CS-GY 9223 D: Lecture something
Linear Programming

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IMPROVING GRADIENT DESCENT

We now have a good understanding of gradient descent.

Number of iterations for ϵ error:

	G-Lipschitz	β-smooth
R bounded start	$O\left(\frac{G^2R^2}{\epsilon^2}\right)$	$O\left(\frac{\beta R^2}{\epsilon}\right)$
α-strong convex	$O\left(\frac{G^2}{\alpha\epsilon}\right)$	$O\left(\frac{\beta}{\alpha}\log(1/\epsilon)\right)$

How do we use this understanding to design faster algorithms?

ACCELERATION

Nesterov's accelerated gradient descent:

- $\mathbf{x}^{(1)} = \mathbf{y}^{(1)} = \mathbf{z}^{(1)}$
- For $t = 1, \ldots, T$
  - $\mathbf{y}^{(t+1)} = \mathbf{x}^{(t)} - \frac{1}{\beta}\nabla f(\mathbf{x}^{(t)})$
  - $\mathbf{x}^{(t+1)} = \left(1 + \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)\mathbf{y}^{(t+1)} + \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\left(\mathbf{y}^{(t+1)} - \mathbf{y}^{(t)}\right)$

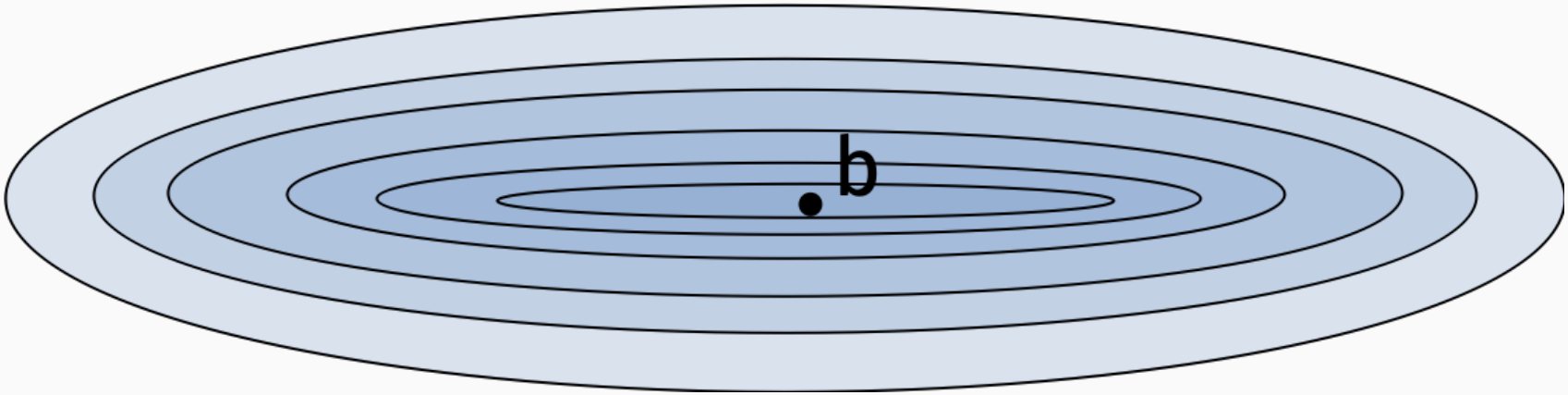
Theorem (AGD for β-smooth, α-strongly convex.)

Let f be a β-smooth and α-strongly convex function. If we run AGD for T steps we have:

$$f(\mathbf{x}^{(t)}) - f(\mathbf{x}^*) \leq \kappa e^{-(t-1)\sqrt{\kappa}}\left[f(\mathbf{x}^{(1)}) - f(\mathbf{x}^*)\right]$$

Corollary: If $T = O\left(\sqrt{\kappa}\log(\kappa/\epsilon)\right)$ achieve error ϵ.

INTUITION BEHIND ACCELERATION



Level sets of $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$.

Other terms for similar ideas:

- Momentum
- Heavy-ball methods

What if we look back beyond two iterates?

