Nonlinear Optimization

Steepest Descent and Quasi-Newton methods

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Methods that avoid calculating the Hessian

- A disadvantage with the Newton method is that the Hessian has to be
  - derived and implemented, which may introduce blunders,
  - calculated, which requires $\mathcal{O}(n^2)$ operations,
  - stored, which require storage for $n^2/2$ elements,
  - "inverted", which requires $\mathcal{O}(n^3)$ operations.

- However, provided we use a global stratey, we may replace the Hessian in the Newton equation
$$\nabla^2 f(x_k)p = -\nabla f(x_k)$$
with any positive definite matrix B_k, i.e.
$$B_k p = -\nabla f(x_k).$$
and still get global convergence.
- Some methods calculate hessian approximations based on first- or second-order derivatives, e.g. are

Gauss-Newton	$B_k = J(x_k)^T J(x_k)$,
Trust-region	$B_k = \nabla^2 f(x_k) + \lambda I$,
Levenberg-Marquardt	$B_k = J(x_k)^T J(x_k) + \lambda I$.

- Other methods calculate their hessian approximations without any derivative information. Two such methods are called *Steepest Descent* and *Quasi-Newton*.

Steepest Descent

- The *steepest-descent* method uses the simplest Hessian approximation
$$B_k = I \quad \Rightarrow \quad p_k = -\nabla f(x_k).$$
- This approximation produce a cheap calculation of the search direction.

- However, the convergence rate is linear with a convergence constant C bounded from above by

$$C_{sup} = \left(\frac{\kappa(Q)-1}{\kappa(Q)+1}\right)^2,$$

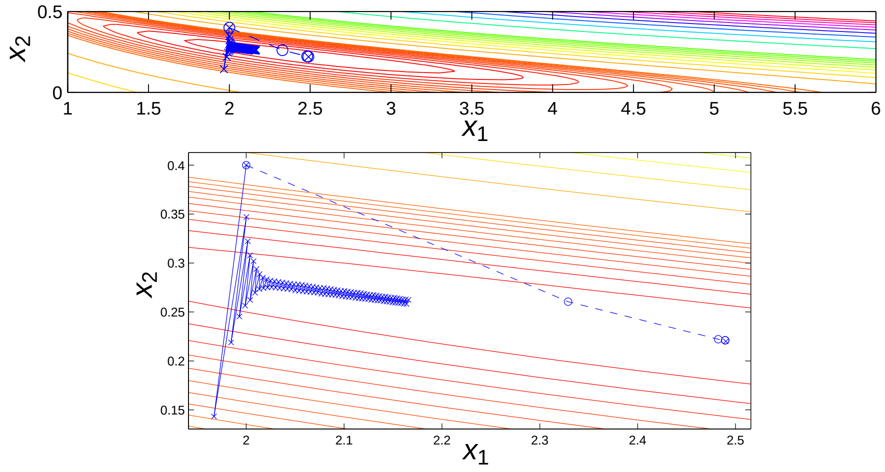
where $Q = \nabla^2 f(x^*)$ is the true hessian and $\kappa(Q)$ is the condition number of Q.

- The convergence rate will be poor even for moderate condition numbers.

$\kappa(Q)$	1	10	100	1000	10000
C	0	0.6694	0.9608	0.9960	0.9996

- **The steepest-descent method should only be used for problems that are known to be well-conditioned.**

Gauss-Newton and the Steepest-descent method for the antelope problem ($\kappa(Q) \approx 500$).



Quasi-Newton methods

- Quasi-Newton methods use a sequence of symmetric positive definite matrices that approximate the hessian (or the inverse hessian).
- For every iteration, the next (inverse) hessian approximation is calculated by *updating* the current approximation.
- Each update is constructed to include the curvature information computed in the last step, i.e. the next (inverse) hessian should behave as the true (inverse) hessian over the last step.
- This condition is called *the secant condition*.

