Adaptive Optimization Methods for Machine Learning and Signal Processing

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Part III/IV: Adaptive first-order methods

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First Order Methods

Goal:

$$\min_{x \in \mathcal{X}} f(x)$$

Update rule:

$$x_{t+1} \;=\; x_t - \eta_t g_t \;; \quad \text{where} \quad \mathbb{E}[g_t | x_t] = \nabla f(x_t)$$

Output:

$$\bar{x}_T \;=\; \bar{x}_T(x_1, g_1, \ldots, x_t, g_t)$$

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After T iterations,

$$\text{err}_T = f(\bar{x}_T) - f(x^*)$$

Ensure low err_T in *expectation* or *with high probability*

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Performance Measure in Non-convex case:

After T iterations,

$$\text{err}_T = \|\nabla f(\bar{x}_T)\|^2$$

Ensure low err_T in *expectation* or *with high probability*

Geometric & Statistical Properties

- G: scale of (stochastic) gradients, $G := \max_t \|g_t\|$
- L: smoothness-Lipschitz continuity of gradients, $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$
- σ^2: variance of gradient noise, $\mathbb{E}[\|g_t - \nabla f(x_t)\|^2 | x_t] \leq \sigma^2$
  Noiseless (a.k.a determinstic) case: $\sigma = 0$
- D: distance of initial point to optimum, $\|x_1 - x^*\|$

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Prior knowledge:

◦ Problem parameters, G, L, σ^2, D **should be known in advance** to obtain the optimal rates

◦ These parameters are also required in order to efficiently parallelize the learning process

Geometric & Statistical Properties $\Rightarrow$ Convergence

Convex objective function

gradient oracle	Smoothness	**GD/SGD**
deterministic/stochastic	non-smooth	$\mathcal{O}\left(\frac{GD}{\sqrt{T}}\right)$
deterministic	smooth	$\mathcal{O}\left(\frac{LD^2}{T}\right)$
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Today:

Adaptive methods that obtain **optimal rates** without any prior knowledge
⇒ efficient and practical parallelization

Benefits of Adaptivity

- Does not require prior knowledge
- Saves expensive hyperparameter tuning
- Adapts to local structure
- Enables efficient & practical Parallelization

Large Batch Training & Parallelization

Minibatch SGD Update rule:

$$x_{t+1} = x_t - \eta_t g_t \; ; \quad \text{where } g_t \text{ is a gradient estimate based on } m \text{ samples}$$

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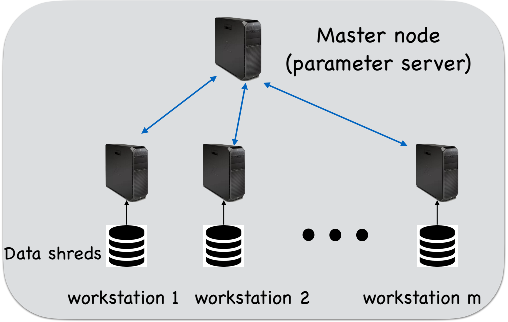

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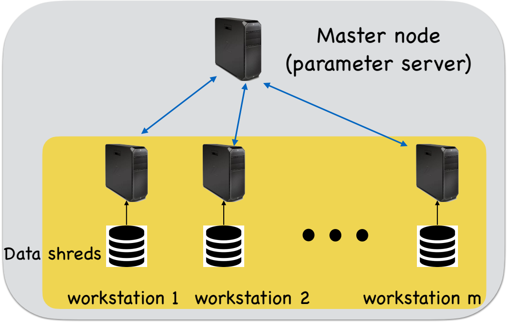

Parallel SGD using Large Batch

- Use large batch size b & Distribute computation of gradient estimate across machines

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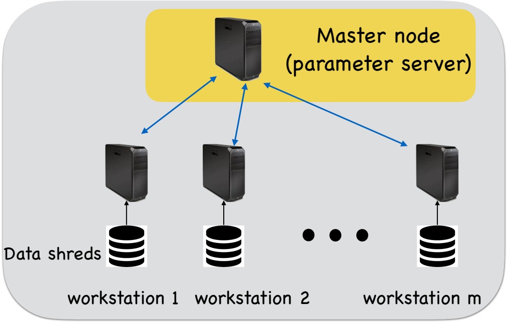

Parallel SGD using Large Batch

- Use large batch size m & Distribute computation of gradient estimate across machines
- Master node collects estimates, updates & communicates weights

When Do we Benefit From Parallelization? (when do m machines are better than a single one?)