PRECONDITIONING

Main idea: Instead of minimizing $f(\mathbf{x})$, find another function $g(\mathbf{x})$ with the same minimum but which is better suited for first order optimization (e.g., has a smaller conditioner number).

Claim: Let $h(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}^d$ be an invertible function. Let $g(\mathbf{x}) = f(h(\mathbf{x}))$. Then

$$\min_{\mathbf{x}} f(\mathbf{x}) = \min_{\mathbf{x}} g(\mathbf{x}) \quad \text{and} \quad \arg\min_{\mathbf{x}} f(\mathbf{x}) = h\left(\arg\min_{\mathbf{x}} g(\mathbf{x})\right).$$

First Goal: We need $g(\mathbf{x})$ to still be convex.

Claim: Let $\mathbf{P}$ be an (invertible) $d \times d$ matrix and let $g(\mathbf{x}) = f(\mathbf{P}\mathbf{x})$.

$g(\mathbf{x})$ is always convex.

If $\mathbf{y}^* = \arg\min g(\mathbf{y})$, then $\mathbf{x}^* = \mathbf{P}\mathbf{y}^*$ minimizes $f(\mathbf{x})$.

Second Goal:

$g(\mathbf{x})$ should have better condition number κ than $f(\mathbf{x})$.

High dimensional chain rule:

$$\text{If } g(\mathbf{x}) = f(\mathbf{P}\mathbf{x}), \qquad \nabla^2 g(\mathbf{x}) = \nabla^2 \mathbf{P}^T f(\mathbf{P}\mathbf{x})\mathbf{P}.$$

Recall that the condition number is equal to:

$$\max_{\mathbf{x}} \frac{\lambda_{\max}\left(\nabla^2 g(\mathbf{x})\right)}{\lambda_{\min}\left(\nabla^2 g(\mathbf{x})\right)}$$

Example:

- $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$. $\nabla f(\mathbf{x}) = 2\mathbf{A}^T\mathbf{A}$. $\kappa_f = \frac{\lambda_1(\mathbf{A}^T\mathbf{A})}{\lambda_d(\mathbf{A}^T\mathbf{A})}$.
- $g(\mathbf{x}) = \|\mathbf{A}\mathbf{P}\mathbf{x} - \mathbf{b}\|_2^2$. $\nabla g(\mathbf{x}) = 2\mathbf{P}^T\mathbf{A}^T\mathbf{A}\mathbf{P}$ $\kappa_g = \frac{\lambda_1(\mathbf{P}^T\mathbf{A}^T\mathbf{A}\mathbf{P})}{\lambda_d(\mathbf{P}^T\mathbf{A}^T\mathbf{A}\mathbf{P})}$.

Ideal preconditioner: Choose P so that $\mathbf{P}^T\mathbf{A}^T\mathbf{A}\mathbf{P} = \mathbf{I}$. For example, could set $P = \sqrt{(\mathbf{A}^T\mathbf{A})^{-1}}$. But obviously this is too expensive to compute.

DIAGONAL PRECONDITIONER

Third Goal: $\mathbf{P}$ should be easy to compute.

Many, many problem specific preconditioners are used in practice. There design is usually a heuristic process.

Example: Diagonal preconditioner for least squares problems.

- Let $\mathbf{D} = \text{diag}(\mathbf{A}^T\mathbf{A})$
- Want $\mathbf{P}\mathbf{A}^T\mathbf{A}\mathbf{P}$ to be close to identity $\mathbf{I}$.
- Let $\mathbf{P} = \sqrt{\mathbf{D}^{-1}}$

$\mathbf{P}$ is often called a Jacobi preconditioner. Often works very well in practice!