The secant condition

- The one-dimensional secant method uses the approximation

$$\begin{aligned} f''(x_k) &\approx \frac{f'(x_k)-f'(x_{k-1})}{x_k - x_{k-1}}, \\ f''(x_k)(x_k - x_{k-1}) &\approx f'(x_k) - f'(x_{k-1}). \end{aligned}$$

- In multiple dimensions this corresponds to

$$\nabla^2 f(x_k)(x_k - x_{k-1}) \approx \nabla f(x_k) - \nabla f(x_{k-1}).$$

- From this we obtain the *secant equation*

$$B_k(x_k - x_{k-1}) = \nabla f(x_k) - \nabla f(x_{k-1}).$$

- With substitutions

$$s_k = x_{k+1} - x_k, y_k = \nabla f(x_{k+1}) - \nabla f(x_k),$$

  we obtain

$$B_{k+1} s_k = y_k.$$

- If $H_k = B_k^{-1}$, the secand equation becomes

$$H_{k+1} y_k = s_k.$$

- The hessian approximation B_k has $n^2/2$ independent elements, but the secant equation has only n equations.
- Thus, several updating schemes are possible.

Properties of Quasi-Newton methods

- An example of a Quasi-Newton update formula is

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k}$$

- This formula illustrates several key features with quasi-Newton approximations.
  - The new approximation B_{k+1} is found by *updating* the old approximation B_k.
  - As a starting approximation $B_0 = I$ may be used, but if a better approximation is available at a small cost, it should be used.

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  - The secant condition will be satisfied indepedently of how B_k is chosen:

$$\begin{aligned} B_{k+1} s_k &= B_k s_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k} s_k \\ &= B_k s_k + \frac{(y_k - B_k s_k)((y_k - B_k s_k)^T s_k)}{(y_k - B_k s_k)^T s_k} \\ &= B_k s_k + (y_k - B_k s_k) = y_k. \end{aligned}$$

  - The new approximation B_{k+1} can be obtained using $\mathcal{O}(n^2)$ operations since the update only involves vector products.

- The number of operations needed to calculate the search direction depends on the choice of update formula.
  - If a B_k update formula is used, the solution of the secant equation needs $\mathcal{O}(n^3)$ operations.
  - Update formulas for the cholesky factors $LL^T = B_k$ exist that reduce the number of operations to $\mathcal{O}(n^2)$.
  - Another $\mathcal{O}(n^2)$ solution is if we use an update formula for H_k. The search direction may then be calculated from

$$p_k = H_k(-\nabla f_k).$$

- Thus, the total time complexity of one iteration of a Quasi-Newton method can be reduced to $\mathcal{O}(n^2)$ compared to $\mathcal{O}(n^3)$ for e.g. Newton and Trust-region methods.

Common Quasi-Newton methods

- The most widely used Quasi-Newton formula is known as BFGS (Broyden-Fletcher-Goldfarb-Shanno):

$$B_{k+1} = B_k - \frac{(B_k s_k)(B_k s_k)^T}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}.$$

- BFGS preserves symmetry and positive definiteness if $y_k^T s_k > 0$, which may be satisfied with a line search using the Wolfe condition.
- The corresponding update formula for H_k is

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T,$$

where $\rho_k = 1/(y_k^T s_k)$.

- One of the first Quasi-Newton formulas was DFP (Davidon-Fletcher-Powell):

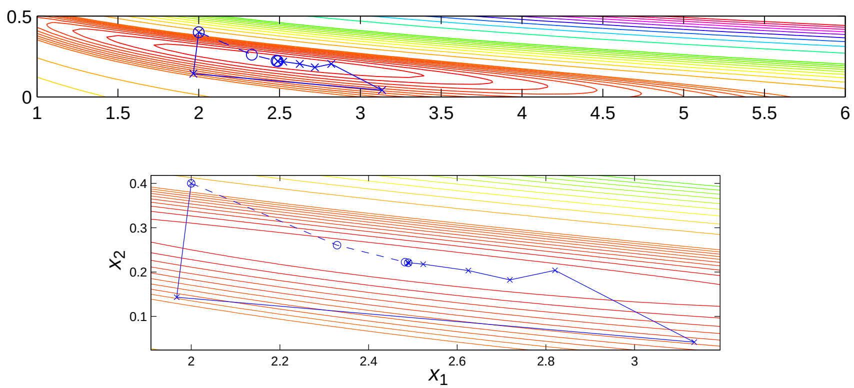
$$B_{k+1} = (I - \rho_k y_k s_k^T) B_k (I - \rho_k s_k y_k^T) + \rho_k y_k y_k^T,$$

and

$$H_{k+1} = H_k - \frac{(H_k y_k)(H_k y_k)^T}{y_k^T H_k y_k} + \frac{s_k s_k^T}{y_k^T s_k}.$$

where $\rho_k = 1/(y_k^T s_k)$.

