Optimization in the “Big Data” Regime 2: SVRG & Tradeoffs in Large Scale Learning.

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Announcements...

- Work on your project milestones
  - read/related work summary
  - some empirical work

Today:

- Review: optimization of finite sums, (dual) coordinate ascent
- New: SVRG (for sums of loss functions);
  Tradeoffs in large scale learning
  How do we optimize in the "big data" regime?

Machine Learning and the Big Data Regime...

goal: find a *d*-dim parameter vector which minimizes the loss on *n* training examples.

- have *n* training examples $(x_1, y_1), \ldots (x_n, y_n)$
- have parametric a classifier $h(x, w)$, where w is a d dimensional vector.

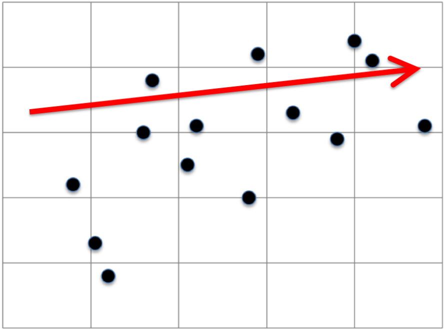
$$\min_w L(w) \text{ where } L(w) = \sum_i \text{loss}(h(x_i, w), y_i)$$

- "Big Data Regime": How do you optimize this when *n* and *d* are large? memory? parallelization?

Can we obtain linear time algorithms to find an ϵ-accurate solution?
i.e. find $\hat{w}$ so that

$$L(\hat{w}) - \min_w L(w) \le \epsilon$$

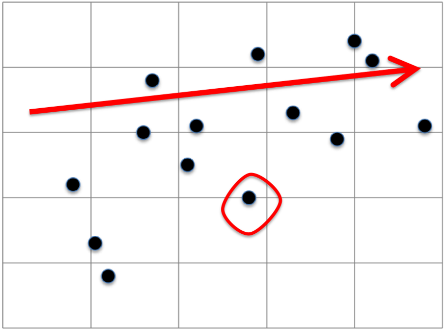
Review: Stochastic Gradient Descent (SGD)



- SGD update rule: at each time t,

$$\text{sample a point } (x_i, y_i)$$
$$w \leftarrow w - \eta(w \cdot x_i - y_i)x_i$$

Review: Stochastic Gradient Descent (SGD)



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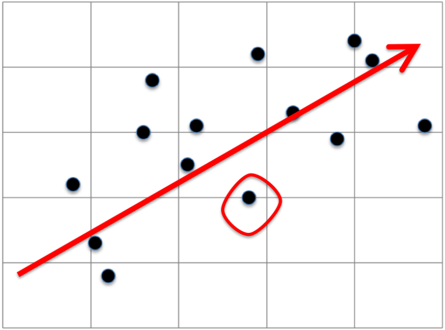


- SGD update rule: at each time t,

$$\text{sample a point } (x_i, y_i)$$
$$w \leftarrow w - \eta(w \cdot x_i - y_i)x_i$$

- Problem: even if $w = w_*$, the update changes w.
  Rate: convergence rate is $O(1/\epsilon)$, with decaying η

  simple algorithm, light on memory, but poor convergence rate

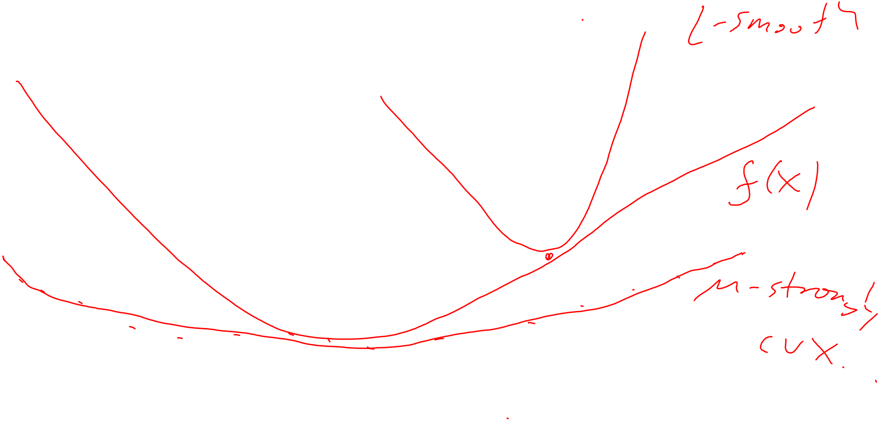
SDCA advantages/disadvantages

- What about more general convex problems? e.g.

$$\min_w L(w) \text{ where } L(w) = \sum_i \mathrm{loss}(h(x_i, w), y_i)$$

  - the basic idea (formalized with duality) is pretty general for convex $\mathrm{loss}(\cdot)$.
  - works very well in practice.
- memory: SDCA needs $O(n + d)$ memory, while SGD is only $O(d)$.
- What about an algorithm for non-convex problems?
  - SDCA seems heavily tied to the convex case.
  - Is there an algo that is highly accurate in the convex case *and* sensible in the non-convex case?

