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Quick Recap: Nonlinear Conjugate Gradient Methods

Extension of the linear CG to work for non-linear (optimization) problems. In the first pass (Fletcher-Reeves' Algorithm), we simply replaced all instances of the residual $\bar{r}_k$ by the gradient of the objective $\nabla f(\bar{x}_k)$, and the step length $\alpha_k$ is calculated by a linesearch.

We looked at some modifications, and arrived at the Polak-Ribièrè PR+CG algorithm, where the $\beta$ of Fletcher-Reeves is modified

$$
\beta_{k+1}^{FR} = \frac{\nabla f_{k+1}^T \nabla f_{k+1}}{\nabla f_k^T \nabla f_k} \quad \rightarrow \quad \beta_{k+1}^{PR} = \frac{\nabla f_{k+1}^T (\nabla f_{k+1} - \nabla f_k)}{\nabla f_k^T \nabla f_k}
$$

and the final $\beta$ is $\beta_{k+1}^+ = \max(\beta_{k+1}^{PR}, 0)$.

Finally, periodic restarting, when

$$
\frac{\nabla f_k^T \nabla f_{k-1}}{\nabla f_k^T \nabla f_k} \geq \nu \sim 0.1
$$

was introduced in order to ensure good convergence.
We know (e.g. from Lecture #5) that Newton’s method has great local convergence properties. Once we get close to the minimizer $\bar{x}^*$ convergence is quadratic.

This convergence requires that we start “close enough” to $\bar{x}^*$ — in regions far away, where the objective is not convex, all bets are off and the behavior can be quite erratic; we cannot guarantee convergence at all!

**Our present goal:**

$\Rightarrow$ To design a Newton-based method which is robust and efficient in “all” cases.
The Newton Step

We get the Newton step from the symmetric $n \times n$ linear system

$$\nabla^2 f(\bar{x}_k) \bar{p}_k^N = -\nabla f(\bar{x}_k)$$

For global convergence the Newton direction must be a descent direction, this is true if the Hessian ($\nabla^2 f(\bar{x}_k)$) is positive definite.

If the Hessian is not positive definite, the Newton direction may be an ascent direction and/or extremely long (division by almost zero).

We look at two approaches: The first uses the conjugate gradient method, and gives us the “Newton-CG” methods for both line-search and trust-region methods; the second strategy involves modifying the Hessian so that it becomes “sufficiently positive definite,” yielding the “modified Newton method.”
As always, we want to keep the computational cost down.

In Newton-CG, this is accomplished by terminating the computation before an exact solution to

$$\nabla^2 f(\bar{x}_k)\bar{p}_k^N = -\nabla f(\bar{x}_k),$$

has been found. Thus we get and approximation $\bar{p}_k \approx \bar{p}_k^N$, hence the name “inexact Newton methods.”

We would like to exploit any special sparsity structure in the Hessian in order to solve the linear problem as efficiently as possible.

For now, we assume we have access to the Hessian in analytical form. We will cover this final issue soon.
Inexact Newton Steps

If we settle for an inexact (approximate) solution of

$$\nabla^2 f(\bar{x}_k)\bar{p}^N_k = -\nabla f(\bar{x}_k),$$

then we need a measure of how close our approximate solution $\bar{p}_k$ is to the exact Newton direction... Another use of the residual

$$\bar{r}_k = \nabla^2 f(\bar{x}_k)\bar{p}_k + \nabla f(\bar{x}_k).$$

Usually we do not want the termination condition for the inexact solution to depend on the size of $f$, hence are interested in the relative size of the residual, and say that an approximate solution is good enough when

**Termination criterion:**

$$\|\bar{r}_k\| \leq \eta_k \|\nabla f(\bar{x}_k)\|, \quad \eta_k \in (0, 1)$$

The sequence $\{\eta_k\}$ is known as a **forcing sequence**.
Selection of the forcing sequence greatly impacts how fast the overall algorithm converges, as illustrated in the following results:

