Optimization in the “Big Data” Regime

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Announcements...

- HW2 due Mon.
- Work on your project milestones
  - read/related work summary
  - some empirical work

Today:

- Review: discuss classical optimization
- New: How do we optimize in the “big data” regime, with large sample sizes and large dimension? Bridge classical to modern optimization.
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 $h_\theta(x, w)$, 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 $\epsilon$-accurate solution?

i.e. find $\hat{w}$ so that

$$
L(\hat{w}) - \min_w L(w) \leq \epsilon
$$
Goal: algorithms to get fixed target accuracy $\epsilon$.

Review: classical optimization viewpoints

A modern view: can be bridge classical optimization to modern problems?

- Dual Coordinate Descent Methods
- Stochastic Variance Reduced Gradient method (SVRG)
Abstraction: Least Squares

\[
\min_w L(w) \text{ where } L(w) = \sum_{i=1}^{n} (w \cdot x_i - y_i)^2 + \lambda \|w\|^2
\]

How much computation time is required to get \(\epsilon\) accuracy?

- \(n\) points, \(d\) dimensions.
- “Big Data Regime”: How do you optimize this when \(n\) and \(d\) are large?
- More general case: Optimize sums of convex (or non-convex functions?)
  - some guarantees will still hold

Aside: think of \(x\) as a large feature representation.
Review: Direct Solution

\[ \min_w L(w) \text{ where } L(w) = \sum_{i=1}^{n} (w \cdot x_i - y_i)^2 + \lambda \|w\|^2 \]

solution:

\[ w = (X^\top X + \lambda I)^{-1} X^\top Y \]

where \( X \) be the \( n \times d \) matrix whose rows are \( x_i \), and \( Y \) is an \( n \)-dim vector.

numerical solution: the “backslash” implementation.

time complexity: \( O(nd^2) \) and memory \( O(d^2) \)

Not feasible due to both time and memory.
Review: Gradient Descent (and Conjugate GD)

$$\min_w L(w) \text{ where } L(w) = \sum_{i=1}^{n} (w \cdot x_i - y_i)^2 + \lambda \|w\|^2$$

- $n$ points, $d$ dimensions,
- $\lambda_{\text{max}}, \lambda_{\text{min}}$ are max and min eigs. of “design matrix” $\frac{1}{n} \sum_i x_i x_i^\top$
- # iterations and computation time to get $\epsilon$ accuracy:
  - Gradient Descent (GD):
    $$\frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} \log 1/\epsilon, \quad \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} nd \log 1/\epsilon$$
  - Conjugate Gradient Descent:
    $$\sqrt{\frac{\lambda_{\text{max}}}{\lambda_{\text{min}}}} \log 1/\epsilon, \quad \sqrt{\frac{\lambda_{\text{max}}}{\lambda_{\text{min}}}} nd \log 1/\epsilon$$
- memory: $O(d)$

Better runtime and memory, but still costly.
SGD update rule: at each time $t$,

sample a point $(x_i, y_i)$

$$w \leftarrow w - \eta (w \cdot x_i - y_i) x_i$$
SGD update rule: at each time \( t \),

sample a point \((x_i, y_i)\)

\[
\mathbf{w} \leftarrow \mathbf{w} - \eta (\mathbf{w} \cdot x_i - y_i)x_i
\]
Review: Stochastic Gradient Descent (SGD)

- **SGD update rule**: at each time $t$,

$$w \leftarrow w - \eta(w \cdot x_i - y_i)x_i$$

- **Problem**: even if $w = w_*$, the update changes $w$.

- **Rate**: convergence rate is $O(1/\epsilon)$, with decaying $\eta$

  simple algorithm, light on memory, but poor convergence rate
λ_{\text{min}} \text{ is the min eig. of } \frac{1}{n} \sum_i x_i x_i^\top

Suppose gradients are bounded by \( B \).

To get \( \epsilon \) accuracy:

# iterations to get \( \epsilon \)-accuracy:

\[
\frac{B^2}{\lambda_{\text{min}} \epsilon}
\]

Computation time to get \( \epsilon \)-accuracy:

\[
\frac{dB^2}{\lambda_{\text{min}} \epsilon}
\]
Regression in the big data regime?

\[ \min_w L(w) \]

How much computation time is required to get \( \epsilon \) accuracy?

"Big Data Regime": How do you optimize this when \( n \) and \( d \) are large?

- Can we ‘fix’ the instabilities of SGD?

Let’s look at (regularized) linear regression.

- Convex optimization: All results can be generalized to smooth+strongly convex loss functions.

