Modern Optimization Techniques

Lucas Rego Drumond

Information Systems and Machine Learning Lab (ISMLL)
Institute of Computer Science
University of Hildesheim, Germany

Stochastic Gradient Descent

Outline

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1. Unconstrained Optimization

2. Stochastic Gradient Descent

3. Choosing the right step size

4. Stochastic Gradient Descent on Practice

Gradient Descent

procedure GradientDescent
input: f_0
  Get initial point $\mathbf{x}$
  repeat
    Get Step Size μ
    $\mathbf{x} := \mathbf{x} - \mu \nabla f_0(\mathbf{x})$
  until convergence
  return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

Outline

Practical Example: Household Spending

Suppose we have the following data about different households:

- Number of workers in the household (a_1)
- Household composition (a_2)
- Region (a_3)
- Gross normal weekly household income (a_4)
- **Weekly household spending** (y)

We want to creat a model of the weekly household spending

Practical Example: Household Spending

If we have data about m households, we can represent it as:

$$A_{m,n} = \begin{pmatrix} 1 & a_{1,2} & \dots & a_{1,n} \\ 1 & a_{2,2} & \dots & a_{2,n} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & a_{m,2} & \dots & a_{m,n} \end{pmatrix} \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

We can model the household consumption is a linear combination of the household features with parameters $\mathbf{x}$:

$$\hat{y}_i = \mathbf{x}^T \mathbf{a_i} = x_0 1 + x_1 a_{i,1} + x_2 a_{i,2} + x_3 a_{i,3} + x_4 a_{i,4}$$

Least Square Problem Revisited

The following least square problem

$$\text{minimize} \quad ||A\mathbf{x} - \mathbf{y}||_2^2$$

Can be rewritten as

$$\text{minimize} \quad \sum_{i=1}^{m} (\mathbf{x}^T \mathbf{a_i} - y_i)^2$$

$$A_{m,n} = \begin{pmatrix} 1 & a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} \\ 1 & a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & a_{m,1} & a_{m,2} & a_{m,3} & a_{m,4} \end{pmatrix} \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

The Gradient Descent update rule

For the problem

$$\text{minimize} \quad \sum_{i=1}^{m} (\mathbf{x}^T \mathbf{a_i} - y_i)^2$$

The the gradient $\nabla f_0(\mathbf{x})$ of the objective function is:

$$\nabla_{\mathbf{x}} f_0(\mathbf{x}) = 2 \sum_{i=1}^{m} (\mathbf{x}^T \mathbf{a_i} - y_i)\mathbf{a_i}$$

The Gradient Descent update rule is then:

$$\mathbf{x} \rightarrow \mathbf{x} - \mu \left(2 \sum_{i=1}^{m} (\mathbf{x}^T \mathbf{a_i} - y_i)\mathbf{a_i} \right)$$

The Gradient Descent update rule

We need to “see“ all the data before updating $\mathbf{x}$

$$\mathbf{x} \rightarrow \mathbf{x} - \mu \left(2 \sum_{i=1}^{m} (\mathbf{x}^T \mathbf{a_i} - y_i)\mathbf{a_i} \right)$$

Can we make any progress before iterating over all the data?

Decomposing the objective function

The objective function

$$f_0(\mathbf{x}) = \sum_{i=1}^{m} (\mathbf{x}^T \mathbf{a_i} - y_i)^2$$

Can be expressed as a function of the objective on each data point $(\mathbf{a}, y)$:

$$g(\mathbf{x}, i) = (\mathbf{x}^T \mathbf{a_i} - y_i)^2$$

So that

$$f_0(\mathbf{x}) = \sum_{i=1}^{m} g(\mathbf{x}, i)$$

A simpler update rule

Now that we have

$$f_0(\mathbf{x}) = \sum_{i=1}^{m} g(\mathbf{x}, i)$$

We can define the following update rule

- Pick a random instance $i \sim \text{Uniform}(1, m)$
- Update $\mathbf{x}$

$$\mathbf{x} \rightarrow \mathbf{x} + \mu \left(-\nabla_{\mathbf{x}} g(\mathbf{x}, i)\right)$$

Stochastic Gradient Descent (SGD)

procedure StochasticGradiendDescent
input: f_0, μ
    Get initial point $\mathbf{x}$
    repeat
        for $i \in 1, \ldots, m$ **do**
            $\mathbf{x} \rightarrow \mathbf{x} - \mu \nabla g(\mathbf{x}, i)$
        end for
    until convergence
    return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

