5374 Fall 2022
Numerical Linear Algebra

Lecture 27

Gradient descent

The **Gradient Descent** algorithm (fixed number of steps $= k_0$)

Initial guess

Given z,
r := b - Az
is called
"the residual"

$\boldsymbol{z} = \boldsymbol{z}_0$

$\boldsymbol{v} = \boldsymbol{v}_0$

$\texttt{for}\ k = 1, \ldots, k_0$:

$\quad \boldsymbol{v} \leftarrow \boldsymbol{b} - \mathrm{A}\boldsymbol{z}$

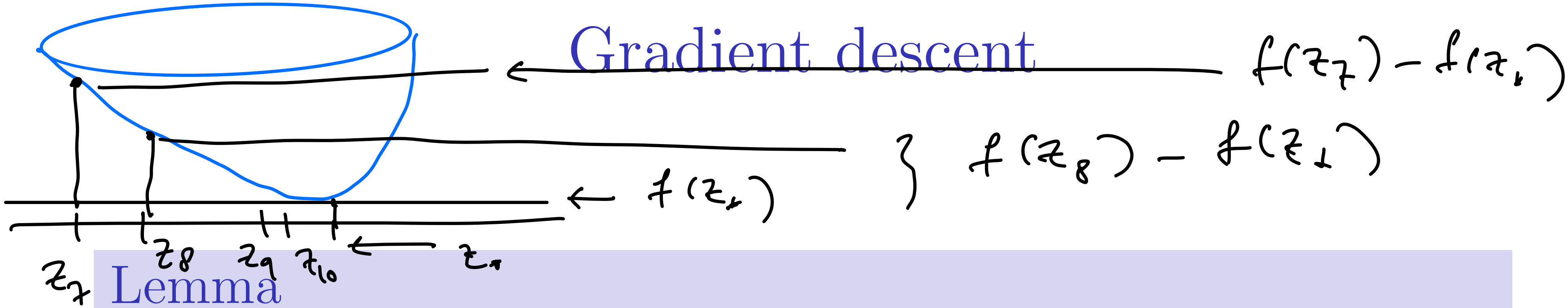
(This is from the formula for a line search with v=r)

$\quad \alpha \leftarrow (\boldsymbol{v}, \boldsymbol{v})/(\mathrm{A}\boldsymbol{v}, \boldsymbol{v})$

$\quad \boldsymbol{z} \leftarrow \boldsymbol{z} + \alpha \boldsymbol{v}$

$\texttt{return}\ \boldsymbol{z}$

Gradient descent



Lemma

Let A be positive and $\boldsymbol{z}_*$ the solution to $A\boldsymbol{z}_* = \boldsymbol{b}$, and $\{\boldsymbol{z}_k\}_k$ a sequence generated by Gradient Descent, then

$$f(\boldsymbol{z}_k) - f(\boldsymbol{z}_*) \leq \left(1 - \frac{1}{\mathrm{cond(A)}}\right)(f(\boldsymbol{z}_{k-1}) - f(\boldsymbol{z}_*))$$

In particular

$$f(\boldsymbol{z}_k) - f(\boldsymbol{z}_*) \leq \left(1 - \frac{1}{\mathrm{cond(A)}}\right)^k (f(\boldsymbol{z}_0) - f(\boldsymbol{z}_*))$$

This inequality ultimately produces an estimate for $\|z_k - z_*\| / \|z_*\|$. How?

Gradient descent

Lastly, observe that

$$f(\boldsymbol{z}_k) - f(\boldsymbol{z}_*) = \frac{1}{2}(\mathrm{A}(\boldsymbol{z}_k - \boldsymbol{z}_*), \boldsymbol{z}_k - \boldsymbol{z}_*)$$

The lemma says LHS $\to 0$ as $k \to \infty$, and thus RHS $\to 0$ as well

If A were diagonal, $A = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$

Then

$$= \frac{1}{2}\left(\lambda_1 (z_k - z_*)_1^2 + \cdots + \lambda_n (z_k - z_*)_n^2 \right)$$

