) is naturally supported through shared-memory random access for multithreaded speedups (e.g., in [17], which used OpenMP to speed up the TRON-SVM quantities in Table 1 within Percolator), the non-contiguous nature of this operation leads to misaligned (i.e., not coalesced) device memory which prevents optimal GPU use. Furthermore, as noted in Section 4.2, large memory transfers between host and device are expensive, hindering approaches where \(I\) is first computed then a randomly accessed submatrix is created on the host and transferred to the device.

To overcome this challenge, we first make use of the insight that, prior to computing \(f_{\text{LR}}(w)\), the active set \(I\) may be computed and stored entirely on the device. With \(I\) on the device, the submatrix \(X_I\) may be efficiently computed within device memory. Computing \(I\) and \(X_I\) on the device entirely decouples these variables from host-side compute and accomplishes all simultaneous optimizations listed in Section 4.2. The major operations of the resulting GPU-optimized solver, called TRON-SVM-GPU, are listed in Table 4.

### Decreasing GPU-memory utilization via mixed-architecture speedups.

In TRON-SVM-GPU, the device memory required to decouple \(X_I\) from host-side compute proves prohibitive for extremely large-scale proteomics datasets. To remedy this, the mixed-architecture solver, TRON-SVM-MIX, utilizes the GPU for heavy lifting before using multithreading for efficient random access to \(X_I\); (after \(I\) is computed) during TRON’s conjugate gradient procedure. Thus, TRON-SVM-MIX utilizes much
less GPU memory than TRON-SVM-GPU, at the expense of some speed due to fewer operations being run on the device. The major operations of TRON-SVM-MIX are listed in Table 4.

6 Results and Discussion

All experiments were run on a dual Intel Xeon Gold 5118 compute node with 48 computational threads, an NVIDIA Tesla V100 GPU, and 768 GB of memory.

Speedups for sparse features. The TRON-LR GPU-optimized and mixed-architecture solvers (described in Section 4.2) are referred to as TRON-LR-GPU and TRON-LR-MIX, respectively. TRON-LR-GPU, TRON-LR-MIX, and TRON-LR-GPU0 were all developed based on LIBLINEAR v2.30. Single-threaded LIBLINEAR tests were run using v2.30. The multithread-optimized version of TRON-LR described in [30], referred to herein as TRON-LR-CPU, was tested using multi-core LIBLINEAR v2.30. All single-threaded TRON-LR implementations (i.e., TRON-LR-GPU0, TRON-LR-GPU, and the single-threaded optimized version of TRON-LR in standard LIBLINEAR) were run with the same command line parameters: `-c 4 -e 0.1 -s 0`. Multithreaded implementations were run with the additional flag `-nr i`, specifying the use of `i` compute threads. As is standard practice, wallclock times were measured as the minimum reported times over ten runs. Training times were measured within LIBLINEAR as the time elapsed calling tron.obj.tron(). Six datasets of varying statistics (i.e., number of features, instances, and nonzero elements) were downloaded from https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/ and used to benchmark the TRON-LR solvers (statistics for each dataset are listed in Appendix D).

The speedups for all methods are displayed in Figure 1. TRON-LR-GPU significantly outperforms the multithread-optimized TRON-LR-CPU and the direct GPU implementation, TRON-LR-GPU0, across all datasets and threads. The mixed-architecture TRON-LR-MIX further improves upon TRON-LR-GPU performance in each dataset for all threads used, leading to over tenfold speedups in training time on half of the presented datasets. We note that, due to thread scheduling overhead, multithreaded methods experience diminished performance for large numbers of threads in Figures 1a,1b,1f. However, the presented GPU optimizations consistently provide the best speedups when both multithreading is not used and when multithreading is overutilized.