Using m machines in parallel:

- Variance decreases: $\sigma_m = \sigma_1 / \sqrt{m}$
- At every iteration T we use minibatchsize $\propto m$ gradients $\Rightarrow$ #Samples $= mT$

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Plugging this back to the rates we have seen before:

- Non-accelerated stochastic methods, m machines,

$$\text{err}^{(\text{m})}(T) \leq \frac{L}{T} + \frac{\sigma_1}{\sqrt{mT}} \quad \Rightarrow \quad m \leq (\#\text{Samples})^{1/2} \quad \text{(Effective Parallelization)}$$

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- Accelerated stochastic methods, m machines,

$$\text{err}^{(m)}(T) \leq \frac{L}{T^2} + \frac{\sigma_1}{\sqrt{mT}} \Rightarrow m \leq (\#\text{Samples})^{3/4} \quad \text{(Effective Parallelization)}$$

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Issue

- Achieving optimal rates (& parallelization) requires tuning according to m, L, σ, D $\Rightarrow$ Impractical!
- Next: Adaptive Accelerated methods to the rescue

A classical approach: Line-search

○ High level Idea: at every step tune the learning rate until a “good" condition holds (e.g. sufficient decrease)

- Long history: Backtracking, Armijo, steepest descent...
- Nesterov has designed an accelerated and adaptive line search method[1]
- has extensions to primal-dual optimization[2]

Issues

- Line search methods are **inappropriate for stochastic** case!
- must set accuracy a priori

[1] Y. Nesterov, “Universal Gradient Methods for Convex Optimization Problems,” Mathematical Programming, 2015.

[2] A. Yurtsever, Q. Tran-Dinh, and V. Cevher, “A Universal Primal-Dual Convex Optimization Framework,” NeurIPS, 2015.

Another Approach: Polyak Stepsize

Update rule:

$$x_{t+1} \;=\; x_t - \eta_t \nabla f(x_t) \;;\quad t = 1 \ldots T$$

Polyak stepsize:

$$\eta_t = \frac{f(x_t) - f(x^*)}{\|g_t\|^2}$$

- Adaptivity: GD with Polyak stepsize is **adaptive**[1,2]. Nevertheless...
  - it is **inappropriate for stochastic** case!
  - requires prior knowledge of $f(x^*)$
  - does not obtain accelerated rates

[1] B. T. Polyak, "Introduction to optimization," Optimization Software, Inc., New York, 1987.

[2] E. Hazan, S. Kakade, "Revisiting the Polyak step size," arXiv, 2019.

The curious case of AdaGrad[1]

Algorithm: General SGD

1: **Input:** Iterations T; x_1
2: **for** $t = 1, ..., T$ **do**
3: Obtain a gradient estimate g_t
4: $x_{t+1} = x_t - \eta_t g_t$
5: **end for**
6: **Output:** $\bar{x}_T = \frac{1}{T}\sum_{t=1}^T x_t$

AdaGrad (scalar) [1]

$$\eta_t = D / \sqrt{\sum_{\tau=1}^{t} \|g_\tau\|^2}$$

AdaGrad's Adaptivity

- Non-smooth stochastic case:

$$\text{err}_T \leq GD/\sqrt{T}$$

- Smooth stochastic case:

$$\text{err}_T \leq LD^2/T + \sigma D/\sqrt{T}$$

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AdaGrad does not accelerate! $\Rightarrow$ Not ideal for parallelization

[1] J. Duchi, E. Hazan, and Y. Singer, "Adaptive subgradient methods for online learning and stochastic optimization," JMLR, 2011.

Towards an Accelerated Adaptive Method

◦ AdaGrad adapts to smoothness and noise but does not accelerate

AdaGrad: $\text{err}_T \leq LD^2/T + \sigma D/\sqrt{T}$

Optimal Accelerated rate: $\text{err}_T \leq LD^2/T^2 + \sigma D/\sqrt{T}$

Q: Can we design a method that is both **adaptive and accelerates**?

