SGDLibrary: A MATLAB library for stochastic gradient descent algorithms

Hiroyuki Kasai

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Abstract

We consider the problem of finding the minimizer of a function \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) of the form
\[
\min_{w \in \mathbb{R}^d} f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w).
\]
This problem has been studied intensively in recent years in machine learning research field. One typical but promising approach for large-scale data is stochastic optimization algorithm. SGDLibrary is a flexible, extensible and efficient pure-Matlab library of a collection of stochastic optimization algorithms. The purpose of the library is to provide researchers and implementers a comprehensive evaluation environment of those algorithms on various machine learning problems.

1 Introduction

This work aims to facilitate research on stochastic optimization for large-scale data. We particularly address a regularized empirical loss minimization problem defined as
\[
\min_{w \in \mathbb{R}^d} f(w) := \frac{1}{n} \sum_{i=1}^{n} f_i(w) = \frac{1}{n} \sum_{i=1}^{n} L(w, x_i, y_i) + \lambda R(w),
\]
where \( w \in \mathbb{R}^d \) represents the model parameter and \( n \) denotes the number of samples. \( L(w, x_i, y_i) \) is the loss function and \( R(w) \) is the regularizer with the regularization parameter \( \lambda \geq 0 \). Widely diverse machine learning models fall into this problem. Considering \( L(w, x_i, y_i) = (w^T x_i - y_i)^2 \), \( x_i \in \mathbb{R}^d \), \( y_i \in \mathbb{R} \) and \( R(w) = \|w\|_2^2 \), this results in L2-norm regularized linear regression problem (a.k.a. ridge regression) for \( n \) training samples \( (x_1, y_1), \ldots, (x_n, y_n) \). In case of the binary classification problem with the desired class label \( y_i \in \{+1, -1\} \) and \( R(w) = \|w\|_1 \), L1-norm regularized logistic regression (LR) problem is obtained as \( f_i(w) = \log(1 + \exp(-y_i w^T x_i)) + \lambda \|w\|_1 \), which encourages the sparsity of the solution of \( w \). Other problems are matrix completion, support vector machines (SVM), and sparse principal components analysis, to name but a few.

Full gradient decent (GD) with a step size \( \eta \) is the most straightforward approach for (1) as
\[
\min_{w \in \mathbb{R}^d} \{ \frac{1}{2n} \sum_{i=1}^{n} \|w - w_{k-1}\|^2 + \langle \nabla f(w_{k-1}), w \rangle \},
\]
where the update reduces to \( w^k \leftarrow w^{k-1} - \nabla f(w^{k-1}) \). However, this is expensive especially when \( n \) is extremely large. In fact, one needs a sum of \( n \) calculations of the inner product \( w^T x_i \) of \( d \)-dimensional vectors, leading to \( O(nd) \) cost overall per iteration. For this issue, a popular and effective alternative is stochastic gradient descent update as
\[
\min_{w \in \mathbb{R}^d} \{ \frac{1}{2n} \|w - w^{k-1}\|^2 + \langle v_k, w \rangle \},
\]
where \( v_k \) is a random vector. A popular choice for this is to set as \( v^k = \nabla f_i(w^{k-1}) \) for \( n \)-th sample uniformly at random, which is called stochastic gradient descent.

*Graduate School of Informatics and Engineering, The University of Electro-Communications, Tokyo, Japan (kasai@is.uec.ac.jp).
descent (SGD). Its update rule is $w^k \leftarrow w^{k-1} - \eta v^k$. Actually, SGD assumes an unbiased estimator of the full gradient as $E_i[\nabla f_i(w^k)] = \nabla f(w^k)$. As the update rule clearly represents, the calculation cost is independent of $n$, resulting in $O(d)$. Mini-batch SGD uses $v^k = 1/|S_k|\sum_{i \in S_k} \nabla f_i(w^{k-1})$, where $S_k$ is the set of samples of size $|S_k|$. Also, SGD needs a diminishing stepsize algorithm to guarantee the convergence, which causes a severe slow convergence rate. To accelerate this rate, we have two active research directions in machine learning; Variance reduction (VR) techniques \cite{1,2,3,4,5} explicitly or implicitly exploit a full gradient estimation to reduce the variance of noisy stochastic gradient, leading to superior convergence properties. We can regard this approach as a hybrid algorithm of GD and SGD. Another promising direction is to modify deterministic second-order algorithms into stochastic settings, and solves the potential problem of first-order algorithms for ill-conditioned problems. A direct extension of quasi-Newton (QN) is known as online BFGS \cite{6}. Its variants include regularized version (RES) \cite{7}, limited memory version (oLBFGS) \cite{6,8}, stochastic QN (SQN) \cite{9}, incremental QN \cite{10}, and non-convex version \cite{11}. Lastly, hybrid algorithms of the stochastic QN algorithm with VR are proposed \cite{12,13}. Others include \cite{14,15,16}.