- Non-convex optimization: some ideas generalize.
Duality (without Duality)

\[
\begin{align*}
    w &= (X^T X + \lambda I)^{-1} X^T Y \\
    &= X^T (XX^T + \lambda I)^{-1} Y \\
    &:= \frac{1}{\lambda} X^T \alpha
\end{align*}
\]

where \( \alpha = (I + XX^T/\lambda)^{-1} Y \).

- **idea:** let’s compute the n-dim vector \( \alpha \).
- let’s do this with coordinate ascent
SDCA: stochastic dual coordinate ascent

\[ G(\alpha_1, \alpha_2, \ldots, \alpha_n) = \frac{1}{2} \alpha^T (I + XX^T / \lambda) \alpha - Y^T \alpha \]

the minimizer of \( G(\alpha) \) is

\[ \alpha = (I + XX^T / \lambda)^{-1} Y \]

SDCA:
- start with \( \alpha = 0 \).
- choose coordinate \( i \) randomly, and update:

\[ \alpha_i = \arg\min_z G(\alpha_1, \ldots, \alpha_{i-1}, z, \ldots, \alpha_n) \]

- easy to do as we touch just one datapoint.
- return \( w = \frac{1}{\lambda} X^T \alpha \).
SDCA: the algorithm

\[ G(\alpha_1, \alpha_2, \ldots, \alpha_n) = \frac{1}{2} \alpha^\top (I + XX^\top / \lambda) \alpha - Y^\top \alpha \]

- start with \( \alpha = 0, \ w = \frac{1}{\lambda} X^\top \alpha \).
- choose coordinate \( i \) randomly, and compute difference:
  \[ \Delta \alpha_i = \frac{(y_i - w \cdot x_i) - \alpha_i}{1 + \|x_i\|^2 / \lambda} \]
- update:
  \[ \alpha_i \leftarrow \alpha_i + \Delta \alpha_i, \quad w \leftarrow w + \frac{1}{\lambda} x_i \cdot \Delta \alpha_i \]
- return \( w = \frac{1}{\lambda} X^\top \alpha \).
Guarantees: speedups for the big data regime

- $n$ points, $d$ dimensions, $\lambda_{av}$ average eigenvalue

Computation time to get $\epsilon$ accuracy gradient descent: (Shalev-Shwartz & Zhang ’12)

- GD vs SDCA:

$$\frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} n d \log \frac{1}{\epsilon} \rightarrow \left(n + d \frac{\lambda_{av}}{\lambda_{\text{min}}} \right) d \log \frac{1}{\epsilon}$$

- conjugate GD vs acceleration+SDCA.
  One can accelerate SDCA as well. (Frosting, Ge, K., Sidford, 2015)
Comparisons to GD

- both algorithms touch one data point at a time, with same computational cost per iteration.
- SDCA has “learning rate” which adaptive to the data point.
- GD has convergence rate of $1/\epsilon$ and SDCA has $\log 1/\epsilon$ convergence rate.
- memory: SDCA: $O(n + d)$, SGD: $O(d)$
- SDCA: can touch points in any order.
SDCA advantages/disadvantages

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

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

- the basic idea (formalized with duality) is pretty general for convex loss(·).
- 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.
- would an algo that is highly accurate in the convex case and sensible in the non-convex case.
(another idea) Stochastic Variance Reduced Gradient (SVRG)

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

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

2 corrected SGD: initialize $w \leftarrow \tilde{w}_s$. for $m$ steps,

sample a point $(x, y)$

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

3 update and repeat: $\tilde{w}_{s+1} \leftarrow w$. 
(another idea) Stochastic Variance Reduced Gradient (SVRG)

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

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

2. **corrected SGD**: initialize $w \leftarrow \tilde{w}_s$. for $m$ steps,

   sample a point $(x, y)$
   $$ w \leftarrow w - \eta \left( \nabla \text{loss}(w, (x, y)) - \nabla \text{loss}(\tilde{w}_s, (x, y)) + \nabla L(\tilde{w}_s) \right) $$

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

Two ideas:
- If $\tilde{w} = w_*$, then no update.
- unbiased updates: blue term is mean 0.
Guarantees of SVRG

- $n$ points, $d$ dimensions, $\lambda_{av}$ average eigenvalue

Computation time to get $\epsilon$ accuracy gradient descent: (Johnson & Zhang ’13)
- GD vs SDCA:
  $$\frac{\lambda_{max}}{\lambda_{min}} n d \log \frac{1}{\epsilon} \rightarrow \left( n + d \frac{\lambda_{av}}{\lambda_{min}} \right) d \log \frac{1}{\epsilon}$$

- conjugate GD vs ??
  $$\sqrt{\frac{\lambda_{max}}{\lambda_{min}}} n d \log \frac{1}{\epsilon} \rightarrow ??$$

- memory: $O(d)$