Quasi-Newton Methods

Lecture 4, Continuous Optimisation
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Notes by Dr Raphael Hauser (hauser@comlab.ox.ac.uk)

Newton-Raphson direction $d_k = n_f(x_k) := -\left(D^2 f(x_k)\right)^{-1} \nabla f(x_k)$.

- Takes $\simeq n$ function evaluations to compute $\nabla f(x_k)$ and $\simeq n^2$ function evaluations to compute $D^2 f(x_k)$.
- Once these matrices have been computed it takes $O(n^3)$ computer operations to solve the following linear system for d_k,
$$D^2 f(x_k)\, d_k = -\nabla f(x_k).$$
- Q-quadratic convergence.

Recall from Lecture 3

Steepest-descent direction $d_k := -\nabla f(x_k)$.

- Takes $\simeq n$ function evaluations (of f) to compute.
- Q-linear convergence.

Ideally, one would like a search-direction that combines the cheapness of $-\nabla f(x_k)$ with the fast convergence of $n_f(x_k)$.

In reality, we need to strike a balance between work per iteration and convergence speed.

Quasi-Newton methods are clever mechanisms that achieve such a balance.

Let $\mathcal{C}(f)$ be the cost of one function evaluation of f. Then the following shows the trade-off between computational cost and convergence speed,

	cost per iteration	convergence rate
Steepest descent	$O\big(n\mathcal{C}(f)\big)$	Q-linear
Quasi-Newton	$O\big(n^2 + n\mathcal{C}(f)\big)$	Q-superlinear
Newton-Raphson	$O\big(n^3 + n^2\mathcal{C}(f)\big)$	Q-quadratic

Motivation of Quasi-Newton Updates:

The Newton-Raphson step is defined by

$$x_{k+1} - x_k = n_f(x_k) = -\big(D^2 f(x_k)\big)^{-1} \nabla f(x_k).$$

Assume an approximation $B_k \approx D^2 f(x_k)$ of the Hessian is available. Then an approximate Newton-Raphson step is given by the *quasi-Newton update*

$$d_k = -B_k^{-1} \nabla f(x_k).$$

This update is well-defined when B_k is nonsingular, and in particular when B_k is positive definite symmetric.

In this case the update is also motivated by the fact that

$$x_k + d_k = x_k - B_k^{-1} \nabla f(x_k).$$

is the global minimiser of the following *quadratic model* of f,

$$p(x) = f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2}(x - x_k)^{\mathsf{T}} B_k (x - x_k).$$

- B_k is only an approximation of $D^2 f(x_k)$. Therefore we use d_k as a search direction rather than an exact update.
- A line-search then yields a new quasi-Newton iterate

$$x_{k+1} = x_k + \alpha_k d_k.$$

- Q-N algorithms specify methods for cheaply computing a new approximate Hessian $B_{k+1} \simeq D^2 f(x_{k+1})$. This computation should only use the quantities $B_k, \nabla f(x_k)$ and $\nabla f(x_{k+1})$.

Algorithm 1: Generic Quasi-Newton Method.

S0 Choose a starting point $x_0 \in \mathbb{R}^n$, a nonsingular $B_0 \in S^n$ (often the choice is $B_0 = I$), and a termination tolerance $\epsilon > 0$. Set $k = 0$.

S1 If $\|\nabla f(x_k)\| \leq \epsilon$ then stop and output x_k as an approximate local minimiser of f. Else go to **S2**.

S2 Compute the quasi-Newton search direction $d_k = -B_k^{-1}\nabla f(x_k)$.

S3 Perform a practical line-search for the minimisation of $\phi(\alpha) = f(x_k + \alpha d_k)$: find a step length α_k that satisfies the Wolfe conditions and compute the new iterate $x_{k+1} = x_k + \alpha_k d_k$.

S4 Compute the new approximate Hessian B_{k+1} according to the specified rule.

S5 Replace k by $k + 1$ and go to **S1**.

A Wish List of Properties of B_k

P1: B_k should be nonsingular, so that **S2** is well-defined.

P2: B_k should be such that d_k is a descent direction, so that **S3** is well-defined.

P3: B_k should be symmetric, as Hessians are symmetric matrices.

Properties P1–P3 can be satisfied by requiring that B_k be positive definite symmetric: P1 and P3 are trivially true, and P2 follows from

$$\langle \nabla f(x_k), d_k \rangle = -\nabla f(x_k)^{\mathsf{T}} B_k^{-1} \nabla f(x_k) < 0,$$

unless $\nabla f(x_k) = 0$.

