Stochastic Gradient Descent

Log-logistic dose-response curve

Lucas Støjko Andersen

University of Copenhagen

November 3, 2022

Stochastic Gradient Descent

Online learning

Assume $L(X, \theta)$ is a loss function we then minimize the expected loss

$$H(\theta) = E(L(X, \theta)). \tag{1}$$

If differentiation and expectation can interchange then

$$\nabla H(\theta) = E(\nabla L(X, \theta)) \tag{2}$$

and if $X_1, X_2, \ldots$ are i.i.d. then $\nabla L(X_i, \theta)$ is an unbiased estimator of $E(\nabla L(X, \theta))$. We then perform gradient descent using sampled $L(X_i, \theta)$:

$$\theta_{n+1} = \theta_n - \gamma_n \nabla L(X_{n+1}, \theta_n). \tag{3}$$

where $\gamma_n > 0$ is a learning rate.

Stochastic Gradient Descent

Batch learning

We replace H with

$$H_N(\theta) = \frac{1}{N} \sum_{i=1}^{N} L(X_i, \theta) \tag{4}$$

and minimize H_N instead. We sample from the empirical distribution of the observations and use the online learning approach.

Implementation of Stochastic Gradient Descent

```
SGD_1 <- function(par0,
                  loss_gr,
                  N,
                  gamma0 = 1,
                  maxit = 15,
                  loss = NULL,
                  cb = NULL) {
  if(is.numeric(gamma0)) {
    if(length(gamma0) == 1) {
      gamma <- rep(gamma0, maxit)
    } else {
      gamma <- c(gamma0, rep(gamma0[length(gamma0)], maxit - length(gamma0)))
    }
  } else if (is.function(gamma0)) {
    gamma <- gamma0(1:maxit)
  } else {
    stop("gamma0 must be a numeric or a function.")
  }
  par <- par0
  for(i in 1:maxit) {
    index <- sample(N)
    for(j in 1:N) {
      gr <- loss_gr(par, index[j])
      par <- par - gamma[i] * gr
    }
    if(!is.null(cb)) cb()
    par0 <- par
  }
  par
}
```

Log-logistic dose-response curve

For $\alpha, \beta, \gamma, \rho \in \mathbb{R}$ consider

$$f(x \mid \alpha, \beta, \gamma, \rho) = \gamma + \frac{\rho - \gamma}{1 + e^{\beta \log(x) - \alpha}}. \tag{5}$$

Let $Y_i = f(X_i \mid \alpha, \beta, \gamma, \rho) + \varepsilon_i$ with $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ independent.

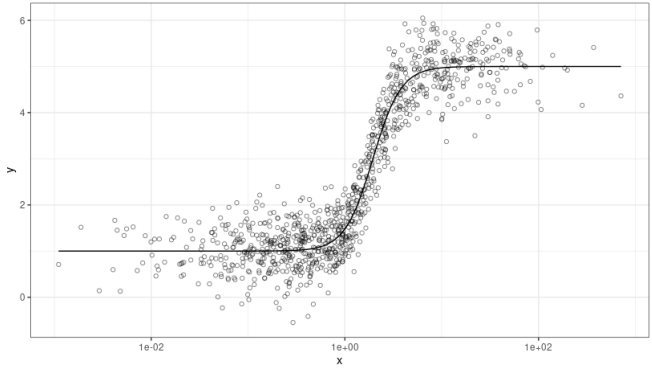
We generate $\log X_i$ from $\mathcal{N}(0, \omega^2)$ and generate Y_i by the above. We aim to minimize the empirical loss

$$\frac{1}{N} \sum_{i=1}^{N} (Y_i - f(X_i \mid \alpha, \beta, \gamma, \rho))^2. \tag{6}$$

Log-logistc dose-response curve

Plot of generated data

With $\omega = 2$, $\sigma = 0.5$, $\alpha = 2$, $\beta = 3$, $\gamma = 5$ and $\rho = 1$ we plot the generated data for 1.000 observations.