DIAGONAL PRECONDITIONER

```
A =

    -734     1    33    9111     0
     -31    -2   108    5946   -19
     232    -1   101    3502    10
     426     0   -65   12503     9
    -373     0    26    9298     0
    -236    -2   -94    2398    -1
    2024     0  -132   -6904   -25
   -2258    -1    92   -6516     6
    2229     0     0   11921   -22
     338     1    -5  -16118   -23
```

```
>> cond(A'*A)

ans =

   8.4145e+07
```

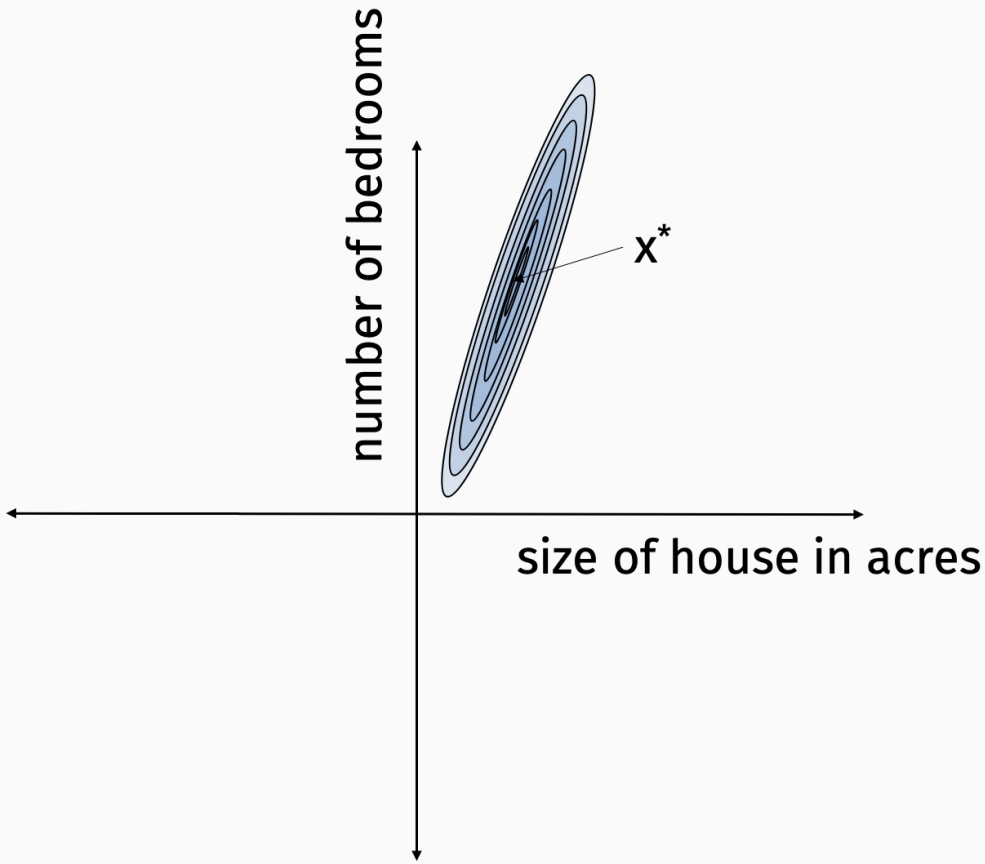
```
>> P = sqrt(inv(diag(diag(A'*A))));
>> cond(P*A'*A*P)

ans =

   10.3878
```

DIAGONAL PRECONDITIONER INTUITION

$g(\mathbf{x}) = f(\|\mathbf{APx} - \mathbf{b}\|_2^2)$ is the same least squares problem as $f(\mathbf{x}) = \|\mathbf{Ax} - \mathbf{b}\|_2^2$, but with each feature (column of $\mathbf{A}$) scaled differently. The i^{th} column is scaled by P_{ii}.



Feature scaling can have a huge impact on conditioning.