The performance of stochastic optimization algorithms is strongly influenced not only by the distribution of data but also by the stepsize algorithm. Therefore, we often encounter results that are completely different from those in papers in every experiment. Consequently, an evaluation framework to test and compare the algorithms at hand is crucially important for fair and comprehensive experiments. SGDLibrary is a flexible, extensible and efficient pure-Matlab library of a collection of stochastic optimization algorithms. The purpose of the library is to provide researchers and implementers a collection of state-of-the-arts stochastic optimization algorithms that solve a variety of large-scale optimization problems. SGDLibrary provides easy access to many solvers and problem examples including, for example, linear/non-linear regression problems and classification problems. This also provides some visualization tools to show classification results and convergence behaviors. To the best of my knowledge, no report of the literature describes a comprehensive experimental environment specialized for stochastic optimization algorithms. The code is available in \url{https://github.com/hiroyuki-kasai/SGDLibrary}.

## 2 Software architecture

The software architecture of SGDLibrary follows a typical module-based architecture, which separates problem descriptor and optimization solver. To use the library, the user selects one problem descriptor of interest and no less than one optimization solvers to be compared.

**Problem descriptor:** The problem descriptor, denoted as problem, specifies the problem of interest with respect to $w$, noted as $w$ in the library. The user does nothing other than calling a problem definition function, for instance, \texttt{logistic\_regression()} for L2-norm regularized LR problem. Each problem definition includes the functions necessary for solvers; (i) (full) cost function $f(w)$, (ii) mini-batch stochastic derivative $v = 1/|S|\sum_{i \in S} \nabla f_i(w)$ for the set of samples $S$, which is denoted as \texttt{indices}. (iii) stochastic Hessian for \texttt{indices}, and (iv) stochastic Hessian-vector product for a vector $v$ and \texttt{indices}. The build-in problems include L2-norm regularized multidimensional linear regression, L2-norm regularized linear SVM, L2-norm regularized LR, L2-norm regularized softmax classification (multinomial LR), L1-norm multidimensional linear regression, and L1-norm LR. The problem descriptor provides additional specific functions that are necessary for the problem. For example, the LR problem includes the prediction and the classification accuracy calculation function.

**Optimization solver:** The optimization solver implements the main routine of the stochastic optimization algorithm. Once the optimization solver function is called with one selected problem
descriptor **problem** as the first argument, it solves the optimization problem by calling the corresponding functions via **problem**, such as the cost function and the stochastic gradient calculation function. Calling the solver function with the selected problem *mutually binds* the two of them. The supported optimization solvers in the library are listed up based on the categorized groups as; (i) **SGD methods**: Vanilla SGD \(^{[17]}\), SGD with classical momentum, SGD with classical momentum with Nesterov’s accelerated gradient \(^{[18]}\), AdaGrad \(^{[14]}\), RMSProp, AdaDelta, Adam, AdaMax (ii) **Variance reduction (VR) methods**: SVRG \(^{[1]}\), SAG \(^{[2]}\), SAGA \(^{[4]}\), SARAH \(^{[5]}\), (iii) **Second-order methods**: SQN \(^{[15]}\), oBFGS-Inf \(^{[6,8]}\), oBFGS-Lim (oLBFGS) \(^{[6,8]}\), Reg-oBFGS-Inf (RES) \(^{[7]}\), Damp-oBFGS-Inf \(^{[11]}\), (iv) **Second-order method with VR**: SVRG-LBFGS \(^{[13]}\), SS-SVRG \(^{[13]}\), SVRG-SQN \(^{[12]}\), (v) **Else**: BB-SGD \(^{[16]}\), SVRG-BB. The solver also receives optional parameters as the second argument, which forms a **struct**, designated as **options** in the library. It contains elements such as the maximum number of epochs, the batch size, and the stepsize algorithm with an initial stepsize. Finally, the solver returns to the caller the final solution \(w\) and rich statistic information, which are, for instance, the histories of the cost function value, optimality gap, and the number of gradient calculations.

**Others**: SGDLibrary accommodates a *user-defined* stepsize algorithm. This accommodation is achieved by setting as **options.stepsizefun=@my_stepsize_alg**, which is delivered to solvers. Additionally, when the regularizer \(R(w)\) in the minimization problem \(^{[1]}\) is a non-smooth regularizer such as L1-norm regularizer \(\|w\|_1\), the solver calls the *proximal operator* as **problem.prox(w,stepsize)**, which is the wrapper function defined in each problem. L1-norm regularized LR problem, for example, calls *soft-threshold* function as \(w = \text{prox}(w,\text{stepsize}) = \text{soft_thresh}(w,\text{stepsize} \cdot \lambda)\), where \(\text{stepsize}\) is the stepsize \(\eta\) and \(\lambda\) is the regularization parameter \(\lambda > 0\).

### 3 Tour of the SGDLibrary

We embark on a tour of SGDLibrary exemplifying L2-norm regularized LR problem. The LR model generates \(n\) pairs of \((x_i,y_i)\) for a (unknown) model parameter \(w\), where \(x_i\) is an input \(d\)-dimensional feature vector and \(y_i \in \{-1,1\}\) is the binary class label, as \(P(y_i|x_i,w) = \frac{1}{1+\exp(-y_i w^T x_i)}\). Then, the problem seeks the unknown parameter \(w\) that fits the regularized LR model to the generated data \((x_i,y_i)\). This problem is cast as a minimization problem as \(\min f(w) := \frac{1}{n} \sum_{i=1}^{n} \log[1 + \exp(-y_i w^T x_i)] + \frac{\lambda}{2} \|w\|^2\). The code for this particular problem is in Listing 1.

```matlab
% generate synthetic 300 samples of dimension 3 for logistic regression
d = logistic_regression_data_generator(300,3);

% define logistic regression problem
problem = logistic_regression(d.x_train,d.y_train,d.x_test,d.y_test);

% set initial value
options.w_init = d.w_init;

% set initial stepsize
options.step_init = 0.01;

% set verbose mode
options.verbose = 2;

% perform SGD solver
[w_sgd, info_sgd] = sgd(problem, options);

% perform SVRG solver
[w_svrg, info_svrg] = svrg(problem, options);

% display cost vs. number of gradient evaluations
display_graph('grad_calc_count','cost',{'SGD','SVRG'},...
    [w_sgd,w_svrg],[info_sgd,info_svrg]);
```