L smooth and μ-strongly convex case



Review: Stochastic Gradient Descent

- Suppose $L(w)$ is μ strongly convex.
- Suppose each loss $\mathrm{loss}(\cdot)$ is L-smooth
- To get ϵ accuracy:
  - # iterations to get ϵ-accuracy:

    $$\frac{L}{\mu\epsilon}$$

    (see related work for precise problem dependent parameters)
  - Computation time to get ϵ-accuracy:

    $$\frac{L}{\mu\epsilon}d$$

    (assuming $O(d)$ cost pre gradient evaluation.)

(another idea) Stochastic Variance Reduced Gradient (SVRG)

1. exact gradient computation: at stage s, using $\widetilde{w}_s$, compute:

$$\nabla L(\widetilde{w}_s) = \frac{1}{n} \sum_{i=1}^{n} \nabla \mathrm{loss}(h(x_i, \widetilde{w}_s), y_i)$$

2. variance reduction $+$ SGD: initialize $w \leftarrow \widetilde{w}_s$. for m steps,

   sample a point (x, y)

   $$w \leftarrow w - \eta \left(\nabla \mathrm{loss}(h(x, w), y) - \nabla \mathrm{loss}(h(x, \widetilde{w}_s), y) + \nabla L(\widetilde{w}_s) \right)$$

3. update and repeat: $\widetilde{w}_{s+1} \leftarrow w$.

Properties of SVRG

- M is constant !!

- unbiased updates: What is the mean of the blue term?

$$\mathbb{E}[\nabla \mathrm{loss}(h(x,\widetilde{w}_s),y) - \nabla L(\widetilde{w}_s)] =?$$

0 !!

  where the expectation is for a random sample (x, y).
- If $\widetilde{w} = w_*$, then no update.
- Memory is $O(d)$.
- No “dual” variables.
  Applicable to non-convex optimization.

Guarantees of SVRG

∘ L is smoothness of loss(w)

∘ μ is str. convexity of $L(w)$

$\frac{L}{\mu} n \log \frac{1}{\varepsilon}$

- set $m = L/\mu$.
- # of gradient computations to get ϵ accuracy:

$$\left(n + \frac{L}{\mu}\right) \log 1/\epsilon$$

$\frac{L}{\mu \varepsilon}$

Comparisons

same as SDCA

- a gradient evaluation is at point (x, y).
  - SVRG: # of gradient computations to get ϵ accuracy:

$$\left(n + \frac{L}{\mu}\right) \log 1/\epsilon$$

  - # of gradient evaluations for batch gradient descent:

$$n\frac{\tilde{L}}{\mu} \log 1/\epsilon$$

  where $\tilde{L}$ is the smoothness of $L(w)$.
  - # of gradient computations for SGD:

$$\frac{L}{\mu\epsilon}$$

Non-convex comparisons

- How many gradient evaluations does it take to find *w* so that:

$$\|\nabla L(w)\|^2 \leq \epsilon^2$$

  (i.e. ”close” to a stationary point)

- Rates: the number of gradient evaluations, at a point (x, y), is:
  - GD: $O(n/\epsilon)$
  - SGD: $O(1/\epsilon^2)$
  - SVRG: $O(n + n^{2/3}/\epsilon)$

SDCA is great :)

Does SVRG work well in practice?

ok.

Tradeoffs in Large Scale Learning.

- Many issues sources of “error”
- approximation error: our choice of a hypothesis class
- estimation error: we only have *n* samples
- optimization error: computing exact (or near-exact) minimizers can be costly.
- How do we think about these issues?

The true objective

- hypothesis map $x \in \mathcal{X}$ to $y \in \mathcal{Y}$.
- have n training examples $(x_1, y_1), \ldots (x_n, y_n)$ sampled i.i.d. from $\mathcal{D}$.
- Training objective: have a set of parametric predictors $\{h(x, w) : w \in \mathcal{W}\}$,

$$\min_{w \in \mathcal{W}} \hat{L}_n(w) \text{ where } \hat{L}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \text{loss}(h(x_i, w), y_i)$$

- True objective: to generalize to $\mathcal{D}$,

$$\min_{w \in \mathcal{W}} L(w) \text{ where } L(w) = \mathbb{E}_{(X,Y) \sim \mathcal{D}} \text{loss}(h(X, w), Y)$$

Optimization: Can we obtain linear time algorithms to find an ϵ-accurate solution? i.e. find $\hat{h}$ so that

$$L(\hat{w}) - \min_{w \in \mathcal{W}} L(w) \le \epsilon$$

Definitions

- Let h^* is the *Bayes optimal hypothesis*, over all functions from $\mathcal{X} \rightarrow \mathcal{Y}$.

$$h^* \in \mathrm{argmin}_h L(h)$$

- Let w^* is the *best in class hypothesis*

$$w^* \in \mathrm{argmin}_{w \in \mathcal{W}} L(w)$$

- Let w_n be the *empirical risk minimizer:*

$$w_n \in \mathrm{argmin}_{w \in \mathcal{W}} \hat{L}_n(w)$$

- Let $\tilde{w}_n$ be what our algorithm returns.