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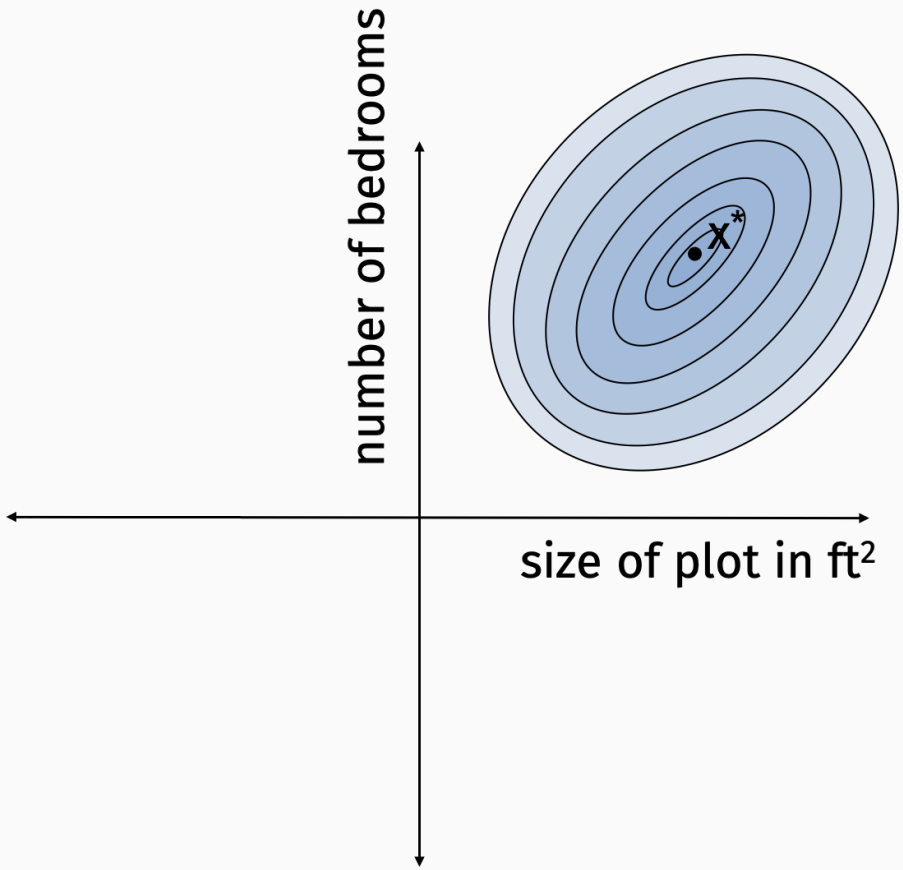


Feature scaling can have a huge impact on conditioning.

Another view: If $g(\mathbf{x}) = f(\mathbf{P}\mathbf{x})$ then $\nabla g(\mathbf{x}) = \mathbf{P}^T \nabla f(\mathbf{P}\mathbf{x})$.

$\nabla g(\mathbf{x}) = \mathbf{P} \nabla f(\mathbf{P}\mathbf{x})$ when $\mathbf{P}$ is symmetric.

Gradient descent on g:

- For $t = 1, \ldots, T$,
  - $\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \eta \mathbf{P} \left[\nabla f(\mathbf{P}\mathbf{x}^{(t)}) \right]$

Gradient descent on g:

- For $t = 1, \ldots, T$,
  - $\mathbf{y}^{(t+1)} = \mathbf{y}^{(t)} - \eta \mathbf{P}^2 \left[\nabla f(\mathbf{y}^{(t)}) \right]$

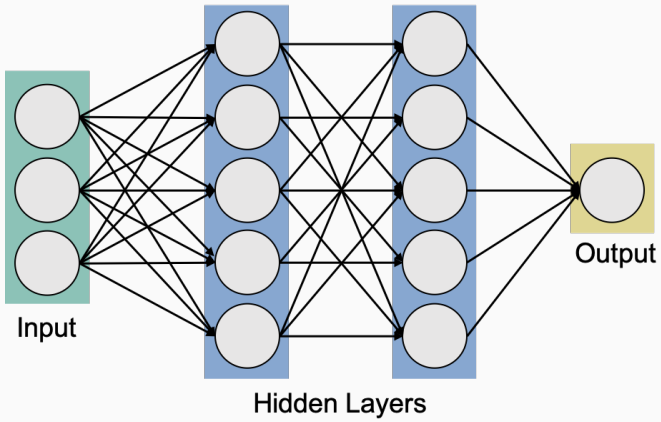
When $\mathbf{P}$ is diagonal, this is just gradient descent with a different step size for each parameter!