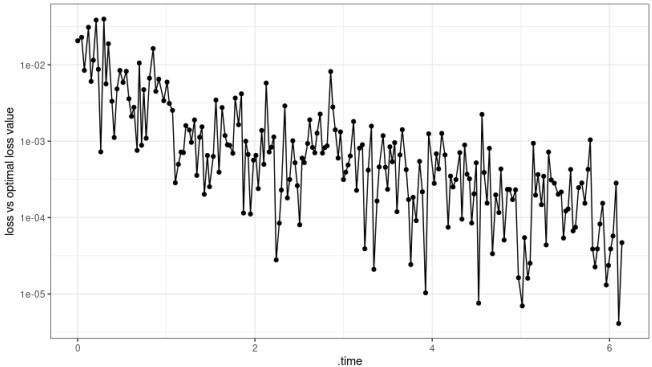
Result of Stochastic Gradient Descent

```
opt_value <- optim(c(2, 3, 5, 1), log_loss(X, Y))$value
SGD_tracer <- tracer("par")
SGD_1(c(-1, 6, 3, 3),
        log_gradient(X, Y),
        N = length(X),
        gamma0 = decay_scheduler(gamma0 = 0.5, gamma1 = 0.01, n1 = 200),
        maxit = 200,
        loss = log_loss(X, Y),
        cb = SGD_tracer$tracer)
```

$$\theta_{\mathsf{SGD}} = (1.815715, 2.797085, 5.006571, 0.959967)$$
$$\theta_{\mathsf{optim}} = (1.820240, 2.789082, 5.001176, 0.965572)$$

Result of Stochastic Gradient Descent

Plot of loss value of optim vs SGD



Abstracting the Implementation of SGD

```
SGD <- function(par0,
                loss_gr,
                N,
                batch,
                epoch,
                gamma0 = 1,
                maxit = 15,
                loss,
                cb = NULL) {
  if(is.numeric(gamma0)) {
    if(length(gamma0) == 1) {
      gamma <- rep(gamma0, maxit)
    } else {
      gamma <- c(gamma0, rep(gamma0[length(gamma0)], maxit - length(gamma0)))
    }
  } else if (is.function(gamma0)) {
    gamma <- gamma0(1:maxit)
  } else {
    stop("gamma0 must be a numeric or a function.")
  }
  for(i in 1:maxit) {
    index <- batch(N)
    par <- epoch(par0, index, loss_gr, gamma[i])
    if(!is.null(cb)) cb()
    par0 <- par
  }
  par
}
```

Batch Implementation

```
batch_random <- function(batch_size = NULL, replace = FALSE) {
  if(!is.null(batch_size)) batch_size <- as.integer(batch_size)
  function(N) {
    if(is.null(batch_size)) batch_size <<- N
    if(batch_size <= N) return(sample(N, batch_size, replace = replace))
    sample(N, batch_size, replace = TRUE)
  }
}
```

Another Batch Implementation

```
batch_random_chunk <- function(size,
                               chunks = 1L,
                               replace = FALSE,
                               shuffle = FALSE) {
  shuffle_index <- NULL
  force(shuffle)
  function(N) {
    if(shuffle & is.null(shuffle_index)) rand_indicies <- sample(N)
    max_chunk <- max(1, floor(N / size) - 1)
    if(is.infinite(chunks)) chunks <- max_chunk
    if(chunks <= max_chunk) {
      chunk_id <- sample(1:max_chunk, replace = replace)
    } else {
      chunk_id <- sample(1:max_chunk, chunks, replace = TRUE)
    }
    index <- numeric(chunks * size)
    if(is.null(shuffle_index)) {
        for(i in seq_along(chunk_id)) {
          index[((i - 1) * size + 1):(i * size)] <-
          ((chunk_id[i] - 1) * size + 1):(chunk_id[i] * size)
        }
    } else {
        for(i in seq_along(chunk_id)) {
          index[((i - 1) * size + 1):(i * size)] <-
            shuffle_index[((chunk_id[i] - 1) * size + 1):(chunk_id[i] * size)]
        }
    }
    index
  }
}
```