Loss decomposition

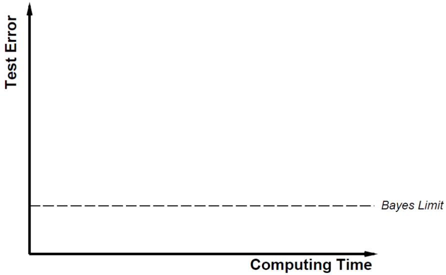
- Observe:

$$\begin{aligned} L(\tilde{w}_n) - L(h^*) = \quad & L(w^*) - L(h^*) && \text{Approximation error} \\ & + L(w_n) - L(w^*) && \text{Estimation error} \\ & + L(\tilde{w}_n) - L(w_n) && \text{Optimization error} \end{aligned}$$

- Three parts which determine our performance.
- Optimization algorithms with “best” accuracy dependencies on $\hat{L}_n$ may not be best.
  Forcing one error to decrease much faster may be wasteful.

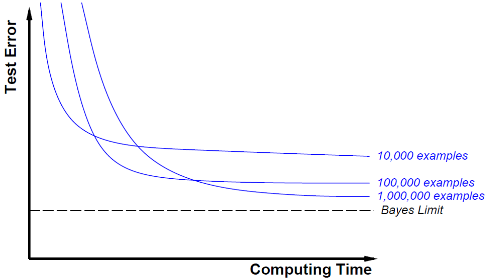
Time to a fixed accuracy

test error versus training time



Comparing sample sizes

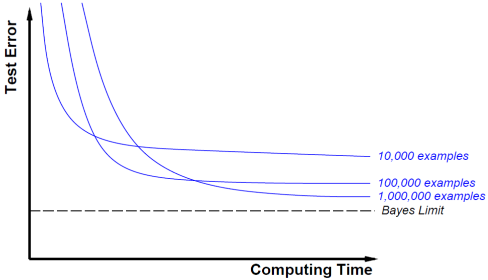
test error versus training time



- Vary the number of examples

Comparing sample sizes and models

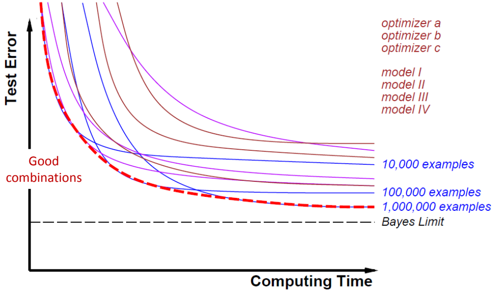
test error versus training time



- Vary the number of examples

Optimal choices

test error versus training time



- Optimal combination depends on training time budget.

Estimation error: simplest case

- Measuring a mean:
$$L(\mu) = \mathbb{E}(\mu - y)^2$$
The minima is at $\mu = \mathbb{E}[y]$.
- With n samples, the Bayes optimal estimator is the sample mean: $\hat{\mu}_n = \frac{1}{n}\sum_i y_i$.
- The error is:
$$\mathbb{E}[L(\hat{\mu}_n)] - L(\mathbb{E}[y]) = \frac{\sigma^2}{n}$$
σ^2 is the variance and the expectation is with respect to the n samples.
- How many samples do we need for ϵ error?

Let's compare:

- SGD: Is $O(1/\epsilon)$ reasonable?
- GD: Is $\log 1/eps$ needed?
- SDCA/SVRG: These are also $\log 1/eps$ but much faster.

Statistical Optimality

- Can generalize as well as the sample minimizer, w_n? (without computing it exactly)
- For a wide class of models (linear regression, logistic regression, etc), we have that the estimation error is:

$$\mathbb{E}[L(w_n)] - L(w^*) = \frac{\sigma^2_{\mathrm{opt}}}{n}$$

where σ^2_{opt} is a problem dependent constant.

- What is the computational cost of achieving exactly this rate? say for large n?

Averaged SGD

- SGD:

$$w_{t+1} \leftarrow w_t - \eta_t \nabla \mathrm{loss}(h(x, w_t), y)$$

- An (asymptotically) optimal algo:
  - Have η_t go to 0 (sufficiently slowly)
  - (iterate averaging) Maintain the a running average:

$$\overline{w_n} = \frac{1}{n} \sum_{t \leq n} w_t$$

  - (Polyak & Juditsky, 1992) for large enough n and with one pass of SGD over the dataset:

$$\mathbb{E}[L(\overline{w_n})] - L(w^*) \overset{n \to \infty}{=} \frac{\sigma_{\mathrm{opt}}^2}{n}$$

Acknowledgements

Some slides from “Large-scale machine learning revisited”, Leon Bottou 2013.