**Theorem**

Suppose that the gradient $\nabla f(\bar{x})$ is continuously differentiable in a neighborhood $\mathcal{N}$ of a minimizer $\bar{x}^*$, and assume that the Hessian $\nabla^2 f(\bar{x}^*)$ is positive definite. Consider the iteration $\bar{x}_{k+1} = \bar{x}_k + \bar{p}_k$ where $\bar{r}_k(\bar{p}_k)$ satisfies

$$\|\bar{r}_k\| \leq \eta_k \|\nabla f(\bar{x}_k)\|, \quad \eta_k \in (0, 1)$$

and assume that $\eta_k \leq \eta$ for some $\eta \in [0, 1)$. Then, if the starting point $\bar{x}_0$ is sufficiently near $\bar{x}^*$, the sequence $\{\bar{x}_k\}$ converges to $\bar{x}^*$ linearly. That is, for all sufficiently large $k$ we have

$$\|\bar{x}_{k+1} - \bar{x}^*\| \leq c \|\bar{x}_k - \bar{x}^*\|$$

for some constant $c \in (0, 1)$.
The preceding theorem is neither very exiting, nor very useful (on its own).

The restriction on the forcing sequence is very mild, we are basically just requiring that we make *some* progress in solving the linear system

\[ \nabla^2 f(\bar{x}_k)\bar{p}_k^N = -\nabla f(\bar{x}_k). \]

Likewise, the result — **linear convergence** — is good news, but hardly anything that causes us to throw a party!

However, by **carefully selecting** the forcing sequence we get a slightly more exciting result...
Suppose that the conditions of the previous theorem hold, and assume that the iterates $\{\bar{x}_k\}$ generated by the inexact Newton method converge to $\bar{x}^*$. Then the rate of convergence is \textbf{superlinear} if $\eta_k \to 0$, and \textbf{quadratic} if $\eta_k = O(\|\nabla f(\bar{x}_k)\|)$.

Now we know exactly how hard we have to work at solving the linear systems in order to achieve certain convergence rates, \textit{e.g.}

$$\eta_k = \min \left(10^{-3}, \sqrt{\|\nabla f(\bar{x}_k)\|}\right) \quad \text{Superlinear Convergence}$$

$$\eta_k = \min \left(10^{-3}, \|\nabla f(\bar{x}_k)\|\right) \quad \text{Quadratic Convergence}$$

\textbf{Note:} These results are still \textit{local} — we still have to figure out how to make our algorithms work if not started “close” to $\bar{x}^*$. 
We now have the pieces necessary to build **robust Newton methods** with good performance characteristics: first on the menu — the line search Newton-CG method:

**Getting the search direction $\bar{p}_k$:**

We apply the linear Conjugate Gradient (CG) method to the Newton equations

$$\nabla^2 f(\bar{x}_k) \bar{p}_k^N = -\nabla f(\bar{x}_k),$$

and require that the solution satisfies a termination test of the type

$$\|\bar{r}_k\| \leq \eta_k \|\nabla f(\bar{x}_k)\|, \quad \eta_k \in (0, 1).$$

However, if the Hessian is not positive definite this may break...
If/When the Hessian is not positive definite we may enter a region of negative curvature; when we do, the CG iteration is terminated in order to guarantee that the generated $\bar{p}_k$ is a descent direction:

In search-direction-search, we set $A = \nabla^2 f(\bar{x}_k)$, $\bar{b} = -\nabla f(\bar{x}_k)$ and then start the CG-iteration:

1. The starting point is set to $\bar{x}^{(0)} = 0$
2. If a (CG-internal) search direction $\bar{p}^{(i)}$ generated by the CG-iteration satisfies

$$
\left[ \bar{p}^{(i)} \right]^T A \left[ \bar{p}^{(i)} \right] \leq 0,
$$

then, if ($i == 0$), set $\bar{x}^{(0)} = \bar{b} = -\nabla f(\bar{x}_k)$ [Steepest Descent] and return, otherwise stop immediately and return $\bar{x}^{(i)}$.

