First TRIPODS Summer School
Stochastic Gradient Descent, AdaGrad, & Co.

Francesco Orabona, Boston University

Content:

- Stochastic Gradient Descent
- Adaptive Stepsizes
- AdaGrad

Sources:

- See papers in the text

Disclaimer

- We will only see the easy proofs, that means strong assumptions will be used
- Stronger results do exist, but the proofs are long and boring

Unconstrained Convex Optimization

Unconstrained convex optimization problem

$$\min_{\boldsymbol{w} \in \mathbb{R}^d} \qquad f(\boldsymbol{w})$$

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$\boldsymbol{w}$ is a global minimizer if and only if $\nabla f(\boldsymbol{w}) = \mathbf{0}$

Unfortunately, can't always find closed-form solution to system of equations $\nabla f(\boldsymbol{w}) = \mathbf{0}$ $\Rightarrow$ Resort to iterative methods to find a solution.

Gradient descent for differentiable objectives

- Start with some initial $\boldsymbol{w}_1 \in \mathbb{R}^d$
- For $t = 1, 2, \ldots$ until some stopping condition is satisfied
  - Compute gradient of f at $\boldsymbol{w}_t$:
  $$\boldsymbol{g}_t := \nabla f(\boldsymbol{w}_t)$$
  - Update:
  $$\boldsymbol{w}_{t+1} := \boldsymbol{w}_t - \eta_t \boldsymbol{g}_t$$
- Output: $\boldsymbol{w}_T$

Subgradient Descent

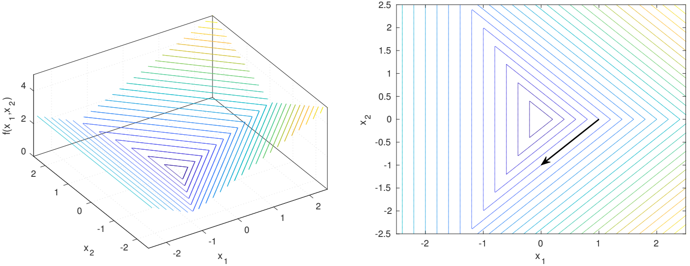
Subgradient Descent

- Start with some initial $\boldsymbol{w}_1 \in \mathbb{R}^d$
- For $t = 1, 2, \ldots, T$
  - Get subgradient $\boldsymbol{g}_t$ of f at $\boldsymbol{w}_t$, i.e. $\boldsymbol{g}_t \in \partial f(\boldsymbol{w}_t)$
  - Update:

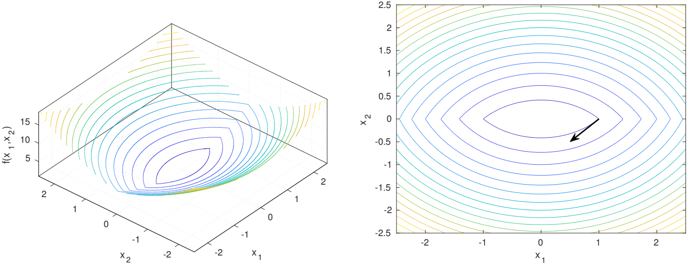
$$\boldsymbol{w}_{t+1} := \boldsymbol{w}_t - \eta_t \boldsymbol{g}_t$$

- Output: $\boldsymbol{w}_T$ or $\bar{\boldsymbol{w}} = \frac{1}{T} \sum_{t=1}^{T} \boldsymbol{w}_t$