Listing 1: Demonstration code for logistic regression problem

First, we generate train/test datasets \(d\) using **logistic_regression_data_generator()**, where the input feature vector is with \(n = 300\) and \(d = 3\). \(y_i \in \{-1,1\}\) is its class label. The LR prob-
lem is defined properly by calling `logistic_regression()`, which internally contains the functions for cost value, the gradient and the Hessian. This is stored in `problem`. Then, we execute optimization solvers, i.e., SGD and SVRG, by calling solver functions, i.e., `sgd()` and `svrg()` with `problem` and `options` after setting some options into the `options` struct. They return the final solutions of \( \{w_{\text{sgd}}, w_{\text{svrg}}\} \) and the statistics information \( \{\text{info}_{\text{sgd}}, \text{info}_{\text{svrg}}\} \). Finally, `display_graph()` visualizes the behavior of the cost function values in terms of the number of gradient evaluations. It is noteworthy that each algorithm requires a different number of evaluations of samples in each epoch. Therefore, it is common to use this value to evaluate the algorithms instead of the number of iterations. An illustrative result is presented in Figure 1(a). Figures 1(b) and 1(c) are also generated, respectively, by the same `display_graph()` and another function `display_classification_result()` specialized for the classification problems. Consequently, SGDLibrary provides other rich visualization tools.

![Figure 1: Results of L2-norm regularized logistic regression problem.](image)
A  

Supported stochastic optimization solvers

Table 1 summarizes the supported stochastic optimization algorithms and configurations.

| Algorithm Name | Solver   | Sub_mode | Other Options | Reference |
|----------------|----------|----------|---------------|-----------|
| SGD            | sgd.m    |          |               | [17]      |
| SGD-CM         | sgd_cm.m | CM       |               |           |
| SGD-CM-NAG     | sgd_cm.m | CM-NAG   |               | [18]      |
| AdaGrad        | adagrad.m| AdaGrad  |               | [14]      |
| RMSProp        | adagrad.m| RMSProp  |               | [19]      |
| AdaDelta       | adagrad.m| AdaDelta |               | [20]      |
| Adam           | adam.m   | Adam     |               | [21]      |
| AdaMax         | adam.m   | AdaMax   |               | [21]      |
| SVRG           | svrg.m   |          |               | [1]       |
| SAG            | sag.m    | SAG      |               | [2]       |
| SAGA           | sag.m    | SAGA     |               | [4]       |
| SARAH          | sarah.m  |          |               | [5]       |
| SARAH-Plus     | sarah.m  | Plus     |               | [5]       |
| SQN            | slbfgs.m | SQN      |               | [9]       |
| oBFGS-Inf      | obfgs.m  | Inf-mem  |               | [6]       |
| oLBFGS-Lim     | obfgs.m  | Lim-mem  |               | [6]       |
| Reg-oBFGS-Inf  | obfgs.m  | Inf-mem  | delta ≠ 0     | [7]       |
| Damp-oBFGS-Inf | obfgs.m  | Inf-mem  | delta ≠ 0 & damped=true | [11]  |
| IQN            | iqn.m    |          |               | [10]      |
| SVRG-SQN       | slbfgs.m | SVRG-SQN |               | [12]      |
| SVRG-LBFGS     | slbfgs.m | SVRG-LBFGS |             | [13]      |
| SS-SVRG        | subsamp  | _svrg.m  |               | [13]      |
| BB-SGD         | bb_sgd.m |          |               | [16]      |
| SVRG-BB        | svrg_bb.m|          |               | [22]      |
B Directory and file structure

The tree structure below represents the directory and file structure of SGDLibrary.

/  
  ├── README.md                  Readme file
  │   └── run_me_first.m          First script to run
  │   └── demo.m                  Demonstration script to check library
  │   └── demo_ext.m              Demonstration script to check library
  │   └── sgdlibrary_version.m    Version and release date information
  │   └── LICENSE.txt             License file
  │   └── problem/                Problem definitions
  │       └── sgd_solver/         Stochastic optimization solvers
  │       └── sgd_test/           Test scripts to use this library
  │       └── plotter/            Tools for plotting
  │       └── tool/              Auxiliary tools
  │       └── gd_solver/          Gradient descent optimization solver files
  │       └── gd_test/            Test scripts for gradient descent solvers
C How to use SGDLibrary

C.1 First to do

Run run_me_first for path configurations.

```matlab
>> run_me_first;
#########################################################
### Welcome to SGDLibrary (version:1.0.12, released:29-Sep-2017) ###
#########################################################
```

Now, we are ready to use the library. Just execute demo for the simplest demonstration of this library. This is the case of L2-norm regularized logistic regression problem.

```matlab
>> demo;
```

The cost function values every iteration of two algorithms are shown in the Matlab command window. Additionally, the convergence plots of the cost function values are shown as in Figure 2.