This also avoids that the quasi-Newton method gets attracted to any point but a local minimiser.

Question: Is this a problem when $D^2 f(x_k) \not\succ 0$?

The wish-list continues . . .

P4: B_{k+1} should be computable by "recycling" the quantities

$$\nabla f(x_{k+1}), \nabla f(x_k), \ldots, \nabla f(x_0), d_k, \alpha_k \text{ and possibly } B_k.$$

Crucial observation: the gradient change

$$\gamma_k := \nabla f(x_{k+1}) - \nabla f(x_k)$$

yields information about the Hessian change $D^2 f(x_{k+1}) - D^2 f(x_k)$.

Let $\delta_k := \alpha_k d_k$ be the chosen update.

The search direction d_k was motivated by the fact that the gradient change predicted by the quadratic model

$$p(x) = f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2}(x - x_k)^{\mathsf{T}} B_k (x - x_k)$$

is

$$\begin{aligned} \nabla f(x_k + d_k) - \nabla f(x_k) &\approx \nabla p(x_k + d_k) - \nabla p(x_k) \\ &= \nabla f(x_k) + B_k d_k - \nabla f(x_k) \\ &= -\nabla f(x_k). \end{aligned} \tag{1}$$

In other words, it is predicted that $x_k + d_k$ is exactly a stationary point of f.

But p is only a *locally* valid model of f and the new iterate x_{k+1} is obtained via a line search.

The true gradient change

$$\gamma_k = \nabla f(x_{k+1}) - \nabla f(x_k)$$

differs from the prediction (1).

A clever way to incorporate γ_k into the Hessian approximations is to choose B_{k+1} so that the quadratic model

$$h(x) = f(x_k) + \langle \nabla f(x_k), (x - x_k) \rangle + \frac{1}{2}(x - x_k) B_{k+1} (x - x)$$

would have correctly predicted the observed gradient change:

$$\gamma_k = \nabla f(x_{k+1}) - \nabla f(x_k) = \nabla h(x_{k+1}) - \nabla h(x_k) = \nabla f(x_k) + B_{k+1}\delta_k - \nabla$$

In other words, B_{k+1} should be chosen such that

$$B_{k+1}\delta_k = \gamma_k \tag{2}$$

holds true. (2) is called the *secant condition*.

The wish-list continues . . .

P5: B_{k+1} should be *close* to B_k in a well-defined sense, so that B_k can converge to $D^2 f(x^*)$ and d_k is allowed to become the Newton-Raphson step asymptotically.

A straightforward idea to define a notion of closeness is by use of a matrix norm: $d(B_{k+1}, B_k) = \|B_{k+1} - B_k\|$.

However, it is often more useful to characterise closeness by keeping the rank of $B_{k+1} - B_k$ as low as possible.

Symmetric Rank-1 Updates (SR1)

The method we are about to describe satisfies some but not all of the properties P1–P6.

P3 and P5 can be satisfied by requiring that B_{k+1} is a rank-1 update of B_k: we want to select some vector u and set

$$B_{k+1} = B_k + uu^{\mathsf{T}}. \tag{3}$$

If B_0 is symmetric, this guarantees that B_k is symmetric for all k, and $\text{rank}(B_{k+1} - B_k) = 1$.

Low rank updates will automatically guarantee that the last property on our wish list is satisfied as well:

P6: The choice of B_k should be such that the overall work per iteration is at most of order $O(n^2)$, to gain a substantial speed-up over the $O(n^3)$ computer operations needed to perform a Newton-Raphson step.

The choice of u is fixed when P4 is satisfied through the secant condition

$$B_{k+1}\delta_k = \gamma_k, \tag{4}$$

where $\delta_k = x_{k+1} - x_k = \alpha_k d_k$ and $\gamma_k = \nabla f(x_{k+1}) - \nabla f(x_k)$ as before.

