Optimization for Machine Learning
CS-439

Lecture 11: Gradient free and adaptive methods

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Chapter XI.1

Zero-Order Optimization

Look mom no gradients!

Can we optimize $\min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x})$ without access to gradients?

meet the newest fanciest optimization algorithm,...
Random search

pick a random direction $\mathbf{d}_t \in \mathbb{R}^d$

$$\gamma := \operatorname*{argmin}_{\gamma\in\mathbb{R}} f(\mathbf{x}_t + \gamma\mathbf{d}_t) \qquad \text{(line-search)}$$

$$\mathbf{x}_{t+1} := \mathbf{x}_t + \gamma\mathbf{d}_t$$

Convergence Rate for Derivative-free Random Search

Theorem: Converges same as gradient descent - up to a slow-down factor d.

Proof. Assume that f is a L-smooth convex, differentiable function. For any γ, by smoothness, we have:

$$f(\mathbf{x}_t + \gamma \mathbf{d}_t) \leq f(\mathbf{x}_t) + \gamma\, \mathbf{d}_t^\top \nabla f(\mathbf{x}_t) + \frac{\gamma^2 L}{2} \|\mathbf{d}_t\|^2$$

Minimizing the upper bound, there is a step size $\bar{\gamma}$ for which

$$f(\mathbf{x}_t + \bar{\gamma} \mathbf{d}_t) \leq f(\mathbf{x}_t) - \frac{1}{L} \Big(\frac{\mathbf{d}_t^\top}{\|\mathbf{d}_t\|} \nabla f(\mathbf{x}_t) \Big)^2$$

The step size γ we actually took (based on f directly) can only be better:

$$f(\mathbf{x}_t + \gamma \mathbf{d}_t) \leq f(\mathbf{x}_t + \bar{\gamma} \mathbf{d}_t) \ .$$

Taking expectations, and using the Lemma $\mathbb{E}_{\mathbf{r}} (\mathbf{r}^\top \mathbf{g})^2 = \frac{1}{d} \|\mathbf{g}\|^2$ for $\mathbf{r} \sim$ sphere $\subseteq \mathbb{R}^d$:

$$\mathbb{E}[f(\mathbf{x}_t + \gamma \mathbf{d}_t)] \leq \mathbb{E}[f(\mathbf{x}_t)] - \frac{1}{Ld} \mathbb{E}[\|\nabla f(\mathbf{x}_t)\|^2] \ .$$

Convergence Rate for Derivative-free Random Search

Same as what we obtained for gradient descent,
now with an **extra factor of d**. d can be huge!!!

Can do the same for different function classes, as before

- For convex functions, we get a rate of $\mathcal{O}(dL/\varepsilon)$.
- For strongly convex, we get $\mathcal{O}(dL/\mu \log(1/\varepsilon))$.

Always d times the complexity of gradient descent on the function class.

credits to Moritz Hardt

Without the Linear Search: Two Function Evaluations

Without the line search, when a function can be evaluated at two points per iteration, a gradient estimate can be obtained by

$$g_\alpha(\mathbf{x}) = \frac{f(\mathbf{x} + \alpha\mathbf{u}) - f(\mathbf{x})}{2\alpha}\mathbf{u} \tag{1}$$

where $\mathbf{u}$ is a random direction sample from the normal distribution $N(0, I_d)$. This can be then used as a gradient estimate in the gradient descent update.

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta_t g_\alpha(\mathbf{x}_t) \tag{2}$$

A simplified analysis: We show a preliminary analysis of the algorithm at the limit of $\alpha \to 0$. Assuming the function f is differentiable, we have,

$$g_0(\mathbf{x}) = \left(\nabla f(\mathbf{x})^\top \mathbf{u}\right) \mathbf{u} \tag{3}$$

Simplified Analysis of the Two Function Evaluation

First note that the gradient estimate is unbiased, i.e., $\mathbb{E}[g_0(\mathbf{x})] = \nabla f(\mathbf{x})$. Hence, this Eq. (2) is equivalent to stochastic gradient descent. Next, note second moment can be bounded as follows:

$$\mathbb{E}[\|g_0(\mathbf{x})\|^2] = \mathbb{E}[\|\mathbf{u}\|^2 \nabla f(\mathbf{x})^\top \mathbf{u}\mathbf{u}^\top \nabla f(\mathbf{x})] = \nabla f(\mathbf{x})^\top \mathbb{E}[\|\mathbf{u}\|^2 \mathbf{u}\mathbf{u}^\top] \nabla f(\mathbf{x}).$$