$(\lambda_0 = \min\{\lambda_1, \ldots, \lambda_n\})$ $$\geq \frac{1}{2} \lambda_0 \left((z_k - z_*)_1^2 + \cdots + (z_k - z_*)_n^2 \right)$$

$$= \frac{1}{2} \lambda_0 \| z_k - z_* \|^2$$

(In general A is diagonalizable and the conclusion still holds)

Gradient descent

If $\lambda_0 =$ smallest eigenvalue of A, we have

$$\frac{1}{2}(\mathrm{A}(\boldsymbol{z}_k - \boldsymbol{z}_*), \boldsymbol{z}_k - \boldsymbol{z}_*) \geq \frac{\lambda_0}{2}|\boldsymbol{z}_k - \boldsymbol{z}_*|^2$$

and thus $z_k \to z_*$ in the limit.

We can do even better! We can say how fast the convergence happens. We have

$$\frac{1}{2}\lambda_0 \|z_k - z_*\|^2 \leq f(z_k) - f(z_*) \quad \text{(by the lemma)}$$

$$\leq \left(1 - \frac{1}{\mathrm{cond}(A)}\right)^k \left(f(z_0) - f(z_*)\right)$$

Gradient descent

Let's look only at $z_0 = 0$, then

$$\frac{1}{2}\lambda_0 \|z_k - z_*\|^2 \leq \left(1 - \frac{1}{\operatorname{cond}(A)}\right)^k \left(-f(z_*)\right)$$

Well, $f(z_*) = \frac{1}{2}(Az_*, z_*) - (b, z_*)$. Since

$Az_* = b$, $\quad f(z_*) = \frac{1}{2}(Az_*, z_*) - (Az_*, z_*)$

$$= -\frac{1}{2}(Az_*, z_*)$$

$$\Rightarrow \quad |f(z_*)| = -f(z_*) = \frac{1}{2}(Az_*, z_*)$$

$$\leq \frac{1}{2}\Lambda_0 \|z_*\|^2$$

where $\quad \Lambda_0 = \max\{\lambda_1, \dots, \lambda_n\}$

(Here, $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A)

Gradient descent

What we have, is

$$\cancel{\frac{1}{2}}\lambda_0 \|z_k - z_*\|^2 \le \left(1 - \frac{1}{\mathrm{cond}(A)}\right)^k \cancel{\frac{1}{2}}\Lambda_0 \|z_*\|^2$$

Since $\mathrm{cond}(A) = \dfrac{\Lambda_0}{\lambda_0}$,

$$\|z_k - z_*\|^2 \le \left(1 - \frac{1}{\mathrm{cond}(A)}\right)^k \mathrm{cond}(A)\, \|z_*\|^2$$

$$\Longrightarrow \quad \frac{\|z_k - z_*\|^2}{\|z_*\|^2} \le \left(1 - \frac{1}{\mathrm{cond}(A)}\right)^k \mathrm{cond}(A)$$

The square of the relative error after k stages of gradient descent.

Gradient descent

In conclusion,

$$\frac{\|z_k - z_*\|}{\|z_*\|} \leq \mathrm{cond}(A)^{\frac{1}{2}} \left(1 - \frac{1}{\mathrm{cond}(A)}\right)^{\frac{k}{2}}$$

Suppose we want the RHS to be $\leq \varepsilon$,

how big should k be?

Gradient descent

For a moment, write $c = \mathrm{cond}(A)$, give $\varepsilon > 0$, we want to find the first $k \in \mathbb{N}$ such that

$$c^{\frac{1}{2}}\left(1 - \frac{1}{c}\right)^{\frac{k}{2}} \le \varepsilon$$

$$e^{\frac{k}{2}\log\left(1-\frac{1}{c}\right)} = \frac{\varepsilon}{c^{1/2}}$$

$$\frac{k}{2}\log\left(1-\frac{1}{c}\right) = \log\left(\varepsilon/c^{1/2}\right)$$

$$k = \frac{2\log\left(\varepsilon/c^{1/2}\right)}{\log\left(1-\frac{1}{c}\right)} = \frac{2\log\left(c^{1/2}/\varepsilon\right)}{\log\left(\frac{c}{c-1}\right)}$$

$$k \sim 2c\log(c^{1/2}/\varepsilon)$$

$$\log\left(\frac{c}{c-1}\right) = \log\left(1+\frac{1}{c}+O\left(\frac{1}{c^2}\right)\right) = \frac{1}{c} + O\left(\frac{1}{c^2}\right)$$

$$\Longrightarrow \quad k \sim 2\,\frac{\log\left(c^{1/2}/\varepsilon\right)}{\frac{1}{c}} = 2c\log\left(c^{1/2}/\varepsilon\right)$$

