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:

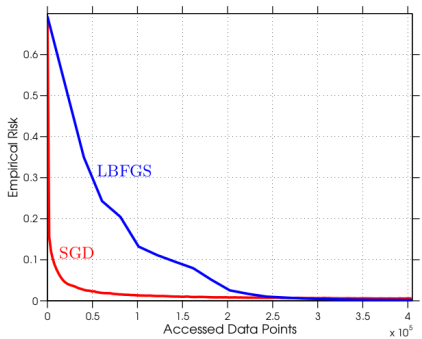
$$\boldsymbol{w}_{k+1} \leftarrow \boldsymbol{w}_k - \alpha_k \nabla R_n(\boldsymbol{w}_k) = \boldsymbol{w}_k - \frac{\alpha_k}{n} \sum_{i=1}^{n} \nabla f_i(\boldsymbol{w}_k)$$

- 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 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

Rate of Convergence

Let $\{x_k\}$ be a sequence in $\mathbb{R}^n$ that converges to x^*.
The convergence is said to be **Q-linear** (quotient-linear) if there is a constant $r \in (0, 1)$ such that

$$\frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} \leq r \qquad \text{for all } k \text{ sufficiently large}$$

ie, the distance to the solution x^* decreases at each iteration by at least a constant factor bounded away from 1 (ie, < 1).

Example:
sequence $\{1 + (0.5)^k\}$ converges Q-linearly to 1, with rate $r = 0.5$.

Rate of Convergence

The convergence is said to be **Q-superlinear** if

$$\lim_{k\to\infty} \frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} = 0$$

Example: the sequence $\{1 + k^{-k}\}$ converges superlinearly to 1.

An even more rapid convergence rate:
The convergence is said to be **Q-quadratic** if

$$\frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^2} \leq M \qquad \text{for all } k \text{ sufficiently large}$$

where M is a positive constant, not necessarily less than 1.
Example: the sequence $\{1 + (0.5)^{2^k}\}$.
The values of r and M depend not only on the algorithm but also on the properties of the particular problem.
Regardless of these values a quadratically convergent sequence will always eventually converge faster than a linearly convergent sequence.

Rate of Convergence

Superlinear convergence (quadratic, cubic, quartic, etc) is regarded as fast and desirable, while sublinear convergence is usually impractical.

- Quasi-Newton methods for unconstrained optimization typically converge Q-superlinearly
- Newton's method converges Q-quadratically under appropriate assumptions.
- Steepest descent algorithms converge only at a Q-linear rate, and when the problem is ill-conditioned the convergence constant r in is close to 1.

Rate of Convergence

A slightly weaker form of convergence:
overall rate of decrease in the error, rather than the decrease over each individual step of the algorithm.
We say that convergence is **R-linear** (root-linear) if there is a sequence of nonnegative scalars $\{v_k\}$ such that

$$\|x_k - x^*\| \leq \{v_k\} \text{ for all } k, \text{ and } \{v_k\} \text{ converges Q-linearly to zero.}$$

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**

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

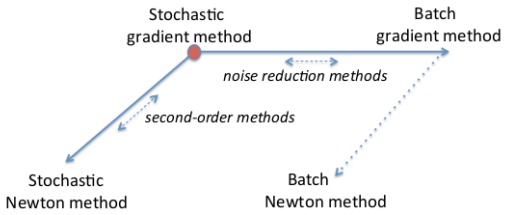
neither the per-iteration cost nor the right-hand side depends on the sample set size n

- 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

Mini-batch 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

Outline

Theoretical Analysis — Preliminaries

convergence properties and worst-case iteration complexity bounds.

$$F(\boldsymbol{w}) = \begin{cases} R_n(\boldsymbol{w}) = \frac{1}{n}\sum_{i=1}^{n} f_i(\boldsymbol{w}) & \text{Empirical Risk} \\ R(\boldsymbol{w}) = \mathbb{E}_{\xi}[f(\boldsymbol{w};\xi)] & \text{Expected Risk} \end{cases}$$

sampling uniformly with replacement from training set $\rightsquigarrow R_n$
sampling with $P(\xi)$ with replacement from training set $\rightsquigarrow R$.