AdaGrad with Importance Weights

Update rule:

$$x_{t+1} = x_t - \eta_t \alpha_t g_t \quad \text{(Weighted Gradients)}$$

Output:

$$\bar{x}_T \propto \sum_{t=1}^{T} \alpha_t x_t \quad \text{(Weighted Average)}$$

Weighted Learning rate:

$$\eta_t = D / \sqrt{\sum_{\tau=1}^{t} \alpha_\tau^2 \|g_\tau\|^2}$$

AcceleGrad[1] Exploiting the linear coupling idea[2]

Algorithm: AcceleGrad for unconstrained optimization

1: **Input:** Iterations T; $y_0, z_0 \in \mathbb{R}^p$
2: **for** $t = 0, \ldots, T-1$ **do**
3: Obtain a gradient estimate g_t at x_t
4: $\alpha_t \approx t+1$
5: $\eta_t = D / \sqrt{G^2 + \sum_{\tau=0}^{t} \alpha_\tau^2 \|g_\tau\|^2}$
6: $x_{t+1} = \frac{1}{\alpha_t} z_t + (1 - \frac{1}{\alpha_t}) y_t,$
9: **end for**
10: **Output:** $\bar{y}_T \propto \sum_{t=1}^{T} \alpha_{t-1} y_t$

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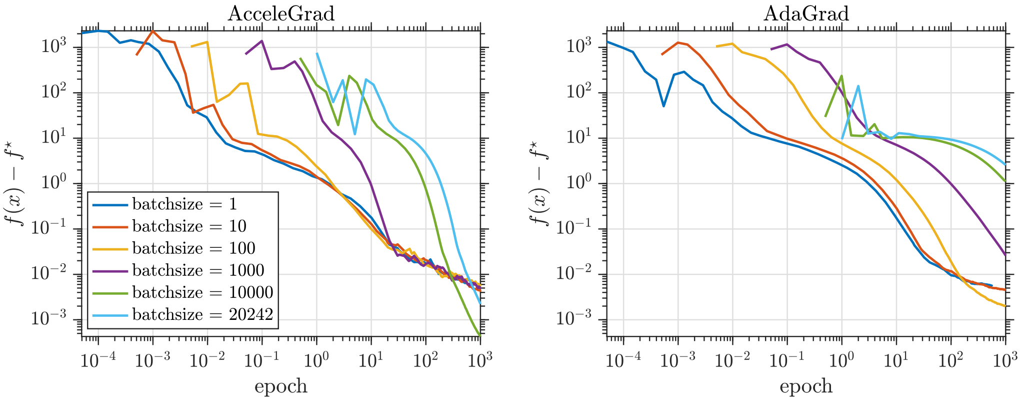
Comments

1. AcceleGrad does not require L, σ, but requires G, D
2. Cannot handle constraints!
3. Optimal Accelerated guarantees up to $\log T$ factors!
   $\Rightarrow$ practical and effective parallelization

[1] K.Y. Levy, A. Yurtsever, and V. Cevher, "Online adaptive methods, universality and acceleration," NeurIPS 2018.
[2] L. Orecchia and Z. Allen-Zhu, "Linear coupling: An ultimate unification of gradient and mirror descent," arXiv:1407.1537, 2014.

Logistic regression

- Data: RCV1
- Oracle: stochastic updates, different mini-bathcsize



Towards an Accelerated Adaptive Method

Next, new techniques for achieving adaptive acceleration for constrained problems,

- Adaptive Learning rate ✓
- Importance weighting ✓
- Mirror Prox updates $\Longleftarrow$
- Querying gradients at **averages**

Nemirovski's Mirror Prox

Mirror Prox update:

$$x_{t+1} \; = \; x_t - \eta_t h_t$$

"Good" hints:

$$\text{when } h_t \;\approx\; \nabla f(x_{t+1}) \quad \Rightarrow \quad \text{better performance}$$

Nemirovski's Mirror Prox[1]

Mirror Prox method

1. Standard GD update: $x_{t+\frac{1}{2}} = x_t - \eta_t \nabla f(x_t)$
2. Taking a hint: $h_t = \nabla f(x_{t+\frac{1}{2}})$
3. Optimistic update: $x_{t+1} = x_t - \eta_t h_t$

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Intuition:

when f is smooth $h_t \approx \nabla f(x_{t+1}) \Rightarrow$ better performance
when f is non-smooth h_t might not help, but is **does not hurt** to use it

[1] A. Nemirovski, "Prox-method with rate of convergence O(1/t) for variational inequalities with lipschitz continuous monotone operators and smooth convex-concave saddle point problems.", SIAM Journal on Optimization, 2004.