Multiplying (3) by δ_k and substituting the result into (4), we find

$$(u^{\mathsf{T}}\delta_k)u = \gamma_k - B_k\delta_k. \tag{5}$$

Multiplying the transpose of this equation by δ_k, we obtain

$$(u^{\mathsf{T}}\delta_k)^2 = (\gamma_k - B_k\delta_k)^{\mathsf{T}}\delta_k. \tag{6}$$

Equation (5) shows that

$$u = \frac{\gamma_k - B_k\delta_k}{u^\mathsf{T}\delta_k}.$$

Therefore, (3) and (6) imply that the updating rule should be as follows,

$$\begin{aligned} B_{k+1} &= B_k + \frac{(\gamma_k - B_k\delta_k)(\gamma_k - B_k\delta_k)^\mathsf{T}}{(u^\mathsf{T}\delta_k)^2} \\ &= B_k + \frac{(\gamma_k - B_k\delta_k)(\gamma_k - B_k\delta_k)^\mathsf{T}}{(\gamma_k - B_k\delta_k)^\mathsf{T}\delta_k}. \end{aligned} \tag{7}$$

Note that since $\gamma_k = \nabla f(x_{k+1}) - \nabla f(x_k)$ and $\delta_k = \alpha_k d_k$, we can compute the SR1 update from the "recycled" information referred to in P4.

What about property P6?

- Once d_k is known, computing $\alpha_k, x_{k+1}, \nabla f(x_{k+1}), \gamma_k$ and δ_k is very cheap.
- The total work for computing the updated matrix B_{k+1} from B_k and d_k is of order $O(n^2)$.
- However, in order to compute d_k we need to solve the linear system of equations

  $$B_k d_k = -\nabla f(x_k), \tag{8}$$

  which takes $O(n^3)$ time!

When B_{k+1} is computed via the updating rule (7) Algorithm 1 is called the *symmetric rank 1 method* (or SR1).

This method was independently suggested by Broyden, Davidson, Fiacco-McCormick, Murtagh-Sargent, and Wolfe in 1967-69.

The updates of the SR1 method are very simple to compute, but they have the drawback that B_k is not always positive definite and d_k might not always be defined or be a descent direction.

Moreover, $(\gamma_k - B_k\delta_k)^\mathsf{T}\delta$ can be close to zero which leads to very large updates.

A way out of the dilemma . . .

Theorem 1: Sherman–Morrison–Woodbury formula. If $B \in \mathbb{R}^{n\times n}$ and $U, V \in \mathbb{R}^{n\times p}$ are matrices then

$$(B + UV^\mathsf{T})^{-1} = B^{-1} - B^{-1}U(I + V^\mathsf{T}B^{-1}U)^{-1}V^\mathsf{T}B^{-1}.$$

See the new problem set for a proof.

The usefulness of this formula is quickly understood:

- Suppose we knew $H_k = B_k^{-1}$. Then, applying the Sherman-Morrison-Woodbury formula to $B_+ = B_{k+1}$, $B = B_k$, $U = u = (\gamma_k - B_k\delta_k)$ and $V = U^\mathsf{T}$ (that is, $p = 1$ in this case), we find

$$\begin{aligned} H_{k+1} &= (B_+)^{-1} \\ &= B^{-1} - B^{-1}u\Big(1 + u^\mathsf{T}B^{-1}u\Big)^{-1}u^\mathsf{T}B^{-1} \\ &= H_k + \frac{(\delta_k - H_k\gamma_k)(\delta_k - H_k\gamma_k)^\mathsf{T}}{(\delta_k - H_k\gamma_k)^\mathsf{T}\gamma_k}. \end{aligned}$$

- Thus, H_{k+1} is just a rank 1 update of H_k.
- Since we assumed H_k known, computing $d_k = -H_k\nabla f(x_k)$ now takes only $O(n^2)$ work.
- Furthermore, H_{k+1} is computed from H_k in $O(n^2)$ time.

If the algorithm is started with $B_0 = \mathrm{I}$, then $H_0 = \mathrm{I}$ is known, and every iteration takes $O(n^2)$ work. B_k need not be formed.

It is possible to analyse the local convergence of the SR1 method and show that the method converges superlinearly in a neighbourhood of a local minimiser of f.

Thus, if the SR1 method is properly implemented, it can combine convergence speeds similar to those of the Newton-Raphson method with a lower complexity.

However, B_k is not guaranteed to stay positive definite, so P2 is not satisfied!

The Broyden-Fletcher-Goldfarb-Shanno Method:

$BFGS$ updates are defined by

$$B_{k+1} = B_k + \frac{B_k\delta_k\delta_k^\mathsf{T}B_k}{\delta_k^\mathsf{T}B_k\delta_k} + \frac{\gamma_k\gamma_k^\mathsf{T}}{\gamma_k^\mathsf{T}\delta_k}.$$

- Rank-2 updates.
- Has all the properties of SR1, but stays positive definite if $B_0 \succ 0$.
- The most successful and widely used quasi-Newton method.
- Motivation more difficult, see Lecture Notes 4.

Reading Assignment: Download and read Lecture-Note 4.