Subgradient Descent is not a Descent Method

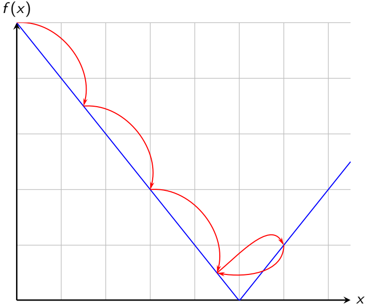


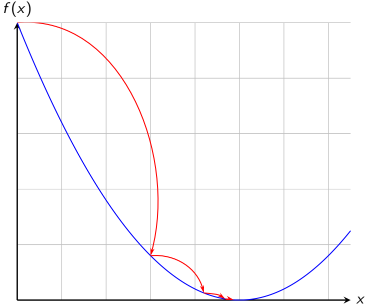
3D plot (left) and level sets (right) of $f(\boldsymbol{x}) = \max[-x_1, x_1 - x_2, x_1 + x_2]$



3D plot (left) and level sets (right) of $f(\boldsymbol{x}) = \max[x_1^2 + (x_2+1)^2, x_1^2 + (x_2-1)^2]$

Decreasing Stepsizes/Learning Rates





The effect of a constant stepsize on non-differentiable (left) and smooth (right) functions

Stochastic Subgradient Descent

- Start with some initial $\boldsymbol{w}_1 \in \mathbb{R}^d$
- For $t = 1, 2, \ldots, T$
  - Get stochastic subgradient $\boldsymbol{g}_t$ of f at $\boldsymbol{w}_t$ such that
    $$\mathbb{E}[\boldsymbol{g}_t] \in \partial f(\boldsymbol{w}_t)$$
  - Update:
    $$\boldsymbol{w}_{t+1} := \boldsymbol{w}_t - \eta_t \boldsymbol{g}_t$$
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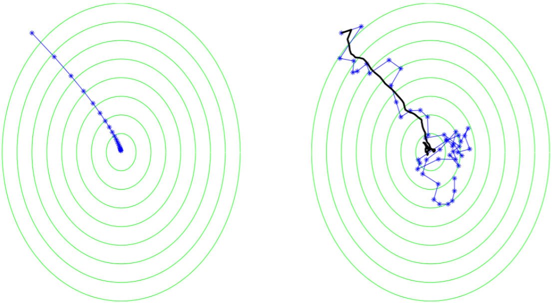
SGD is More "Unstable"



Analyzing SGD for Convex Functions (1)

For any sequence of $\boldsymbol{g}_1, \cdots, \boldsymbol{g}_T$, any $\eta_1, \cdots, \eta_T > 0$, and any $\boldsymbol{w}^\star$, we have

$$\eta_t \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t \rangle = \frac{\|\boldsymbol{w}_t - \boldsymbol{w}^\star\|^2 - \|\boldsymbol{w}_{t+1} - \boldsymbol{w}^\star\|^2}{2} + \frac{\eta^2}{2}\|\boldsymbol{g}_t\|^2$$

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Considering a constant stepsize η, diving by η, and summing we have

$$\sum_{t=1}^{T} \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t \rangle = \frac{\|\boldsymbol{w}_1 - \boldsymbol{w}^\star\|^2 - \|\boldsymbol{w}_{T+1} - \boldsymbol{w}^\star\|^2}{2\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \|\boldsymbol{g}_t\|^2$$

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Assume that $\|\boldsymbol{g}_t\| \leq L$ for all t, $\boldsymbol{w}_1 = \boldsymbol{0}$, and that $\|\boldsymbol{w}^\star\| \leq B$ we obtain

$$\sum_{t=1}^{T} \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t \rangle \leq \frac{B^2}{2\eta} + \frac{\eta L^2 T}{2}$$

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In particular, for $\eta = \sqrt{\frac{B^2}{L^2 T}}$ we get

$$\sum_{t=1}^T \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t \rangle \leq BL\sqrt{T}$$

Analyzing SGD for Convex Functions (2)

Taking expectation of both sides w.r.t. the randomness of choosing $\boldsymbol{g}_1, \cdots, \boldsymbol{g}_T$ we obtain:

$$\mathbb{E}_{\boldsymbol{g}_1, \cdots, \boldsymbol{g}_T}\left[\sum_{t=1}^{T} \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t \rangle\right] \leq BL\sqrt{T}$$