Epoch Implementation

```
epoch_batch <- function(mini_batch_size = 1) {
  function(par0, index, loss_gr, gamma) {
    mini_batch_size <- min(length(index), mini_batch_size)
    M <- floor(length(index) / mini_batch_size)
    par <- par0
    for(i in 1:M) {
      mini_batch_index <- ((i - 1) * mini_batch_size + 1):(i * mini_batch_size)
      gr <- loss_gr(par, index[mini_batch_index])
      par <- par - gamma * gr
    }
    par
  }
}

epoch_full <- function() {
  function(par0, index, loss_gr, gamma) {
    for(i in 1:length(index)) {
      gr <- loss_gr(par0, index[i])
      par0 <- par0 - gamma * gr
    }
    par0
  }
}
```

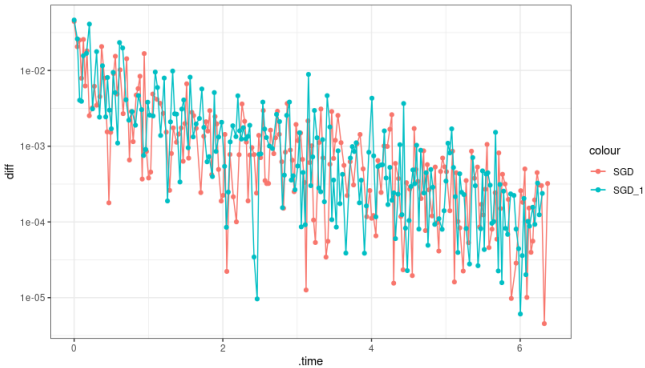
Testing Against the First Implementation

```
SGD_tracer2 <- tracer("par")
SGD(par0 = c(-1, 6, 3, 3),
    loss_gr = log_gradient(X, Y),
    N = length(X),
    batch = batch_random(),
    epoch = epoch_full(),
    gamma0 = decay_scheduler(gamma0 = 1, gamma1 = 0.2, n1 = 200),
    loss = log_loss(X, Y),
    maxit = 200,
    cb = SGD_tracer2$tracer)
```

The abstract implementation yields

$$\theta_{\mathsf{SGD}} = (1.8175899, 2.7902753, 4.9934073, 0.9892618). \tag{7}$$

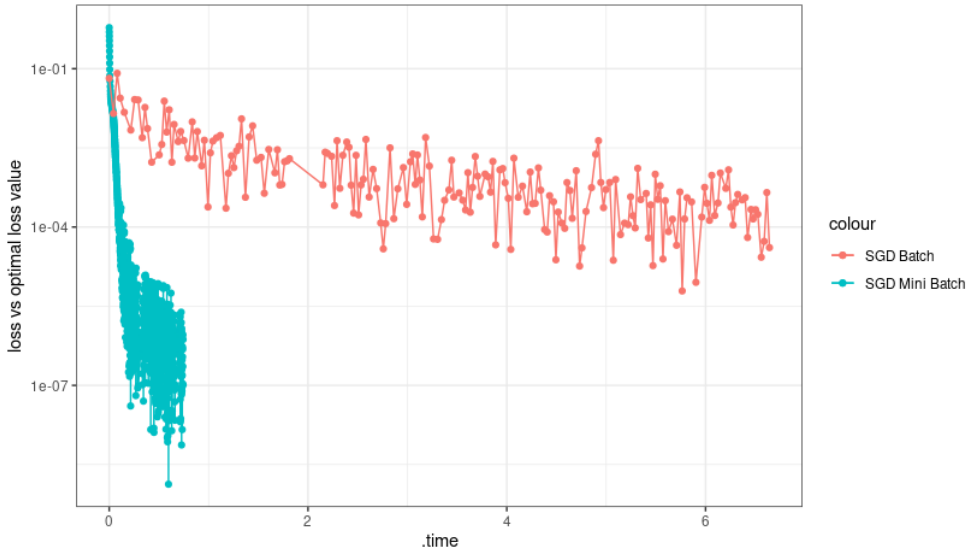
Testing Against the First Implementation



Mini Batch vs Batch

```
SGD_tracer3 <- tracer("par")
SGD(par0 = c(-1, 6, 3, 3),
    loss_gr = log_gradient(X, Y),
    N = length(X),
    batch = batch_random(),
    epoch = epoch_batch(100),
    gamma0 = decay_scheduler(gamma0 = 1, gamma1 = 0.1, n1 = 1000),
    maxit = 1000,
    loss = log_loss(X, Y),
    cb = SGD_tracer3$tracer)
```