Gradient descent

For a moment, write $c = \mathrm{cond}(A)$, give $\varepsilon > 0$, we want to find the first $k \in \mathbb{N}$ such that

$$c\left(1 - \frac{1}{c}\right)^{\frac{k}{2}} \leq \varepsilon$$

$$k \sim 2c\log(c^{1/2}/\varepsilon)$$

<u>Example</u>: If $c = 100$, and we want ℓ decimals of precision (or the relative error say) then $\varepsilon = 10^{-\ell}$

$$\Longrightarrow \quad k = \left\lceil 2\,100 \log\left(10/10^{-\ell}\right)\right\rceil = \left\lceil 200 \log\left(10^{\ell+1}\right)\right\rceil$$

$$= 200\cdot(\ell+1)$$

Gradient descent

What's remarkable about this estimate is its independence on the dimension n, showing that a n dimensional equation with n large but good condition number can be effectively solved in relatively few steps.

In summary
Gradient Descent:

- Involves minimizing $f(\boldsymbol{z}) := \frac{1}{2}(\mathrm{A}\boldsymbol{z}, \boldsymbol{z}) - (\boldsymbol{b}, \boldsymbol{z})$

- Line searches to minimize $f(\boldsymbol{z})$,

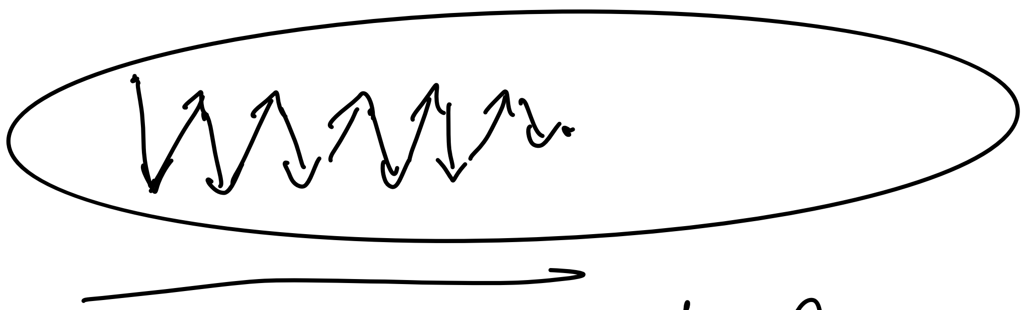
$$\operatorname{argmin}_\alpha f(\boldsymbol{z} + \alpha \boldsymbol{v}) = -\frac{(\mathrm{A}\boldsymbol{z} - \boldsymbol{b}, \boldsymbol{v})}{(\mathrm{A}\boldsymbol{v}, \boldsymbol{v})} = \frac{(\boldsymbol{r}, \boldsymbol{v})}{(\mathrm{A}\boldsymbol{v}, \boldsymbol{v})}$$

- Gradient descent consists in taking $\boldsymbol{v} = -\nabla f(\boldsymbol{z}) = \boldsymbol{r}$

- $\#\{\text{iterations for rel. error} \leq \varepsilon\} \sim \mathrm{cond}(A) \log(\mathrm{cond}(A)^{1/2}/\varepsilon)$

