A Krylov method for solving symmetric systems arising in optimization

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Symmetric system of linear equations

Consider

$$Hx + c = 0,$$

for $x \in \mathbb{R}^n$. Assume $H = H^T \in \mathbb{R}^{n\times n}$ and $c \neq 0$.

Motivation: KKT systems arising in optimization, $H = H^T$, in general indefinite

General idea: Generate linearly independent vectors $\{q_k\}$ based on H and c.

Krylov subspaces

Consider

$$\mathcal{K}_0(c, H) = \{0\},$$

$$\mathcal{K}_k(c, H) = span\{c, Hc, H^2c, \dots, H^{k-1}c\}, \quad k = 1, 2, \dots.$$

With $q_0 = c$, then one sequence of l.i. vectors may be generated as

$$q_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^{\perp}, k = 1, \dots, r,$$

such that $q_k \neq 0$ for $k < r$ and $q_r = 0$. (r is the minimum index k for which $q_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^{\perp} = \{0\}$)

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Krylov vectors

The *Krylov vectors* $\{q_0, q_1, \dots, q_{r-1}\}$, with $q_0 = c$

- form an orthogonal, hence linearly independent, basis of $\mathcal{K}_r(c, H)$
- are each uniquely determined up to a nonzero scaling
- may be expressed as,

$$q_k = \sum_{j=0}^{k} \delta_k^{(j)} H^j c, \quad k = 1, \dots, r$$

where $\{\delta_k^{(j)}\}_{j=0}^{k}$ are uniquely determined up to a common non-zero scaling.

Not sufficient to just have q_k and it is not convenient to have a representation using all $\{\delta_k^{(j)}\}$!

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Triples

Let

$$q_k = H\Big(\underbrace{\sum_{j=1}^{k} \delta_k^{(j)} H^{j-1} c}_{=:\, y_k \in \mathcal{K}_k(c,H)}\Big) + \underbrace{\delta_k^{(0)}}_{=:\, \delta_k} c = Hy_k + \delta_k c$$

Each Krylov vector q_k may be associated with a triple (q_k, y_k, δ_k).

Possible to continue the recursion, and let

$$y_k = Hy_k^{(1)} + \delta_k^{(1)} c, \quad \text{with}$$

$$y_k^{(1)} = \sum_{j=2}^{k} \delta_k^{(j)} H^{j-2} c \in \mathcal{K}_{k-1}(c,H), \quad k = 2, \ldots, r.$$

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How to generate the Krylov vectors?

Given $q_0 = c$, let

$$q_{k+1} \leftarrow \alpha_k \Big(- Hq_k + \frac{q_k^T H q_k}{q_k^T q_k} q_k + \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}} q_{k-1} \Big),$$

where α_k, $k = 0, \ldots, r$ are free and non-zero.

How to generate the triples?

Given $y_0 = 0$ and $\delta_0 = 1$, let

$$y_{k+1} \leftarrow \alpha_k \Big(- q_k + \frac{q_k^T H q_k}{q_k^T q_k} y_k + \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}} y_{k-1} \Big),$$

$$\delta_{k+1} \leftarrow \alpha_k \Big(\frac{q_k^T H q_k}{q_k^T q_k} \delta_k + \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}} \delta_{k-1} \Big),$$

where α_k, $k = 0, \ldots, r$ are free and non-zero.

Remarks on the recursions for the triples

- Given $(q_0, y_0, \delta_0) = (c, 0, 1)$, generate the triples (q_k, y_k, δ_k), $k = 1, \ldots, r$, for which $q_k = Hy_k + \delta_k c$
- One matrix-vector multiplication, Hq_k, for each k
- It holds that $y_k \neq 0$, $k = 1, \ldots, r$.
- Note that $\{\alpha_k\}$ is explicitly undecided
- What happens for $k = r$, i.e. $(q_r, y_r, \delta_r) = (0, y_r, \delta_r)$?