SGD and the least squares

We have

$$f_0(\mathbf{x}) = \sum_{i=1}^{m} g(\mathbf{x}, i)$$

with

$$g(\mathbf{x}, i) = (\mathbf{x}^T \mathbf{a_i} - y_i)^2$$

The update rule is

$$\nabla_{\mathbf{x}} g(\mathbf{x}, i) = 2(\mathbf{x}^T \mathbf{a_i} - y_i)\mathbf{a_i}$$

$$\mathbf{x} \rightarrow \mathbf{x} - \mu \left(2(\mathbf{x}^T \mathbf{a_i} - y_i)\mathbf{a_i} \right)$$

SGD vs. GD

procedure SGD
input: f_0, μ
    Get initial point $\mathbf{x}$
    repeat
        for $i \in 1, \ldots, m$ **do**
            $\mathbf{x} \rightarrow \mathbf{x} - \mu \nabla g(\mathbf{x}, i)$
        end for
    until convergence
    return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

procedure GradientDescent
input: f_0
    Get initial point $\mathbf{x}$
    repeat
        Get Step Size μ
        $\mathbf{x} := \mathbf{x} - \mu \nabla f_0(\mathbf{x})$
    until convergence
    return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

SGD vs. GD - Least Squares

procedure SGD
input: f_0, μ
Get initial point $\mathbf{x}$
repeat
for $i \in 1, \ldots, m$ **do**
$$\mathbf{x} \rightarrow \mathbf{x} - \mu \left(2(\mathbf{x}^T \mathbf{a_i} - y_i)\mathbf{a_i}\right)$$
end for
until convergence
return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

procedure GD
input: f_0
Get initial point $\mathbf{x}$
repeat
Get Step Size μ
$$\mathbf{x} \rightarrow \mathbf{x} - \mu \left(2 \sum_{i=1}^{m} (\mathbf{x}^T \mathbf{a_i} - y_i)\mathbf{a_i}\right)$$
until convergence
return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

Outline

Choosing the step size for SGD

- The step size μ is a crucial parameter to be tuned
- Given the low cost of the SGD update, using line search for the step size is a bad choice
- Possible alternatives:
  - Fixed step size
  - Armijo principle
  - Bold-Driver
  - Adagrad

Real World Dataset: Body Fat prediction

We want to estimate the percentage of body fat based on various attributes:

- Age (years)
- Weight (lbs)
- Height (inches)
- Neck circumference (cm)
- Chest circumference (cm)
- Abdomen 2 circumference (cm)
- Hip circumference (cm)
- Thigh circumference (cm)
- Knee circumference (cm)
- ...

http://lib.stat.cmu.edu/datasets/bodyfat

Real World Dataset: Body Fat prediction

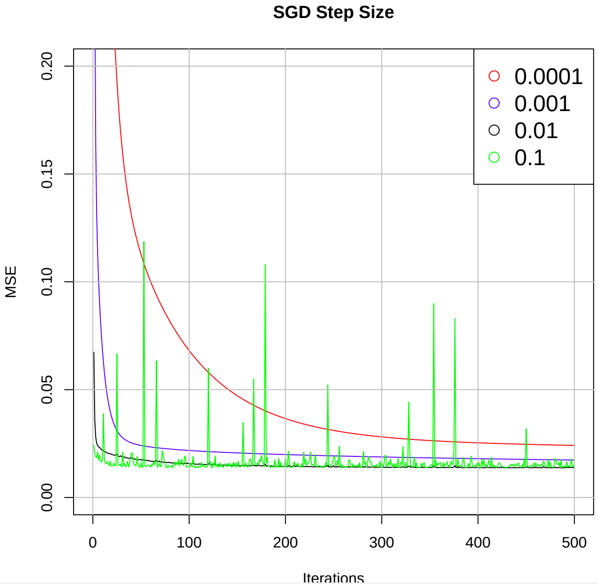
The data is represented it as:

$$A_{m,n} = \begin{pmatrix} 1 & a_{1,1} & a_{1,2} & \dots & a_{1,n} \\ 1 & a_{2,1} & a_{2,2} & \dots & a_{2,n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & a_{m,1} & a_{m,2} & \dots & a_{m,n} \end{pmatrix} \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

with $m = 252$, $n = 14$
We can model the percentage of body fat y is a linear combination of the body measurements with parameters $\mathbf{x}$:

$$\hat{y}_i = \mathbf{x}^T \mathbf{a_i} = x_0 1 + x_1 a_{i,1} + x_2 a_{i,2} + \ldots + x_n a_{i,n}$$

