Stochastic Gradient Descent

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[1]Slides based on Lecture 2a from David Rosenberg's course material.

Gradient Descent for Empirical Risk - Scaling Issues

Gradient Descent for Empirical Risk and Averages

- Suppose we have a hypothesis space of functions $\mathcal{F} = \{f_w : \mathcal{X} \to \mathcal{A} \mid w \in \mathrm{R}^d\}$
  - Parameterized by $w \in \mathrm{R}^d$.
- ERM is to find w minimizing

$$\hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(f_w(x_i), y_i)$$

- Suppose $\ell(f_w(x_i), y_i)$ is differentiable as a function of w.
- Then we can do gradient descent on $\hat{R}_n(w)$...

Gradient Descent: How does it scale with n?

- At every iteration, we compute the gradient at current w:

$$\nabla \hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \nabla_w \ell(f_w(x_i), y_i)$$

- We have to touch all n training points to take a single step. $[O(n)]$
- Will this scale to "big data"?
- Can we make progress without looking at all the data?

Stochastic Gradient Descent

“Noisy” Gradient Descent

- We know gradient descent works.
- But the gradient may be slow to compute.
- What if we just use an estimate of the gradient?
- Turns out that can work fine.
- **Intuition**:
    - Gradient descent is an interative procedure anyway.
    - At every step, we have a chance to recover from previous missteps.

Minibatch Gradient

- The **full gradient** is

$$\nabla \hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n} \nabla_w \ell(f_w(x_i), y_i)$$

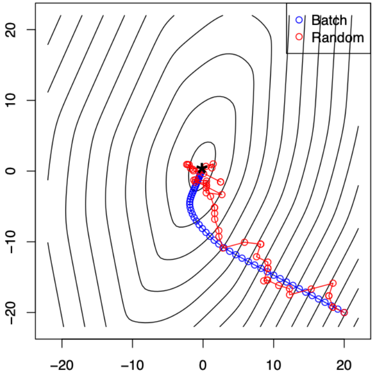
- It's an average over the **full batch** of data $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- Let's take a random subsample of size N (called a **minibatch**):

$$(x_{m_1}, y_{m_1}), \ldots, (x_{m_N}, y_{m_N})$$

- The **minibatch gradient is**

$$\nabla \hat{R}_N(w) = \frac{1}{N}\sum_{i=1}^{N} \nabla_w \ell(f_w(x_{m_i}), y_{m_i})$$

Batch vs Stochastic Methods



(Slides adapted from Ryan Tibshirani)

Rule-of-thumb for stochastic methods:

- Stochastic methods work well far from the optimum
- But struggles close the the optimum

Minibatch Gradient

- What can we say about the minibatch gradient? It's random. What's its expectation?

$$
\begin{aligned}
\mathbb{E}\left[\nabla \hat{R}_N(w)\right] &= \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}\left[\nabla_w \ell(f_w(x_{m_i}), y_{m_i})\right] \\
&= \mathbb{E}\left[\nabla_w \ell(f_w(x_{m_1}), y_{m_1})\right] \\
&= \sum_{i=1}^{n}\mathbb{P}(m_1 = i)\,\nabla_w \ell(f_w(x_i), y_i) \\
&= \frac{1}{n}\sum_{i=1}^{n}\nabla_w \ell(f_w(x_i), y_i) \\
&= \nabla \hat{R}_n(w)
\end{aligned}
$$

Minibatch Gradient Properties

- Minibatch gradient is an **unbiased estimator** for the [full] batch gradient:

$$\mathbb{E}\left[\nabla \hat{R}_N(w)\right] = \nabla \hat{R}_n(w)$$

- The bigger the minibatch, the better the estimate.

$$\frac{1}{N}\mathrm{Var}\left[\nabla \hat{R}_1(w)\right] = \mathrm{Var}\left[\nabla \hat{R}_N(w)\right]$$

