Adaptive Subgradient Methods for Stochastic Optimization

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Outline

- Stochastic (sub)gradient methods
 - Formulations
 - Limitations
- Adaptive stochastic (sub)gradient methods (AdaGrad)
 - Formulations
 - Interpretations
 - Theoretical Guarantees
- Empirical comparison

Stochastic (Sub)gradient Methods

Notations

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w_t - model parameter at the t\text{-th} step
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$$g_{t}$$
 - (sub)gradient at the t -th step, i.e. $g_{t} \in \partial_{w} f_{t}\left(w\right)$

 \mathcal{W} - feasible domain for w

 η_0 - learning rate

Stochastic (sub)gradient method (SGD¹)

$$w_{t+1} = \Pi_{\mathcal{W}} (w_t - \eta_0 g_t) = \underset{w \in \mathcal{W}}{\operatorname{argmin}} \|w - (w_t - \eta_0 g_t)\|_2^2$$
 (1)

- ullet Tricky to find a good learning rate η_0
- Implicitly presumes the data geometry to be isotropic

¹strictly speaking, SGD is subsumed by stochastic subgradient methods

Limitation of SGD

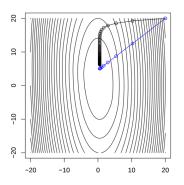


Figure : SGD (black) may suffer from inappropriate isotropic assumption about the data geometry

—Is it possible to probe the underlying geometry during stochastic updates, and carry out correction in favor of SGD?

http://www.stat.cmu.edu/~ryantibs/convexopt-S15/lectures/ 14-newton.pdf

AdaGrad - A Geometric Interpretation

AdaGrad [Duchi et al., 2011]:

Making SGD adaptive to the data geometry

$$w_{t+1} = \prod_{W}^{G_t^{\frac{1}{2}}} \left(w_t - \eta_0 G_t^{-\frac{1}{2}} g_t \right)$$

$$= \underset{w \in \mathcal{W}}{\operatorname{argmin}} \left\| w - \left(w_t - \eta_0 G_t^{-\frac{1}{2}} g_t \right) \right\|_{G^{\frac{1}{2}}}^{2}$$
(3)

where $G_t := \sum_{\tau=0}^t g_\tau g_\tau^\top$ is a covariance matrix estimated from historical subgradients for 2nd-order correction

• Similar in spirit to quasi-Newton SGD [Bordes et al., 2009]—

$$w_{t+1} = \Pi_{\mathcal{W}}^{\tilde{H}_t} \left(w_t - \eta_0 \tilde{H}_t^{-1} g_t \right) \tag{4}$$

• But is more widely applicable, e.g., to nonsmooth problems

AdaGrad - Approximation

Full AdaGrad:
$$w_{t+1} = \overset{G_t^{\frac{1}{2}}}{\Pi_{\mathcal{W}}} \left(w_t - \eta_0 G_t^{-\frac{1}{2}} g_t \right)$$

- ullet Problem: $G_t^{rac{1}{2}}$ is computationally impractical for large p.
- Workaround: replace G_t with its diagonal:

$$w_{t+1} = \Pi_{\mathcal{W}}^{\operatorname{diag}(G_t)^{\frac{1}{2}}} \left(w_t - \eta_0 \operatorname{diag}(G_t)^{-\frac{1}{2}} g_t \right)$$
 (5)

$$= \prod_{\mathcal{W}}^{\operatorname{diag}(G_t)^{\frac{1}{2}}} \left(w_t - \eta_t' \odot g_t \right) \tag{6}$$

 $\eta_t' \in \mathbb{R}^p$: learning rates adapted to different dimensions

$$\eta'_{t,j} = \frac{\eta_0}{\sqrt{\sum_{t=0}^t g_{\tau,j}^2}} \qquad j = 1, 2, \dots p$$
 (7)

AdaGrad - An Alternative Interpretation

Per-feature learning rate:
$$\eta_{t,j}' = \eta_0 / \sqrt{\sum_{\tau=0}^t g_{\tau,j}^2}$$

AdaGrad takes notice of infrequent features by associating them with relatively larger learning rates during optimization

- The j-th feature is rare $\implies g_{\tau,j} = 0$ with a high probability $\implies \eta'_{t,j} = \frac{\eta_0}{\sqrt{\sum_{\tau=0}^t g_{\tau,j}^2}}$ is large
- Infrequent features are usually more predictive!

Heuristics that emphasize rare features: TF-IDF (preprocessing)

AdaGrad - Guarantees

Let $\mathcal{W} = \{w : ||w||_{\infty} \le 1\}$ and $R(t) = \sum_{\tau=0}^{t} [f_{\tau}(w_{\tau}) - f_{\tau}(w^{*})].$ With diagonal approximation²

$$R_{ada}(t) \le 2\sqrt{2} \times \sum_{j=1}^{p} \left[\sum_{\tau=0}^{t} g_{\tau,j}^{2} \right]^{\frac{1}{2}}$$
 (8)

while
$$R_{sgd}(t) \le 2\sqrt{2} \times p \left[\sum_{j=1}^{p} \sum_{\tau=0}^{t} g_{\tau,j}^2 \right]^{\frac{1}{2}}$$
 (9)

AdaGrad has a tighter bound over SGD:

$$\sum_{j=1}^{p} \left[\sum_{\tau=0}^{t} g_{\tau,j}^{2} \right]^{\frac{1}{2}} \leq_{Cauchy's} \left(p \sum_{j=1}^{p} \sum_{\tau=0}^{t} g_{\tau,j}^{2} \right)^{\frac{1}{2}} \leq p \left[\sum_{j=1}^{p} \sum_{\tau=0}^{t} g_{\tau,j}^{2} \right]^{\frac{1}{2}}$$
(10)

²See [Duchi et al., 2011] for proof details.

Other Popular Methods

A non-exhaustive list

- Momentum [Rumelhart et al., 1988]
- NAG: Nesterov's accelerated gradient [Nesterov et al., 1994]
- AdaDelta: AdaGrad refined [Zeiler, 2012]
- Rprop & Rmsprop [Tieleman and Hinton, 2012]: Ignoring the magnitude of gradient

Demos ³

- Animation 0
- Animation 1
- Animation 2
- Animation 3

³https://www.reddit.com/r/MachineLearning/comments/2gopfa/ visualizing_gradient_optimization_techniques/cklhott

Takeaways

AdaGrad is a variant of SGD which

- Adaptively adjusts to data geometry
- Adaptively determines learning rates for different dimensions

Advantages of AdaGrad

- Easy to implement and tends to work well in practice.
- Not sensitive to the initial learning rate (η_0) .
- Generic, backed up by nice theoretical guarantees.

Reference I



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