SGD - Fixed Step Size on the Body Fat dataset



Bold Driver Heuristic

- The Bold Driver Heuristic makes the assumption that smaller step sizes are needed when closer to the optimum
- It adjusts the step size based on the value of $f_0(\mathbf{x}^t) - f_0(\mathbf{x}^{t-1})$
- If the value of $f_0(\mathbf{x})$ grows, the step size must decrease
- If the value of $f_0(\mathbf{x})$ decreases, the step size can be larger for faster convergence

Bold Driver Heuristic - Update Rule

We have

$$f_0(\mathbf{x}) = \sum_{i=1}^{m} g(\mathbf{x}, i)$$

We need to define an increase factor γ and a decay factor ν

- For each epoch
- Evaluate the objective function $f_0(\mathbf{x}^{t-1})$
- Cycle through the whole data and update the parameters
- Evaluate the objective function $f_0(\mathbf{x}^{t})$
- if $f_0(\mathbf{x}^{t}) < f_0(\mathbf{x}^{t-1})$ then $\mu \rightarrow \gamma\mu$
- else $f_0(\mathbf{x}^{t}) > f_0(\mathbf{x}^{t-1})$ then $\mu \rightarrow \nu\mu$

Widely used values: $\gamma = 1.05$ and $\nu = 0.5$

SGD with Bold Driver

procedure BoldDriverSGD
input: f_0, μ, γ and ν
  Get initial point $\mathbf{x}$
  repeat
    $\epsilon^{t-1} \rightarrow f_0(\mathbf{x})$
    for $i \in 1, \ldots, m$ **do**
      $\mathbf{x} \rightarrow \mathbf{x} - \mu \nabla g(\mathbf{x}, i)$
    end for
    $\epsilon^{t} \rightarrow f_0(\mathbf{x})$
    if $\epsilon^{t} < \epsilon^{t-1}$ **then**
      $\mu \rightarrow \nu\mu$
    else
      $\mu \rightarrow \gamma\mu$
    end if
  until convergence
  return $\mathbf{x}$, $f_0(\mathbf{x})$

Considerations

- Works well for a range of problems
- The initial μ just need to be large enough
- γ and ν needs to be adusted
- May lead to faster convergence rates

AdaGrad

- Adagrad adjusts the step size for each parameter to be optimized
- It uses information about the past gradients
- Leads to faster convergence
- Less sensitive to the choice of the step size

AdaGrad - Update Rule

We have

$$f_0(\mathbf{x}) = \sum_{i=1}^{m} g(\mathbf{x}, i)$$

Update rule:

- Pick a random instance $i \sim \text{Uniform}(1, m)$
- Compute the gradient $\nabla_{\mathbf{x}} g(\mathbf{x}, i)$
- Update the gradient history $\mathbf{h} \rightarrow \mathbf{h} + \nabla_{\mathbf{x}} g(\mathbf{x}, i) \circ \nabla_{\mathbf{x}} g(\mathbf{x}, i)$
- The step size for parameter $\mathbf{x}_i$ is $\frac{\mu}{\sqrt{h_i}}$
- Update

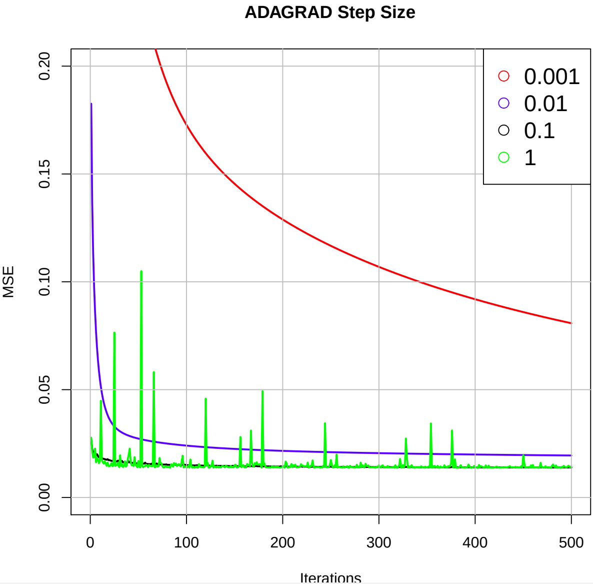
$$\mathbf{x} \rightarrow \mathbf{x} - \frac{\mu}{\sqrt{\mathbf{h}}} \circ (\nabla_{\mathbf{x}} g(\mathbf{x}, i))$$