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The law of total expectation: for every two random variables α, β, and a function h, $\mathbb{E}_\alpha[h(\alpha)] = \mathbb{E}_\beta E_\alpha[h(\alpha)|\beta]$. Therefore

$$\mathbb{E}_{\boldsymbol{g}_1, \cdots, \boldsymbol{g}_T}[\langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t\rangle] = \mathbb{E}_{\boldsymbol{g}_1, \cdots, \boldsymbol{g}_{t-1}}\mathbb{E}_{\boldsymbol{g}_t, \cdots, \boldsymbol{g}_T}[\langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t\rangle | \boldsymbol{g}_1, \cdots, \boldsymbol{g}_{t-1}]$$

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Once we know $\boldsymbol{g}_1, \cdots, \boldsymbol{g}_{t-1}$ the value of $\boldsymbol{w}_t$ is not random, hence,

$$\begin{aligned}\mathbb{E}_{\boldsymbol{g}_t,\cdots,\boldsymbol{g}_T}[\langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t\rangle|\boldsymbol{g}_1,\cdots,\boldsymbol{g}_{t-1}] &= \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \mathbb{E}_{\boldsymbol{g}_t,\cdots,\boldsymbol{g}_T}[\boldsymbol{g}_t]\rangle \\ &= \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \mathbb{E}_{\boldsymbol{g}_t}[\boldsymbol{g}_t]\rangle \\ &= \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \nabla f(\boldsymbol{w}_t)\rangle\end{aligned}$$

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By the defintion of subgradient, this means

$$\mathbb{E}_{\boldsymbol{g}_1,\cdots,\boldsymbol{g}_T}\left[\sum_{t=1}^{T}(f(\boldsymbol{w}_t) - f(\boldsymbol{w}^\star))\right] \leq BL\sqrt{T}$$

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Very slow convergence, but very low per-step complexity!

- $$\min_{\boldsymbol{w} \in \mathcal{F}} L_S(w) \text{ where } L_S(\boldsymbol{w}) = \frac{1}{m} \sum_{i=1}^{m} \ell(p(\boldsymbol{w}, \boldsymbol{x}_i), y_i)$$

Stochastic Gradient Descent for Machine Learning

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- We just showed that this is good enough!

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- In expectation, nothing changes for any choice of n, but...
- ...the variance decreases with n
- ...the time to calculate the approximation grows with n

SGD Guarantee for Convex ERM Problems

Corollary

Consider a convex ERM problem, L-Lipschitz and with the domain of diameter B. Then, if we run the SGD method for minimizing $L_S(\boldsymbol{w})$ with T iterations and with $\eta = \sqrt{\frac{B^2}{L^2 T}}$, then the output of SGD satisfies:

$$\mathbb{E}[L_S(\bar{\boldsymbol{w}})] \leq \min_{\boldsymbol{w} \in \mathcal{F}} L_S(\boldsymbol{w}) + \frac{BL}{\sqrt{T}}$$

In words, we minimize the empirical risk (but, we still have to hope that this will give us small true risk...)

Learning *Directly* with Stochastic Gradient Descent

- Consider a learning problem
- Recall: our goal is to (probably approximately) solve:

$$\min_{\boldsymbol{w} \in \mathcal{F}} L_{\mathcal{D}}(\boldsymbol{w}) \text{ where } L_{\mathcal{D}}(\boldsymbol{w}) = \mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}[\ell(p(\boldsymbol{w},\boldsymbol{x}),y)]$$

- So far, learning was based on the empirical risk, $L_S(\boldsymbol{w})$

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- So far, learning was based on the empirical risk, $L_S(\boldsymbol{w})$
- Can we minimize directly $L_{\mathcal{D}}(\boldsymbol{w})$?

