Parameter-free Online Optimization Part 1

Francesco Orabona Ashok Cutkosky

ICML 2020

■ Most of the algorithms we know/use in machine learning have parameters

- Most of the algorithms we know/use in machine learning have parameters
 - E.g. regularization parameter in LASSO, *k* in *k*-Nearest Neighbourhood, topology of the networks in deep learning

- Most of the algorithms we know/use in machine learning have parameters
 - E.g. regularization parameter in LASSO, *k* in *k*-Nearest Neighbourhood, topology of the networks in deep learning
- Most of the time, a large enough validation set can be used to tune the parameters

- Most of the algorithms we know/use in machine learning have parameters
 - E.g. regularization parameter in LASSO, *k* in *k*-Nearest Neighbourhood, topology of the networks in deep learning
- Most of the time, a large enough validation set can be used to tune the parameters
- But, at what computational price? Are they really necessary?

- Most of the algorithms we know/use in machine learning have parameters
 - E.g. regularization parameter in LASSO, *k* in *k*-Nearest Neighbourhood, topology of the networks in deep learning
- Most of the time, a large enough validation set can be used to tune the parameters
- But, at what computational price? Are they really necessary?
- Are you ignoring some computational/sample complexities?

- Most of the algorithms we know/use in machine learning have parameters
 - E.g. regularization parameter in LASSO, *k* in *k*-Nearest Neighbourhood, topology of the networks in deep learning
- Most of the time, a large enough validation set can be used to tune the parameters
- But, at what computational price? Are they really necessary?
- Are you ignoring some computational/sample complexities?
- When is the last time you needed to tune the learning rate to invert a matrix?

How ML Should Be

- No parameters to tune
- No humans in the loop
- Some guarantees

How ML Should Be

- No parameters to tune
- No humans in the loop
- Some guarantees
- Sometimes this is possible
- This tutorial is about a method to achieve it in many interesting cases



Learning Rates are Unavoidable?

- Let's consider an example
- You have 11 real numbers $y_1, \dots y_{11}$
- We want to solve $\min_{x} \sum_{i=1}^{11} |x y_i|$
- You might use SGD
- It will converge, but you have to set a learning rate...

Learning Rates are Unavoidable?

- Let's consider an example
- You have 11 real numbers $y_1, ..., y_{11}$
- We want to solve $\min_{x} \sum_{i=1}^{11} |x y_i|$
- You might use SGD
- It will converge, but you have to set a learning rate...
- Alternative: you just need the median, so sort the numbers and pick the one in the middle...

Outline of the Tutorial

- Part 1: Stochastic and Online Convex Optimization
- Part 2: Parameter-free Convex Optimization
- Part 3: More Adaptivity and Applications
- Part 4: Implementation, Experiments, Open Problems

Learning Objectives

- Explain the problems behind learning rates
- Intuition behind recent parameter-free approaches
- Stripped-down algorithms and proofs
- Trick&tips for practical implementations

Overall, democratize these new methods and expand the number of people working in this field

Outline of the Tutorial

- Part 1: Stochastic and Online Convex Optimization
- Part 2: Parameter-free Convex Optimization
- Part 3: More Adaptivity and Applications
- Part 4: Implementation, Experiments, Open Problems

Stochastic Optimization of Convex Functions

We want to solve the problem

$$\min_{\mathbf{x}\in X} F(\mathbf{x}),$$

where F is a convex function

- We will also assume F to be G-Lipschitz, i.e., $|F(x) F(y)| \le G||x y||$
- For the most part of this tutorial, we will not assume much more than this

Stochastic Gradients

- We have access to an first-order stochastic oracle
- It gives us noisy estimate g_t of the gradient of F in a point x_t
- We will assume unbiasedness: $\mathbb{E}[\boldsymbol{g}_t|\boldsymbol{g}_1,\ldots,\boldsymbol{g}_{t-1}] = \nabla F(\boldsymbol{x}_t)$

Most of the things we say work also for non-diffentiable functions using subgradients

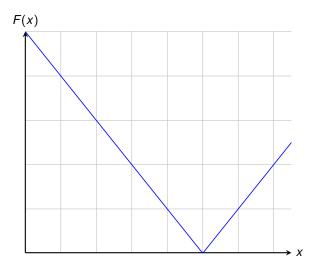
The Most Used Algorithm in ML: SGD

- The simplest algorithm that we can use in our setting is <u>Stochastic Gradient</u> <u>Descent</u> (SGD)
- Iteratively it moves in the negative direction of the gradient:

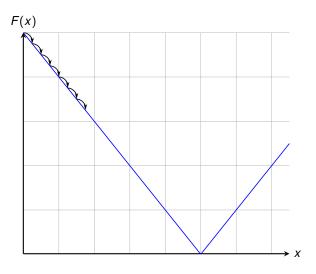
$$\boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \eta_t \boldsymbol{g}_t$$

- \blacksquare η_t is the learning rate or step size
- Choosing the correct learning rate is a black art...
- Why is it so difficult?