C.2 Simplest usage example: 4 steps!

The code of demo.m is shown in Listing 2.

```
1 % generate synthetic 300 samples of dimension 3 for logistic regression
2 d = logistic_regression_data_generator(300,3);
3
4 % define logistic regression problem
5 problem = logistic_regression(d.x_train,d.y_train,d.x_test,d.y_test);
6
7 options.w_init = d.w_init; % set initial value
8 options.step_init = 0.01; % set initial stepsize
9 options.verbose = 2; % set verbose mode
10 [w_sgd, info_sgd] = sgd(problem, options); % perform SGD solver
11 [w_svrg, info_svrg] = svrg(problem, options); % perform SVRG solver
12
13 % display cost vs. number of gradient evaluations
14 display_graph(['grad_calc_count', 'cost', {'SGD', 'SVRG'}],...
Figure 2: Result of L2-norm regularized logistic regression problem.

Listing 2: Demonstration code for the logistic regression problem

Let us take a closer look at the code above bit by bit. The procedure has only 4 steps!

**Step 1: Generate data**
First, we generate datasets including train set and test set using a data generator function `logistic_regression_data_generator()`. The output includes train & test set and an initial value of the solution $w$.

```matlab
% generate synthetic 300 samples of dimension 3 for logistic regression
d = logistic_regression_data_generator(300,3);
```

Listing 3: Code for data generation.

**Step 2: Define problem**
The problem to be solved should be defined properly from the supported problems. `logistic_regression()` provides the comprehensive functions for a logistic regression problem. This returns the cost value by $\text{cost}(w)$, the gradient by $\text{grad}(w)$ and the hessian by $\text{hess}(w)$ when given $w$. These are essential for any gradient descent algorithms.

```matlab
% define logistic regression problem
problem = logistic_regression(d.x_train,d.y_train,d.x_test,d.y_test);
```

Listing 4: Code for problem definition.

**Step 3: Perform solver**
Now, you can perform optimization solvers, i.e., SGD and SVRG, calling solver functions, i.e., `sgd()` function and `svrg()` function, after setting some optimization options as the `options` struct.

```matlab
options.w_init = d.w_init;               % set initial value
options.step_init = 0.01;               % set initial stepsizes
options.verbose = 2;                   % set verbose mode
[w_sgd, info_sgd] = sgd(problem, options);            % perform SGD solver
[w_svrg, info_svrg] = svrg(problem, options);         % perform SVRG solver
```

Listing 5: Code for optimization solver execution.
They return the final solutions of $w$ and the statistics information that include the histories of the epoch numbers, the cost function values, norms of gradient, the number of gradient evaluations and so on.

**Step 4: Show result**

Finally, `display_graph()` provides output results of decreasing behavior of the cost values in terms of the number of gradient evaluations. Note that each algorithm needs different number of evaluations of samples in each epoch. Therefore, it is common to use this number to evaluate stochastic optimization algorithms instead of the number of iterations.

```matlab
13  % display cost vs. number of gradient evaluations
display_graph('grad_calc_count','cost',{'SGD','SVRG'},...
               {w_sgd,w_svrg},{info_sgd,info_svrg});
```

Listing 6: Code for showing results.
D  Problem definition

This specifies the problem of interest with respect to $w$, noted as $w$ in the library. The user does nothing other than calling a problem definition function.

The build-in problems in the library include

- L2-norm regularized multidimensional linear regression
- L2-norm regularized linear support vector machines (SVM)
- L2-norm regularized logistic regression (LR)
- L2-norm regularized softmax classification (multinomial LR)
- L1-norm regularized multidimensional linear regression
- L1-norm regularized logistic regression (LR)

Each problem definition contains the functions necessary for solvers;

- $\text{cost}(w)$: calculate full cost function $f(w)$,
- $\text{grad}(w,\text{indices})$: calculate mini-batch stochastic derivative $v = 1/|S| \nabla f_{i \in S}(w)$ for the set of samples $S$, which is noted as $\text{indices}$.
- $\text{hess}(w,\text{indices})$: calculate stochastic Hessian for $\text{indices}$.
- $\text{hess}_\text{vec}(w, v, \text{indices})$: calculate stochastic Hessian-vector product for $v$ and $\text{indices}$.

We illustrate the code of the definition of L2-norm regularized linear regression function as an example. Listing 7 shows its entire code of linear_regression() function.