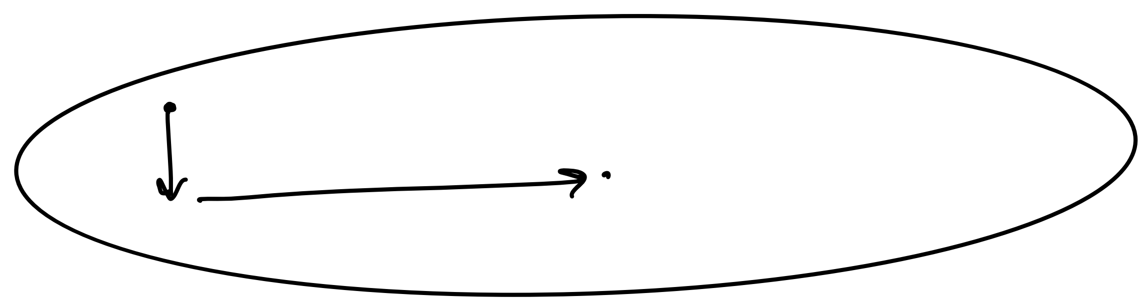
The Conjugate Gradient Method

$$f(\boldsymbol{z}) = f(\boldsymbol{z}_*) + \frac{1}{2}(\mathrm{A}(\boldsymbol{z} - \boldsymbol{z}_*), \boldsymbol{z} - \boldsymbol{z}_*)$$



(too much zigzag'ing if A has a bad condition number)

What we would like to happen...



Conjugate gradient

We introduce an auxiliary inner product

$$(\boldsymbol{x}, \boldsymbol{y})_{\mathrm{A}} := (\mathrm{A}\boldsymbol{x}, \boldsymbol{y}), \quad \|\boldsymbol{x}\|_{\mathrm{A}} := \sqrt{(\boldsymbol{x}, \boldsymbol{x})_{\mathrm{A}}}$$

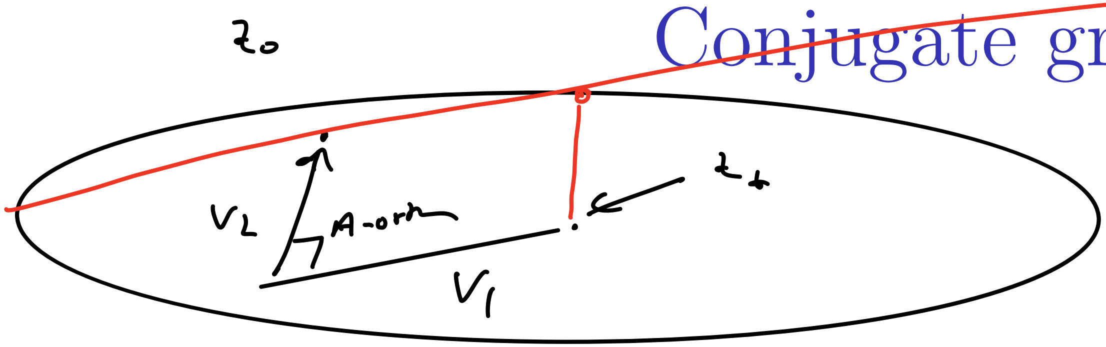
In the context of scientific computing, when two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ are orthogonal with respect to this inner product they are said to be A-conjugate.

Conjugate gradient

Observe, that in terms of $\|\cdot\|_{\mathrm{A}}$, we have

$$f(\boldsymbol{z}) = f(\boldsymbol{z}_*) + \frac{1}{2}\|\boldsymbol{z} - \boldsymbol{z}_*\|_{\mathrm{A}}^2$$

Conjugate gradient



Let $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n$ be a basis made out of A-conjugate vectors

$$(\boldsymbol{v}_i, \boldsymbol{v}_j)_{\mathrm{A}} = 0 \text{ whenever } i \neq j$$

As they form a basis, given some initial guess $\boldsymbol{z}_0$, we can write

$$\boldsymbol{z}_0 - \boldsymbol{z}_* = \alpha_1 \boldsymbol{v}_1 + \ldots + \alpha_n \boldsymbol{v}_n$$

for some (at the moment, unknown) numbers $\alpha_1, \ldots, \alpha_n$.