3. The approximate Newton step $\bar{p}_k \overset{\text{def}}{=} \bar{x}^{(i)}$. 

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Practical Newton Methods — (12/18)
Algorithm: “CG-core”

Given $A$, $\bar{b}$, $\eta^{(\kappa)}$, $\bar{x}^{CG}_0$: $\bar{r}_0 = A\bar{x}^{CG}_0 - \bar{b}$, $\bar{p}_0 = -\bar{r}_0$, $k = 0$

while ( $\|\bar{r}_k\| > \eta^{(\kappa)}\|\bar{b}\|$ )

$$
\alpha_k = \frac{\bar{r}_k^T \bar{r}_k}{\bar{p}_k^T A \bar{p}_k},
$$

if $\bar{p}_k^T A \bar{p}_k \leq 0$, $k > 0$ return ($\bar{x}^{CG}_k$)

$$
\bar{x}^{CG}_{k+1} = \bar{x}^{CG}_k + \alpha_k \bar{p}_k
$$

if $\bar{p}_k^T A \bar{p}_k \leq 0$, $k = 0$ return ($\bar{x}^{CG}_{k+1}$)

$$
\bar{r}_{k+1} = \bar{r}_k + \alpha_k A \bar{p}_k
$$

$$
\beta_{k+1} = \frac{\bar{r}_{k+1}^T \bar{r}_{k+1}}{\bar{r}_k^T \bar{r}_k},
$$

Save numerator for next iteration!

$$
\bar{p}_{k+1} = -\bar{r}_{k+1} + \beta_{k+1} \bar{p}_k
$$

end-while ( $k = k + 1$ )

The $\bar{p}_k$’s are CG-internal search directions, not to be confused with the search direction for the optimization algorithm!
**Note:** If the CG-core algorithm encounters a direction of negative curvature in the first iteration, the steepest descent direction is used.

Given $\bar{x}_0$: $k = 0$

while ( $\bar{x}_k$ is not a minimum )

$\bar{p}^{N-CG}_k = \text{CG-core}(A = \nabla^2 f(\bar{x}_k), \bar{b} = -\nabla f(\bar{x}_k), \eta^{(k)} = \eta_k, \bar{x}^{CG}_0 = \bar{0})$

$\alpha^{LS}_k = \text{linesearch}(\bar{p}^{N-CG}_k, ...)$

$\bar{x}_{k+1} = \bar{x}_k + \alpha^{LS}_k \bar{p}^{N-CG}_k$

end-while ( $k = k + 1$ )

Where we specify $\eta_k$ as discussed earlier, and the linesearch is such that $\alpha_k$ satisfies the Wolfe, Strong Wolfe, Goldstein, or Armijo backtracking conditions.
Comments:

- Nothing is stopping us from basing this on the preconditioned version of CG, in fact that is probably the right thing to do (see other comments)!

- Line Search Newton-CG (LS-N-CG) is well suited for large problems.

- LS-N-CG has one minor weakness — If/When the Hessian is nearly singular, the Newton-CG direction can be excessively long resulting in many function evaluations in the linesearch.

- This weakness is greatly alleviated by preconditioning, i.e. implementing LS-N-PCG(M).
Sometimes it is desirable to use a direct linear algebra technique, *i.e.* an efficient cousin of Gaussian Elimination, to solve the Newton equations

\[
\nabla^2 f(\bar{x}_k) \bar{p}_k^N = -\nabla f(\bar{x}_k).
\]

If/When the Hessian is not positive definite (or close to singular), it can be modified either before or **during** the solution process so that in effect we solve

\[
\left[ \nabla^2 f(\bar{x}_k) + E_k \right] \bar{p}_k^N = -\nabla f(\bar{x}_k),
\]

where the Hessian modification $E_k$ is chosen so that the resulting matrix is sufficiently positive definite.
Algorithm: Line Search Newton with Modification

Given $\bar{x}_0$: $k = 0$

while ( $\bar{x}_k$ is not a minimum )

\[ B_k = \text{factorize}(\nabla^2 f(\bar{x}_k) + E_k) \]
\[ \bar{p}^{N-mod}_k = -B_k^{-1} \nabla f(\bar{x}_k) \]
\[ \alpha_{k}^{LS} = \text{linesearch}(\bar{p}^{N-mod}_k, \ldots) \]
\[ \bar{x}_{k+1} = \bar{x}_k + \alpha_{k}^{LS} \bar{p}^{N-mod}_k \]

end-while ( $k = k + 1$ )

Where the linesearch is such that $\alpha_k$ satisfies the Wolfe, Strong Wolfe, Goldstein, or Armijo backtracking conditions.

The factorization algorithm is such that $E_k = 0$ if $\nabla^2 f(\bar{x}_k)$ is sufficiently positive definite; otherwise chosen so that $B_k$ is sufficiently positive definite.

We save the details of Hessian modification for next lecture...