Convergence result

Recall: $q_k = Hy_k + \delta_k c$, for all k. For $k = r$ it holds that $q_r = 0$, hence

$$0 = q_r = Hy_r + \delta_r c$$

Theorem

Let (q_k, y_k, δ_k), $k = 0, \dots, r$, be given the recursions then,

(1) *If $\delta_r \neq 0$, then $Hx_r + c = 0$ for $x_r = (1/\delta_r)y_r$, so that $c \in \mathcal{R}(H)$ and x_r solves $Hx + c = 0$.*

(2) *If $\delta_r = 0$, then $Hy_r = 0$, $c^T y_r \neq 0$ so that $c \notin \mathcal{R}(H)$ and $Hx + c = 0$ has no solution.*

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A Krylov algorithm

Generate triples (q_k, y_k, δ_k) until $q_r = 0$. Then examine if $\delta_r \neq 0$ or $\delta_r = 0$.

Choice of α_k non-zero is arbitrary. Our choice: α_k such that $||y_{k+1}|| = ||c||$, $(y_{k+1} \neq 0, \forall k \geq 0)$

Example

Let

$$c = \begin{pmatrix} 3 & 2 & 1 & 0 & -1 & -2 & -3 \end{pmatrix}^T, \quad H = diag(c),$$

Then $Hx + c = 0$ is compatible, with optimal solution $x^* = \begin{pmatrix} -1 & -1 & -1 & 0 & -1 & -1 & -1 \end{pmatrix}^T$.

Note that H is indefinite.

Krylov algorithm on example problem

```
q = 3.0000   -9.0000    2.2678   -2.7046    0.2648   -0.2445    0.0000
    2.0000   -4.0000   -2.2678    5.4912   -1.0591    1.4673         0
    1.0000   -1.0000   -2.2678    2.3768    1.3239   -3.6681         0
         0         0         0         0         0         0         0
   -1.0000   -1.0000    2.2678    2.3768   -1.3239   -3.6681         0
   -2.0000   -4.0000    2.2678    5.4912    1.0591    1.4673         0
   -3.0000   -9.0000   -2.2678   -2.7046   -0.2648   -0.2445   -0.0000

y =      0   -3.0000    3.4017   -0.9015   -2.2241   -0.0815    2.1602
         0   -2.0000    1.5119    2.7456   -2.8419    0.7336    2.1602
         0   -1.0000    0.3780    2.3768   -0.9885   -3.6681    2.1602
         0         0         0         0         0         0         0
         0    1.0000    0.3780   -2.3768   -0.9885    3.6681    2.1602
         0    2.0000    1.5119   -2.7456   -2.8419   -0.7336    2.1602
         0    3.0000    3.4017    0.9015   -2.2241    0.0815    2.1602

d = 1.0000         0   -2.6458         0    2.3123         0   -2.1602
```

Some results on $\{\delta_k\}$

If $q_k \neq 0$ and $\delta_k = 0$, then

- $\delta_{k+1} \neq 0$
- $\delta_{k-1}\delta_{k+1} < 0$

If $H \succeq 0$, then

- $\delta_k \neq 0$, for all $k < r$
- if $\delta_k > 0$ and $\delta_{k+1} \neq 0$, then $\delta_{k+1} > 0$ iff $\alpha_k > 0$

With $\delta_0 = 1$ and $\alpha_k > 0$ it holds that

- for $H \succeq 0$, $\delta_k > 0$, for all $k < r$ and $\delta_r \geq 0$

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Connection to the method of conjugate gradients

Obtain CG as a special case of the Krylov method for exactly the choice of α_k such that (q_k, y_k, δ_k) may be denoted by $(g_k, x_k, 1)$.
(This particular α_k is the same as the steplength when CG is derived a linesearch method for minimizing over expanding subpaces)
Note:

- For $H \succeq 0$ and $Hx + c = 0$ compatible, it will be ok since $\delta_k \neq 0$ for all k
- For $H \succeq 0$ and $Hx + c = 0$ incompatible, CG will fail in the last iteration, only then will $\delta_r = 0$

This choice of scaling will fail for $\delta_k = 0$.

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Extension of the Krylov method

- The Krylov method gives a certificate incompatibility if $Hx + c = 0$ is not compatible
- Next extend the Krylov method, using the triples (q_k, y_k, δ_k), to obtain, in each step, a minimum-residual solution x_k^{MR} and in the final step get the minimum-residual solution of minimum Euclidean norm.

Minimum residual solution

Let x_k^{MR} be defined as a solution to

$$\min_{x \in \mathcal{K}_k(c,H)} ||Hx + c||_2^2$$

and the corresponding residual $g_k^{MR} = Hx_k^{MR} + c$.