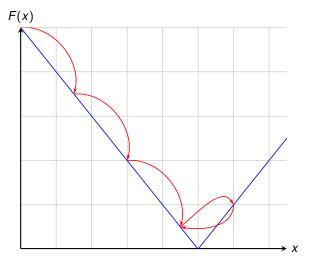
Minimize F(x) = |x - 10|



First Problem: The Learning Rate Sets Your Maximum Precision

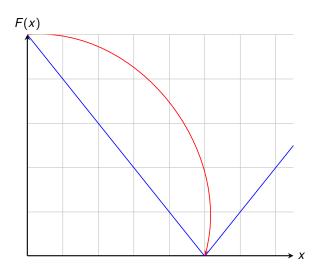


First Problem: The Learning Rate Sets Your Maximum Precision



riangle If you want to converge at least in the limit, learning rates cannot be fixed

One Jump?

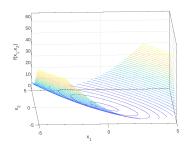


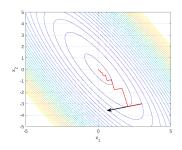
No One Jump!

- First, in the stochastic setting, line search is not possible because you do not have the exact gradient nor can you exactly compute the function value
 - You need strong assumptions (and parameters...) to make stochastic line search work [Paquette&Scheinberg, arXiv'18; Vaswani et al., NeurlPS'19]

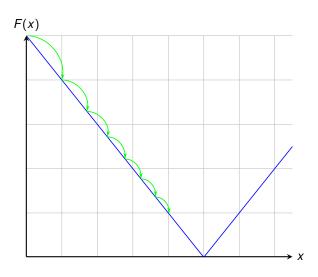
No One Jump!

- First, in the stochastic setting, line search is not possible because you do not have the exact gradient nor can you exactly compute the function value
 - You need strong assumptions (and parameters...) to make stochastic line search work [Paquette&Scheinberg, arXiv'18; Vaswani et al., NeurIPS'19]
- Even in 2d, the gradients does not necessarily point towards the minimum



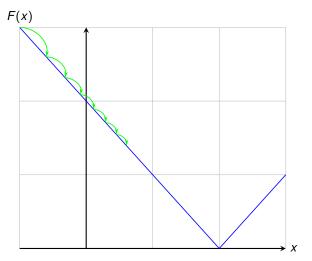


Solution: Decreasing Learning Rates



Second Problem: Distance to the Optimum

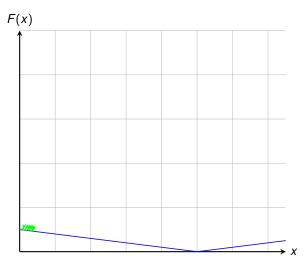
Starting from -5, our choice of the learning rate is not good anymore!



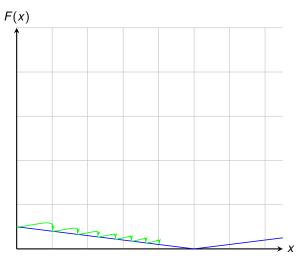
Optimal learning rate depends on distance from the optimum

Third Problem: Scale

Changing the function to 0.1|x - 10| again ruins the convergence



What About "Adaptive" Algorithms?



AdaGrad adapts to the scale of <u>each</u> coordinate, but does not adapt to distance from the optimum!

Take Home Messages on Learning Rates

Learning rates...

- ...must decrease
- ...depend on the distance to the optimal solution
- ...depend on the scale

- Use a decreasing learning rate, $\eta_t = \frac{\alpha}{\sqrt{t}}$
- Convergence after T iterations is $\mathcal{O}\left(\frac{1}{\sqrt{T}}\left(\frac{\|\mathbf{x}^{\star}-\mathbf{x}_1\|^2}{\alpha}+\alpha \mathbf{G}^2\right)\right)$
- **x*** is the best solution
- G the bound on the norm of the stochastic gradients

- Use a decreasing learning rate, $\eta_t = \frac{\alpha}{\sqrt{t}}$
- Convergence after T iterations is $\mathcal{O}\left(\frac{1}{\sqrt{T}}\left(\frac{\|\mathbf{x}^{\star}-\mathbf{x}_1\|^2}{\alpha}+\alpha \mathbf{G}^2\right)\right)$
- \mathbf{x}^{\star} is the best solution
- G the bound on the norm of the stochastic gradients
- The optimal learning rate is with $\alpha = \frac{\|\mathbf{x}^\star \mathbf{x}_1\|}{G}$ that would give a rate of $\mathcal{O}\left(\frac{G\|\mathbf{x}^\star \mathbf{x}_1\|}{\sqrt{T}}\right)$