Conjugate gradient

As we recalled a moment ago, we have

$$\begin{aligned} f(\boldsymbol{z}_0) &= f(\boldsymbol{z}_*) + \tfrac{1}{2}(A(\boldsymbol{z}_0 - \boldsymbol{z}_*), \boldsymbol{z}_0 - \boldsymbol{z}_*) \\ &= f(\boldsymbol{z}_*) + \tfrac{1}{2}\||\boldsymbol{z}_0 - \boldsymbol{z}_*\|_A^2 \end{aligned}$$

Since $\boldsymbol{z}_0 - \boldsymbol{z}_* = \alpha_1 \boldsymbol{v}_1 + \ldots + \alpha_n \boldsymbol{v}_n$ and the $\boldsymbol{v}_i$ are A-orthogonal,

$$f(\boldsymbol{z}_0) = f(\boldsymbol{z}_*) + \tfrac{1}{2}\|\boldsymbol{v}_1\|_{\mathrm{A}}^2 \alpha_1^2 + \ldots + \tfrac{1}{2}\|\boldsymbol{v}_n\|_{\mathrm{A}}^2 \alpha_n^2$$

Conjugate gradient

Line searches

It is wortwhile to check what would happen if we perform consecutive line searches in the directions $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n$, starting from $\boldsymbol{z}_0$

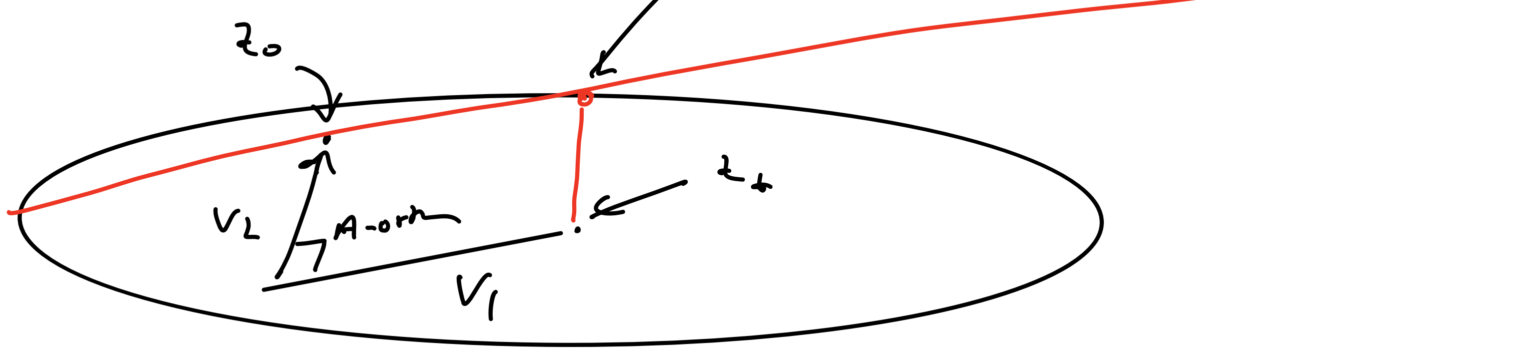
Observe that

$$f(\boldsymbol{z}_0 + s\boldsymbol{v}_1) = f(\boldsymbol{z}_*) + \frac{1}{2}\|\boldsymbol{v}_1\|_{\mathrm{A}}^2(\alpha_1 + s)^2 + \ldots + \frac{1}{2}\|\boldsymbol{v}_n\|_{\mathrm{A}}^2 \alpha_n^2$$

It is clear that the minimum is achieved for $s = -\alpha_1$, so that

z_1

$$\boldsymbol{z}_1 = \boldsymbol{z}_* + \alpha_2\boldsymbol{v}_2 + \ldots + \alpha_n\boldsymbol{v}_n$$



Conjugate gradient

Line searches

Now, performing a line search at $\boldsymbol{z}_1$ in the direction $\boldsymbol{v}_2 \ldots$

$$f(\boldsymbol{z}_1 + s\boldsymbol{v}_2) = f(\boldsymbol{z}_*) + \frac{1}{2}\|\boldsymbol{v}_2\|_{\mathrm{A}}^2(\alpha_2 + s)^2 + \ldots + \frac{1}{2}\|\boldsymbol{v}_n\|_{\mathrm{A}}^2\alpha_n^2$$

Now the minimum is achieved for $s = -\alpha_2$, so

$$\boldsymbol{z}_2 = \boldsymbol{z}_1 - s_2\boldsymbol{v}_2 = \boldsymbol{z}_* + \alpha_3\boldsymbol{v}_3 + \ldots + \alpha_n\boldsymbol{v}_n$$