```
function Problem = linear_regression (x_train, y_train, x_test, y_test, lambda)
    d = size(x_train, 1);
    n_train = length(y_train);
    n_test = length(y_test);

    Problem.name = @( ) 'linear_regression';
    Problem.dim = @( ) d;
    Problem.samples = @( ) n_train;
    Problem.lambda = @( ) lambda;
    Problem.hessain_w_independent = @( ) true;
    Problem.x_norm = @( ) sum(x_train.^2,1);
    Problem.x = @( ) x_train;

    % define cost function
    Problem.cost = @cost;
    function f = cost(w)
        f = sum((w'*x_train - y_train).^2)/(2*n_train) + lambda/2*w'*w;
    end

    % define stochastic gradient
    Problem.grad = @grad;
    function g = grad(w, indices)
        residual = w'*x_train(:,indices) - y_train(indices);
        g = x_train(:,indices) * residual'/length(indices) + lambda*w;
    end
```

% define full gradient
Problem.full_grad = @full_grad;
function g = full_grad(w)
g = grad(w, 1:n_train);
end

% define stochastic hessian
Problem.hess = @hess;
function h = hess(w, indices)
    h = 1/length(indices) * x_train(:,indices) * (x_train(:,indices)') + lambda * eye(d);
end

% define full hessian
Problem.full_hess = @full_hess;
function h = full_hess(w)
    h = hess(w, 1:n_train);
end

% define stochastic hessian-vector
Problem.hess_vec = @hess_vec;
function hv = hess_vec(w, v, indices)
    hv = 1/length(indices) * x_train(:,indices) * ...
        ((x_train(:,indices)'*v)) + lambda*v;
end

% define prediction function
Problem.prediction = @prediction;
function p = prediction(w)
p = w' * x_test;
end

% define mse calculation function
Problem.mse = @mse;
function e = mse(y_pred)
e = sum((y_pred-y_train).^2)/(2*n_train);
end

Listing 7: Demonstration code for linear regression problem.

We explain line-by-line of Listing 7 below; Listing 8 defines the cost calculation function cost() with respect to \( w \).

% define cost function
Problem.cost = @cost;
function f = cost(w)
f = sum((w'*x_train-y_train).^2)/(2*n_train) + lambda/(2*w'*w);
end

Listing 8: Cost function code for linear regression problem.

Listing 9 defines the stochastic gradient calculation function grad() with respect to \( w \) for indices. full_grad() calculates the full gradient estimation.

% define stochastic gradient
Problem.grad = @grad;
function g = grad(w, indices)
    residual = w'*x_train(:,indices)-y_train(indices);
end
Listing 9: Gradient calculation function code for linear regression problem.

Listing 10 defines the stochastic Hessian calculation function hess() with respect to \( w \) for \( \text{indices} \). full_hess() calculates the full Hessian estimation.

Listing 10: Hessian calculation function code for linear regression problem.

Listing 11 defines the stochastic Hessian-vector product calculation function hess_vec() with respect to \( w \) and a vector \( v \) for \( \text{indices} \).

Listing 11: Hessian-vector product calculation function code for linear regression problem.

The problem descriptor also provides some specific functions that are necessary for a particular problem. For example, the linear regression problem predicts the class for test data based on the model parameter that is trained by a stochastic optimization algorithm. Then, the final classification are calculated. Therefore, the regression problem equips the prediction and the mean squares error (MSE) calculation functions.

- prediction\((w)\)
- mse\((y_{\text{pred}})\)

Listing 12 shows the prediction function prediction from the final solution \( w \), and the MSE calculation function mse.
% define mse calculation function
Problem.mse = @mse;
function e = mse(y_pred)
    e = sum((y_pred-y_test).^2)/(2*n_test);
end

Listing 12: Prediction and MSE calculation code for linear regression problem.

Meanwhile, in case of the logistic regression problem, the final classification are calculated. Therefore, the regression problem equips the prediction and the prediction accuracy calculation functions.

- prediction(w)

- accuracy(y_pred)

Listing 13 illustrates the binary-class prediction function prediction with the final solution w, and prediction accuracy calculation function accuracy with the predicted classes.

% define prediction function
Problem.prediction = @prediction;
function p = prediction(w)
    p = sigmoid(w' * x_test);
    class1_idx = p>0.5;
    class2_idx = p<=0.5;
    p(class1_idx) = 1;
    p(class2_idx) = -1;
end

% define prediction accuracy calculation function
Problem.accuracy = @accuracy;
function a = accuracy(y_pred)
    a = sum(y_pred == y_test)/n_test;
end

Listing 13: Prediction and prediction accuracy calculation code for logistic regression problem.

The last example is the softmax regression problem case. This case also contains the prediction function prediction and the prediction accuracy calculation function accuracy as shown in Listing 14.

% define prediction function
Problem.prediction = @prediction;
function max_class = prediction(w)
    w_mat = reshape(w, [d n_classes]);
    p = w_mat' * x_test;
    [~, max_class] = max(p, [], 1);
end

% define prediction accuracy calculation function
Problem.accuracy = @accuracy;
function a = accuracy(class_pred)
    [~, class_test] = max(y_test, [], 1);
    a = sum(class_pred == class_test) / n_test;
end

Listing 14: Prediction and prediction accuracy calculation code for softmax regression problem.
E  Solver definition

This implements the main routine of the stochastic optimization solver. The optimization solver solves an optimization problem by calling the corresponding functions via the problem definition, such as \( \text{cost}(w) \), \( \text{grad}(w,\text{indices}) \), and possibly \( \text{hess}(w,\text{indices}) \). The final optimal solution \( w \) and the statistic information are returned. The latter is stored as the info struct. See also Appendix [H].

This section illustrates the definition of the SGD function \( \text{sgd}() \) as an example. The entire code of \( \text{sgd}() \) is shown in Listing 15.

Listing 15: Demonstration code for SGD solver.

