Modern Optimization Techniques

2. Unconstrained Optimization / 2.2. Stochastic Gradient Descent

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Outline

Outline

Unconstrained Convex Optimization

$$\arg\min_{x \in \operatorname{dom} f} f(x)$$

- $\operatorname{dom} f \subseteq \mathbb{R}^N$ is convex and open (unconstrained optimization)
  - e.g., $\operatorname{dom} f = \mathbb{R}^N$
- f is convex

Stochastic Gradient

Gradient Descent makes use of the gradient

$$\nabla f(x)$$

Stochastic Gradient Descent: makes use of Stochastic Gradient only:

$$g(x) \sim p(g \in \mathbb{R}^N \mid x), \quad \mathbb{E}_p(g(x)) = \nabla f(x)$$

- for each point $x \in \mathbb{R}^N$:
  random variable over $\mathbb{R}^N$ with distribution p (conditional on x)
- on average yields the gradient (at each point)

Stochastic Gradient / Example: Big Sums

f is a "big sum":

$$f(x) = \frac{1}{C} \sum_{c=1}^{C} f_c(x)$$

with f_c convex, $\quad c = 1, \ldots, C$

g is the gradient of a random summand:

$$p(g \mid x) := \text{Unif}(\{\nabla f_c(x) \mid c = 1, \ldots, C\})$$

Stochastic Gradient / Example: Least Squares

$$\min_{x\in\mathbb{R}^N} f(x) := ||Ax-b||_2^2$$

- will find solution for $Ax = b$ if there is any (then $||Ax-b||_2 = 0$)
- otherwise will find the x where the difference $Ax - b$ of left and right side is as small as possible (in the squared L2 norm)
- is a big sum:

$$f(x) := ||Ax-b||_2^2 = \sum_{m=1}^{M}((Ax)_m - b_m)^2 = \sum_{m=1}^{M}(A_{m,.}x - b_m)^2$$

$$= \frac{1}{M}\sum_{m=1}^{M} f_m(x), \quad f_m(x) := M(A_{m,.}x - b_m)^2$$

- stochastic gradient g:
  - gradient for a random component m

Stochastic Gradient / Example: Supervised Learning

$$\min_{\theta \in \mathbb{R}^P} f(x) := \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, \hat{y}(x_n, \theta)) + \lambda ||\theta||_2^2$$

- where
  - $(x_n, y_n) \in \mathbb{R}^M \times \mathbb{R}^T$ are N training samples,
  - $\hat{y}$ is a parametrized model, e.g., logistic regression

    $$\hat{y}(x; \theta) := (1 + e^{-\theta^T x})^{-1}, \quad P := M, T := 1$$

  - ℓ is a loss, e.g., negative binomial loglikelihood:

    $$\ell(y, \hat{y}) := -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

  - $\lambda \in \mathbb{R}_0^+$ is the regularization weight.
- will find parametrization with best trade-off between low loss and low model complexity

Stochastic Gradient / Example: Supervised Learning (2/2)

$$\min_{\theta \in \mathbb{R}^P} f(x) := \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, \hat{y}(x_n, \theta)) + \lambda ||\theta||_2^2$$

- where
  - $(x_n, y_n) \in \mathbb{R}^M \times \mathbb{R}^T$ are N training samples,
  - ...
- is a big sum:

$$f(\theta) := \frac{1}{N} \sum_{n=1}^{N} f_n(\theta), \quad f_n(\theta) := \ell(y_n, \hat{y}(x_n, \theta)) + \lambda ||\theta||_2^2$$

- stochastic gradient g:
  - gradient for a random sample n

Outline

Stochastic Gradient Descent

- the very same as Gradient Descent
- but use stochastic gradient $g(x)$ instead of exact gradient $\nabla f(x)$ in each step

```
min-sgd(f, p, x^(0), μ, K):
  for k := 1, ..., K:
    draw g^(k-1) ~ p(g | x)
    Δx^(k-1) := -g^(k-1)
    μ^(k-1) := μ(f, x^(k-1), Δx^(k-1))
    x^(k) := x^(k-1) + μ^(k-1) Δx^(k-1)
    if converged(...):
      return x^(k)
  raise exception "not converged in K iterations"
```

where

- p (distribution of the) stochastic gradient of f

Stochastic Gradient Descent / For Big Sums

```
min-sgd((f_c)_{c=1,...,C}, (∇f_c)_{c=1,...,C}, x^(0), μ, K):
  for k := 1, ..., K:
    draw c^(k−1) ∼ Unif(1, ..., C)
    g^(k−1) := ∇f_{c^(k−1)}(x^(k−1))
    Δx^(k−1) := −g^(k−1)
    μ^(k−1) := μ(f, x^(k−1), Δx^(k−1))
    x^(k) := x^(k−1) + μ^(k−1) Δx^(k−1)
    if converged(...):
      return x^(k)
  raise exception "not converged in K iterations"
```

where

- $(f_c)_{c=1,\ldots,C}$ objective function summands, $f := \frac{1}{C}\sum_{c=1}^{C} f_c$
- $(\nabla f_c)_{c=1,\ldots,C}$ gradients of the objective function summands