- Use a decreasing learning rate, $\eta_t = \frac{\alpha}{\sqrt{t}}$
- Convergence after T iterations is $\mathcal{O}\left(\frac{1}{\sqrt{T}}\left(\frac{\|\mathbf{x}^{\star}-\mathbf{x}_1\|^2}{\alpha}+\alpha \mathbf{G}^2\right)\right)$
- \mathbf{x}^* is the best solution
- G the bound on the norm of the stochastic gradients
- The optimal learning rate is with $\alpha = \frac{\|\mathbf{x}^\star \mathbf{x}_1\|}{G}$ that would give a rate of $\mathcal{O}\left(\frac{G\|\mathbf{x}^\star \mathbf{x}_1\|}{\sqrt{T}}\right)$
- ...but you don't know **x***...

- Use a decreasing learning rate, $\eta_t = \frac{\alpha}{\sqrt{t}}$
- Convergence after T iterations is $\mathcal{O}\left(\frac{1}{\sqrt{T}}\left(\frac{\|\mathbf{x}^{\star}-\mathbf{x}_1\|^2}{\alpha}+\alpha \mathbf{G}^2\right)\right)$
- \mathbf{x}^* is the best solution
- G the bound on the norm of the stochastic gradients
- The optimal learning rate is with $\alpha = \frac{\|\mathbf{x}^\star \mathbf{x}_1\|}{G}$ that would give a rate of $\mathcal{O}\left(\frac{G\|\mathbf{x}^\star \mathbf{x}_1\|}{\sqrt{T}}\right)$
- ...but you don't know **x***...
- Only if the domain is bounded, you can (loosely) upper bound $\|\mathbf{x}^* \mathbf{x}_1\|$
 - Not-a-solution solution: Assume your domain is bounded or bounded iterates

I Hate Learning Rates

- Finding the right one is critical!
- The only existing solution: tries different learning rates



Theorem

lacksquare $\mathcal{O}\left(\frac{G\|\mathbf{x}^{\star}-\mathbf{x}_{1}\|}{\sqrt{T}}\right)$ cannot be achieved, unless we know $\|\mathbf{x}^{\star}-\mathbf{x}_{1}\|$

Theorem

- lacksquare $\mathcal{O}\left(\frac{G\|\mathbf{x}^{\star}-\mathbf{x}_1\|}{\sqrt{T}}\right)$ cannot be achieved, unless we know $\|\mathbf{x}^{\star}-\mathbf{x}_1\|$
- we can achieve $\mathcal{O}\left(\frac{G\|\mathbf{x}^{\star}-\mathbf{x}_1\|}{\sqrt{T}}\sqrt{\log(G\|\mathbf{x}^{\star}-\mathbf{x}_1\|\sqrt{T}+1)}+\frac{1}{T}\right)$

Theorem

- lacksquare $\mathcal{O}\left(\frac{G\|\mathbf{x}^{\star}-\mathbf{x}_1\|}{\sqrt{T}}\right)$ cannot be achieved, unless we know $\|\mathbf{x}^{\star}-\mathbf{x}_1\|$
- we can achieve $\mathcal{O}\left(\frac{G\|\mathbf{x}^{\star}-\mathbf{x}_1\|}{\sqrt{T}}\sqrt{\log(G\|\mathbf{x}^{\star}-\mathbf{x}_1\|\sqrt{T}+1)}+\frac{1}{T}\right)$
- $\bullet \text{ or } \mathcal{O}\left(\frac{G\|\boldsymbol{x}^{\star}-\boldsymbol{x}_{1}\|}{\sqrt{T}}\sqrt{\log(G\|\boldsymbol{X}^{\star}-\boldsymbol{X}_{1}\|+1)}+\tfrac{1}{\sqrt{T}}\right)$

Theorem

- lacksquare $\mathcal{O}\left(\frac{G\|\mathbf{x}^{\star}-\mathbf{x}_1\|}{\sqrt{7}}\right)$ cannot be achieved, unless we know $\|\mathbf{x}^{\star}-\mathbf{x}_1\|$
- we can achieve $\mathcal{O}\left(\frac{G\|\mathbf{x}^* \mathbf{x}_1\|}{\sqrt{T}}\sqrt{\log(G\|\mathbf{x}^* \mathbf{x}_1\|\sqrt{T} + 1)} + \frac{1}{T}\right)$
- or $O\left(\frac{G\|\mathbf{x}^{\star} \mathbf{x}_1\|}{\sqrt{T}}\sqrt{\log(G\|\mathbf{x}^{\star} \mathbf{x}_1\| + 1)} + \frac{1}{\sqrt{T}}\right)$

- The logarithmic term is the price you have to pay because you don't know how far is the optimal solution
- Think of it as the complexity of binary searching for the optimal learning rate

Our Tools

- Before solving this problem, we need some tools
- We will use Online Convex Optimization algorithms
- Online Optimization ≠ Stochastic Optimization
- Online Optimization is actually more general than Stochastic Optimization!