ADAPTIVE STEPSIZES

Less clear how to set P for general optimization problems where the Hessian is changing, but lots of heuristic algorithms based on this idea:

- AdaGrad, AdaDelta
- RMSprop
- Adam optimizer

(Pretty much all of the most widely used optimization methods for training neural networks.)



COORDINATE DESCENT

Main idea: Trade slower convergence (more iterations) for cheaper iterations.

Stochastic Gradient Descent: When $f(\mathbf{x}) = \sum_{i=1}^{n} f_i(\mathbf{x})$, approximate $\nabla f(\mathbf{x})$ with $\nabla f_i(\mathbf{x})$ for randomly chosen i.

Main idea: Trade slower convergence (more iterations) for cheaper iterations.

Stochastic Coordinate Descent: Only compute a single random entry of $\nabla f(\mathbf{x})$ on each iteration:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \frac{\partial f}{\partial x_2}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_d}(\mathbf{x}) \end{bmatrix} \qquad \nabla_i f(\mathbf{x}) = \begin{bmatrix} 0 \\ \frac{\partial f}{\partial x_i}(\mathbf{x}) \\ \vdots \\ 0 \end{bmatrix}$$

Update: $\mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^{(t)} - \eta \nabla_i f(\mathbf{x}^{(t)})$.

When $\mathbf{x}$ has d parameters, computing $\nabla_i f(\mathbf{x})$ sometimes costs just a $1/d$ fraction of what it costs to compute $\nabla f(\mathbf{x})$

Example: $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$ for $\mathbf{A} \in \mathbb{R}^{n \times d}, \mathbf{x} \in \mathbb{R}^d, \mathbf{b} \in \mathbb{R}^n$.

- $\nabla f(\mathbf{x}) = 2\mathbf{A}^T\mathbf{A}\mathbf{x} - 2\mathbf{A}^T\mathbf{b}$.
- $\nabla_i f(\mathbf{x}) = 2\left[\mathbf{A}^T\mathbf{A}\mathbf{x}\right]_i - 2\left[\mathbf{A}^T\mathbf{b}\right]_i$.

Computing full gradient takes $O(nd)$ time. Can we do better here?

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- $\nabla_i f(\mathbf{x}) = 2\left[\mathbf{A}^T\mathbf{A}\mathbf{x}\right]_i - 2\left[\mathbf{A}^T\mathbf{b}\right]_i$.

- $\mathbf{A}\mathbf{x}^{(t+1)} = \mathbf{A}\left(\mathbf{x}^{(t)} + c \cdot \mathbf{e}_i\right)$ — $O(n)$ time
- $2\left[\mathbf{A}^T\left(\mathbf{A}\mathbf{x}^{(t+1)} - \mathbf{b}\right)\right]_i$ — $O(n)$ time

Stochastic Coordinate Descent:

- Choose number of steps T and step size η.
- For $t = 1, \ldots, T$:
  - Pick random $j \in 1, \ldots, d$ uniformly at random.
  - $\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \eta \nabla_j f(\mathbf{x}^{(i)})$
- Return $\hat{\mathbf{x}} = \frac{1}{T} \sum_{t=1}^{T} \mathbf{x}^{(t)}$.

Theorem (Stochastic Coordinate Descent convergence)

Given a G-Lipschitz function f with minimizer $\mathbf{x}^*$ and initial point $\mathbf{x}^{(1)}$ with $\|\mathbf{x}^{(1)} - \mathbf{x}^*\|_2 \leq R$, SCD with step size $\eta = \frac{1}{Rd}$ satisfies the guarantee:

$$\mathbb{E}[f(\hat{\mathbf{x}}) - f(\mathbf{x}^*)] \leq \frac{2GR}{\sqrt{T/d}}$$

Often it doesn't make sense to sample i uniformly at random:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -.5 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 10 \\ 42 \\ -11 \\ -51 \\ 34 \\ -22 \end{bmatrix}$$

Select indices i proportional to $\|\mathbf{a}_i\|_2^2$:

$$\Pr[\text{select index } i \text{ to update}] = \frac{\|\mathbf{a}_i\|_2^2}{\sum_{j=1}^{d} \|\mathbf{a}_j\|_2^2} = \frac{\|\mathbf{a}_i\|_2^2}{\|\mathbf{A}\|_F^2}$$

Let's analyze this approach.