```plaintext
function \([w, \text{infos}] = \text{sgd}(\text{problem}, \text{in_options})\)
    n = \text{problem}.samples(); \quad % \text{number of samples}

    % set options
    local_options = [];
    options = \text{mergeOptions}(\text{get_default_options}(\text{problem}.dim()), local_options);
    options = \text{mergeOptions}(options, in_options);

    % initialize
    iter = 0; epoch = 0; grad_calc_count = 0;
    w = options.w_init;
    num_of_bachces = \text{floor}(n/\text{options}.batch_size);

    % store first statistics infos
    \text{infos} = \text{store Infos}(\text{problem}, w, options, [], epoch, grad_calc_count, 0);

    % outer loop
    \text{s_time} = \text{tic}();
    \text{while} (\text{optgap} > \text{options}.tol_optgap) \&\& (\text{epoch} < \text{options}.max_epoch)
        perm_idx = \text{randperm}(n); \quad % permute samples

        % inner loop
        for \( j = 1 : \text{num_of_bachces} \)
            step = options.stepsizefun(iter, options); \quad % step-size

            s_index = \((j-1)\times\text{options}.batch_size+1\);
            indice_j = perm_idx(s_index : s_index + \text{options}.batch_size - 1);

            grad = \text{problem}.grad(w, indice_j); \quad % calculate gradient

            w = w - step * grad; \quad % update w

            \text{if isfield(\text{problem},'prox')} \quad % proximal operator
                w = \text{problem}.prox(w, step);
            \text{end}

            iter = iter + 1;
        \text{end}

        grad_calc_count = grad_calc_count + \text{num_of_bachces} \times \text{options}.batch_size;
        epoch = epoch + 1;

        % store statistics infos
        \text{infos} = \text{store Infos}(\text{problem}, w, options, \text{infos}, epoch, ...
            grad_calc_count, \text{toc}(\text{s_time}));
    \text{end}
end
```
We explain line-by-line of Listing 15 below.

We first set option parameters as a `options` struct. The solver merges the local default options `local_options`, the default options `get_default_options()` that are commonly used in all solvers, and the input options `in_options`. This is shown in Listing 16.

```matlab
% set options
local_options=[];
options=mergeOptions(get_default_options(problem.dim()),local_options);
options=mergeOptions(options,in_options);
```

Listing 16: Optional parameter configuration code for SGD solver.

Next, the initial statistics data are collected by `store_infos` function as shown in Listing 17 before entering the main optimization routine. The statistics data are also collected at the end of every epoch, i.e., outer iteration, as Listing 18. See also Appendix H.

```matlab
% store first statistics infos
infos=store_infos(problem,w,options,[],epoch,grad_calc_count,0);

% store statistics infos
infos=store_infos(problem,w,options,infos,epoch,...
grad_calc_count,toc(s_time));
```

Listing 17: Initial statistics data collection code for SGD solver.

The code in Listing 19 shows the calculation of the stepsize. If the user does not specify his/her user-defined stepsize algorithm, the solver calls a default stepsize algorithm function with `options` parameter. This parameter contains the stepsize algorithm type, the initial stepsize and so on. Otherwise, the user-defined stepsize algorithm is called. See also Appendix G.

```matlab
step=options.stepsizefun(iter,options); % step-size
```

Listing 19: Stepsize calculation code for SGD solver.

Listing 20 illustrates the code for the stochastic gradient calculation, where `indice_j` is calculated from the number of the inner iteration, `j`, and the batch size `options.batch_size`.

```matlab
s_index=(j-1)*options.batch_size+1;
indice_j=perm_idx(s_index:s_index+options.batch_size-1);
grad=problem.grad(w, indice_j); % calculate gradient
```

Listing 20: Stochastic gradient calculation code for SGD solver.

Finally, the model parameter `w` is updated using the calculated stepsize `step` and the stochastic gradient `grad` as Listing 21.

```matlab
w=w-step*grad; % update w
```

Listing 21: Mode parameter update code for SGD solver.
F Default stepsize algorithms

SGDLibrary supports four stepsize algorithms. This can be switched by the setting option struct such as `options.step_alg='decay-2'`. After $\eta_0$ (= `options.step_init` and $\lambda$ (= `options.lambda`) are properly configured, we can use one of the following algorithms according to the total inner iteration number $k$ as;

- **fix**: This case uses below;
  \[ \eta = \eta_0. \]

- **decay**: This case uses below;
  \[ \eta = \frac{\eta_0}{1 + \eta_0 \lambda k}. \]

- **decay-2**: This case uses below;
  \[ \eta = \frac{\eta_0}{1 + k}. \]

- **decay-3**: This case uses below;
  \[ \eta = \frac{\eta_0}{\lambda + k}. \]

SGDLibrary also accommodates a user-defined stepsize algorithm. See the next section.
SGDLibrary allows the user to define a new user-defined stepsize algorithm. This is done by setting as `options.stepsizefun = @my_stepsize_alg`, which is delivered to solvers via their input arguments. The illustrative example code is shown in Listing 22.