Mini Batch vs Batch



Comparison to Gradient Descent Algorithm

```
GD <- function(par0,
               loss,
               loss_gr,
               d = 0.8,
               c = 0.1,
               gamma0 = 1,
               maxit = 500,
               stop_criteria = NULL,
               backtrack = TRUE,
               cb = NULL) {
  for(i in 1:maxit) {
    if(backtrack) value <- loss(par0)
    grad <- loss_gr(par0)
    h_prime <- sum(grad^2)
    gamma <- gamma0
    par <- par0 - gamma * grad
    if(backtrack) {
      while(loss(par) > value - c * gamma * h_prime) {
        gamma <- d * gamma
        par <- par0 - gamma * grad
      }
    }
    if(!is.null(cb)) cb()
    if(!is.null(stop_criteria)) {
      if(stop_criteria(par, par0, loss_gr, loss)) break
    }
    par0 <- par
  }
  if(i == maxit)
    warning("Maximal number, ", maxit, ", of iterations reached")
  par
}
```

Stopping criteria

```
stop_parm <- function(epsilon, k) {
  force(epsilon)
  force(k)
  n <- 0
  function(par0, par, loss_gr, loss) {
    if(norm(par0 - par, "2") <
       epsilon * (norm(par0, "2") + epsilon)) {
      n <<- n + 1
    } else {
      n <<- 0
    }
    n == k
  }
}
```

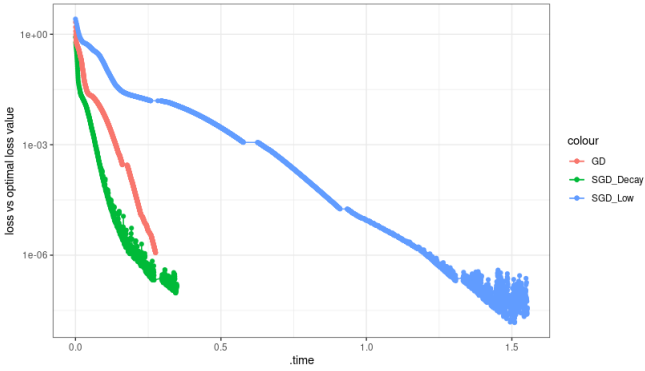
SGD vs. GD

```
GD_tracer <- tracer("par", N = 0)
GD(par0 = c(-1, 6, 3, 3),
   loss = log_loss(X, Y),
   loss_gr = log_gradient(X, Y),
   gamma0 = 1,
   maxit = 100000,
   stop_criteria = stop_parm(1e-5, 3),
   backtrack = FALSE,
   cb = GD_tracer$tracer)
```

SGD vs. GD

```
SGD_tracer4 <- tracer("par", N = 0)
SGD(par0 = c(-1, 6, 3, 3),
    loss_gr = log_gradient(X, Y),
    N = length(X),
    batch = batch_random(),
    epoch = epoch_batch(200),
    gamma0 = decay_scheduler(gamma0 = 1, gamma1 = 0.05, a = 2, n1 = 1000),
    maxit = 100000,
    stop_criteria = stop_parm(1e-5, 3),
    cb = SGD_tracer4$tracer)

SGD_tracer5 <- tracer("par", N = 0)
SGD(par0 = c(-1, 6, 3, 3),
    loss_gr = log_gradient(X, Y),
    N = length(X),
    batch = batch_random(),
    epoch = epoch_batch(200),
    gamma0 = 0.1,
    maxit = 100000,
    stop_criteria = stop_parm(1e-5, 3),
    cb = SGD_tracer5$tracer)
```

SGD vs. GD


1e+00
1e-03
1e-06
loss vs optimal loss value
0.0
0.5
1.0
1.5
.time
colour
GD
SGD_Decay
SGD_Low