SGD / For Big Sums / Epochs

min-sgd$((f_c)_{c=1,\ldots,C},\ (\nabla f_c)_{c=1,\ldots,C},\ x^{(0)},\ \mu,\ K)$:
  $\mathcal{C} := (1, 2, \ldots, C)$
  $x^{(0,C)} := x^{(0)}$
  for $k := 1, \ldots, K$:
    randomly shuffle $\mathcal{C}$
    $x^{(k,0)} := x^{(k-1,C)}$
    for $i = 1, \ldots, C$:
      $g^{(k,i-1)} := \nabla f_{c_i}(x^{(k,i-1)})$
      $\Delta x^{(k,i-1)} := -g^{(k,i-1)}$
      $\mu^{(k,i-1)} := \mu(f, x^{(k,i-1)}, \Delta x^{(k,i-1)})$
      $x^{(k,i)} := x^{(k,i-1)} + \mu^{(k,i-1)} \Delta x^{(k,i-1)}$
  return $x^{(K,C)}$

where

- $(f_c)_{c=1,\ldots,C}$ objective function summands, $f := \frac{1}{C} \sum_{c=1}^{C} f_c$
- ...

Theorem (Convergence of Gradient Descent) [review]

If

(i) f is strongly convex,

(ii) the initial sublevel set $S := \{x \in \text{dom}\, f \mid f(x) \leq f(x^{(0)})\}$ is closed,

(iii) an exact line search is used,

then gradient descent converges, esp.

$$f(x^{(k)}) - p^* \leq (1 - \frac{m}{M})^k \; (f(x^{(0)}) - p^*)$$

$$||x^{(k)} - x^*||^2 \leq (1 - \frac{m}{M})^k \frac{||(\nabla f(x^{(0)}))||^2}{m^2}$$

Theorem (Convergence of SGD)

If

(i) f is strongly convex ($||\nabla^2 f(x)|| \succeq mI, m \in \mathbb{R}^+$),

(ii) the expected squared norm of its stochastic gradient g is uniformly bounded ($\exists G \in \mathbb{R}_0^+ \; \forall x : \mathbb{E}(||g(x)||^2) \leq G^2$) and

(iii) the step size $\mu^{(k)} := \frac{1}{m(k+1)}$ is used,

then SGD converges, esp.

$$\mathbb{E}_p(||x^{(k)} - x^*||^2) \leq \frac{1}{k+1} \max\{||x^{(0)} - x^*||^2, \frac{G^2}{m^2}\}$$

Convergence of SGD / Proof

$$f(x^*) - f(x) \geq \nabla f(x)^T (x^* - x) + \frac{m}{2} ||x^* - x||^2 \quad \text{str. conv. (i)}$$

$$f(x) - f(x^*) \geq \nabla f(x^*)^T (x - x^*) + \frac{m}{2} ||x - x^*||^2 = \frac{m}{2} ||x^* - x||^2$$

summing both yields

$$0 \geq \nabla f(x)^T (x^* - x) + m||x^* - x||^2$$

$$\nabla f(x)^T (x - x^*) \geq m||x^* - x||^2 \qquad (1)$$

$$\begin{aligned}
&\mathbb{E}(||x^{(k)} - x^*||^2) \\
&= \mathbb{E}(||x^{(k-1)} - \mu^{(k-1)} g^{(k-1)} - x^*||^2) \\
&= \mathbb{E}(||x^{(k-1)} - x^*||^2) - 2\mu^{(k-1)} \mathbb{E}((g^{(k-1)})^T (x^{(k-1)} - x^*)) + (\mu^{(k-1)})^2 \mathbb{E}(||g^{k-1}||^2) \\
&= \mathbb{E}(||x^{(k-1)} - x^*||^2) - 2\mu^{(k-1)} \mathbb{E}(\nabla f(x^{(k-1)})^T (x^{(k-1)} - x^*)) + (\mu^{(k-1)})^2 \mathbb{E}(||g^{k-1}||^2) \\
&\overset{(ii),(1)}{\leq} \mathbb{E}(||x^{(k-1)} - x^*||^2) - 2\mu^{(k-1)} m \mathbb{E}(||x^* - x^{(k-1)}||^2) + (\mu^{(k-1)})^2 G^2 \\
&= (1 - 2\mu^{(k-1)} m) \mathbb{E}(||x^{(k-1)} - x^*||^2) + (\mu^{(k-1)})^2 G^2 \qquad (2)
\end{aligned}$$