For normal distribution $N(0, I_d)$, we have $\mathbb{E}[\|\mathbf{u}\|^2 \mathbf{u}\mathbf{u}^\top] \preccurlyeq (d+3) I_d$, hence we can write the second moment as:

$$\mathbb{E}[\|g_0(\mathbf{x})\|^2] \leqslant (d+3)\|\nabla f(\mathbf{x})\|^2.$$

In the case of stochastic gradient descent, we have studied the convergence with stochastic gradient oracle $E[\|g_t\|^2] \leqslant B$. Here, we have a *better* control on the second moment which we use in the following analysis.

Analysis of the Two Function Evaluation Method

For a L-smooth convex function f with optimum at $\mathbf{x}_*$, using the vanilla analysis,

$$\begin{aligned}\mathbb{E}[\|\mathbf{x}_{t+1} - \mathbf{x}_*\|^2 &= \|\mathbf{x}_t - \mathbf{x}_*\|^2 - 2\eta_t \mathbb{E}[g_0(\mathbf{x}_t)]^\top (\mathbf{x}_t - \mathbf{x}_*) + \eta_t^2 \mathbb{E}[\|g_0(\mathbf{x}_t)\|^2] \\ &\leq \|\mathbf{x}_t - \mathbf{x}_*\|^2 - 2\eta_t \mathbb{E}[\nabla f(\mathbf{x}_t)]^\top (\mathbf{x}_t - \mathbf{x}_*) + (d+3)\eta_t^2 \|\nabla f(\mathbf{x}_t)\|^2.\end{aligned}$$

With smoothness, we have $\|\nabla f(\mathbf{x}_t)\|^2 \leq 2L(f(\mathbf{x}_t) - f(\mathbf{x}_*))$. With convexity, we have $f(\mathbf{x}_t) - f(\mathbf{x}_*) \leq \nabla f(\mathbf{x}_t)^\top (\mathbf{x}_t - \mathbf{x}_*)$.

$$\mathbb{E}[\|\mathbf{x}_{t+1} - \mathbf{x}_*\|^2] \leq \|\mathbf{x}_t - \mathbf{x}_*\|^2 - 2\eta_t(1-(d+3)\eta_t L)(f(\mathbf{x}_t)-f(\mathbf{x}_*))$$

$$2\eta_t(1 - (d+3)\eta_t L)(f(\mathbf{x}_t) - f(\mathbf{x}_*)) \leq \|\mathbf{x}_t - \mathbf{x}_*\|^2 - \mathbb{E}[\|\mathbf{x}_{t+1} - \mathbf{x}_*\|^2],$$

$$\sum_{t=0}^{T} 2\eta_t(1 - (d+3)\eta_t L)\mathbb{E}[(f(\mathbf{x}_t) - f(\mathbf{x}_*))] \leq \|\mathbf{x}_0 - \mathbf{x}_*\|^2 - \mathbb{E}[\|\mathbf{x}_{t+1} - \mathbf{x}_*\|^2].$$

With a stepsize $\eta_t = \eta < \frac{1}{(d+3)L}$, we get a rate of convergence of $\mathcal{O}(d/T)$.

(Extra) Beyond Simplified Analysis

For the general case of gradient estimate $g_\alpha(\mathbf{x})$, a similar analysis can be following by computing the expectation and second moment as

$$\mathbb{E}[g_\alpha(\mathbf{x})] = \nabla f(\mathbf{x}) + \mathcal{O}(\alpha),$$
$$\mathbb{E}[\|g_\alpha(\mathbf{x})\|^2] \leqslant \mathcal{O}(\|\nabla f(\mathbf{x})\|^2 + \alpha^2).$$

The analysis can be followed as before with the correction terms involving α. For a careful analysis, refer to the paper [DJWW15].

Applications for Derivative-free Random Search

Applications

- can be used for **Reinforcement learning**
- memory and communication advantages: never need to store a gradient
- hyperparameter optimization, and other difficult problems like discrete optimization problems
- finding adversarial examples

Reinforcement Learning

$$\mathbf{s}_{t+1} = f(\mathbf{s}_t, \mathbf{a}_t, \mathbf{e}_t)\,.$$

where $\mathbf{s}_t$ is the state of the system, $\mathbf{a}_t$ is the control action, and $\mathbf{e}_t$ is some random noise. We assume that f is fixed, but unknown.