Conjugate gradient

Line searches

Repeating this argument, after k steps (with $k < n$) we have

$$\boldsymbol{z}_k = \boldsymbol{z}_* + \alpha_{k+1}\boldsymbol{v}_{k+1} + \ldots + \alpha_n \boldsymbol{v}_n$$

and, at the n-th step

$$\boldsymbol{z}_n = \boldsymbol{z}_*.$$

That is, **if rounding errors are not a problem**, we would find the **exact** solution $\boldsymbol{z}_*$ after no more than n line searches.

Conjugate gradient

Selecting the search directions

We are all left with generating the search directions $\boldsymbol{v}_k$ so that they are pairwise conjugate (= orthogonal with respect to $(,)_A$)

We cannot take $\boldsymbol{v}_k = -\nabla f(\boldsymbol{z}_k)$ (cannot expect $(A\boldsymbol{v}_i, \boldsymbol{v}_j) = 0$)

However, we can progressively modify these $\boldsymbol{v}$'s, setting, first

$$\boldsymbol{v}_1 = \boldsymbol{r}_1 = \boldsymbol{b} - \mathrm{A}\boldsymbol{z}_0$$

and defining (recursively) for $k = 2, \ldots, n$

$$\boldsymbol{v}_k = \boldsymbol{r}_k - \left(\begin{array}{l} \text{the } A\text{-orthogonal projection of } \boldsymbol{r}_k \\ \text{onto the space spanned by } \boldsymbol{v}_1, \ldots, \boldsymbol{v}_{k-1} \end{array} \right)$$

recall,

$r_k = b - Az_k$

Conjugate gradient

Selecting the search directions

$\left(r_k = b - A x_k = -\nabla f(x_k) \right)$

With better notation, we will take $\boldsymbol{v}_k = \mathrm{P}_{k-1}\boldsymbol{r}_k$, where

$$\mathrm{P}_{k-1} = \begin{array}{l}\text{A-orthogonal projection onto} \\ \text{the complement of } \boldsymbol{v}_1, \ldots, \boldsymbol{v}_{k-1}\end{array}$$

This means that for any $\boldsymbol{x} \in \mathbb{R}^n$ and $k = 2, \ldots, n$

$$\mathrm{P}_{k-1}\boldsymbol{x} = \boldsymbol{x} - \sum_{j=1}^{k-1} \frac{(\boldsymbol{v}_j, \boldsymbol{x})_{\mathrm{A}}}{(\boldsymbol{v}_j, \boldsymbol{v}_j)_{\mathrm{A}}} \boldsymbol{v}_j$$

Conjugate gradient

Selecting the search directions

$$
\begin{aligned}
\boldsymbol{v}_k &= -\mathrm{P}_{k-1}\nabla Q(\boldsymbol{z}_k) \\
&= \mathrm{P}_{k-1}\boldsymbol{r}_k \\
&= \boldsymbol{r}_k - \sum_{j=1}^{k-1} \frac{(\boldsymbol{v}_j, \boldsymbol{r}_k)_{\mathrm{A}}}{(\boldsymbol{v}_j, \boldsymbol{v}_j)_{\mathrm{A}}} \boldsymbol{v}_j
\end{aligned}
$$

Conjugate gradient

Selecting the search directions

Lemma

For the sequences $\boldsymbol{z}_k$, $\boldsymbol{r}_k$ in the CGM, we have

$$(\boldsymbol{r}_{k-1}, \boldsymbol{v}_j) = 0 \text{ for } 1 \leq j \leq k-2$$

In particular, for $k = 2, \ldots, n$, the following holds

$$\boldsymbol{v}_k = \boldsymbol{r}_k - \frac{(\boldsymbol{v}_{k-1}, \boldsymbol{r}_k)_{\mathrm{A}}}{(\boldsymbol{v}_{k-1}, \boldsymbol{v}_{k-1})_{\mathrm{A}}} \boldsymbol{v}_{k-1}$$