Nemirovski's Mirror Prox[1]

- Mirror Prox also works in stochastic case

Mirror Prox method

1. Standard GD update: $x_{t+\frac{1}{2}} = x_t - \eta_t g_t$
2. Taking a hint: h_t
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where,

$$\mathbb{E}[g_t|x_t] = \nabla f(x_t) \quad \& \quad \mathbb{E}[h_t|x_t] = \nabla f(x_{t+\frac{1}{2}})$$

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Towards an Accelerated Adaptive Method

◦ Combining the techniques below $\Rightarrow$ **adaptive acceleration**

- Adaptive Learning rate ✓
- Importance weighting ✓
- Optimistic updates ✓
- Querying gradients at **averages** ✓

Towards an Accelerated Adaptive Method

Algorithm: AdaGrad

1: **Input:** Iterations T; $x_1 \in \mathcal{X} \subset \mathbb{R}^d$
2: **for** $t = 1, ..., T$ **do**
3: Obtain a gradient estimate g_t at x_t
4: Set:

$$\eta_t = D / \sqrt{\sum_{\tau=1}^{t} \|g_\tau\|^2}$$

5: Update:

$$x_{t+1} = x_t - \eta_t g_t$$

6: **end for**
7: **Output:** $\bar{x}_T \propto \sum_{t=1}^{T} x_t$

- Adaptive Learning rate ✓
- Importance weighting
- Optimistic updates
- Querying gradients at **averages**

Towards an Accelerated Adaptive Method

Algorithm: Weighted AdaGrad

Input: Iterations T; $x_1 \in \mathcal{X} \subset \mathbb{R}^d$
for $t = 1, ..., T$ **do**
Set weight $\alpha_t = t$
Obtain a gradient estimate g_t at x_t
Set:

$$\eta_t \;=\; D/\sqrt{\sum_{\tau=1}^{t} \alpha_\tau^2 \|g_\tau\|^2}$$

Update:

$$x_{t+1} \;=\; x_t - \eta_t \alpha_t g_t$$

end for
Output: $\bar{x}_T \;\propto\; \sum_{t=1}^{T} \alpha_t x_t$

- Adaptive Learning rate ✓
- Importance weighting ✓
- Optimistic updates
- Querying gradients at **averages**

Towards an Accelerated Adaptive Method

Algorithm: Mirror Prox Weighted AdaGrad

Input: Iterations T; $x_1 \in \mathcal{X} \subset \mathbb{R}^d$

for $t = 1, ..., T$ **do**

Set weight $\alpha_t = t$

Obtain a gradient estimate g_t at x_t

Set:

$$\eta_t = D / \sqrt{1 + \sum_{\tau=1}^{t-1} \alpha_\tau^2 \|g_\tau - h_\tau\|^2}$$

Update:

$$x_{t+\frac{1}{2}} = x_t - \eta_t \alpha_t g_t$$

Compute h_t an unbiased gradient estimate at $x_{t+\frac{1}{2}}$

$$x_{t+1} = x_t - \eta_t \alpha_t h_t$$

end for

Output: $\bar{x}_T \propto \sum_{t=1}^T \alpha_t x_t$

UnixGrad - Universal eXtra Gradient method

Algorithm: UnixGrad[1] = Anytime Optimistic Weighted AdaGrad

Input: Iterations T; $x_1 \in \mathcal{X} \subset \mathbb{R}^d$, weights $\alpha_t = t$

for $t = 1, ..., T$ **do**

Obtain a gradient estimate g_t at $\bar{x}_t \propto \alpha_t x_t + \sum_{\tau=1}^{t-1} \alpha_\tau x_{\tau+\frac{1}{2}}$

Set:

$$\eta_t = D / \sqrt{1 + \sum_{\tau=1}^{t-1} \alpha_\tau^2 \|g_\tau - h_\tau\|^2}$$