We search for a control 'policy'

$$\mathbf{a}_t := \pi(\mathbf{a}_1, \ldots, \mathbf{a}_{t-1}, \mathbf{s}_0, \ldots, \mathbf{s}_t)\,.$$

which takes a trajectory of the dynamical system and outputs a new control action. Want to maximize overall reward

$$\begin{aligned} \max_{\mathbf{a}_t}\ & \mathbb{E}_{\mathbf{e}_t}\Big[\sum_{t=0}^{N} R_t(\mathbf{s}_t, \mathbf{a}_t)\Big] \\ \text{s.t.}\ \ & \mathbf{s}_{t+1} = f(\mathbf{s}_t, \mathbf{a}_t, \mathbf{e}_t) \\ & (\mathbf{s}_0 \text{ given}) \end{aligned}$$

Examples: Simulations, Games (e.g. Atari), Alpha Go

Chapter XI.2

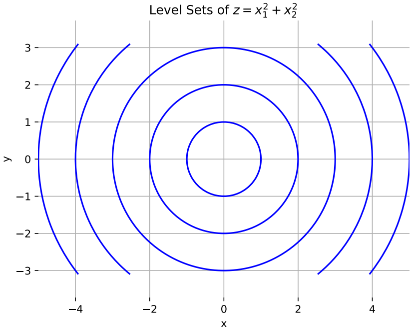
Adaptive Methods

Some problems with GD

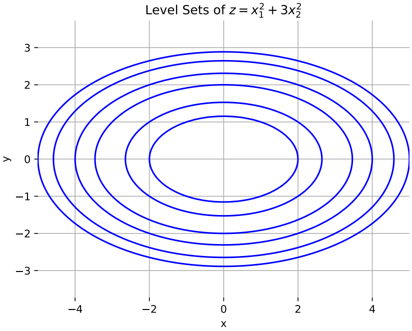
Conside the following function:

$$f(\mathbf{x}) = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix} \begin{bmatrix} \mu & 0 \\ 0 & L \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}$$

The level sets of the functions for different choices of μ and L can be seen as follows:



(a) Circular level sets when $L, \mu = 1$



(b) Elliptical level sets when $L, \mu = 3, 1$

Some problems with GD

- For skewed functions, $\mu << L$, the level sets are ellipses, in these cases GD can be very slow along some directions.
- A solution to this problem is to use a preconditioner P.

Preconditioned Gradient Descent

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta_t P_t \nabla f(\mathbf{x}_t),$$

for some semi-definite matrix P_t which is often called as preconditioner.

Intuition: Consider a function $g(\mathbf{y}) = f(R\mathbf{y})$, for some matrix R, now gradient descent on g is given by:

$$\begin{aligned}
\mathbf{y}_{t+1} &= \mathbf{y}_t - \eta_t \nabla g(\mathbf{y}_t) = \mathbf{y}_t - \eta_t R^\top \nabla f(R\mathbf{y}_t), \\
R\mathbf{y}_{t+1} &= R\mathbf{y}_t - \eta_t R R^\top \nabla f(R\mathbf{y}_t) \\
\mathbf{x}_{t+1} &= \mathbf{x}_t - \eta_t R R^\top \nabla f(\mathbf{x}_t).
\end{aligned}$$

Hence, we can choose $P_t = RR^\top$, and the preconditioned gradient descent is equivalent to the gradient descent on the function $g(\mathbf{y}) = f(R\mathbf{y})$.

How to choose the preconditioner?

- The optimal preconditioner is the inverse of the Hessian, $P = (\nabla^2 f(\mathbf{x}))^{-1}$ (similar to the Newton method).
- However, for a function f in d-dimensional space, the Hessian is a $d \times d$ matrix, making its inversion computationally expensive and often impractical.
- As a result, practical approaches rely on approximations, such as using a diagonal matrix to estimate the Hessian.

Adagrad

Adagrad is an adaptive variant of SGD.