Specialization of SCD to $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$:

Randomized Coordinate Descent (Strohmer, Vershynin 2007 / Leventhal, Lewis 2018)

- For iterate $\mathbf{x}^{(t)}$, let $\mathbf{r}^{(t)}$ be the residual:

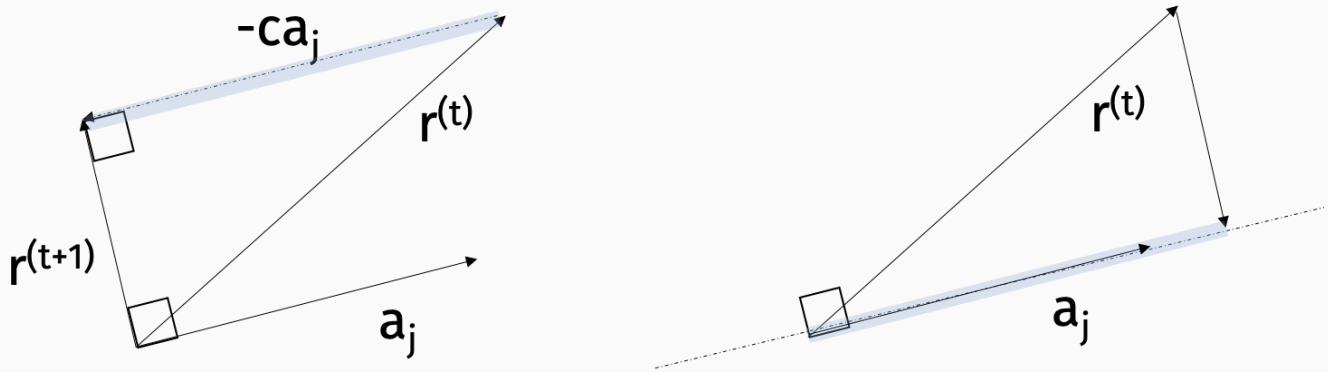
$$\mathbf{r}^{(t)} = \mathbf{A}\mathbf{x}^{(t)} - \mathbf{b}$$

- $\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - c\mathbf{e}_j$.
- $\mathbf{r}^{(t+1)} = \mathbf{r}^{(t)} - c\mathbf{a}_j$. Here $\mathbf{a}_j$ is the i^{th} column of $\mathbf{A}$.

Typically c depends on fixed learning rate. Here we will choose it optimally – similar idea to gradient descent with line search.

What choice for c minimizes $\|\mathbf{r}^{(t+1)}\|_2^2$?

- $\|\mathbf{r}^{(t+1)}\|_2^2 = \|\mathbf{r}^{(t)} - c\mathbf{a}_j\|_2^2$
- Requires projecting $\mathbf{r}^{(t)}$ onto perpendicular of $\mathbf{a}_j$.



- $c = \dfrac{\mathbf{a}_j^T \mathbf{r}^{(t)}}{\|\mathbf{a}_j\|_2^2}$

Note that $\|\mathbf{r}^{(t+1)}\|_2^2 = \|\mathbf{r}^{(t)}\|_2^2 - \|c\mathbf{a}_j\|_2^2 = \|\mathbf{r}^{(t)}\|_2^2 - \dfrac{(\mathbf{a}_j^T \mathbf{r}^{(t)})^2}{\|\mathbf{a}_j\|_2^2}$

Specialization of SCD to $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$:

Randomized Coordinate Descent

- Choose number of steps T.
- Let $\mathbf{x}^{(1)} = \mathbf{0}$ and $\mathbf{r}^{(1)} = \mathbf{b}$.
- For $t = 1, \ldots, T$:
  - Pick random $j \in 1, \ldots, d$. Index j is selected with probability proportional to $\|\mathbf{a}_j\|_2^2 / \|\mathbf{A}\|_F^2$.
  - Set $c = \mathbf{a}_j^T \mathbf{r}^{(t)} / \|\mathbf{a}_j\|_2^2$
  - $\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - c\mathbf{e}_j$
  - $\mathbf{r}^{(t+1)} = \mathbf{r}^{(t)} - c\mathbf{a}_j$
- Return $\mathbf{x}^{(T)}$.