SGD vs. GD

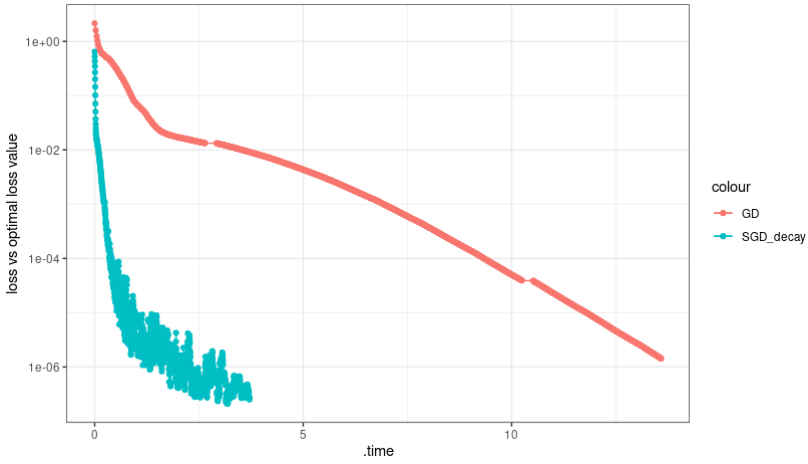
Large Sample Size

Generate 100.000 samples.

```
GD_tracer2 <- tracer("par", N = 0)
GD(par0 = c(-1, 6, 3, 3),
   loss = log_loss(X_big, Y_big),
   loss_gr = log_gradient(X_big, Y_big),
   gamma0 = 1,
   maxit = 10000,
   stop_criteria = stop_parm(1e-5, 3),
   backtrack = FALSE,
   cb = GD_tracer2$tracer)

SGD_tracer5 <- tracer("par", N = 0)
SGD(par0 = c(-1, 6, 3, 3),
    loss_gr = log_gradient(X_big, Y_big),
    N = length(X_big),
    batch = batch_random(10000, replace = TRUE),
    epoch = epoch_batch(1000),
    gamma0 = decay_scheduler(gamma0 = 1, gamma1 = 0.01, a = 2, n1 = 1000),
    stop_criteria = stop_parm(1e-5, 3),
    maxit = 10000,
    cb = SGD_tracer5$tracer)
```

SGD vs. GD

Large Sample Size

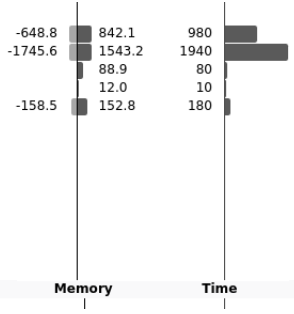


Profiling SGD Implementation Using `profvis` Package

```
  for(i in 1:maxit) {
    index <- batch(N)
    par <- epoch(par0, index, loss_gr, gamma[i])
    if(!is.null(cb)) cb()
    if(!is.null(stop_criteria)) {
      if(stop_criteria(par, par0, loss_gr, loss)) break
    }
    par0 <- par
  }
  if(!is.null(stop_criteria) & maxit == i) {
    warning("Maximum number of iterations ", i, " reached.")
  }
  par
}
```

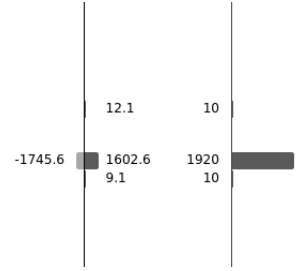
.R

log_loss <- function(x, y) {



Profiling SGD Implementation Using `profvis` Package

```
epoch_batch <- function(mini_batch_size = 1) {
  function(par0, index, loss_gr, gamma) {
    mini_batch_size <- min(length(index), mini_batch_size)
    M <- floor(length(index) / mini_batch_size)
    par <- par0
    for(i in 1:M) {
      mini_batch_index <- ((i - 1) * mini_batch_size + 1):(i *
mini_batch_size)
      gr <- loss_gr(par, index[mini_batch_index])
      par <- par - gamma * gr
    }
    par
  }
}
```



Implementation of Gradient Using Rcpp

```
#include <Rcpp.h>

using namespace Rcpp;

// [[Rcpp::export]]
NumericVector gradient_rcpp(NumericVector par,
                            NumericVector x,
                            NumericVector y) {
  int N = x.size();
  NumericVector gr(4);
  for(int i = 0; i < N; ++i) {
    double elogx, da, db, dg, dr, yf, logx;
    logx = std::log(x[i]);
    elogx = std::exp(par[1] * logx - par[0]);
    dr = 1 / (1 + elogx);
    dg = 1 - dr;
    da = elogx * (par[3] - par[2]) * dr * dr;
    db = -da * logx;
    yf = y[i] - par[2] - (par[3] - par[2]) * dr;
    gr[0] -= da * yf / 2;
    gr[1] -= db * yf / 2;
    gr[2] -= dg * yf / 2;
    gr[3] -= dr * yf / 2;
  }
  return gr / N;
}
```

