Stochastic Gradient Method

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Why should I bother to learn this stuff?

- Main algorithm principle for training machine learning model, and in particular deep neural network
- $\Longrightarrow$ useful for
  - understanding how the library train ML models
  - specialization in optimization
  - specialization in machine learning

Contents

The optimization problem

We consider the following optimization problem

$$\underset{x \in \mathbb{R}^p}{\text{Min}} \qquad F(x) := \mathbb{E}\Big[f(x, \xi)\Big]$$

where ξ is a random variable.

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Computing the gradient

$$F(x) := \mathbb{E}\Big[f(x, \xi)\Big]$$

Under some regularity conditions (e.g. $f(\cdot, \xi)$ differentiable, $\dfrac{\partial f(x, \cdot)}{\partial x}$ Lipschitz, and ξ integrable) we have

$$\nabla F(x) = \mathbb{E}\left[\frac{\partial f}{\partial x}(x, \xi)\right]$$

This is obvious if ξ is finitely supported : $\mathrm{supp}(\xi) = \{\xi_i\}_{i \in [N]}$, and $p_i := \mathbb{P}(\xi = \xi_i)$,

$$\nabla F(x) = \frac{\partial}{\partial x}\left(\sum_{i \in [N]} p_i f(x, \xi_i)\right) = \sum_{i \in [N]} p_i \frac{\partial}{\partial x} f(x, \xi_i)$$

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Standard continuous optimization method

Thus, we are looking at

$$\underset{x \in \mathbb{R}^p}{\text{Min}}\ F(x)$$

where F is a (strongly) convex differentiable function if $f(\cdot, \xi)$ is, and we know how to compute its gradient.

Thus, we should be able to solve our problem through the method presented in earlier courses:

- gradient algorithm
- conjugate gradient
- Newton / Quasi-Newton

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Computing the gradient is costly

For a given solution $x \in \mathbb{R}^p$ computing the gradient

$$\nabla F(x) = \mathbb{E}\left[\frac{\partial f(x, \xi)}{\partial x}\right]$$

is costly as it requires computing a multidimensional integral (if ξ admits a density), or a large sum.

Indeed, in most machine learning applications, we consider that ξ is uniformly distributed over the data (*empirical risk minimization*), thus computing the gradient requires a pass over every sample in the dataset.

Datasets of size $N > 10^6$ are common.

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Estimating the gradient

Instead of using a true gradient

$$g^{(k)} = \nabla F(x^{(k)})$$

we can use a *statistical estimator* of the gradient

$$\hat{g}^{(k)} \rightsquigarrow g^{(k)} = \mathbb{E}\Big[\frac{\partial f(x^{(k)}, \xi)}{\partial x}\Big]$$

The most standard estimator being

$$\hat{g}^{(k)} = \frac{\partial f(x^{(k)}, \xi^{(k)})}{\partial x}$$

where $\xi^{(k)}$ is drawn randomly according to the law of ξ (i.e. it is a random datapoint).

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Pros and Cons

Pros:

- computing $\hat{g}^{(k)} = \frac{\partial f(x^{(k)}, \xi^{(k)})}{\partial x}$ is really easy
- we do not need to spend lots of time early to get a precise gradient
- we can stop whenever we want (do not need a full pass on the data)

Cons:

- $\hat{g}^{(k)}$ is a noisy estimator of the gradient
- requires a new convergence theory
- $x^{(k+1)} := x^{(k+1)} - \alpha \hat{g}^{(k)}$ generally does not converge almost surely to the optimal solution as this makes a noisy trajectory

Noisy trajectory

- At optimality we should have $\nabla F(x^\sharp) = 0$
- It doesnot mean that $\frac{\partial f(x^\sharp, \xi^{(k)})}{\partial x}$ equals 0 !
- In particular there is no reason for $\hat{g}^{(k)}$ to be eventually small, only its expectation should be small!

- $\rightsquigarrow$ we generally use either:
  - decreasing step e.g. $\alpha^{(k)} = \frac{\alpha^{(0)}}{k}$
  - average points $\bar{x}^{(k)} = \frac{1}{k} \sum_{\kappa \leq k} x^{(\kappa)}$

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Mini-batch version

- $\hat{g}^{(k)} = \frac{\partial f(x^{(k)},\xi^{(k)})}{\partial x}$ is an easy-to-compute but noisy estimator of the gradient
- $\hat{g}^{(k)} = \frac{1}{N} \sum_{i \in [N]} \frac{\partial f(x^{(k)},\xi_i)}{\partial x}$ is a long (full batch) to compute but perfect estimator
- minibatch aims at a middle ground: randomly draw a sample S of realizations of $\boldsymbol{\xi}$, and use $\hat{g}^{(k)} = \frac{1}{|S|} \sum_{\xi \in S} \frac{\partial f(x^{(k)},\xi)}{\partial x}$

Video explanation

A video explaining why the stochastic gradient might be efficient
`https://www.youtube.com/watch?v=UmathvAKj80` (3')
Some adaptations of the stochastic gradient method are presented in the following video: `https://www.youtube.com/watch?v=NE88eqLngkg` (15')

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What you have to know

- That for a stochastic problem gradient step requires to compute an expectation
- That stochastic gradient do not compute the true gradient, but only an estimator of the gradient

What you really should know

- gradient algorithm (or more advanced version) is faster in term of number of iterations
- stochastic gradient needs more iteration, but each is faster

What you have to be able to do

- dive in the scientific litterature on the subject if you need to implement this type of algorithm