Convergence of SGD / Proof (2/2)

induction over k: $k := 0$:

$$||x^{(0)} - x^*||^2 \leq \frac{1}{1} L, \quad L := \max\{||x^{(0)} - x^*||^2, \frac{G^2}{m^2}\}$$

$k > 0$:

$$\begin{aligned}
\mathbb{E}(||x^{(k)} - x^*||^2) &\overset{(2)}{\leq} (1 - 2\mu^{(k-1)} m)\mathbb{E}(||x^{(k-1)} - x^*||^2) + (\mu^{(k-1)})^2 G^2 \\
&\overset{(iii)}{=} (1 - \frac{2}{k})\mathbb{E}(||x^{(k-1)} - x^*||^2) + \frac{G^2}{m^2 k^2} \\
&\overset{\text{ind.hyp.}}{\leq} (1 - \frac{2}{k})\frac{1}{k} L + \frac{G^2}{m^2 k^2} \\
&\overset{\text{def. } L}{\leq} (1 - \frac{2}{k})\frac{1}{k} L + \frac{1}{k^2} L \\
&= \frac{k-2}{k^2} L + \frac{1}{k^2} L = \frac{k-1}{k^2} L \leq \frac{1}{k+1} L
\end{aligned}$$

Outline

1. Stochastic Gradients
2. Stochastic Gradient Descent (SGD)
3. More on Line Search: Bold Driver
4. More on Line Search: AdaGrad

Choosing the step size for SGD

- The step size μ is a crucial parameter of gradient descent
- Given the low cost of the SGD update,
  using exact line search for the step size is a bad choice
- Possible alternatives:
  - Fixed step size
  - Exponentially decreasing step size
  - Backtracking / Armijo principle
  - Bold-Driver
  - Adagrad

Example: 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

Example: Body Fat prediction

The data is represented it as:

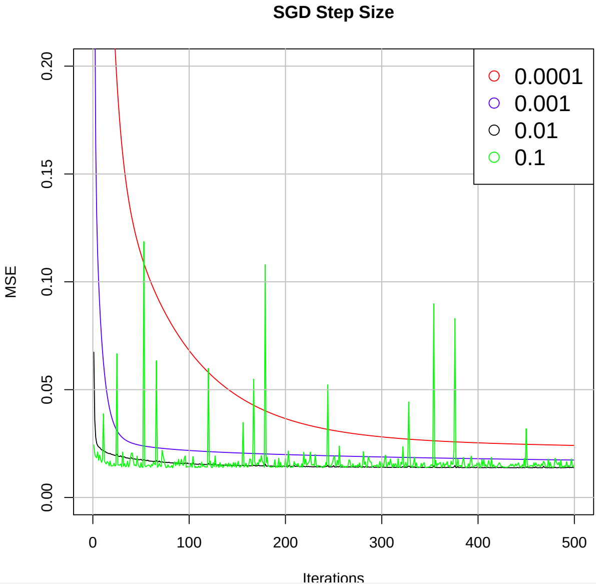
$$A = \begin{pmatrix} 1 & a_{1,1} & a_{1,2} & \dots & a_{1,M} \\ 1 & a_{2,1} & a_{2,2} & \dots & a_{2,M} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & a_{N,1} & a_{N,2} & \dots & a_{N,M} \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$

with $N = 252$, $M = 14$

We can model the percentage of body fat y
as a linear combination of the body measurements with parameters $\mathbf{x}$:

$$\hat{y}_n = \mathbf{x}^T \mathbf{a_n} = x_0 1 + x_1 a_{n,1} + x_2 a_{n,2} + \ldots + x_M a_{n,M}$$

SGD - Fixed Step Size on the Body Fat dataset



Bold Driver Heuristic

- idea: use smaller step sizes closer to the minimum.
- adjust step size based on the value of $f(\mathbf{x}^{(k)}) - f(\mathbf{x}^{(k-1)})$
- if the value of $f(\mathbf{x})$ grows,
  the step size must decrease
- if the value of $f(\mathbf{x})$ decreases,
  the step size can increase for faster convergence
- adapt stepsize only **once after each epoch**,
  not for every (inner) iteration.