Speedups for dense features. The TRON GPU solvers described in Section 5—the GPU-optimized TRON-SVM-GPU and the mixed-architecture TRON-SVM-MIX—are compared against the multithread-optimized versions of TRON (referred to as TRON-SVM-CPU) and L2-SVM-MFN.
Reported runtimes are the minimum wall-clock times measured over five runs for the Kim dataset and three runs for the Wilhelm dataset. The original Percolator SVM learning runtimes (collected using Percolator v3.04.0) were 14.4 hours and 4.4 days for the Kim and Wilhelm datasets, respectively. Speedups for both datasets are illustrated in Figure 2. For the Kim dataset, speedup results for all discussed methods are illustrated in Figure 2a. For the Wilhelm dataset, total Tesla V100 memory (16 GB) is exceeded for TRON-SVM-GPU. However, the reduced memory requirements of TRON-SVM-MIX allow GPU speedups for this massive dataset (illustrated in Figure 2b).

Both GPU solvers greatly accelerate Percolator SVM learning while dominating previously proposed multithreaded speedups. For the Kim dataset, TRON-SVM-MIX and TRON-SVM-GPU achieve 6.6 and 7.4 fold speedups, respectively, over Percolator’s current SVM learning engine. For the Wilhelm dataset, TRON-SVM-MIX achieves a 5.4 fold speedup while being notably efficient using few system threads—withe at most 16 threads, TRON-SVM-MIX improves the average training time of TRON-SVM-CPU and $L_2$-SVM-MFN by 50% and 70%, respectively. Together, these two solvers present versatile trade-offs for different compute environments; when the dataset does not exceed the GPU memory, TRON-SVM-GPU offers superior performance. However, when onboard GPU memory is limited, a small portion of speed may be traded for much less memory consumption by using TRON-SVM-MIX. Furthermore, when the number of computational threads is also limited, TRON-SVM-MIX offers significantly better (and more stable) performance at low numbers of utilized threads compared to the purely multithreaded solvers TRON-SVM-CPU and $L_2$-SVM-MFN.

### 7 Conclusions and Future Work

In this work, we’ve shown that by using general GPU-optimization principles, excellent speedups may be enjoyed by algorithms which natively resist GPU optimization. For the widely used TRON algorithm, we’ve presented several GPU-optimized solvers for both sparse and dense feature sets of $L_2$-regularized primal problems. Using a single GPU, these solvers were shown to dominate recently proposed speedups for logistic regression (within LIBLINEAR) and SVM classification for state-of-the-art proteomics analysis (within Percolator). Furthermore, for sparse features, we’ve shown how multithreading may compliment GPU optimizations and, for memory-restrictive dense
features, how multithreading may relieve device-memory requirements while allowing substantial GPU speedups. The former optimizations achieve over an order-of-magnitude speedup on half of the presented datasets (and an average 9.3 fold speedup on all datasets), while the latter optimizations decrease massive-scale biological analysis time from 4.4 days down to just 19.7 hours.

There are significant avenues for future work. We plan to extend GPU-optimized TRON implementations to use general gradient and Hessian-vector product information computed in automatic differentiation [4] packages such as PyTorch [37] and TensorFlow [1], which utilize second-order primal solvers (such as L-BFGS) to optimize losses while relying on GPU compute for optimal performance. Furthermore, we plan to apply the presented GPU-optimization principles to speed up other fast machine learning solvers [21, 2, 45, 29, 25, 26] which, like TRON, are natively designed to rely on sequential dependencies of variables.

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A GPU speedups training a logistic regression classifier in PyTorch

A binary logistic regression classifier was implemented in PyTorch (v1.4.0) and trained over the rcv1 dataset to illustrate the speed ups possible using a GPU (Nvidia Tesla V100) versus only multithreading (24 CPU threads using an Intel Xeon Gold 5118). Speedups were tested for both batch gradient descent (with a 0.001 learning rate) and L-BFGS. The rcv1 dataset was downloaded from https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary/rcv1_train.binary.bz2. Gradient descent converged after 3,000 iterations and L-BFGS converged after 100 iterations. For reference, a logistic regression classifier was trained using single-threaded TRON (as implemented in scikit-learn v0.20.4). All code is available in pyTorchLogisticRegression_rcv1.py.