Online Learning

- **■** In each round, output $x_t \in X$
- Pay $\ell_t(\boldsymbol{x}_t)$
- Receive $\boldsymbol{g}_t = \nabla \ell_t(\boldsymbol{x}_t)$
- 4 Update \mathbf{x}_{t+1}

Online Learning

- 1 In each round, output $\mathbf{x}_t \in X$
- Pay $\ell_t(\boldsymbol{x}_t)$
- Receive $\boldsymbol{g}_t = \nabla \ell_t(\boldsymbol{x}_t)$
- 4 Update \mathbf{x}_{t+1}

Choose \mathbf{x}_t before observing ℓ_t

Online Learning

- **■** In each round, output $\mathbf{x}_t \in X$
- Pay $\ell_t(\boldsymbol{x}_t)$
- Receive $\boldsymbol{g}_t = \nabla \ell_t(\boldsymbol{x}_t)$
- 4 Update \mathbf{x}_{t+1}

Choose \mathbf{x}_t before observing ℓ_t No assumptions on how ℓ_t is generated!

Online Learning

- In each round, output $\mathbf{x}_t \in X$
- 2 Pay $\ell_t(\mathbf{x}_t)$
- No assumptions on how ℓ_t is generated! Receive $\mathbf{g}_t = \nabla \ell_t(\mathbf{x}_t)$

Choose \mathbf{x}_t before observing ℓ_t

4 Update \mathbf{x}_{t+1}

Regret minimization

$$\min_{\boldsymbol{x}_1,...,\boldsymbol{x}_T \in X} \ \sum_{t=1}^T \ell_t(\boldsymbol{x}_t) \qquad \text{equivalently} \qquad \min_{\boldsymbol{x}_1,...,\boldsymbol{x}_T \in X} \ \underbrace{\sum_{t=1}^T \ell_t(\boldsymbol{x}_t) - \sum_{t=1}^T \ell_t(\boldsymbol{x}^\star)}_{\text{Regret}_T(\boldsymbol{x}^\star)}$$

- Typically, we can design Online algorithms where the $Regret_T(\mathbf{x}^*) = O(\sqrt{T})$
- Harder setting, easier analysis, same results:)

[Cesa-Bianchi&Lugosi, 2006; Shalev-Shwartz, 2012; Hazan, 2016; Orabona, arXiv'19]

From Online to Stochastic (or Batch) Optimization

- 1: **for** t = 1 **to** T **do**
- 2: Get \mathbf{x}_t from Online Learning Algorithm
- 3: Receive stochastic gradient \boldsymbol{g}_t such that $\mathbb{E}_t[\boldsymbol{g}_t] = \nabla F(\boldsymbol{x}_t)$
- 4: Pass loss $\ell_t(\mathbf{x}) = \langle \mathbf{g}_t, \mathbf{x} \rangle$ to Online Learning Algorithm
- 5: end for
- 6: **return** $\bar{\boldsymbol{x}}_T = \frac{1}{T} \sum_{t=1}^T \boldsymbol{x}_t$

Theorem

$$\mathbb{E}[F(\bar{\boldsymbol{x}}_{T})] - F(\boldsymbol{x}^{\star}) \leq \frac{\mathbb{E}[Regret_{T}(\boldsymbol{x}^{\star})]}{T}$$

In words: If you have an online algorithm able to work just with <u>linear</u> losses, you have a stochastic optimization algorithm for any convex function!

[Cesa-Bianchi et al., IEEE Trans. Inf. Theory 2004]

Some Famous Online Learning Algorithms

- Online Gradient Descent [Zinkevich, ICML'03]
- AdaGrad [Duchi et al., COLT'10, JMRL'11]
- AMSGrad [Reddi et al., ICLR'18]

These algorithms are designed to work in the adversarial setting and have a $O(\sqrt{T})$ regret bound

Hence, they can also be used as stochastic optimization algorithms with a $O(\frac{1}{\sqrt{T}})$ convergence rate

Summary of Part 1

- Learning rates are difficult to set because they depends on quantities you don't know nor you can easily estimate
- In particular, the additional logarithmic dependency on the distance to the optimal solution is unavoidable
- Online Optimization gives us a set of powerful tools to attack this problem