Bold Driver Heuristic — Update Rule

We need to define

- an **increase factor** $\mu^+ > 1$, e.g. $\mu^+ := 1.05$, and
- a **decay factor** $\mu^- \in (0, 1)$, e.g., $\mu^- := 0.5$.

Step size update rule:

- Cycle through the whole data and update the parameters
- Evaluate the objective function $f(\mathbf{x}^{(k)})$
- if $f(\mathbf{x}^{(k)}) < f(\mathbf{x}^{(k-1)})$ then $\mu \rightarrow \mu^+\mu$
- else $f(\mathbf{x}^{(k)}) > f(\mathbf{x}^{(k-1)})$ then $\mu \rightarrow \mu^-\mu$
- different from the bold driver heuristics for batch gradient descent, there is no way to evaluate $f(x + \mu\Delta x)$ for different μ.
  - stepsize μ is adapted once after the step has been done

Bold Driver

stepsize-bd($\mu, f_{\text{new}}, f_{\text{old}}, \mu^+, \mu^-$):
    if $f_{\text{new}} < f_{\text{old}}$
        $\mu := \mu^+ \mu$
    else
        $\mu := \mu^- \mu$
    return μ

where

- μ stepsize of last update
- $f_{\text{new}}, f_{\text{old}} = f(x^k), f(x^{k-1})$ function values before and after the last update
- μ^+, μ^- stepsize increase and decay factors

Considerations

- works well for a range of problems
- initial μ just needs to be large enough
- μ^+ and μ^- have to be adjusted to the problem at hand
  - often used values: $\mu^+ = 1.05$ and $\mu^- = 0.5$
- may lead to faster convergence

Outline

AdaGrad

- idea: adjust the step size
  individually for each variable to be optimized
- use information about past gradients
- often leads to faster convergence
- does not have parameters
  - such as μ^+ and μ^- for Bold Driver
- update stepsize for every inner iteration

AdaGrad - Update Rule

We have

$$\mathbf{g}(x) \sim p(\mathbf{g} \in \mathbb{R}^N \mid x), \quad \mathbb{E}_p(\mathbf{g}(x)) = \nabla f(x)$$

Update rule:

- Update the gradient square history

$$\mathbf{G}^{2,\text{next}} := \mathbf{G}^2 + \mathbf{g}(x) \odot \mathbf{g}(x)$$

- The step size for variable $\mathbf{x}_n$ is

$$\mu_n := \frac{\mu_0}{\sqrt{\mathbf{G^2}_n} + \epsilon}$$

- Update

$$\mathbf{x}^{\text{next}} := \mathbf{x} - \mu \odot \mathbf{g}(x)$$

$$\text{i.e., } \mathbf{x}_n^{\text{next}} := \mathbf{x}_n - \frac{\mu_0}{\sqrt{\mathbf{G^2}_n} + \epsilon}(g(x))_n$$

$\odot$ denotes the elementwise product, $\mathbf{G^2}$ a variable name, not a square.

AdaGrad

stepsize-adagrad$(\mathbf{g}, \mathbf{G^2}; \mu_0, \epsilon)$:

$\quad \mathbf{G^2} := \mathbf{G^2} + \mathbf{g} \circ \mathbf{g}$

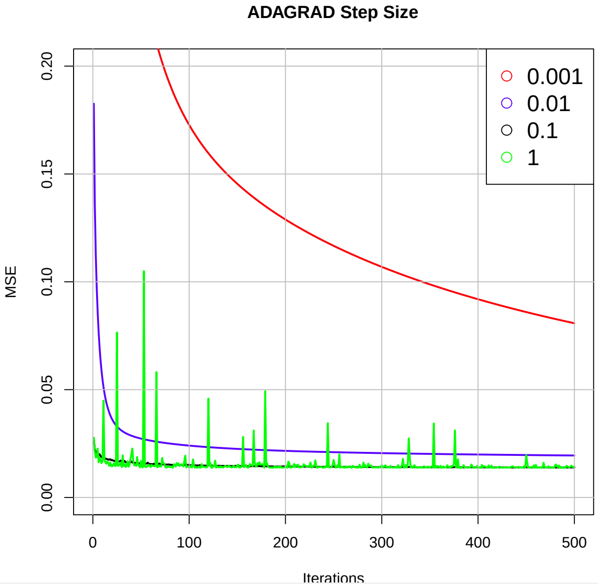
$\quad \mu_n := \frac{\mu_0}{\sqrt{\mathbf{G^2}_n + \epsilon}}$ for $n = 1, \ldots, N$