Update:

$$x_{t+\frac{1}{2}} = x_t - \eta_t \alpha_t g_t$$

Compute h_t an unbiased gradient estimate at $\bar{x}_{t+\frac{1}{2}} \propto \alpha_t x_{t+\frac{1}{2}} + \sum_{\tau=1}^{t-1} \alpha_\tau x_{\tau+\frac{1}{2}}$

$$x_{t+1} = x_t - \eta_t \alpha_t h_t$$

end for

Output: $\bar{x}_{T+\frac{1}{2}} \propto \sum_{t=1}^{T} \alpha_t x_{t+\frac{1}{2}}$

[1] A. Kavis, K.Y. Levy, F. Bach, and V. Cevher, "Unixgrad: A universal, adaptive algorithm with optimal guarantees for constrained optimization." NIPS, 2019.

UnixGrad - an Adaptive Accelerated Optimal Method

- UnixGrad ensures optimal guarantees,
  1. $\mathcal{O}\left(GD/\sqrt{T}\right)$ - non-smooth deterministic/stochastic
  2. $\mathcal{O}\left(LD^2/T^2\right)$ - smooth deterministic case
  3. $\mathcal{O}\left(LD^2/T^2 + \sigma D/\sqrt{T}\right)$ - smooth stochastic case

- Comments:
  - UnixGrad adapts to G, L, σ^2, but requires a bound on D
  - UnixGrad can be applied to **constrained** problems
  - No guarantees for non-convex problems!

[1] A. Kavis, K.Y. Levy, F. Bach, and V. Cevher, "Unixgrad: A universal, adaptive algorithm with optimal guarantees for constrained optimization." NIPS, 2019.

Neural network training: ADAM vs. AcceleGrad

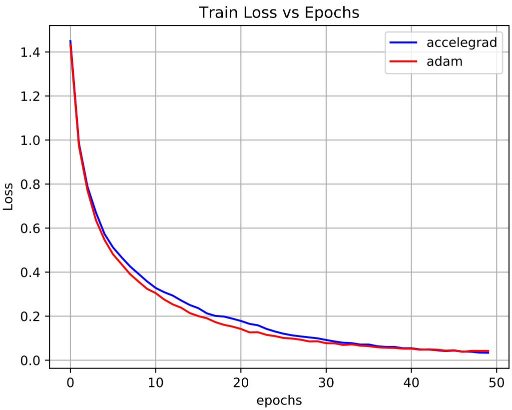

Figure: Resnet classifier optimization (train loss)

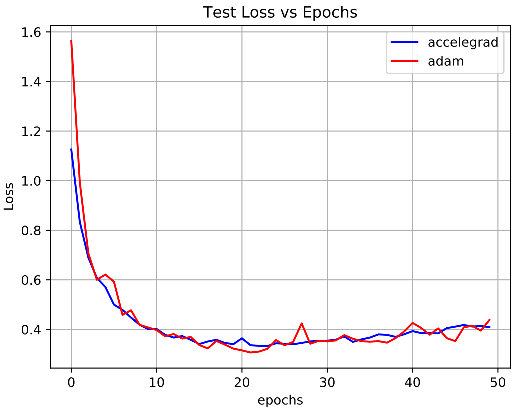

Figure: Resnet classifier optimization (test loss)

Conclusions

◦ Adaptive accelerated methods ⇒ practical and efficient acceleration. Still...lots of interesting questions.

Adaptive methods for non-convex problems,

- AdaGrad adapts to smoothness and noise in non-convex problems[1].
  Can we design an accelerated adaptive method?
- Can we design adaptive methods that provide stronger guarantees rather than stationarity?
- Is there a prevalent non-convex structure that we can adaptively exploit? (other than smoothness and noise)

Strong-convexity is a property that often arises in regularized problems, Simple algorithms automatically adapt to strong convexity under broad assumptions

- GD achieves linear rate with $\eta = 1/L$, & SGD achieves $\mathcal{O}(1/T)$-rate with $\eta_t = \mathcal{O}(1/t)$
- PDHG achieves linear rate under metric subregularity[2,3,4]

◦ Adaptive methods are promising but are not yet truly universal...

- AdaGrad/Accelegrad/UniXgrad does not adapt to strong convexity
- Adam-type does not adapt to strong convexity
- MetaGrad comes close but is not universal yet[5]

◦ Still seeking one algorithm to rule them all!

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