$\circ$ denotes the elementwise product

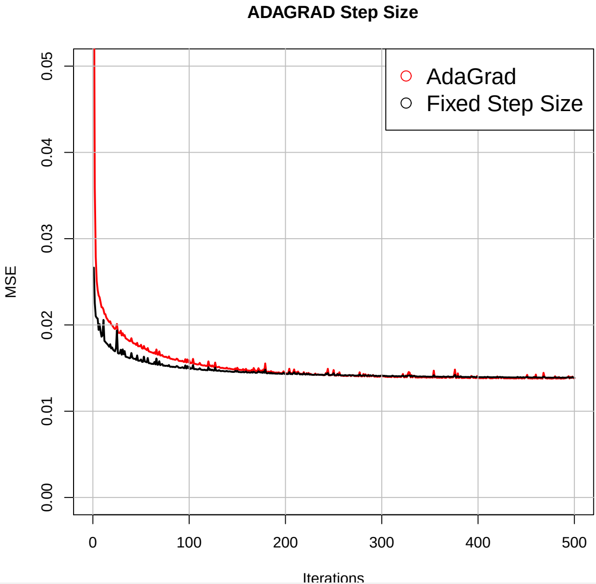
SGD with Adagrad

procedure ADAGRADSGD
input: f_0, μ
  Get initial point $\mathbf{x}$
  $\mathbf{h} \rightarrow \mathbf{0}$
  repeat
    for $i \in 1, \ldots, m$ **do**
      $\mathbf{h} \rightarrow \mathbf{h} + \nabla_{\mathbf{x}} g(\mathbf{x}, i) \circ \nabla_{\mathbf{x}} g(\mathbf{x}, i)$
      $\mathbf{x} \rightarrow \mathbf{x} - \frac{\mu}{\sqrt{\mathbf{h}}} \circ \nabla g(\mathbf{x}, i)$
    end for
  until convergence
  return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

AdaGrad Step Size

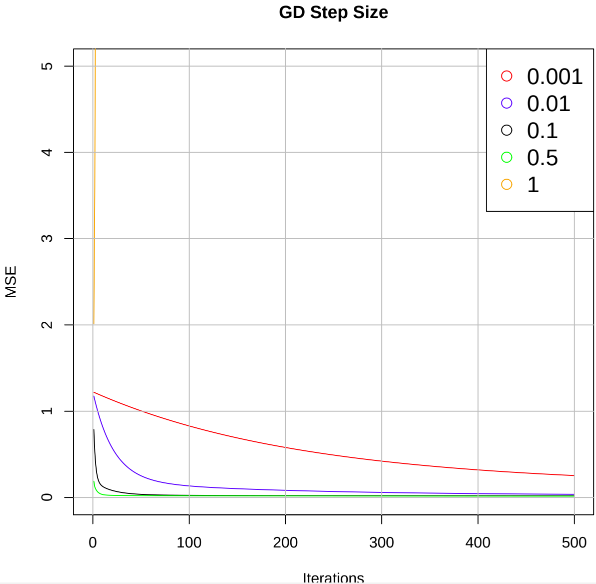


AdaGrad vs Fixed Step Size

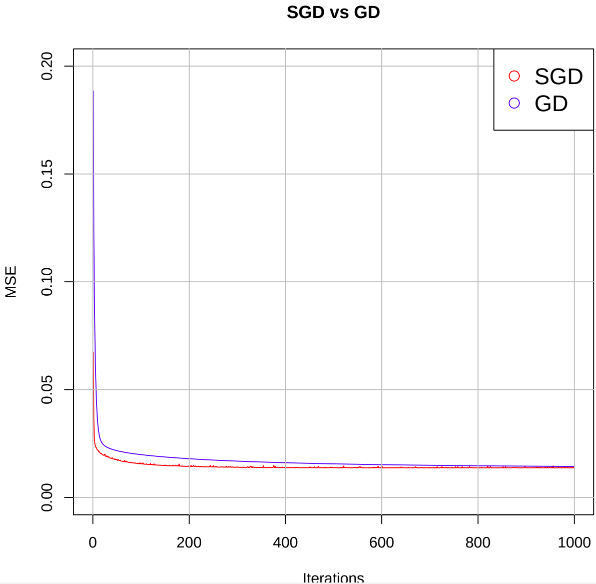


Outline

GD Step Size


GD Step Size
MSE
0
1
2
3
4
5
Iterations
0
100
200
300
400
500
0.001
0.01
0.1
0.5
1

