Stochastic Gradient Descent with Momentum and Line Searches

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Abstract

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1 Introduction

1.1 Optimization problem

$$\min_{w \in \mathbb{R}^p} f(w) = L(w) + \lambda \Omega(w)$$

$$\min \sum_{i=1}^{N} \log\bigl(1 + \exp(-y^{(i)} w^T x^{(i)})\bigr) + \lambda \|w\|^2 \tag{1}$$

where $i = \ldots, N$ are the dataset indices, $y^i \in \{-1, 1\}$ is the response variable corresponding to the negative or positive class, $x^i \in \mathbb{R}^p$ are dataset examples.

$$\nabla f(w) = X^T r + 2\lambda w, \quad r = -y^{(i)} \sigma(-y^{(i)} w^T x^{(i)})$$

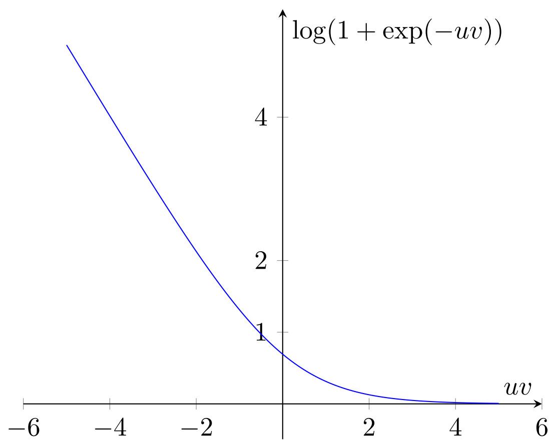
$$\nabla^2 f(w) = X^T D X + 2\lambda I, \quad d_{ii} = \sigma(y^{(i)} w^T x^{(i)}) \sigma(-y^{(i)} w^T x^{(i)})$$

Proposition 1. *Problem* (1) *admits a unique optimal solution.*

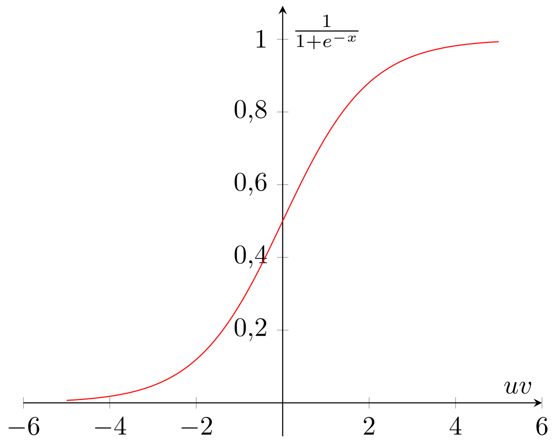
$$X^T = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \ldots & x_p^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \ldots & x_p^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & x_2^{(N)} & \ldots & x_p^{(N)} \end{pmatrix} \in \mathbb{R}^{N \times (p+1)}$$

$$w = \begin{pmatrix} b \\ w_1 \\ w_2 \\ \vdots \\ w_p \end{pmatrix} \in \mathbb{R}^{p+1}$$

$$y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{pmatrix} \in \{-1, 1\}$$



(a) *Log-loss*



(b) *Sigmoid function*

Figure 1: Log-loss and sigmoid function plots

- $uv \gg 0$: the example is labelled correctly
- $uv \ll 0$: the class assigned to the example is the wrong one
- the hessian matrix is positive defined $\forall w$, this means that the objective function, which is quadratic, is coercive and for the continuity that function admits global minimum, so $f(w)$ has finite inferior limit
- the hessian matrix being positive defined implies also that the objective function is strictly convex (on the other hand the loss function is just convex, due to its hessian matrix being positive semi-defined), this implies that if the global minimum exists, that solution is unique
- a global minimum is a point that satisfy $\nabla f(w^*) = 0$, which is a sufficient condition implied by the convexity of the problem, see figure 1a on the preceding page
- the ℓ_2 regularization implies that the objective function is strongly convex, this speeds up the convergence
- further more we can assume that $\nabla f(w)$ is Lipschitz-continuous with constant L

