AI505

Optimization

Optimization in Machine Learning

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Simplified Notation

Let ξ be a random seed or the realization of a single (or a set of) sample $(\boldsymbol{x}, y)$.
For a given $(\boldsymbol{w}, \xi)$ let $f(\boldsymbol{w}; \xi)$ be the composition of the loss function L and the prediction function h
Then:

$$R(\boldsymbol{w}) = \mathbb{E}_{\xi}[f(\boldsymbol{w}; \xi)] \qquad \text{Expected Risk}$$

Let $\{\xi_{[i]}\}_{i=1}^{n}$ be realizations of ξ corresponding to $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$ and $f_i(\boldsymbol{w}) \stackrel{def}{=} f(\boldsymbol{w}; \xi_{[i]})$
Then:

$$R_n(\boldsymbol{w}) \stackrel{def}{=} \frac{1}{n} \sum_{i=1}^{n} f_i(\boldsymbol{w}) \qquad \text{Empirical Risk}$$

Stochastic vs Batch Optimization Methods

Reduction to minimizing R_n, with $\boldsymbol{w}_0 \in \mathbb{R}^d$ given (deterministic problem)

Stochastic Approach: Stochastic Gradient (Robbins and Monro, 1951)

$$\boldsymbol{w}_{k+1} \leftarrow \boldsymbol{w}_k - \alpha_k \nabla f_{i_k}(\boldsymbol{w}_k)$$

i_k is chosen randomly from $\{1, \ldots, n\}$, $\alpha_k > 0$.

- very cheap iteration only on one sample.
- $\{\boldsymbol{w}_k\}$ is a stochastic process determined by the random sequence $\{i_k\}$.
- the direction might not always be a descent but if it is a descent direction in **expectation**, then the sequence $\{\boldsymbol{w}_k\}$ can be guided toward a minimizer of R_n.

Batch Approach: batch gradient, steepest descent, full gradient method:

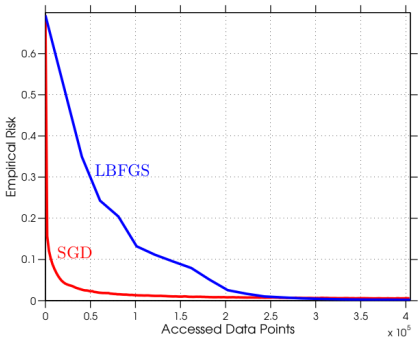
$$\boldsymbol{w}_{k+1} \leftarrow \boldsymbol{w}_k - \alpha_k \nabla R_n(\boldsymbol{w}_k) = \boldsymbol{w}_k - \frac{\alpha_k}{n} \sum_{i=1}^{n} \nabla f_i(\boldsymbol{w}_k)$$

- more expensive
- can use all deterministic gradient-based optimization methods
- the sum structure opens up to parallelization

Analogues in simulation: stochastic approximation (SA) and sample average approximation (SAA)

Stochastic Gradient

- In case of redundancy using all of the sample data in every iteration is inefficient
- Comparison of the performance of a batch L-BFGS method on number of evaluations of a sample gradient $\nabla f_{i_k}(\boldsymbol{w}_k)$. Each set of n consecutive accesses is called an **epoch**.
- The batch method performs only one step per epoch while SG performs n steps per epoch.



the fast initial improvement achieved by SG, followed by a drastic slowdown after 1 or 2 epochs, is common in practice

SG more sensitive to α_k and starting point

if more epochs, batch may become better

Theoretical Motivations

- a batch approach can minimize R_n at a fast rate; e.g., if R_n is strongly convex. A batch gradient method, then there exists a constant $\rho \in (0,1)$ such that, for all $k \in \mathbb{N}$, the training error follows **linear convergence**

$$R_n(\boldsymbol{w}_k) - R_n^* \leq \mathcal{O}(\rho^k),$$

- rate of convergence of a basic stochastic method is slower than for a batch gradient; e.g., if R_n is strictly convex and each i_k is drawn uniformly from $\{1, \ldots, n\}$, then for all $k \in \mathbb{N}$, SG satisfies the **sublinear convergence property**

$$\mathbb{E}[R_n(\boldsymbol{w}_k) - R_n^*] = \mathcal{O}(1/k).$$

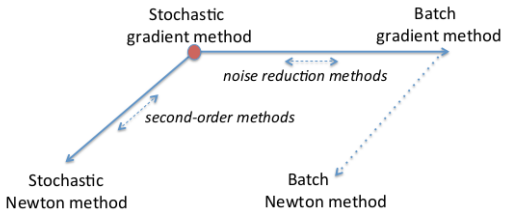
neither the per-iteration cost nor the right-hand side depends on the sample set size n

- in a stochastic optimization setting, SG yields for the expected risk the same convergence rate once substituted $\nabla f_{i_k}(\boldsymbol{w}_k)$ replaced by $\nabla f(\boldsymbol{w}_k; \xi_k)$ with each ξ_k drawn independently according to the distribution P

$$\mathbb{E}[R(\boldsymbol{w}_k) - R^*] = \mathcal{O}(1/k).$$

If $n >> k$ up to iteration k minizming R_n same as minimizing R

Beyond SG: Noise Reduction and Second-Order Methods



- on horizontal axis methods that try to improve rate of convergence
- on vertical axis, methods that try to overcome non-linearity and ill-conditioning

Minibatch Approach small subset of samples, call it $\mathcal{S}_k \subseteq \{1, \ldots, n\}$, chosen randomly in each iteration:

$$\boldsymbol{w}_{k+1} \leftarrow \boldsymbol{w}_k - \frac{\alpha_k}{|\mathcal{S}_k|} \sum_{i \in \mathcal{S}} \nabla f_i(\boldsymbol{w}_k)$$

due to the reduced variance of the stochastic gradient estimates, the method is easier to tune in terms of choosing the stepsizes $\{\alpha_k\}$.
dynamic sample size and gradient aggregation methods, both of which aim to improve the rate of convergence from sublinear to linear