Procedure SG(...);
Choose an initial iterate $\boldsymbol{w}_0$ **for** $k = 0, 1, \ldots$ **do**
- Generate a realization of the random variable xi_k;
- Compute a stochastic vector $g(\boldsymbol{w}_k, \xi_k)$;
- Choose a stepsize $\alpha_k > 0$;
- Set the new iterate as $\boldsymbol{w}_{k+1} \leftarrow \boldsymbol{w}_k - \alpha_k g(\boldsymbol{w}_k, \xi_k)$;

Theoretical Analysis — Preliminaries

ξ_k may represent a single sample or a mini-batch
g may represent a stochastic gradient (biased estimator of $\nabla F(\boldsymbol{w}_k)$ or a stochastic Netwon or quasi-Newton direction).

$$g(\boldsymbol{w}_k, \xi_k) = \begin{cases} \nabla f(\boldsymbol{w}_k; \xi_k) \\ \frac{1}{n_k} \sum_{i=1}^{n_k} \nabla f(\boldsymbol{w}_k; \xi_{k,i}) \\ H_k \frac{1}{n_k} \sum_{i=1}^{n_k} \nabla f(\boldsymbol{w}_k; \xi_{k,i}) \end{cases}$$

H_k a symmetric positive definite scaling matrix
α_k fixed stepsize or diminishing stepsizes
$\boldsymbol{w}_k$ can have influence on the sample selection (active learning)

Convergence Analysis – Assumptions

- Assumption 4.1 Lipschitz-continuous objective gradients
- Assumption 4.3 First and second moment limits. The objective function and SG (Algorithm 4.1) satisfy the following:
  - objective function to be bounded below over the region explored by the algorithm.
  - in expectation, the vector $-g(\boldsymbol{w}_k, \xi_k)$ is a direction of sufficient descent for F from $\boldsymbol{w}_k$ with a norm comparable to the norm of the gradient
  - the variance of $g(\boldsymbol{w}_k, \xi_k)$ is restricted, but in a relatively minor manner.
- Lemma: Markovian manner in the sense that $\boldsymbol{w}_{k+1}$ is a random variable that depends only on the iterate $\boldsymbol{w}_k$, the seed ξ_k, and the stepsize α_k and not on any past iterates.
- Assumption 4.5 Strong convexity. The objective function $F : \mathbb{R}^d \to \mathbb{R}$ is **strongly convex** in that there exists a constant $c > 0$ such that

$$F(\bar{\boldsymbol{w}}) \geq F(\boldsymbol{w}) + \nabla F(w)^T(\bar{\boldsymbol{w}} - \boldsymbol{w}) + \frac{1}{2}c\,\|\bar{\boldsymbol{w}} - \boldsymbol{w}\|_2^2 \qquad \text{for all } (\bar{\boldsymbol{w}}, \boldsymbol{w}) \in \mathbb{R}^d \times \mathbb{R}^d$$

(grows at least quadratically, second derivative $\geq m$, $m \geq 0$) Hence, F has a unique minimizer, denoted as $\boldsymbol{w}^* \in \mathbb{R}^d$ with $F^* \stackrel{def}{=} F(w^*)$.

Convergence Analysis – Results

- Theorem 4.6 (Strongly Convex Objective, Fixed Stepsize).
- Theorem 4.7 (Strongly Convex Objective, Diminishing Stepsizes)
  - role of strong convexity
  - role of initial point
  - trade-offs of mini batches
- Theorem 4.8 (Nonconvex Objective, Fixed Stepsize)
  - While one cannot bound the expected optimality gap as in the convex case, inequality (4.28b) bounds the average norm of the gradient of the objective function observed on $\{\boldsymbol{w}_k\}$ visited during the first K iterations.
  - classical result for the full gradient method applied to nonconvex functions, namely, that the sum of squared gradients remains finite, implying that

$$\{\|\nabla F(\boldsymbol{w}_k)\|_2\} \to 0.$$

- Theorem 4.9 (Nonconvex Objective, Diminishing Stepsizes)
  - for the SG method with diminishing stepsizes, the expected gradient norms cannot stay bounded away from zero
  - the weighted average norm of the squared gradients converges to zero even if the gradients are noisy, i.e., if $M > 0$ one can still conclude that the expected gradient norms cannot asymptotically stay far from zero.