```matlab
function stepsize_alg_demo()
    % generate synthetic 1000 samples of dimension 10
    d = logistic_regression_data_generator(1000,10);

    % define logistic regression problem
    problem = logistic_regression(d.x_train, d.y_train, d.x_test, d.y_test);

    % define user-defined stepsize algorithm
    function step = my_stepalg(iter,options)
        step = options.step_init/(10+iter*0.5);
    end

    options.w_init = d.w_init; % set initial value
    options.step_init = 0.01; % set initial stepsize
    options.step_alg = 'decay'; % set decay stepsize algorithm
    [w_sgd,info_sgd] = sgd(problem, options); % perform SGD solver
    options.stepsizefun = @my_stepalg; % set my_stepalg stepsize algorithm
    [w_sgd_my,info_sgd_my] = sgd(problem, options); % perform SGD solver

    % display cost/optimality gap vs number of gradient evaluations
    display_graph('grad_calc_count','cost',{'SGD (decay)','SGD (My algorithm)'},{w_sgd,w_sgd_my},{info_sgd,info_sgd_my});
end
```

Listing 22: Demonstration code for user-define stepsize algorithm.

Listing 23 defines an example of the user-defined stepsize algorithm named as `my_stepalg`.

```matlab
% define user-defined stepsize algorithm
function step = my_stepalg(iter,options)
    step = options.step_init/(10+iter*0.5);
end
```

Listing 23: Definition code of user-define stepsize algorithm.

Then, the new algorithm function `my_stepalg` is set to the algorithm via `options` value for each solver as shown in Listing 24.

```matlab
options.stepsizefun = @my_stepalg; % set my_stepalg stepsize algorithm
```

Listing 24: Setting code of user-define stepsize algorithm.
H Collect statistics information

The solver automatically collects statistics information every epoch, i.e., outer iteration, via `store_infos()` function. The collected data are stored in `infos` struct, and it is returned to the caller function to visualize the results. The information contain below.

- **iter**: number of iterations
- **time**: elapsed time
- **grad_calc_count**: count of gradient calculations
- **optgap**: optimality gap
- **cost**: cost function value
- **gnorm**: norm of full gradient

Additionally, when a regularizer exists, its value is collected. This provides informative information, for example, the sparsity when $R(w) = \|w\|_1$. Furthermore, the user can collect the history of solution $w$ in every epoch.

The code of `store_infos()` is illustrated in Listing 25.

```matlab
function [infos,f_val,optgap] = store_infos(problem,w,options,infos,...
    epoch,grad_calc_count,elapsed_time)

    % calculation of cost function value
    f_val = problem.cost(w);
    % calculation of norm of full gradient
    gnorm = norm(problem.full_grad(w));
    % calculation of optimality gap
    optgap = f_val - options.f_opt;

    % number of iterations
    infos.iter = [infos.iter epoch];
    % elapsed time
    infos.time = [infos.time elapsed_time];
    % count of gradient calculations
    infos.grad_calc_count = [infos.grad_calc_count grad_calc_count];
    % optimality gap
    infos.optgap = [infos.optgap optgap];
    % cost function value
    infos.cost = [infos.cost f_val];
    % norm of full gradient
    infos.gnorm = [infos.gnorm gnorm];
    % value of regularizer
    if isfield(problem, 'reg')
        reg = problem.reg(w);
        infos.reg = [infos.reg reg];
    end

    % solution w
    if options.store_w
        infos.w = [infos.w w];
    end
end
```

Listing 25: Statistic information collection code.
I Visualizations

SGDLibrary provides various visualization tools, which include

- **display_graph()**: display various graphs such as cost function values vs. the number of gradient evaluations, and the optimality gap vs. the number of gradient evaluations.
- **display_regression_result()**: show regression results for regression problems.
- **display_classification_result()**: show classification results specialized for classification problems.
- **draw_convergence_animation()**: draw convergence behavior animation of solutions.

This section provides illustrative explanations in case of L2-norm regularized logistic regression problem. The entire code is shown in Listing 26.

```matlab
% generate synthetic 300 samples of dimension 2 for logistic regression
d=logistic_regression_data_generator(300,2);

% define problem definitions
problem=logistic_regression(d.x_train,d.y_train,d.x_test,d.y_test);

w_opt=problem.calc_solution(problem,1000); % calculate optimal w
options.f_opt=problem.cost(w_opt); % calculate optimal f
options.store_w=true; % store w for convergence animation
options.w_init=d.w_init; % set initial value
options.step_init=0.01; % set initial stepsize
[w_sgd,info_sgd]=gd(problem,options); % perform SGD solver
[w_svrg,info_svrg]=svrg(problem,options); % perform SVRG solver

% display cost/optimality gap vs number of gradient evaluations
display_graph('grad_calc_count','cost',{'SGD','SVRG'},...
{w_sgd,w_svrg},{info_sgd,info_svrg});
display_graph('grad_calc_count','optimality_gap',{'SGD','SVRG'},...
{w_sgd,w_svrg},{info_sgd,info_svrg});