Stochastic Gradient Descent for Learning

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- Again, we can use a mini-batch

Stochastic Gradient Descent for Learning

$$\min_{\boldsymbol{w} \in \mathcal{F}} L_{\mathcal{D}}(w) \text{ where } L_{\mathcal{D}}(\boldsymbol{w}) = \mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}[\ell(p(\boldsymbol{w},\boldsymbol{x}),y)]$$

- Gradient descent on the true risk: $\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \eta \nabla L_{\mathcal{D}}(\boldsymbol{w}_t)$
- Observe: $\nabla L_{\mathcal{D}}(\boldsymbol{w}_t) = \mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}[\nabla \ell(p(\boldsymbol{w},\boldsymbol{x}),y)]$
- We cannot calculate $\nabla L_{\mathcal{D}}(\boldsymbol{w}_t)$ because we do not know $\mathcal{D}$
- But we can estimate it by $\nabla \ell(p(\boldsymbol{w},\boldsymbol{x}),y)$ for $(\boldsymbol{x},y) \sim \mathcal{D}$
- Again, we can use a mini-batch
- Once again, we already showed that this is good enough!

Corollary

Consider a convex learning problem, L-Lipschitz and with the domain of diameter B. Then, if we run the SGD method to minimize $L_{\mathcal{D}}(\boldsymbol{w})$ with T iterations (i.e. number of examples) and with $\eta = \sqrt{\frac{B^2}{L^2 T}}$, then the output of SGD satisfies:

$$\mathbb{E}[L_{\mathcal{D}}(\bar{\boldsymbol{w}})] \leq \min_{\boldsymbol{w} \in \mathcal{F}} L_{\mathcal{D}}(\boldsymbol{w}) + \frac{BL}{\sqrt{T}}$$

In words, we minimize the true risk!

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- In this view, SGD is computationally optimal [Bottou&Bousquet, NIPS'08]

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Practical Considerations for Convex Problems with Enough Data

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- If you do not want learning rates at all, google "parameter-free online optimization"

Example: Soft-Margin SVM (without Offset)

$$\min_{\boldsymbol{w} \in \mathbb{R}^d} \qquad f(\boldsymbol{w}) := \frac{\lambda}{2} \|\boldsymbol{w}\|_2^2 + \frac{1}{|S|} \sum_{(\boldsymbol{x},y) \in S} [1 - y\langle \boldsymbol{w}, \boldsymbol{x} \rangle]_+$$

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In practice, usually don't have examples with $y\langle \boldsymbol{w}, \boldsymbol{x} \rangle = 1$ *exactly* anyway

Subgradient descent algorithm for soft-margin SVM:

- Start with some initial $\boldsymbol{w}_1 \in \mathbb{R}^d$.
- For $t = 1, 2, \ldots$ until some stopping condition is satisfied

$$\boldsymbol{w}_{t+1} := \boldsymbol{w}_t - \eta_t \left(\lambda \boldsymbol{w}_t + \frac{1}{|S|} \sum_{(\boldsymbol{x},y) \in S} \begin{cases} \boldsymbol{0} & \text{if } 1 - y\langle \boldsymbol{w}_t, \boldsymbol{x} \rangle < 0; \\ -y\boldsymbol{x} & \text{if } 1 - y\langle \boldsymbol{w}_t, \boldsymbol{x} \rangle \geq 0 \end{cases} \right)$$

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- Optimal stepsize $\eta_t = \frac{1}{\lambda t}$ gives the Pegasos algorithm [Shalev-Shwartz et al. ICML'07]

Adaptive Stepsizes

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Nobody wants to tune the learning rates/stepsizes!

Adaptive algorithms:

- AdaGrad [Duchi et al. COLT'10]
- AdaDelta [Zeiler. ArXiv'12]
- RMSProp [Tieleman&Hinton. Coursera slide'12]
- Adam [Kingma&Ba. ICLR'15]
- ...

Let's consider again

$$f\left(\frac{1}{T}\sum_{t=1}^{T} \boldsymbol{w}_t\right) - f(\boldsymbol{w}^\star) \leq \frac{\frac{B^2}{2\eta} + \frac{\eta}{2}\sum_{t=1}^{T} \|\boldsymbol{g}_t\|^2}{T}$$

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- But, we should know the future!