Computational Complexity Analysis

- consider a big data scenario with an infinite supply of training examples, but a **limited computational time budget**. what type of algorithm — e.g., a simple SG or batch gradient method — would provide the best guarantees in terms of achieving a low expected risk
- SG, with its sublinear rate of convergence, is more efficient for large-scale learning than (full, batch) gradient-based methods that have a linear rate of convergence.
- reducing the optimization error $\mathcal{E}_{opt}(H, n, \epsilon)$ (evaluated with respect to R rather than R_n) one might need to make up for the additional computing time by: (i) reducing the sample size n, potentially increasing the estimation error $\mathcal{E}_{est}(H, n)$; or (ii) simplifying the function family $\mathcal{H}$, potentially increasing the approximation error $\mathcal{E}_{app}(\mathcal{H})$.
- carrying out a worst-case analysis on the influence of the sample size nand optimization tolerance ϵ, which together only influence the estimation and optimization errors.
- a stochastic optimization algorithm performs better in terms of expected error, and, hence, makes a better learning algorithm in the sense considered
- a large gap between asymptotical behavior and practical realities.

Remarks

- Fragility of the Asymptotic Performance of SG
  ok if objective function it includes a squared L_2-norm regularizer (related to constant c) but regularization parameter should be lowered when the number of samples increases.

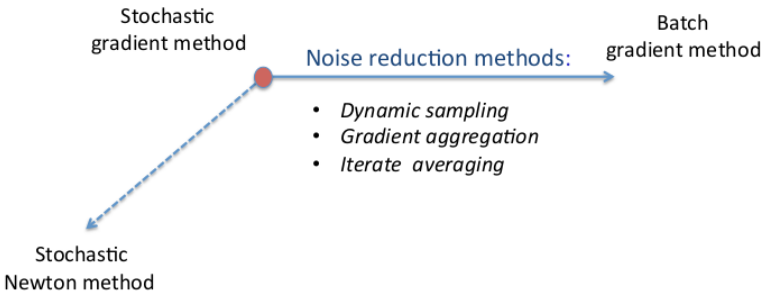
- SG good for GPUs but ill-conditioning erodes efficiency of SG

- Distributed computing not working with basic SG because of too frequent updates of $\boldsymbol{w}$, more promising with mini-batch.

- Alternatives with Faster Convergence: mnimizing empirical risk R_n there is information from previous gradients.
  - gradient aggregation methods
  - dynamic sampling approach

Noise Reduction Methods

SG suffers from the adverse effect of **noisy gradient estimates**. This prevents it from converging to the solution when fixed stepsizes are used and leads to a slow, sublinear rate of convergence when a diminishing stepsize sequence $\{\alpha_k\}$ is employed.



Achieve linear rate of convergence to the optimal value using a fixed stepsize.

- **dynamic sampling methods** achieve noise reduction by gradually increasing the mini-batch size used in the gradient computation, thus employing increasingly more accurate gradient estimates as the optimization process proceeds.

- **Gradient aggregation methods** improve the quality of the search directions by storing gradient estimates corresponding to samples employed in previous iterations, updating one (or some) of these estimates in each iteration, and defining the search direction as a weighted average of these estimates.

Rate of convergence remains sublinear

- **iterate averaging methods** maintain an average of iterates computed during the optimization process and employes a more aggressive stepsize sequence–of order $O(1/\sqrt{k})$ rather than $O(1/k)$.
  It can be shown that the variance of the sequence average iterates is smaller than the variance of the SG iterates.