Pick a stochastic gradient $\mathbf{g}_t$. For all i,

$$\text{Update } [G_t]_i := \sum_{s=0}^{t} ([\mathbf{g}_s]_i)^2$$

$$\text{Diagonal preconditioner: } P_t = \begin{bmatrix} \sqrt{[G_t]_1} & 0 & \cdots & 0 \\ 0 & \sqrt{[G_t]_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{[G_t]_d} \end{bmatrix}^{-1},$$

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma\, P_t\, \mathbf{g}_t, \implies [\mathbf{x}_{t+1}]_i := [\mathbf{x}_t]_i - \frac{\gamma}{\sqrt{[G_t]_i}} [\mathbf{g}_t]_i.$$

Adagrad

- chooses an adaptive, coordinate-wise learning rate
- To select the preconditioner, intutively first the Hessian is approximated by the sum of gradient outer product matrices, $G_t = \sum_{s=0}^{t} \mathbf{g}_s \mathbf{g}_s^\top$ and then only the diagonal enteries are used.
- strong performance in practice; theoretical guarantees for convergence in convex setting with better performance than GD especially for sparse gradients [DHS11]
- However, Adagrad often leads to diminishing learning rates as the aggregates square gradients, G_t, quickly become large.
- Variants: Adadelta, RMSprop, **Adam**

RMSprop

RMSprop is a variant of Adagrad that uses an exponential moving average with a parameter β of the squared gradients instead of the sum.

Pick a stochastic gradient $\mathbf{g}_t$. For all i,

$$\text{Update } [G_t]_i := (\beta)[G_{t-1}]_i + (1-\beta)([\mathbf{g}_t]_i)^2$$
$$\mathbf{x}_{t+1} := [\mathbf{x}_t]_i - \frac{\gamma}{\sqrt{[G_t]_i}}[\mathbf{g}_t]_i.$$

Momentum SGD

Before presenting Adam, lets discuss another momentum variant of SGD a classical technique propsed by Polyak in 1964 to accelerate gradient descent.

pick a stochastic gradient $\mathbf{g}_t$

$$\mathbf{m}_{t+1} := \beta \mathbf{m}_t + (1-\beta)\mathbf{g}_t \qquad \text{(momentum term)}$$

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma \mathbf{m}_{t+1}$$

(standard choice of $\mathbf{g}_t := \nabla f_j(\mathbf{x}_t)$ for sum-structured objective functions $f = \sum_j f_j$)

- momentum from previous gradients
- is a variant of the Nesterov acceleration seen before
- key element of deep learning optimizers, necessary for top accuracy

Polyak Momentum and Nesterov Acceleration

Polyak Momentum

At iteration t,

$$\mathbf{m}_{t+1} = \beta \mathbf{m}_t + \eta \nabla f(\mathbf{x}_t),$$
$$\mathbf{x}_{t+1} = \mathbf{x}_t - \mathbf{m}_{t+1}$$

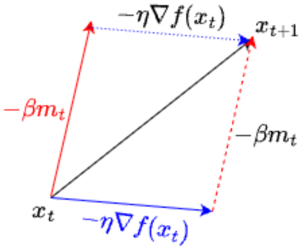


Figure: Aggregating the momentum and the gradient

Nesterov Acceleration

At iteration t,

$$\mathbf{m}_{t+1} = \beta \mathbf{m}_t + \eta \nabla f(\mathbf{x}_t - \beta \mathbf{m}_t),$$
$$\mathbf{x}_{t+1} = \mathbf{x}_t - \mathbf{m}_{t+1}$$

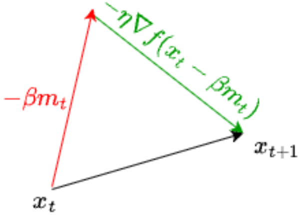


Figure: 'Look ahead' gradient. Add the momentum and take a gradient step from the new position.

Convergence of Momentum and Nesterov Acceleration

- For quadratic functions, both methods converge at an accelerated rate of $\exp\{-{}^{t}/_{\sqrt{\kappa}}\}$, where κ is the condition number of the function.
- For strongly convex functions, Nesterov acceleration converges at a rate of $\exp\{-{}^{t}/_{\kappa}\}$, while Polyak momentum does not provably converge at a faster rate.