Claim

$$\mathbb{E}\|\mathbf{r}^{(t+1)}\|_2^2 = \|\mathbf{r}^{(t)}\|_2^2 - \frac{1}{\|\mathbf{A}\|_F^2}\|\mathbf{A}^T\mathbf{r}^{(t)}\|_2^2$$

Any residual $\mathbf{r}$ can be written as $\mathbf{r} = \mathbf{r}^* + \bar{\mathbf{r}}$ where $\mathbf{r}^* = \mathbf{A}\mathbf{x}^* - \mathbf{b}$ and $\bar{\mathbf{r}} = \mathbf{A}(\mathbf{x}^t - \mathbf{x}^*)$. Note that $\mathbf{A}^T\mathbf{r}^* = 0$ and $\bar{\mathbf{r}} \perp \mathbf{r}^*$.

Claim

$$\mathbb{E}\|\bar{\mathbf{r}}^{(t+1)}\|_2^2 \leq \|\bar{\mathbf{r}}^{(t)}\|_2^2 - \frac{\lambda_{\min}(\mathbf{A}^T\mathbf{A})}{\|\mathbf{A}\|_F^2}$$

$$\mathbb{E}\|\bar{\mathbf{r}}^{(t+1)}\|_2^2 + \|\mathbf{r}^*\|_2^2 \leq \|\bar{\mathbf{r}}^{(t)}\|_2^2 + \|\mathbf{r}^*\|_2^2 - \frac{1}{\|\mathbf{A}\|_F^2}\|\mathbf{A}^T\bar{\mathbf{r}}^{(t)}\|_2^2\|\bar{\mathbf{r}}^{(t)}\|_2^2$$

Exercise: Because $\bar{\mathbf{r}}$ is in the column span of $\mathbf{A}$,

$$\|\mathbf{A}^T\bar{\mathbf{r}}^{(t)}\|_2^2 \geq \lambda_{\min}(\mathbf{A}^T\mathbf{A})\|\bar{\mathbf{r}}^{(t)}\|_2^2$$

Theorem (Randomized Coordinate Descent convergence)

After T steps of RCD with importance sampling run on $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$, we have:

$$\mathbb{E}[f(\mathbf{x}^{(t)}) - f(\mathbf{x}^*)] \leq \left(1 - \frac{\lambda_{\min}(\mathbf{A}^T\mathbf{A})}{\|\mathbf{A}\|_F^2}\right)^t [f(\mathbf{x}^{(0)}) - f(\mathbf{x}^*)]$$

Corollary: After $T = O(\frac{\|\mathbf{A}\|_F^2}{\lambda_{\min}(\mathbf{A}^T\mathbf{A})} \log \frac{1}{\epsilon})$ we obtain error $\epsilon\|\mathbf{b}\|_2^2$.

Is this more or less iterations than the $T = O(\frac{\lambda_{\max}(\mathbf{A}^T\mathbf{A})}{\lambda_{\min}(\mathbf{A}^T\mathbf{A})} \log \frac{1}{\epsilon})$ required for gradient descent to converge?

Recall useful linear algebraic fact:

$$\|\mathbf{A}\|_F^2 = \mathrm{tr}(\mathbf{A}^T\mathbf{A}) = \sum_{i=1}^{d} \lambda_i(\mathbf{A}^T\mathbf{A})$$

$$\lambda_{\max}(\mathbf{A}^T\mathbf{A}) \leq \|\mathbf{A}\|_F^2 \leq d \cdot \lambda_{\max}(\mathbf{A}^T\mathbf{A})$$

For solving $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$,

$$(\#\text{ GD Iterations}) \leq (\#\text{ RCD Iterations}) \leq d \cdot (\#\text{ GD Iterations})$$

But RCD iterations are cheaper by a factor of d.