$\quad$ return $(\mu, \mathbf{G^2})$

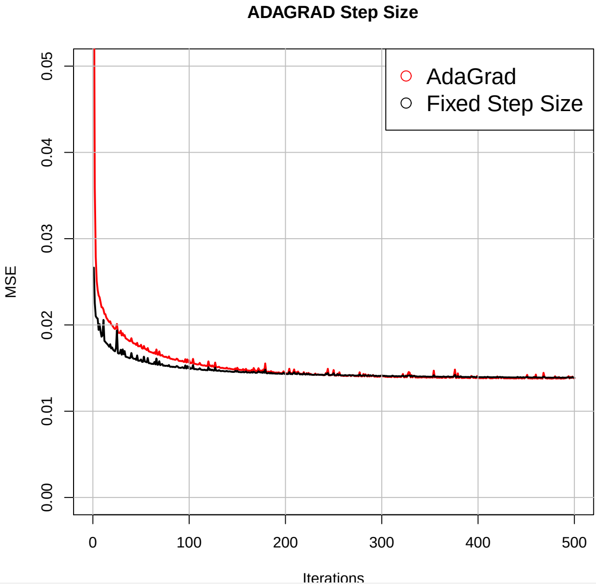
where

- returns a vector of stepsizes, one for each variable
- $\mathbf{g} \sim p(\mathbf{g} \in \mathbb{R}^N \mid \mathbf{x}), \quad \mathbb{E}_p(\mathbf{g}(\mathbf{x})) = \nabla f(x)$ current (stochastic) gradient
- $\mathbf{G}$ past gradient square history
- μ_0 initial stepsize

AdaGrad Step Size



AdaGrad vs Fixed Step Size



Adam

stepsize-adam$(\mathbf{g}, \mathbf{G}, \mathbf{G^2}, t; \mu_0, \beta_1, \beta_2, \epsilon)$:
  $\mathbf{G} := \beta_1 \mathbf{G} + (1-\beta_1)\mathbf{g}$
  $\mathbf{G^2} := \beta_2 \mathbf{G^2} + (1-\beta_2)\mathbf{g} \odot \mathbf{g}$
  $\mu_n := \mu_0 \frac{\mathbf{G}_n/(1-\beta_1^t)}{\sqrt{\mathbf{G^2}_n/(1-\beta_2^t)}+\epsilon}$ for $n = 1, \ldots, N$
  return $(\mu, \mathbf{G}, \mathbf{G^2})$

where

- returns a vector of stepsizes, one for each variable
- $\mathbf{g} \sim p(\mathbf{g} \in \mathbb{R}^N \mid \mathbf{x})$, $\mathbb{E}_p(\mathbf{g}(\mathbf{x})) = \nabla f(x)$ current (stochastic) gradient
- $\mathbf{G}, \mathbf{G^2}$ past gradient and gradient square history
- t iteration
- μ_0 initial stepsize

Note: Adagrad is a special case for $\beta_1 := 0, \beta_2 := \frac{1}{2}$ and iteration-dependent $\mu_0(t) := 2\mu_0^{\text{Adagrad}}/\sqrt{1-0.5^t}$.

Summary

- Stochastic Gradient Descent (SGD) is like Gradient Descent,
  - but instead of the exact gradient uses just a random vector called stochastic gradient
    - with expectation of the true/exact gradient.

- stochastic gradients occur naturally when the objective is a big sum
  - then the gradient of a uniformly random component is a stochastic gradient
  - e.g., objectives for most machine learning problems are big sums over instance-wise losses (and regularization terms).

- SGD converges with a rate of $1/k$ in the number of steps k.

Summary (2/2)

- step size and convergence critera have to be adapted
  - to aggregate over several update steps, e.g., an epoche
  - cannot test for different step sizes (like backtracking)

- Bold driver step size control:
  - update per epoche based on additional function evaluation.

- Adagrad step size control:
  - individual step size for each variable
  - $1/\sum g^2$ for past gradients.

Further Readings

- SGD is not covered in Boyd and Vandenberghe [2004].
- Leon Bottou, Frank E. Curtis, Jorge Nocedal (2016): *Stochastic Gradient Methods for Large-Scale Machine Learning*, ICML 2016 Tutorial, http://users.iems.northwestern.edu/~nocedal/ICML
- Francis Bach (2013): *Stochastic gradient methods for machine learning*, Microsoft Machine Learning Summit 2013, http://research.microsoft.com/en-us/um/cambridge/events/mls2013/downloads/stochastic_gradient.pdf
- for the convergence proof:
  Ji Liu (2014), Notes "Stochastic Gradient Descent",
  http://www.cs.rochester.edu/~jliu/CSC-576-2014fall.html

References

Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge University Press, 2004.