Adam

Adam is a momentum variant of Adagrad

pick a stochastic gradient $\mathbf{g}_t$

$$\mathbf{m}_t := \beta_1 \mathbf{m}_{t-1} + (1-\beta_1)\mathbf{g}_t \qquad \text{(momentum term)}$$

$$[\mathbf{v}_t]_i := \beta_2 [\mathbf{v}_{t-1}]_i + (1-\beta_2)([\mathbf{g}_t]_i)^2 \quad \forall i \qquad \text{(2nd-order statistics)}$$

$$[\mathbf{x}_{t+1}]_i := [\mathbf{x}_t]_i - \frac{\gamma}{\sqrt{[\mathbf{v}_t]_i}} [\mathbf{m}_t]_i \quad \forall i$$

- faster forgetting of older weights
- momentum from previous gradients (see acceleration)
- (simplified version, without correction for initialization of $\mathbf{m}_0, \mathbf{v}_0$)
- strong performance in practice, e.g. for self-attention based networks like transformers

Convergence Issues with Adam

- While RMSprop and Adam solve the problem of diminishing learning rates, they can lead to convergence issues particularly due to the "short-term" memory of the exponential moving average of the squared gradients.
- EMA of the squared gradients approximately limits the update to only a few past gradients. Hence, particularly in the case where a few minibatches provide large gradients, their influence dies out quickly due to the EMA.

Convergence Issues with Adam

Problem Setup: Consider the functions $f_t(x) = \begin{cases} Cx & \text{for } t \bmod 3 = 1, \\ -x & \text{otherwise.} \end{cases}$, for $C > 2$ over the domain $\mathcal{F} = [-1, 1]$. We are interested in the following quantity (regret) over the course of optimization

$$R_T = \frac{1}{T}\sum_{t=1}^{T}(f_t(x_t)) - \frac{1}{T}\min_{x\in\mathcal{F}}\sum_{i=1}^{T} f_t(x)$$

Note that $x = -1$ gives the minimum regret, i.e., $\min\limits_{x\in\mathcal{F}} \sum_{i=1}^{T} f_t(x)$. However, Adam provably converges to highly suboptimal $x = +1$ [RKK18].

Convergence Issues with Adam

Note the gradient of the function $f_t(x)$ is given by:

$$\nabla f_t(x) = \begin{cases} C & \text{for } t \bmod 3 = 1, \\ -1 & \text{otherwise.} \end{cases} \quad ,$$

i.e., one large gradient every 3 iterations. However, the EMA of squared gradients nullify this large gradient. It can be shown that for the update of Adam,

Lemma

Consider the Adam algorithm with appropriate choice of β_1 and β_2 starting with $x_1 = 1$, then

$$x_t = 1 \textit{ for every } t \textit{ such that } t \textit{ mod } 3 = 1$$

Proof can be done by induction following [RKK18].

Convergence Issues with Adam

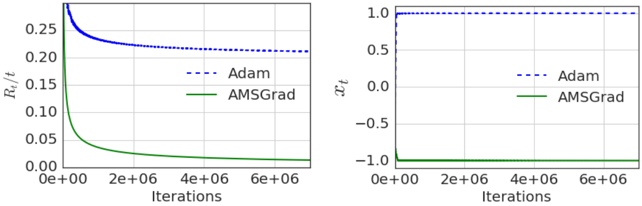


Figure: Non-convergence of ADAM on a simple one dimensional convex problem $f_t(x)$. The second plot shows that ADAM converges to $x = 1$. AMSGrad is the algorithm proposed in [RKK18]. Image is taken from [RKK18].

Chapter XI.3

Efficient variants of SGD

SignSGD

Only use the sign (one bit) of each gradient entry:
SignSGD is a communication efficient variant of SGD.

pick a stochastic gradient $\mathbf{g}_t$

$$[\mathbf{x}_{t+1}]_i := [\mathbf{x}_t]_i - \gamma_t \, sign([\mathbf{g}_t]_i) \qquad \forall i$$

(with possible rescaling of γ_t with $\|\mathbf{g}_t\|_1$)

- communication efficient for distributed training
- convergence issues

ClippedSGD

Clip the gradients to a predefined maximum length $c > 0$.

$$\begin{aligned} &\text{pick a stochastic gradient } \mathbf{g}_t \\ &\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma_t \, clip_c(\mathbf{g}_t) \qquad \forall i \end{aligned}$$

with $clip_c(\mathbf{g}) := \min\left(1, \frac{c}{\|\mathbf{g}\|}\right) \cdot \mathbf{g}$

- used to avoid instabilities in deep learning training (such as LLMs)
- used with differential privacy (adding noise of comparable magnitude)
- convergence non-trivial

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