| Solver                  | CPU training time (s) | GPU training time (s) | GPU Speedup |
|-------------------------|-----------------------|-----------------------|-------------|
| Gradient descent        | 395.58                | 27.05                 | 14.63       |
| L-BFGS                  | 40.56                 | 3.1                   | 13.08       |
| TRON (scikit-learn)     | 0.29                  | –                     | –           |

Table 3: Logistic regression training times, measured in seconds, for the rcv1 dataset. Gradient descent and L-BFGS solvers are implemented in PyTorch, and single-threaded TRON is implemented in scikit-learn.

B Derivation of TRON Hessian-vector products

Consider feature vectors \(x_i \in \mathbb{R}^n, i = 1, \ldots, l\) and label vector \(y \in \{-1, 1\}^l\), and let \(X = [x_1 \ldots x_l]^T\) be the feature matrix. For vectors, index-set subscripts denote subvectors and for matrices, pairs of index-set subscripts denote submatrices. Let \(1\) denote the indicator function.

The general \(L_2\)-regularized objective, which we wish to minimize w.r.t. \(w\), is

\[
    f(w) = \frac{1}{2}w^T w + C \sum_{i=1}^l \ell(w; x_i, y_i),
\]

where \(\frac{1}{2}w^T w\) is the regularization term, \(C > 0\) is a regularization hyperparameter, and \(\ell(w; x_i, y_i)\) is a loss function. When \(\ell(w; x_i, y_i) = \log(1 + \exp(-(y_i w^T x_i)))\), commonly referred to as the logistic loss, minimizing Equation 3 corresponds to learning a classifier using logistic regression. Similarly, minimizing Equation 3 when \(\ell(w; x_i, y_i) = (\max(0, 1 - y_i w^T x_i))^2\), commonly referred to as the L2-SVM or quadratic SVM loss, corresponds to learning a linear SVM classifier. The logistic loss results in an objective function that is twice differentiable and the L2-SVM loss yields a differentiable objective (unlike the hinge loss) with a generalized Hessian [29]). We denote Equation 3 under the logistic loss as \(f_{LR}\) and, under the \(L_2\)-SVM loss, as \(f_{L2}\).

TRON is detailed in Algorithm 2. At each iteration, given the current parameters \(w\) and trust region interval \(\Delta\), TRON considers the following quadratic approximation to \(f(w + d) - f(w)\),

\[
    q(d) = \nabla f(w)^T d + \frac{1}{2}d^T \nabla^2 f(w) d.
\]

A truncated Newton step, confined in the trust region, is then found by solving

\[
    \min_d q(d) \quad \text{s.t. } ||d||_2 \leq \Delta.
\]

If \(q(d)\) is close to \(f(w + d) - f(w)\), \(w\) is updated to \(w + d\) and the trust region interval is increased for the subsequent iteration. Otherwise, \(w\) remains unchanged and the trust region interval is shrunk.

Note that the function evaluation \(f(w)\) must be computed for each new iteration, as well as the gradient and the Hessian for Equation 4. However, Equation 4 involves only a Hessian-vector product, computation of which circumvents loading the entire Hessian into memory. For the logistic loss, we have

\[
    \nabla f_{LR}(w) = w + C \sum_{i=1}^l (b(y_i w^T x_i) - 1)y_i x_i,
\]
Algorithm 2 The TRON algorithm

