Nonlinear conjugate gradient method

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In numerical optimization, the **nonlinear conjugate gradient method** generalizes the conjugate gradient method to nonlinear optimization. For a quadratic function $f(x)$

$$f(x) = \|Ax - b\|^2,$$

the minimum of f is obtained when the gradient is 0:

$$\nabla_x f = 2A^T(Ax - b) = 0.$$

Whereas linear conjugate gradient seeks a solution to the linear equation $A^T Ax = A^T b$, the nonlinear conjugate gradient method is generally used to find the local minimum of a nonlinear function using its gradient $\nabla_x f$ alone. It works when the function is approximately quadratic near the minimum, which is the case when the function is twice differentiable at the minimum and the second derivative is non-singular there.

Given a function $f(x)$ of N variables to minimize, its gradient $\nabla_x f$ indicates the direction of maximum increase. One simply starts in the opposite (steepest descent) direction:

$$\Delta x_0 = -\nabla_x f(x_0)$$

with an adjustable step length α and performs a line search in this direction until it reaches the minimum of f:

$$\alpha_0 := \arg\min_\alpha f(x_0 + \alpha \Delta x_0),$$
$$x_1 = x_0 + \alpha_0 \Delta x_0$$

After this first iteration in the steepest direction Δx_0, the following steps constitute one iteration of moving along a subsequent conjugate direction s_n, where $s_0 = \Delta x_0$:

1. Calculate the steepest direction: $\Delta x_n = -\nabla_x f(x_n)$,
2. Compute β_n according to one of the formulas below,
3. Update the conjugate direction: $s_n = \Delta x_n + \beta_n s_{n-1}$
4. Perform a line search: optimize $\alpha_n = \arg\min_\alpha f(x_n + \alpha s_n)$,
5. Update the position: $x_{n+1} = x_n + \alpha_n s_n$,

With a pure quadratic function the minimum is reached within N iterations (excepting roundoff error), but a non-quadratic function will make slower progress. Subsequent search directions lose conjugacy requiring the search direction to be reset to the steepest descent direction at least every N iterations, or sooner if progress stops. However, resetting every iteration turns the method into steepest descent. The algorithm stops when it finds the minimum, determined when no progress is made after a direction reset (i.e. in the steepest descent direction), or when some tolerance criterion is reached.

Within a linear approximation, the parameters α and β are the same as in the linear conjugate gradient method but have been obtained with line searches. The conjugate gradient method can follow narrow (ill-conditioned) valleys, where the steepest descent method slows down and follows a criss-cross pattern.

Four of the best known formulas for β_n are named after their developers:

- Fletcher–Reeves:[1]

$$\beta_n^{FR} = \frac{\Delta x_n^T \Delta x_n}{\Delta x_{n-1}^T \Delta x_{n-1}}.$$

- Polak–Ribière:[2]

$$\beta_n^{PR} = \frac{\Delta x_n^T (\Delta x_n - \Delta x_{n-1})}{\Delta x_{n-1}^T \Delta x_{n-1}}.$$

- Hestenes–Stiefel:[3]

$$\beta_n^{HS} = \frac{\Delta x_n^T (\Delta x_n - \Delta x_{n-1})}{-s_{n-1}^T (\Delta x_n - \Delta x_{n-1})}.$$

- Dai–Yuan:[4]

$$\beta_n^{DY} = \frac{\Delta x_n^T \Delta x_n}{-s_{n-1}^T (\Delta x_n - \Delta x_{n-1})}..$$

These formulas are equivalent for a quadratic function, but for nonlinear optimization the preferred formula is a matter of heuristics or taste. A popular choice is $\beta = \max\{0, \beta^{PR}\}$, which provides a direction reset automatically.[5]

Algorithms based on Newton's method potentially converge much faster. There, both step direction and length are computed from the gradient as the solution of a linear system of equations, with the coefficient matrix being the exact Hessian matrix (for Newton's method proper) or an estimate thereof (in the quasi-Newton methods, where the observed change in the gradient during the iterations is used to update the Hessian estimate). For high-dimensional problems, the exact computation of the Hessian is usually prohibitively expensive, and even its storage can be problematic, requiring $O(N^2)$ memory (but see the limited-memory L-BFGS quasi-Newton method).

The conjugate gradient method can also be derived using optimal control theory.[6] In this accelerated optimization theory, the conjugate gradient method falls out as a nonlinear optimal feedback controller,

$u = k(x, \dot{x}) := -\gamma_a \nabla_x f(x) - \gamma_b \dot{x}$ for the double integrator system,

$$\ddot{x} = u$$

The quantities $\gamma_a > 0$ and $\gamma_b > 0$ are variable feedback gains.[6]

See also [edit]

- Gradient descent
- Broyden–Fletcher–Goldfarb–Shanno algorithm
- Conjugate gradient method
- L-BFGS (limited memory BFGS)
- Nelder–Mead method
- Wolfe conditions

References [edit]

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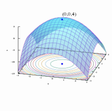

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