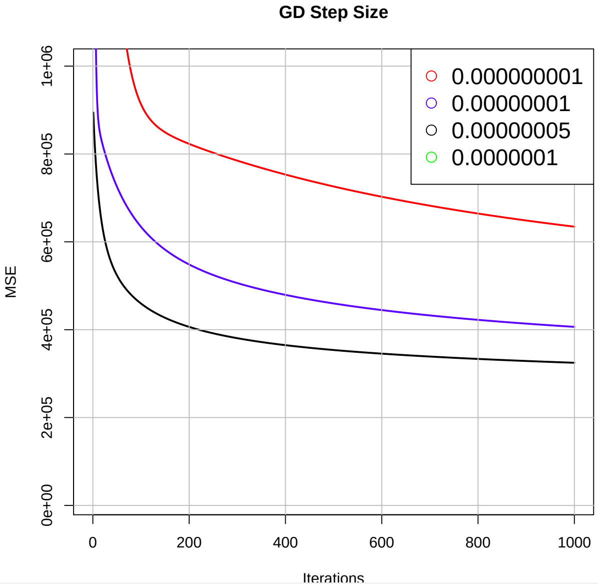
SGD vs GD - Body Fat Dataset



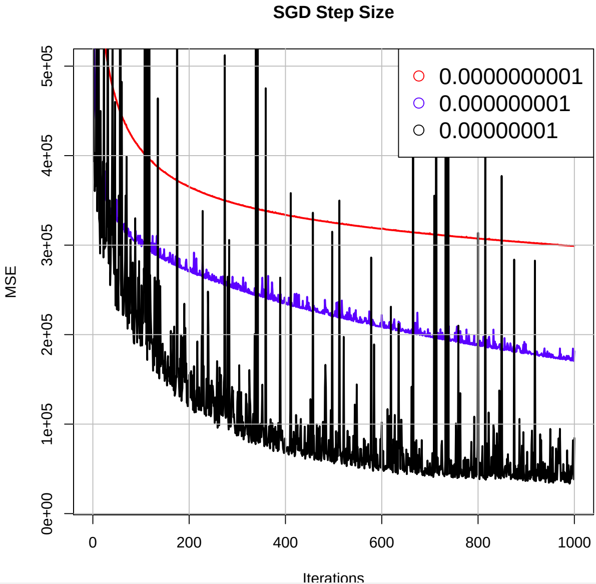
Year Prediction Data Set

- Least Squares Problem
- Prediction of the release year of a song from audio features
- 90 features
- Experiments done on a subset of 1000 instances of the data

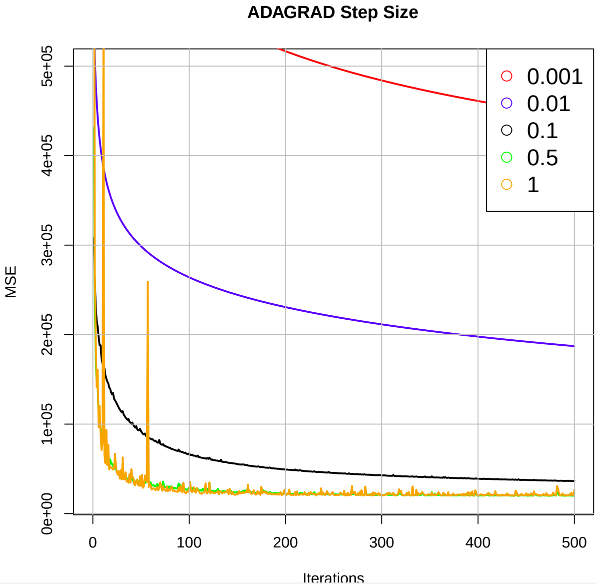
GD Step Size - Year Prediction



SGD Step Size - Year Prediction



AdaGrad Step Size - Year Prediction



AdaGrad vs SGD vs GD - Year Prediction