The vectors x_k^{MR} are are uniquely defined for $k = 0, \ldots, r-1$, and for $k = r$ if $c \in \mathcal{R}(H)$. For the case $k = r$ and $c \notin \mathcal{R}(H)$ there is one degree of freedom for x_r^{MR}.

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Theorem

Given the triples (q_k, y_k, δ_k) then x_k^{MR} is a solution to

$$min_{x \in \mathcal{K}_k(c,H)} ||Hx + c||_2^2$$

if and only if $x_k^{MR} = \sum_{i=0}^{k} \gamma_i y_i$ for some γ_i, $i = 0, \ldots, k$, that are optimal to

$$\begin{array}{ll} min & \frac{1}{2} \sum_{i=0}^{k} \gamma_i^2 q_i^T q_i \\ s.t. & \sum_{i=0}^{k} \gamma_i \delta_i = 1. \end{array}$$

An arbitrary $g \in \mathcal{K}_{k+1}(c, H)$

$$g = \sum_{i=0}^{k} \gamma_i q_i = \sum_{i=0}^{k} \gamma_i (Hy_i + \delta_i c) = H(\sum_{i=0}^{k} \gamma_i y_i) + (\sum_{i=0}^{k} \gamma_i \delta_i) c$$

Theorem cont.

In particular, x_k^{MR} takes the following form:

(a) *For $k < r$, it holds that*

$$x_k^{MR} = \frac{1}{\sum_{j=0}^{k} \frac{\delta_j^2}{q_j^T q_j}} \sum_{i=0}^{k} \frac{\delta_i}{q_i^T q_i} y_i,$$

and $g_k^{MR} = Hx_k^{MR} + c \neq 0$.

(b) *For $k = r$ and $\delta_r \neq 0$,*

$$x_r^{MR} = (1/\delta_r) y_r$$

and $g_r^{MR} = Hx_r^{MR} + c = 0$.

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(b) *For $k = r$ and $\delta_r \neq 0$,*

$$x_r^{MR} = (1/\delta_r) y_r$$

and $g_r^{MR} = Hx_r^{MR} + c = 0$.

Theorem cont.

(c) *For $k = r$ and $\delta_r = 0$, it holds that $x_r^{MR} = x_{r-1}^{MR} + \gamma_r y_r$, where γ_r is an arbitrary scalar, and $g_r^{MR} = Hx_r^{MR} + c = g_{r-1}^{MR} \neq 0$. In addition, x_{r-1}^{MR} and x_r^{MR} solve $\min_{x \in \mathbb{R}^n} ||Hx + c||_2^2$. The particular choice*

$$\gamma_r = -\frac{y_r^T x_{r-1}^{MR}}{y_r^T y_r}$$

Makes x_r^{MR} an optimal solution to $\min_{x \in \mathbb{R}^n} ||Hx + c||_2^2$ of minimum Euclidean norm.

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Recursions for the minimum residual method

Given (q_k, y_k, δ_k) and let $\delta_0^{MR} := \delta_0^2$, $y_0^{MR} := \delta_0 y_0$, and

$$\delta_k^{MR} = \frac{q_k^T q_k}{q_{k-1}^T q_{k-1}} \delta_{k-1}^{MR} + \delta_k^2, \quad y_k^{MR} = \frac{q_k^T q_k}{q_{k-1}^T q_{k-1}} y_{k-1}^{MR} + \delta_k y_k,$$

for $k = 1, \ldots, r$, then

$$x_k^{MR} = \frac{1}{\delta_k^{MR}} y_k^{MR}, \quad k = 0, \ldots, r-1 \text{ and } k = r \text{ if } \delta_r \neq 0,$$

Extended Krylov algorithm

Generate (q_k, y_k, δ_k) as before. Generate δ_k^{MR} and y_k^{MR}, to obtain x_k^{MR}. Until $q_r = 0$. Then examine if $\delta_r \neq 0$ or $\delta_r = 0$.

