Machine Learning (CSE 446): Pratical issues: optimization and learning

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Review

Our running example for the loss minimization problem

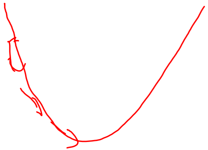
$$\underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} \frac{1}{2} (y_n - \mathbf{w} \cdot \mathbf{x}_n)^2 + \frac{1}{2} \lambda \|\mathbf{w}\|^2$$

- How do we run GD/SGD?

- how do we set the step size? λ? the "mini-batch" size?

We will help with guidance/understanding/theory. Ultimately, we just have try to tune these ourselves to get experience. HW3 will help...

review: GD for the square loss



Data: step sizes $\langle \eta^{(1)}, \dots, \eta^{(K)} \rangle$
Result: parameter $\mathbf{w}$
initialize: $\mathbf{w}^{(0)} = \mathbf{0}$;
for $k \in \{1, \dots, K\}$ **do**
  $\mathbf{w}^{(k)} = \mathbf{w}^{(k-1)} + \eta^{(k)} \left(\frac{1}{N} \sum_n \left(y_n - \mathbf{w}^{(k-1)} \cdot \mathbf{x}_n \right) \mathbf{x}_n \right)$;
end
return $\mathbf{w}^{(K)}$;

$L(w) = \sum \frac{1}{2} \left(y_n - w^{(k-1)} \cdot x_n \right)^2$

Algorithm 1: SGD

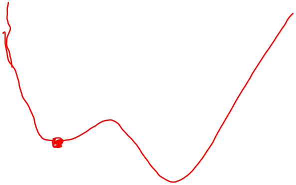
- the term in red is a costly to compute!
- Even by using matrix multiplications (and not explicitly doing the sum), it is often too slow.

Gradient Descent: review

- how do we set the stepsize?
  - Remember: we diverge if the step size is too big!
  - you just set it a little lower (like $1/2$) less than when things start to diverge.
- do we decay it?
  No: GD will converge just fine without decaying the learning rate.
- Is GD a good algorithm?
  GD is often too slow:
  - computing the gradient of the objective function involves a sum over
- Today: SGD/let's sample the gradient!

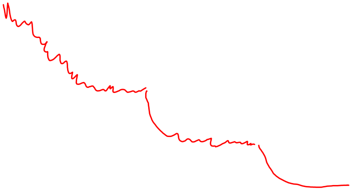
Today

SGD for the square loss



Data: step sizes $\langle \eta^{(1)}, \ldots, \eta^{(K)} \rangle$
Result: parameter $\mathbf{w}$
initialize: $\mathbf{w}^{(0)} = \mathbf{0}$;
for $k \in \{1, \ldots, K\}$ **do**
  Sample $n \sim \text{Uniform}(\{1, \ldots, N\})$;
  $\mathbf{w}^{(k)} = \mathbf{w}^{(k-1)} + \eta^{(k)} \left(y_n - \mathbf{w}^{(k-1)} \cdot \mathbf{x}_n \right) \mathbf{x}_n$;
end
return $\mathbf{w}^{(K)}$;

Algorithm 2: SGD



- the term in red is a "sampled" gradient.

"mini-batch" SGD for the square loss

$L(w) = \frac{1}{2} \sum_{n} (y - w \cdot x)^2$

Data: step sizes $\langle \eta^{(1)}, \ldots, \eta^{(K)} \rangle$
Result: parameter $\mathbf{w}$
initialize: $\mathbf{w}^{(0)} = \mathbf{0}$;
for $k \in \{1, \ldots, K\}$ **do**
  Sample m examples of (x, y) (uniformly at random) from the training set and let $\mathcal{M}$ be the set of these m points;
  $\mathbf{w}^{(k)} = \mathbf{w}^{(k-1)} + \eta^{(k)} \frac{1}{m} \sum_{(x,y) \in \mathcal{M}} \left(y - \mathbf{w}^{(k-1)} \cdot \mathbf{x}\right) \mathbf{x}$;
end
return $\mathbf{w}^{(K)}$;

Algorithm 3: SGD

- the term in red is a lower variance, "sampled" gradient.
- how do we choose m?
  larger m means lower variance but more computation.
- Matrix algebra can make computing the term in red very fast!
  This is critical to get big performance bumps.

SGD: How do we set the step sizes?

- Theory: If you turn down the step sizes at (some prescribed decaying method) then SGD will converge to the right answer.
  The "classical" theory doesn't provide enough practical guidance.
- Practice:
  - starting stepsize: start it "large":
    if it is "too large", then either you diverge (or nothing improves). set it a little less (like $1/4$) less than this point.
  - When do we decay it?
    When your training error stops decreasing "enough".
- HW: you'll need to tune it a little. (a slow approach: sometimes you can just start it somewhat smaller than the "divergent" value and you will find something reasonable.)

SGD: How do we set the mini-batch size m?

- Theory: there are diminishing returns to increasing m.
  - As you grow m, your "improvements" tend to diminish.
  - mini-batch size m "small": you can turn it up and you will find that you are making more progress per update.
  - mini-batch size m "large": you can turn it up and you will make roughly the same amount of progress (so your code will become slower).
- Practice: there are diminishing returns to increasing m.
- How do we set it?
  Easy: just keep cranking it up and eventually you'll see that your code doesn't get any faster.

“regularized” SGD for the square loss, $m = 1$

Data: step sizes $\langle \eta^{(1)}, \ldots, \eta^{(K)} \rangle$
Result: parameter $\mathbf{w}$
initialize: $\mathbf{w}^{(0)} = \mathbf{0}$;
for $k \in \{1, \ldots, K\}$ **do**
  Sample $n \sim \text{Uniform}(\{1, \ldots, N\})$;
  $\mathbf{w}^{(k)} = \mathbf{w}^{(k-1)} + \eta^{(k)} \left(\left(y_n - \mathbf{w}^{(k-1)} \cdot \mathbf{x}_n \right) \mathbf{x}_n - \lambda \mathbf{w} \right)$;
end
return $\mathbf{w}^{(K)}$;

Algorithm 4: SGD

- Regularization has been added: How do we set it?
- we can combine this with mini-batching

Regularization: How do we set it?

- Theory: really just says that λ controls your "model complexity".
  - we DO know that "early stopping" for GD/SGD is (basically) doing L2 regularization for us
  - i.e. if we don't run for too long, then $\|\mathbf{w}\|^2$ won't become too big.
- Practice:
  - Exact methods (like matrix inverse/least squares): always need to regularize or something horrible happens....
  - GD/SGD: sometimes (often ?) it works just fine ignoring regularization
  - Other times we have to tune it on some dev set.
    Fortunately, it is pretty robust to tune, by trying out different "orders of magnitude" guesses.