1: Given $w$, $\Delta$, and $\sigma_0$
2: Calculate $f(w)$ \hspace{1cm} // Critically depends on $z = X^T w$
3: \textbf{while} Not converged \textbf{do}
4: \hspace{1cm} Find $d = \text{argmin}_v q(v) \text{ s.t. } ||v||_2 \leq \Delta$. \hspace{1cm} // Critically depends on $\nabla f(w)$, $\nabla^2 f(w)v$
5: \hspace{1cm} Calculate $f(w + d), \sigma = \frac{f(w) - f(w + d)}{q(d)}$ \hspace{1cm} // Critically depends on $z = X^T (w + d)$
6: \hspace{1cm} \textbf{if} $\sigma > \sigma_0$ \textbf{then}
7: \hspace{1cm} \hspace{1cm} $w \leftarrow w + d$, increase trust region $\Delta$.
8: \hspace{1cm} \textbf{else}
9: \hspace{1cm} \hspace{1cm} Shrink $\Delta$.
10: \hspace{1cm} \textbf{end if}
11: \hspace{1cm} \textbf{end while}

where $h(y_i w^T x_i) = (1 + e^{-y_i w^T x_i})^{-1}$. For the L2-SVM loss, we have

$$\nabla f_{L2}(w) = w + 2C \hat{X}^T \hat{z} = w + 2CX_{I,:}(X_{I,:}w - y_I), \tag{7}$$

where $I \equiv \{i \mid 1 - y_i w^T x_i > 0\}$ is an index set and the operator $:=$ denotes all elements along the corresponding dimension (i.e., all columns in this case). Thus, $X_{I,:}$ is the submatrix of all $X$ rows the indices of which are in $I$.

Equation 5 involves only a single Hessian-vector product, the structure of which is exploited to avoid loading the entire Hessian into memory. For the logistic loss, we have

$$\nabla^2 f_{LR}(w) = \mathcal{I} + CX^T D X, \tag{8}$$

where $D$ is a diagonal matrix with elements $D_{i,i} = h(y_i w^T x_i)(1 - h(y_i w^T x_i))$. Thus, for a vector $v$, the Hessian-vector product is efficiently computed as $\nabla^2 f_{LR}(w)v = v + CX^T(D(Xv))$. For the L2-SVM loss, we have

$$\nabla^2 f_{L2}(w) = \mathcal{I} + 2CX^T DX = \mathcal{I} + 2CX_{I,:}X_{I,:}, \tag{9}$$

where $D$ is a diagonal matrix with elements $D_{i,i} = 1_{i \in I}$. The Hessian-vector product is thus efficiently computed as $\nabla^2 f_{L2}(w)v = v + 2CX_{I,:}X_{I,:}v$.

C Concealing large-memory transfer latency between the host and device

To optimally conceal device-to-host transfer latency while maximizing host and device parallelism, it is necessary to:

(a) Add all dependent device-functions involving the data to be sent to an asynchronous device stream, $s$,

(b) add the transfer of the data from device-to-host to $s$,

(c) run independent host and/or device operations,

(d) synchronize $s$ just prior to running a dependent operation on the host.

(e) Note that if the dependent data needed from the device on the host is a scalar, it may be returned without latency.

The other direction is slightly different. To optimally conceal host-to-device transfer latency while maximizing host and device parallelism, it is necessary to:

(a) launch the transfer on a device stream as soon as the data is available,

(b) add all dependent device-functions involving the data being sent to the device stream.

It is easy to see that algorithms with many sequential dependencies are at odds with these principles (they reveal transfer latency while minimizing host/device parallelism).
## Benchmark Dataset Statistics

| Dataset   | #instances | #features | #nonzeros  |
|-----------|------------|-----------|------------|
| rcv1      | 20,242     | 47,236    | 1,498,952  |
| SUSY      | 5,000,000  | 18        | 88,938,127 |
| HIGGS     | 11,000,000 | 28        | 283,685,620|
| KDD2010-b | 19,264,097 | 29,890,095| 566,345,888|
| url       | 2,396,130  | 3,231,961 | 277,058,644|
| real-sim  | 72,309     | 20,958    | 3,709,083  |
| Kim       | 23,330,311 | 18        | 0          |
| Wilhelm   | 215,282,771| 18        | 0          |

Table 4: Sparse and dense benchmark dataset statistics for TRON-LR and TRON-SVM, respectively.