Recall (the compatible) example:

```
xMR =

         0         0   -1.1108   -1.1108   -0.9953   -0.9953   -1.0000
         0         0   -0.4937   -0.4937   -1.0641   -1.0641   -1.0000
         0         0   -0.1234   -0.1234   -0.3593   -0.3593   -1.0000
         0         0         0         0         0         0         0
         0         0   -0.1234   -0.1234   -0.3593   -0.3593   -1.0000
         0         0   -0.4937   -0.4937   -1.0641   -1.0641   -1.0000
         0         0   -1.1108   -1.1108   -0.9953   -0.9953   -1.0000

delta =

    1.0000         0   -2.6458         0    2.3123         0   -2.1602
```

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         0         0   -0.1234   -0.1234   -0.3593   -0.3593   -1.0000
         0         0         0         0         0         0         0
         0         0   -0.1234   -0.1234   -0.3593   -0.3593   -1.0000
         0         0   -0.4937   -0.4937   -1.0641   -1.0641   -1.0000
         0         0   -1.1108   -1.1108   -0.9953   -0.9953   -1.0000

delta =

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```

An incompatible example

Let

$$\begin{aligned} c &= \quad \begin{pmatrix} 3 & 2 & 1 & 1 & -1 & -2 & -3 \end{pmatrix}^T, \\ H &= diag \begin{pmatrix} 5 & 2 & 1 & 0 & -1 & -2 & -3 \end{pmatrix}, \end{aligned}$$

Note that H is indefinite and the system $Hx + c = 0$ is incompatible.

```
q =
    3.0000  -13.1379    3.5628   -0.8597    0.1063   -0.0181    0.0017   -0.0000
    2.0000   -2.7586   -5.7676    3.9832   -1.3787    0.6372   -0.1470   -0.0000
    1.0000   -0.3793   -3.1464    0.1039    1.8638   -2.5737    1.1021    0.0000
    1.0000    0.6207   -2.8617   -1.7605    2.2573    0.5896   -1.7634   -0.0000
   -1.0000   -1.6207    2.0296    2.7934   -0.6882   -2.4489   -1.4695    0.0000
   -2.0000   -5.2414    1.3007    4.3735    2.1842    1.1548    0.3149   -0.0000
   -3.0000  -10.8621   -3.8286   -2.6032   -0.6658   -0.2082   -0.0367    0.0000

y =
         0   -3.0000    2.4296    0.8844   -1.3331   -0.3574    1.0584   -0.0000
         0   -2.0000   -0.0222    3.7521   -2.9466   -0.2710    1.6899         0
         0   -1.0000   -0.2847    1.8644   -0.3935   -3.1633    2.8655    0.0000
         0   -1.0000   -0.5584    1.5833    0.7502   -3.7018   -0.7931    5.3852
         0    1.0000    0.8320   -1.0329   -1.5691    1.8593    3.2329    0.0000
         0    2.0000    2.2113   -0.4262   -3.3494   -1.1670    1.6060    0.0000
         0    3.0000    4.1379    2.6283   -2.0353   -0.5202    1.7756    0.0000

delta =
    1.0000    0.6207   -2.8617   -1.7605    2.2573    0.5896   -1.7634   -0.0000

xMR =
         0   -0.1588   -0.6633   -0.6143   -0.5995   -0.5998   -0.6000   -0.6000
         0   -0.1059   -0.0228   -0.6647   -1.0640   -1.0371   -1.0000   -1.0000
         0   -0.0529    0.0585   -0.2817   -0.2148   -0.4441   -1.0000   -1.0000
         0   -0.0529    0.1284   -0.1845    0.1376   -0.1481    0.1333   -0.0000
         0    0.0529   -0.1983    0.0407   -0.4178   -0.2588   -1.0000   -1.0000
         0    0.1059   -0.5364   -0.2994   -1.0375   -1.0794   -1.0000   -1.0000
         0    0.1588   -1.0143   -1.1600   -0.9990   -0.9938   -1.0000   -1.0000
```

- Using triples (q_k, y_k, δ_k) such that $q_k = Hy_k + \delta_k c$ (uniquely determined up to a common non-zero scaling)
- A Krylov method for solving a system of linear equations $Hx + c = 0$ for $H = H^T$. Gives a solution $x_r = (1/\delta_r)y_r$ in the compatible case or a certificate of incompatibility
- An extended Krylov method with explicit recursions for y_k^{MR} and δ_k^{MR} to obtain the minimum-residual solution x_k^{MR} in each step. Gives a solution $x_r^{MR} = x_r$ in the compatible case or the minimum-residual solution of minimum Euclidean norm

$$x_r^{MR} = x_{r-1}^{MR} - \frac{y_r^T x_{r-1}^{MR}}{y_r^T y_r} y_r$$

in the incompatible case

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Thank you for your time!

Questions?

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