Conjugate gradient

The **Conjugate Gradient** algorithm

Let $k_0 \leq n$,

$$
\begin{aligned}
&\boldsymbol{z} = \boldsymbol{z}_0 \\
&\boldsymbol{r} = \boldsymbol{b}_0 - \mathrm{A}\boldsymbol{z}_0 \\
&\boldsymbol{v} = \boldsymbol{r} \\
&\texttt{for } k = 1, \ldots, k_0\texttt{:} \\
&\qquad \alpha \leftarrow \frac{(\boldsymbol{r},\boldsymbol{v})}{(\mathrm{A}\boldsymbol{v},\boldsymbol{v})} \\
&\qquad \boldsymbol{z} \leftarrow \boldsymbol{z} + \alpha\boldsymbol{v} \\
&\qquad \boldsymbol{r} \leftarrow \boldsymbol{b} - \mathrm{A}\boldsymbol{z} \\
&\qquad \boldsymbol{v} \leftarrow \boldsymbol{r} - \frac{(\mathrm{A}\boldsymbol{v},\boldsymbol{r})}{(\mathrm{A}\boldsymbol{v},\boldsymbol{v})}\boldsymbol{v} \\
&\texttt{return } \boldsymbol{z}
\end{aligned}
$$

line search in the current direction v

compute new residual

get new search direction by projection r into A-orthogonal complement of current v

Conjugate gradient

Lemma

Let A be positive and $\boldsymbol{z}_*$ the solution to $A\boldsymbol{z}_* = \boldsymbol{b}$, and $\{\boldsymbol{z}_k\}_k$ a sequence generated by Conjugate Gradient, then

$$f(\boldsymbol{z}_k) - f(\boldsymbol{z}_*) \leq 2\left(1 - \frac{2}{\sqrt{\mathrm{cond(A)}} + 1}\right)^k (f(\boldsymbol{z}_0) - f(\boldsymbol{z}_*))$$

From here follows a similar estimate for

$\|z_k - z_*\| / \|z_*\|$

as in gradient descent.

Conjugate gradient

Number of operations

Each iteration of the conjugate gradient method (CGM) has:

- Matrix-vector products: $A\boldsymbol{v}, A\boldsymbol{z}$ ($O(n^2)$ ($O(n)$ if sparse))
- Inner products: $(\boldsymbol{r}, \boldsymbol{v}), (A\boldsymbol{v}, \boldsymbol{v}), (A\boldsymbol{v}, \boldsymbol{r})$ $O(n)$
- Sums/differences $\boldsymbol{z} + \alpha\boldsymbol{v}$, $\boldsymbol{b} - A\boldsymbol{z}, \boldsymbol{r} - \frac{(A\boldsymbol{v},\boldsymbol{r})}{(A\boldsymbol{v},\boldsymbol{v})}\boldsymbol{v}$ $O(n)$

How many FLOPs?

The first • takes $O(n^2)$ FLOPs ($O(n)$ if A is sparse)

The second and third • take $O(n)$ FLOPs

Total (for k_0 iteration) $O(k_0 n^2)$ / $O(k_0 n)$ if spa

Conjugate gradient

Number of operations

Each iteration of the conjugate gradient method (CGM) has:

- Matrix-vector products: $\mathrm{A}\boldsymbol{v}, \mathrm{A}\boldsymbol{z}$
- Inner products: $(\boldsymbol{r}, \boldsymbol{v}), (\mathrm{A}\boldsymbol{v}, \boldsymbol{v}), (\mathrm{A}\boldsymbol{v}, \boldsymbol{r})$
- Sums/differences $\boldsymbol{z} + \alpha\boldsymbol{v}$, $\boldsymbol{b} - \mathrm{A}\boldsymbol{z}, \boldsymbol{r} - \frac{(\mathrm{A}\boldsymbol{v},\boldsymbol{r})}{(\mathrm{A}\boldsymbol{v},\boldsymbol{v})}\boldsymbol{v}$

How many FLOPs?

The first • takes $O(n^2)$ FLOPs ($O(n)$ if A is sparse)

The second and third • take $O(n)$ FLOPs

The analysis of CGM is more delicate, but in general it will perform **much better** than regular gradient descent.