Approximating the Future

- Let's approximate the optimal stepsize with something we can calculate [Auer et al. 2002]
- Instead of $\eta = \frac{B}{\sqrt{\sum_{i=1}^{T} \|\boldsymbol{g}_i\|^2}}$ let's use $\eta_t = \frac{B}{\sqrt{\sum_{i=1}^{t} \|\boldsymbol{g}_i\|^2}}$
- Let's prove that it works!

Adding Projections to the Algorithm

Projected Stochastic Subgradient Descent

- Start with some initial $\boldsymbol{w}_1 \in V$, V convex set
- For $t = 1, 2, \ldots, T$
  - Get stochastic subgradient $\boldsymbol{g}_t$ of f at $\boldsymbol{w}_t$ such that
$$\mathbb{E}[\boldsymbol{g}_t] \in \partial f(\boldsymbol{w}_t)$$
  - Update:
$$\boldsymbol{w}_{t+1} := \Pi_V(\boldsymbol{w}_t - \eta_t \boldsymbol{g}_t)$$
- Output: $\boldsymbol{w}_T$ or $\bar{\boldsymbol{w}} = \frac{1}{T}\sum_{t=1}^{T} \boldsymbol{w}_t$

$$\Pi_V(\boldsymbol{w}) = \arg\min_{\boldsymbol{v} \in V} \|\boldsymbol{w} - \boldsymbol{v}\|_2$$

$$\eta_t \langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t \rangle \leq \frac{\|\boldsymbol{w}_t - \boldsymbol{w}^\star\|^2 - \|\boldsymbol{w}_{t+1} - \boldsymbol{w}^\star\|^2}{2} + \frac{\eta^2}{2} \|\boldsymbol{g}_t\|^2$$

Denote $\Delta_t = \|\boldsymbol{w}_t - \boldsymbol{w}^\star\|^2$, divide by η_t and sum

where we assumed V to have diameter B

Zinchevich's Proof [Zinchevich, ICML'03]

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&= \frac{B^2}{2\eta_T} + \sum_{t=1}^{T}\frac{\eta_t}{2}\|\boldsymbol{g}_t\|^2
\end{aligned}$$

where we assumed V to have diameter B

The Approximation Works

A useful lemma:

$$\sum_{t=1}^{T} \frac{a_t}{\sqrt{\sum_{i=1}^{t} a_t}} \leq 2\sqrt{\sum_{t=1}^{T} a_t}$$

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Hence

$$f\left(\frac{1}{T}\sum_{t=1}^{T} \boldsymbol{w}_t\right) - f(\boldsymbol{w}^\star) \leq \sqrt{2}\frac{B\sqrt{\sum_{t=1}^{T} \|\boldsymbol{g}_t\|^2}}{T}$$

- Only $\sqrt{2}$ worse than knowing the future!
- Similar proof with stochastic subgradients

Adaptation to Subgradients Implies Adaptation to Noise (1)

Let's now assume that

- ∇f is M-Lipschitz $\Rightarrow \|\nabla f(\boldsymbol{w})\|^2 \leq 2M(f(\boldsymbol{w}) - f(\boldsymbol{w}^\star))$
- $\mathbb{E}_t[\boldsymbol{g}_t] = \nabla f(\boldsymbol{w}_t)$
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$$\sum_{t=1}^{T} \mathbb{E}[f(\boldsymbol{w}_t)] - f(\boldsymbol{w}^\star) \leq \sqrt{2}B\sqrt{\sum_{t=1}^{T} \mathbb{E}[\|\boldsymbol{g}_t\|^2]}$$

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&\leq \sqrt{2}B\sqrt{T\sigma^2 + 2M\sum_{t=1}^{T}(\mathbb{E}[f(\boldsymbol{w}_t)] - f(\boldsymbol{w}^\star))}
\end{aligned}
$$