Gauss-Newton and BFGS on the antelope problem.



$$B_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, B_{1..8} = \left\{ \begin{bmatrix} 15 & 105 \\ 105 & 776 \end{bmatrix}, \begin{bmatrix} 6 & 31 \\ 31 & 289 \end{bmatrix}, \begin{bmatrix} 8 & 45 \\ 45 & 398 \end{bmatrix}, \begin{bmatrix} 9 & 66 \\ 66 & 671 \end{bmatrix}, \begin{bmatrix} 10 & 72 \\ 72 & 621 \end{bmatrix}, \right.$$

$$\left. \begin{bmatrix} 10 & 80 \\ 80 & 700 \end{bmatrix}, \begin{bmatrix} 10 & 78 \\ 78 & 691 \end{bmatrix}, \begin{bmatrix} 10 & 75 \\ 75 & 664 \end{bmatrix} \right\}, B_9 = \begin{bmatrix} 10 & 74 \\ 74 & 652 \end{bmatrix}, \nabla^2 f(x^*) = \begin{bmatrix} 10 & 74 \\ 74 & 652 \end{bmatrix}.$$

Convergence properties

- The BFGS method has super-linear convergence, i.e. faster than linear but slower than quadratic.
- The deficit to quadratically convergent methods usually shows only in the few last iterations.
- Thus, for many practical applications, BFGS converges as fast as a Newton method, i.e. it requires approximately the same number of *iterations*.
- Since the BFGS search direction can be calculated in n^2 time vs. n^3 time for the Newton method, the required *execution time* is usually substantially less than Newton.

Termination rules

- Mathematically, a minimization algorithm should terminate with a solution x_k satisfying $\nabla f(x_k) = 0$ and $\nabla^2 f(x_k)$ positive semi-definite.
- Due to e.g. the use of finite arithmetic, no algorithm is guaranteed to satisfy this condition in finite time.
- Instead we will rely on termination rules based on thresholds on e.g. $\|\nabla f(x_k)\|$.

- Consider the *absolute termination criteria*

$$\|\nabla f(x_k)\| \leq \epsilon,$$

  for some $\epsilon > 0$. I.e. we stop when the norm of the gradient falls below a threshold.
- This condition is *scale dependent*, since a change of unit in f would rescale ∇f and affect the strength of the condition.
- E.g. a change of unit from km to m would correspond to a scaling of 10^3.

- A small modification of the absolute termination criteria leads the *relative termination criteria*

$$\|\nabla f(x_k)\| \leq \epsilon |f(x_k)|,$$

  which is not scale dependent.
- However, if $f(x^*) \approx 0$, the relative test will be difficult or even impossible to satisfy due to round-off errors.
- A possible combination is

$$\|\nabla f(x_k)\| \leq \epsilon \left(1 + |f(x_k)|\right).$$

- This test will behave like an absolute test if $f(x_k) \approx 0$, and otherwise like a relative test.

- For least squares problems

$$\min_x f(x) = \frac{1}{2} r(x)^T r(x),$$

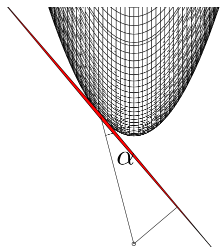
  the test

$$\|Jp\| = \|J(J^T J)^{-1} J^T r\| \leq \epsilon(1 + \|r\|)$$

  may be used instead of the gradient test.
- Since Jp and F belong to the same vector space, the test may be interpreted geometrically.
- The quotient

$$\frac{\|Jp\|}{\|r\|} = \cos\alpha,$$

  describes the angle α between the residual r and the tangent plane at r.



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may be used instead of the gradient test.
- Since Jp and F belong to the same vector space, the test may be interpreted geometrically.
- Close to the solution the residual will approach orthogonality with the tangent plane, i.e.

$$\alpha \to \pi/2 \text{ and } \frac{\|Jp\|}{\|r\|} \to 0.$$