- Tradeoffs of minibatch size:
  - Bigger $N \implies$ Better estimate of gradient, but slower (more data to touch)
  - Smaller $N \implies$ Worse estimate of gradient, but can be quite fast

Convergence of SGD

- For convergence guarantee, use **diminishing step sizes**, e.g. $\eta_k = 1/k$ (dampens noise in step direction)
- Theoretically, GD is much faster than SGD in terms of convergence rate
  - much faster to add a digit of accuracy on the minimum
  - but most of that benefit happens once you're already pretty close
- However, in many ML problems we don't care about optimizing to high accuracy

Step Sizes in Minibatch Gradient Descent

Minibatch Gradient Descent (minibatch size N)

- initialize $w = 0$
- repeat
  - randomly choose N points $\{(x_i, y_i)\}_{i=1}^N \subset \mathcal{D}_n$
  - $w \leftarrow w - \eta \left[\frac{1}{N} \sum_{i=1}^N \nabla_w \ell(f_w(x_i), y_i) \right]$

- For SGD, fixed step size can work well in practice.
- Typical approach: Fixed step size reduced by constant factor whenever validation performance stops improving.
- Other tricks: Bottou (2012), "Stochastic gradient descent tricks"

Summary

- **Gradient descent** or "**full-batch**" **gradient descent**
  - Use full data set of size n to determine step direction
- **Minibatch gradient descent**
  - Use a random subset of size N to determine step direction
- **Stochastic gradient descent**
  - Minibatch with $N = 1$.
  - Use a single randomly chosen point to determine step direction.

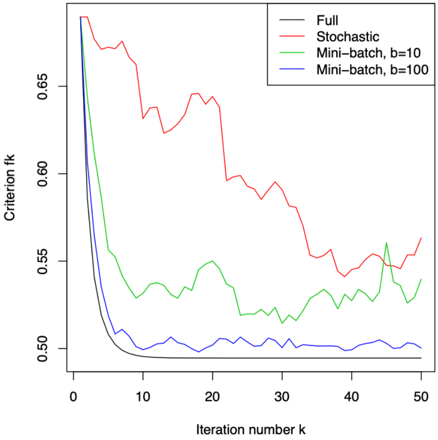
These days terminology isn't used so consistently, so always clarify the [mini]batch size.

SGD is much more efficient in time and memory cost and has been quite successful in large-scale ML.

Practical Comparison of GD vs SGD

Logistic regression with ℓ_2 regularization

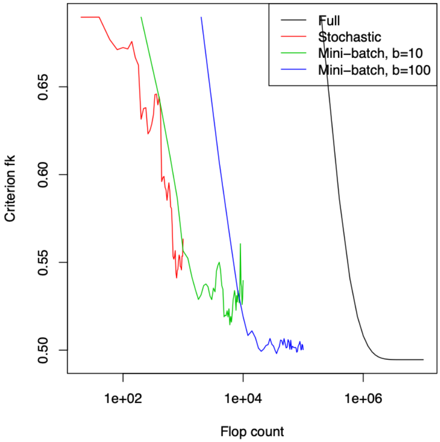
Batch methods converge faster



(Example from Ryan Tibshirani)

Logistic regression with ℓ_2 regularization

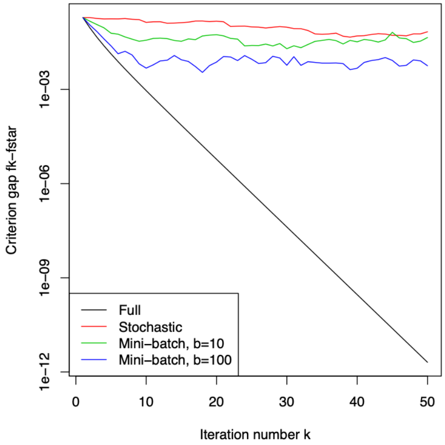
Stochastic methods are computationally more efficient



(Example from Ryan Tibshirani)

Logistic regression with ℓ_2 regularization

Batch methods are much faster close to the optimum



(Example from Ryan Tibshirani)