Implementation of Mini Batch Epoch Using Rcpp Package

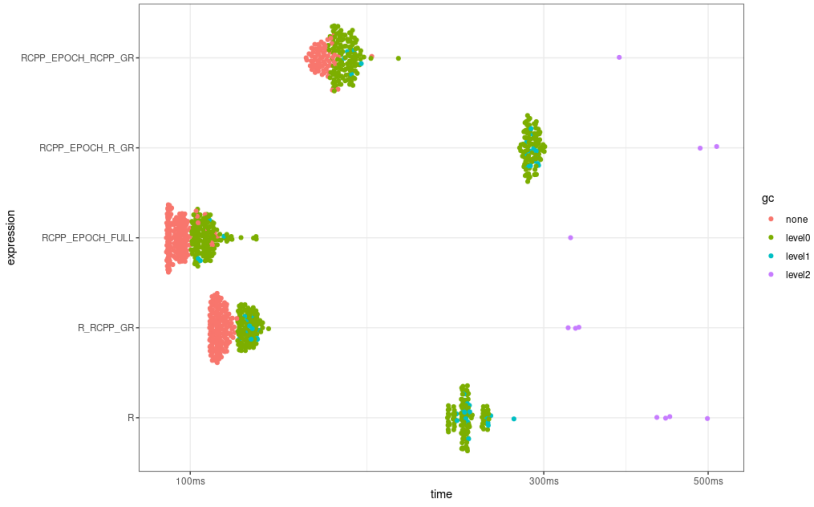
```
// [[Rcpp::export]]
NumericVector epoch_rcpp(NumericVector par0,
                         NumericVector x,
                         NumericVector y,
                         int minisize,
                         double gamma) {
  int n, MAX;
  Range r(0, minisize - 1);

  n = x.size();
  MAX = std::floor(n / minisize);
  NumericVector par = clone(par0);

  for(int i = 0; i < MAX; ++i, r += minisize) {
     par = par - gamma * gradient_rcpp(par, x[r], y[r]);
  }

  return par;
}
```

Implementation of Mini Batch Epoch Using Rcpp Package

Calling Gradient from R

```
// [[Rcpp::export]]
NumericVector epoch_rcpp_partial(NumericVector par0,
                                 NumericVector index,
                                 Function gr,
                                 int minisize,
                                 double gamma) {

  int n = index.size();
  int MAX = std::floor(n / minisize);
  NumericVector par = clone(par0);

  Range r(0, minisize - 1);

  for(int i = 0; i < MAX; ++i, r += minisize) {
    NumericVector gr_tmp = gr(par, index[r]);
    par = par - gamma * gr_tmp;
  }

  return par;
}
```

Benchmark Using bench Package



Epoch Implementation Using R's C API

```
SEXP epoch_batch(SEXP par0, SEXP index, SEXP loss_gr, SEXP gamma, SEXP mbs, SEXP rho) {
  int mbs2, M, n;
  n = length(par0);
  if(INTEGER(mbs)[0] > length(index)) {
    mbs2 = length(index);
  } else {
    mbs2 = INTEGER(mbs)[0];
  }
  M = floor(length(index) / mbs2);
  SEXP gr_call = PROTECT(lang3(loss_gr, R_NilValue, R_NilValue));
  SEXP par = PROTECT(allocVector(REALSXP, n));
  SEXP m_index = PROTECT(allocVector(INTSXP, mbs2));
  int *iptr = INTEGER(index);
  int *miptr = INTEGER(m_index);
  for(int i = 0; i < n; ++i)
    REAL(par)[i] = REAL(par0)[i];
  for(int i = 0; i < M; ++i) {
    for(int j = 0; j < mbs2; ++j)
      miptr[j] = iptr[i * mbs2 + j];
    SETCADR(gr_call, par);
    SETCADDR(gr_call, m_index);
    SEXP gr = eval(gr_call, rho);
    for(int k = 0; k < n; ++k)
      REAL(par)[k] = REAL(par)[k] - REAL(gamma)[0] * REAL(gr)[k];
  }
  UNPROTECT(3);
  return par;
}
```