Adaptation to Subgradients Implies Adaptation to Noise (2)

$$\sum_{t=1}^{T} \mathbb{E}[f(\boldsymbol{w}_t)] - f(\boldsymbol{w}^\star) \le \sqrt{2}B\sqrt{T\sigma^2 + 2M\sum_{t=1}^{T}(\mathbb{E}[f(\boldsymbol{w}_t)] - f(\boldsymbol{w}^\star))}$$

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implies

$$\sum_{t=1}^{T} \mathbb{E}[f(\boldsymbol{w}_t)] - f(\boldsymbol{w}^\star) \leq B\sigma\sqrt{T} + 4MB^2$$

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- If $\sigma > 0$ we will converge as $O(\frac{1}{\sqrt{T}})$
- If $\sigma = 0$ we will converge as $O(\frac{1}{T})$
- The algorithm adapts to the level of noise

Folklore, e.g. [Li&Orabona, ArXiv'18]

AdaGrad

AdaGrad [Duchi et al. COLT'10]

We can think to use the previous stepsize for each single coordinate!
Proof is easy, for each coordinate j we have $\eta_{t,j} = \frac{\sqrt{2}B}{2\sqrt{\sum_{i=1}^{t} g_{i,j}^2}}$

$$\sum_{t=1}^{T}(w_{t,j} - w_j^\star)g_{t,j} \leq \sqrt{2}B_i\sqrt{\sum_{t=1}^{T} g_{t,j}^2}$$

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Summing over the coordinate we have

$$\sum_{t=1}^{T}\langle \boldsymbol{w}_t - \boldsymbol{w}^\star, \boldsymbol{g}_t\rangle = \sum_{j=1}^{d}\sum_{t=1}^{T}(w_{t,j} - w_j^\star)g_{t,j} \leq \sqrt{2}\sum_{j=1}^{d} B_i \sqrt{\sum_{t=1}^{T} g_{t,j}^2}$$

$$\leq \sqrt{2}B_\infty \sum_{j=1}^{d} \sqrt{\sum_{t=1}^{T} g_{t,j}^2}$$

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So, as before,

$$f\left(\frac{1}{T}\sum_{t=1}^{T}\boldsymbol{w}_t\right) - f(\boldsymbol{w}^\star) \leq \frac{\sqrt{2}B_\infty \sum_{j=1}^{d}\sqrt{\sum_{t=1}^{T} g_{t,j}^2}}{T}$$

Is AdaGrad Always a Good Idea?

Adaptive bound

$$f\left(\frac{1}{T}\sum_{t=1}^{T}\boldsymbol{w}_t\right) - f(\boldsymbol{w}^\star) \leq \sqrt{2}\frac{B\sqrt{\sum_{t=1}^{T}\|\boldsymbol{g}_t\|^2}}{T}$$

AdaGrad

$$f\left(\frac{1}{T}\sum_{t=1}^{T}\boldsymbol{w}_t\right) - f(\boldsymbol{w}^\star) \leq \frac{\sqrt{2}B_\infty \sum_{j=1}^{d}\sqrt{\sum_{t=1}^{T} g_{t,j}^2}}{T}$$

- It depends on B vs B_∞ and the gradients
- Hypercubes are better for AdaGrad
- Balls are better for adaptive
- Sparse gradients are better for AdaGrad

AdaGrad is Scale-free

- Having a gradient vector whose coordinates have vastly different magnitude is a problem
  - Bad "condition number"
  - Related to vanishing gradient in DNN
- Important observation: AdaGrad does not depend on the scale of each single coordinate of the gradients!
- AdaGrad is scale-free [Orabona&Pal, ALT'15]

General Recipe for Adaptive Algorithms

- Find a tight convergence bound that depends on an unknown hyperparameter
- Find the optimal setting of that hyperparameter
- Approximate it
- Try to prove a convergence rate for the approximated version