2 Mini-batch gradient descent variants

2.1 Fixed step-size

Mini-batch Gradient Descent with fixed or decreasing step-size

given $w^0 \in \mathbb{R}^n$, $f(w) = \sum_{i=1}^{N} f_i(w)$, $k = 0$ e $\{\alpha_k\} \mid \alpha_k = \alpha \vee \alpha_k = \frac{\alpha_0}{k+1}$
while $(\|\nabla f(w^k)\| > \varepsilon(1 + |f(w)|))$
  shuffle $\{1, \ldots, N\}$ and split $B_1, \ldots, B_{N/M}$ such that $1 < |B_t| = M \ll N$
  set $y_0 = w^k$
  for $t = 1, \ldots, N/M$
    get mini-batch indices from B_t
    approximate true gradient $\nabla f_{i_t}(w) = \frac{1}{M} \sum_{j \in B_t} \nabla f_j(y_{t-1})$
    compute direction $d_t = -\nabla f_{i_t}(y_{t-1})$
    make a (internal) step $y_t = y_{t-1} + \alpha_t d_t$
  end for
  update weights $w^{k+1} = y_{N/M}$
  epoch ends $k = k + 1$
end while

2.2 Stochastic line search

Mini-batch Gradient Descent with Armijo line search

given $w^0 \in \mathbb{R}^{p+1}$, $f(w) = \sum_{i=1}^{N} f_i(w)$, $\gamma \in (0,1)$, $\delta \in (0,1)$, $\alpha_0 \in \mathbb{R}^+$
$k = 0$
while $(\|\nabla f(w^k)\| > \varepsilon(1 + |f(w)|))$
  shuffle $\{1, \ldots, N\}$ and split $B_1, \ldots, B_{N/M}$ such that $1 < |B_t| = M \ll N$
  set $y_0 = w^k$
  for $t = 1, \ldots, N/M$
    get mini-batch indices i_t from B_t
    approximate true gradient $\nabla f_{i_t}(w) = \frac{1}{M} \sum_{j \in B_t} \nabla f_j(y_{t-1})$
    compute direction $d_t = -\nabla f_{i_t}(y_{t-1})$
    $\alpha =$ reset(), $q = 0$
    while $(f_{i_t}(y_{t-1} + \alpha d_t) > f_{i_t}(y_{t-1}) + \gamma \alpha \nabla f_{i_t}(y_{t-1})^T d_t)$
      reduce step-size $\alpha = \delta \alpha$
      rejections counter $q = q + 1$
    end while
    set optimal mini-batch step-size $\alpha_t = \alpha$
    make a (internal) step $y_t = y_{t-1} + \alpha_t d_t$
  end for
  update weights $w^{k+1} = y_{N/M}$
  epoch ends $k = k + 1$
end while

2.3 Fixed momentum term

Mini-batch Gradient Descent with fixed momentum term and fixed step-size

```
given $w^0 \in \mathbb{R}^{p+1}$, $f(w) = \sum_{i=1}^N f_i(w)$, $\gamma \in (0,1), \delta \in (0,1)$, $\{\alpha_k\} = \alpha$, $\beta \in (0,1)$
$k = 0$
while ($\|\nabla f(w^k)\| > \varepsilon(1 + |f(w)|)$)
 shuffle $\{1, \dots, N\}$ and split $B_1, \dots, B_{N/M}$ such that $1 < |B_t| = M \ll N$
 set $y_0 = w^k$, $d_0 = 0$
 for $t = 1, \dots, N/M$
  get mini-batch indices $i_t$ from $B_t$
  approximate true gradient $\nabla f_{i_t}(w) = \frac{1}{M} \sum_{j \in B_t} \nabla f_j(y_{t-1})$
  compute direction $d_t = -\big((1-\beta)\nabla f_{i_t}(y_{t-1}) + \beta d_{t-1}\big)$
  make a (internal) step $y_t = y_{t-1} + \alpha_t d_t$
 end for
 update weights $w^{k+1} = y_{N/M}$
 epoch ends $k = k + 1$
end while
```