When does $\|A\|_F^2 = \text{tr}(A^T A) = d \cdot \lambda_{\max}(A^T A)$?

When does $\|A\|_F^2 = \text{tr}(A^T A) = 1 \cdot \lambda_{\max}(A^T A)$?

Roughly:

Stochastic Gradient Descent performs well when data points (rows) are repetitive.

Stochastic Coordinate Descent performs well when data features (columns) are repetitive.

NON-CONVEX OPTIMIZATION

STATIONARY POINTS

We understand much less about optimizing non-convex functions in comparison to convex functions, but not nothing. In many cases, we're still figuring out the right questions to ask

Definition (Stationary point)

For a differentiable function f, a stationary point is any $\mathbf{x}$ with:

$$\nabla f(\mathbf{x}) = \mathbf{0}$$

local/global minima - local/global maxima - saddle points

Reasonable goal: Find an approximate stationary point $\hat{x}$ with

$$\|\nabla f(\hat{x})\|_2^2 \leq \epsilon.$$

Definition

A differentiable (potentially non-convex) function f is β smooth if for all $\mathbf{x}, \mathbf{y}$,

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \leq \beta \|\mathbf{x} - \mathbf{y}\|_2$$

Corollary: For all $\mathbf{x}, \mathbf{y}$

$$\left|\nabla f(\mathbf{x})^T(\mathbf{x} - \mathbf{y}) - [f(\mathbf{x}) - f(\mathbf{y})]\right| \leq \frac{\beta}{2}\|\mathbf{x} - \mathbf{y}\|_2^2.$$

GRADIENT DESCENT FINDS APPROXIMATE STATIONARY POINTS

Theorem

If GD is run with step size $\eta = \frac{1}{\beta}$ on a differentiable function f with global minimum $\mathbf{x}^*$ then after $T = O(\frac{\beta[f(\mathbf{x}^{(1)}) - f(\mathbf{x}^*)]}{\epsilon})$ we will find an ϵ-approximate stationary point $\hat{\mathbf{x}}$.

- $\nabla f(\mathbf{x}^{(t)})^T(\mathbf{x}^{(t)} - \mathbf{x}^{(t+1)}) - f(\mathbf{x}^{(t)}) + f(\mathbf{x}^{(t+1)}) \leq \frac{\beta}{2}\|\mathbf{x}^{(t)} - \mathbf{x}^{(t+1)}\|_2^2$.
- $f(\mathbf{x}^{(t+1])}) - f(\mathbf{x}^{(t)}) \leq \frac{\beta}{2}\eta^2\|\nabla f(\mathbf{x}^{(t)})\|_2^2 - \eta\|\nabla f(\mathbf{x}^{(t)})\|_2^2$
- $f(\mathbf{x}^{(t+1])}) - f(\mathbf{x}^{(t)}) \leq \frac{-\eta}{2}\|\nabla f(\mathbf{x}^{(t)})\|_2^2$
- $\frac{1}{T}\sum_{t=1}^{T}\frac{\eta}{2}\|f(\mathbf{x}^{(t)})\|_2^2 \leq \frac{1}{T}\sum_{t=1}^{T} f(\mathbf{x}^{(t)}) - f(\mathbf{x}^{(t+1)})$
- $\frac{\eta}{2}\min_t \|f(\mathbf{x}^{(t)})\|_2^2 \leq \frac{1}{T}\left[f(\mathbf{x})^{(1)} - f(\mathbf{x})^{(T)})\right]$

Questions in non-convex optimization

If GD can find a stationary point, are there algorithms which find a stationary point faster using preconditioning, acceleration, stocastic methods, etc.?

Questions in non-convex optimization

What if my function only has global minima and stationary points? Randomized methods (SGD, perturbed gradient methods, etc.) can "escape" stationary points under some minor assumptions.

Example: $\min_x \frac{-x^T A^T A x}{x^T x}$

- **Global minimum**: Top eigenvector of $A^T A$ (i.e., top principal component of A).
- **Stationary points:** All other eigenvectors of A.

Useful for lots of other matrix factorization problems beyond vanilla PCA.