% display classification results
y_pred_sgd=problem.prediction(w_sgd); % predict for SGD
accuracy_sgd=problem.accuracy(y_pred_sgd); % calculate accuracy for SGD
fprintf('Classification accuracy: SGD: %.4f
','SGD',accuracy_sgd);
y_pred_sgd(y_pred_sgd==-1)=2; % convert from {1,-1} to {1,2}
y_pred_sgd(y_pred_sgd==1)=1;
y_pred_svrg = problem.prediction(w_svrg); % predict for SVRG
accuracy_svrg=problem.accuracy(y_pred_svrg); % calculate accuracy for SVRG
fprintf('Classification accuracy: SVRG: %.4f
','SVRG',accuracy_svrg);
y_pred_svrg(y_pred_svrg==-1)=2; % convert from {1,-1} to {1,2}
y_pred_svrg(y_pred_svrg==1)=1;
d.y_train(d.y_train==-1)=2; d.y_train(d.y_train==1)=1;
d.y_test(d.y_test==-1)=2; d.y_test(d.y_test==1)=1;
display_classification_result(problem,{'SGD','SVRG'},
{y_pred_sgd,y_pred_svrg},{w_sgd,w_svrg},...
{accuracy_sgd,accuracy_svrg},...
d.x_train,d.y_train,d.x_test,d.y_test);

draw_convergence_animation(problem,{'SGD','SVRG'},...
{info_sgd.w,info_svrg.w},100,0.1);
```
Listing 26: Demonstration code for result visualization.

First, for the calculation of \textit{optimality gap}, the user needs the optimal solution \(w_{opt}\) beforehand. This is obtained by calling \texttt{problem.calc_solution()} function of the problem definition function. This case uses the L-BFGS solver inside it to obtain the optimal solution under maximum iteration 1000 with a very precise tolerant stopping condition. Then, the optimal cost function value \(f_{opt}\) is calculated from \(w_{opt}\). Listing 27 shows the code.

```matlab
w_opt = problem.calc_solution(problem, 1000); % calculate optimal w
options.f_opt = problem.cost(w_opt); % calculate optimal f
```

Listing 27: Optimal solution and cost function value calculation code.

Then, you obtain the result of the optimality gap by \texttt{display_graph()} as Listing 28. The first argument and the second argument correspond to the values of \(x\)-axis and \(y\)-axis, respectively, in the graph. We can change these values according to the statistics data explained in Appendix H. The third argument represents the list of the algorithm names that are shown in the legend of the graph. The forth parameter indicates the list of the \texttt{info} structs to be shown.

```matlab
% display cost/optimality gap vs number of gradient evaluations
display_graph('grad_calc_count', 'cost', {'SGD', 'SVRG'}, ...
{w_sgd, w_svrg}, {info_sgd, info_svrg});
display_graph('grad_calc_count', 'optimality_gap', {'SGD', 'SVRG'}, ...
{w_sgd, w_svrg}, {info_sgd, info_svrg});
```

Listing 28: Display graph code.

Additionally, in case of L2-norm regularized logistic regression problems, the results of classification accuracy are calculated using the corresponding prediction function \texttt{probrem.prediction()} and the accuracy calculating function \texttt{probrem.accuracy()}. Then, the classification accuracies are illustrated by \texttt{display_classification_result()} function. The code is shown as Listing 29.

```matlab
y_pred_sgd = problem.prediction(w_sgd); % predict for SGD
accuracy_sgd = problem.accuracy(y_pred_sgd); % calculate accuracy for SGD
fprintf('Classification accuracy:%s:%.4f\n','SGD', accuracy_sgd);
y_pred_sgd(y_pred_sgd==-1)=2; % convert from \{-1,1\} to \{1,2\}
y_pred_sgd(y_pred_sgd==1)=1;
y_pred_svrg = problem.prediction(w_svrg); % predict for SVRG
accuracy_svrg = problem.accuracy(y_pred_svrg); % calculate accuracy for SVRG
fprintf('Classification accuracy:%s:%.4f\n','SVRG', accuracy_svrg);
y_pred_svrg(y_pred_svrg==-1)=2; % convert from \{-1,1\} to \{1,2\}
y_pred_svrg(y_pred_svrg==1)=1;
d.y_train(d.y_train==1)=1;
d.y_test(d.y_test==1)=1;
display_classification_result(problem, {'SGD', 'SVRG'}, {w_sgd, w_svrg}, ...
{y_pred_sgd, y_pred_svrg}, {accuracy_sgd, accuracy_svrg}, ...
d.x_train, d.y_train, d.x_test, d.y_test);
```

Listing 29: Display classification results code.

Finally, you can also show a demonstration of \textit{convergence animation}. You need specify additional options before executing solvers as Listing 30.

```matlab
options.store_w = true; % store w for convergence animation
```

Listing 30: Store history of solutions.
Now, the animation of the convergence behavior is shown. The code is shown in Listing 31. It should be noted that `draw_convergence_animation()` is executable when only the dimension $d$ of the parameters is 2. The last parameter for the function, i.e., 0.1 in this example, indicates the speed of the animation.

```matlab
% display convergence animation
draw_convergence_animation(problem, {'SGD', 'SVRG'},
{info_sgd.w, info_svrg.w}, 100, 0.1);
```

Listing 31: Draw convergence animation.

![Convergence Animation](image)

Figure 3: Logistic regression problem.

![Convergence Animation](image)

Figure 4: convergence animation.
J  More results

We show more results for L2-norm regularized linear regression problem, L2-norm softmax classifier problem, and L2-norm regularized linear SVM problem in Figures 5 to 7, respectively.

Figure 5: Linear regression problem.

Figure 6: Softmax classifier problem.
Figure 7: Linear SVM problem.
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