SGD Implementation Using R's C API

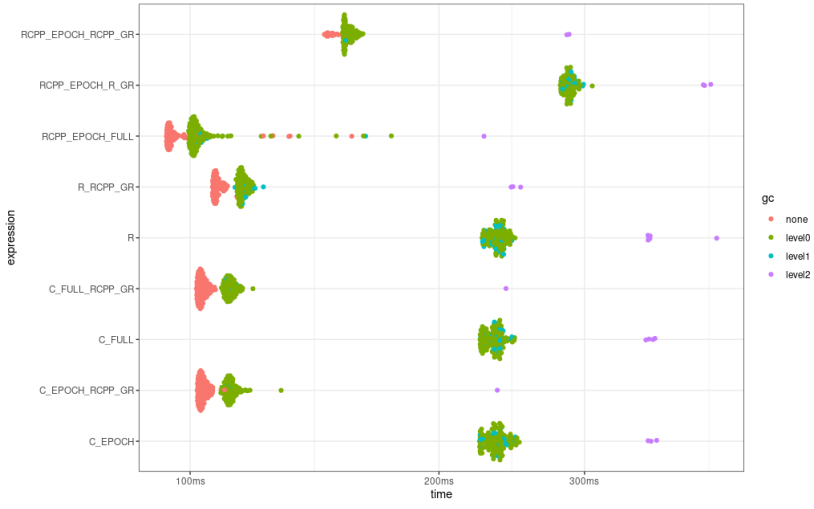
```
#include <Rinternals.h>
#include <R.h>

SEXP sgd(SEXP par0, SEXP loss_gr, SEXP N, SEXP batch, SEXP epoch, SEXP gamma0, SEXP maxit, SEXP rho) {
  int n_maxit = asInteger(maxit);
  double *gam = REAL(gamma0);
  SEXP par = PROTECT(allocVector(REALSXP, length(par0)));
  for(int i = 0; i < length(par0); ++i)
    REAL(par)[i] = REAL(par0)[i];
  SEXP batch_call = PROTECT(lang2(batch, R_NilValue));
  SEXP s, t;
  for(int i = 0; i < n_maxit; ++i) {
    SETCADR(batch_call, N);
    SEXP index = eval(batch_call, rho);
    SEXP gami = PROTECT(ScalarReal(gam[i]));
    t = s = PROTECT(allocList(5));
    SET_TYPEOF(s, LANGSXP);
    SETCAR(t, epoch); t = CDR(t);
    SETCAR(t, par); t = CDR(t);
    SETCAR(t, index); t = CDR(t);
    SETCAR(t, loss_gr); t = CDR(t);
    SETCAR(t, gami);
    par = eval(s, rho);
    UNPROTECT(2);
  }
  UNPROTECT(2);
  return par;
}
```

SGD Implementation Using R's C API

Build shared library using `R CMD SHLIB` command.

```
dyn.load("c/src/sgd_o.o")

epoch_test <- function(mini_batch_size = 1L) {
  function(par0, index, loss_gr, gamma0) {
    .Call("epoch_batch",
          par0,
          index,
          loss_gr,
          gamma0,
          mini_batch_size,
          environment())
  }
}
```

SGD Implementation Benchmark



SGD Implementation Benchmark

```
# A tibble: 9 × 3
  expression           median mem_alloc
  <bch:expr>         <bch:tm> <bch:byt>
1 RCPP_EPOCH_FULL       101ms    35.5MB
2 C_FULL_RCPP_GR        106ms    25.1MB
3 C_EPOCH_RCPP_GR       106ms      25MB
4 R_RCPP_GR             115ms    32.4MB
5 RCPP_EPOCH_RCPP_GR    155ms    48.3MB
6 C_FULL                233ms   198.5MB
7 C_EPOCH               235ms   198.6MB
8 R                     236ms   206.3MB
9 RCPP_EPOCH_R_GR       287ms   225.7MB
```