Quasi-Newton methods

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- variable metric methods
- quasi-Newton methods
- BFGS update
- limited-memory quasi-Newton methods

Basic idea

- Gradient descent method is simple, but it converges slowly.
- Newton's method converges fast, but it need large calculation.
- Can we design algorithms that combine the advantages of fast convergence without calculating the second-order partial derivative matrix and its inverse matrix to construct the search direction for each iteration?

Basic idea

- Gradient descent method is simple, but it converges slowly.
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The gradient descent method and Newton's method can be written as:

$$x^{k+1} = x^k - \lambda_k {H_k}^{-1} \nabla f(x^k).$$

- If $H_k = I$, then it is gradient descent method
- If $H_k = [\nabla^2 f(x^k)]$ and $\lambda_k = 1$, then it is Newton's method.

Variable metric methods

In order to maintain the advantages of Newton's method, we want H_k^{-1} approximate $[\nabla^2 f(x^k)]^{-1}$. $H_k \succ 0$ is approximation of the Hessian at x, chosen to:

- avoid calculation of second derivatives
- simplify computation of search direction

'Variable metric' interpretation

$$\triangle x_k = -H_k^{-1} \nabla f(x^k)$$

is steepest descent direction at x for quadratic norm

$$\|z\|_{H_k} = (z^T H_k z)^{1/2}.$$

Quasi-Newton methods

given starting point $x^{(0)} \in \operatorname{dom} f$, $H_0 \succ 0$

1. compute quasi-Newton direction $\triangle x = -H_{k-1}^{-1} \nabla f(x^{(k-1)})$
2. determine step size t (e.g., by backtracking line search)
3. compute $x^{(k)} = x^{(k-1)} + t \triangle x$
4. compute H_k

- different methods use different rules for updating H in step 4
- can also propagate H_k^{-1} to simplify calculation of $\triangle x$

Broyden-Fletcher-Goldfarb-Shanno (BFGS) update

BFGS update:

$$H_k = H_{k-1} + \frac{yy^T}{y^T s} - \frac{H_{k-1} s s^T H_{k-1}}{s^T H_{k-1} s},$$

where

$$s = x^{(k)} - x^{(k-1)}, \quad y = \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$$

$$H_k^{-1} = \left(I - \frac{sy^T}{y^T s}\right) H_{k-1}^{-1} \left(I - \frac{ys^T}{y^T s}\right) + \frac{ss^T}{y^T s}$$

- note that $y^T s > 0$ for strictly convex f;
- cost of update or inverse update is $O(n^2)$ operations

Positive definiteness

if $y^T s > 0$, BFGS update preserves positive definitess of H_k

Proof: from inverse update formula,

$$v^T H_k^{-1} v = \left(v - \frac{s^T v}{s^T y} y\right)^T H_{k-1}^{-1} \left(v - \frac{s^T v}{s^T y} y\right) + \frac{(s^T v)^2}{y^T s}$$

- if $H_{k-1} \succ 0$, both terms are nonnegative for all v
- second term is zero only if $s^T v = 0$; then first term is zero only if $v = 0$

this ensures that $\triangle x = -H_k^{-1} \nabla f(x^{(k)})$ is a descent direction

Secant condition

the BFGS update satisfies the secant condition $H_k s = y$, i.e.,

$$H_k(x^{(k)} - x^{(k-1)}) = \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$$

Interpretation: define second-order approximation at $x^{(k)}$

$$f_{\mathrm{quad}}(z) = f(x^{(k)}) + \nabla f(x^{(k)})^T(z - x^{(k)}) + \frac{1}{2}(z - x^{(k)})^T H_k(z - x^{(k)})$$

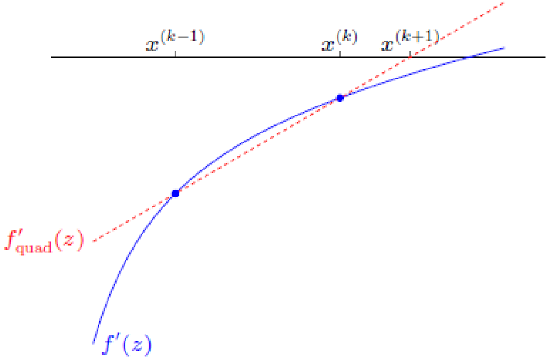
secant condition implies that gradient of f_{quad} agrees with f at $x^{(k-1)}$:

$$\begin{aligned}\nabla f_{\mathrm{quad}}(x^{(k-1)}) &= \nabla f(x^{(k)}) + H_k(x^{(k-1)} - x^{(k)}) \\ &= \nabla f(x^{(k-1)})\end{aligned}$$

Secant method

for $f : R \to R$, BFGS with unit step size gives the secant method

$$x^{(k+1)} = x^{(k)} - \frac{f'(x^{(k)})}{H_k}; \quad H_k = \frac{f'(x^{(k)}) - f'(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}$$



Convergence

Global result

if f is strongly convex, BFGS with backtracking line search converges from any $x^{(0)},\ H_0 \succ 0$

Local convergence

if f is strongly convex and $\nabla^2 f(x)$ is Lipschitz continuous, local convergence is superlinear: for sufficiently large k,

$$\|x^{(k+1)} - x^*\|_2 \leq c_k \|x^{(k)} - x^*\|_2 \to 0$$

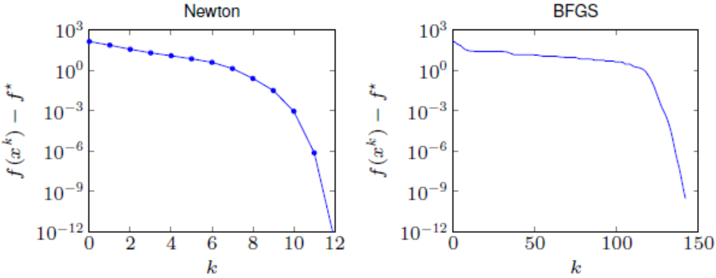
where $c_k \to 0$

(cf., quadratic local convergence of Newton method)

Example

$$\min \quad c^T x - \sum_{i=1}^{m} \log(b_i - a_i^T x)$$

$n = 100, \ m = 500$



- cost per Newton iteration: $O(n^3)$ plus computing $\nabla^2 f(x)$
- cost per BFGS iteration: $O(n^2)$

Square root BFGS update

to improve numerical stability, propagate H_k in factored form $H_k = L_k L_k^T$

- if $H_{k-1} = L_{k-1} L_{k-1}^T$ then $H_k = L_k L_k^T$ with

$$L_k = L_{k-1} \left(I + \frac{(\alpha \widetilde{y} - \widetilde{s})\widetilde{s}^T}{\widetilde{s}^T \widetilde{s}} \right),$$

  where

$$\widetilde{y} = L_{k-1}^{-1} y, \quad \widetilde{s} = L_{k-1} s, \quad \alpha = \left(\frac{\widetilde{s}^T \widetilde{s}}{y^T s} \right)^{1/2}$$

- if L_{k-1} is triangular, cost of reducing L_k to triangular form is $O(n^2)$

Optimality of BFGS update

$X = H_k$ solves the convex optimization problem

$$\begin{aligned} \min \quad & \operatorname{tr}(H_{k-1}^{-1}X) - \log\det(H_{k-1}^{-1}X) - n \\ s.t. \quad & Xs = y \end{aligned}$$

- cost function is nonnegative, equal to zero only if $X = H_{k-1}$
- also known as relative entropy between densities $N(0, X)$, $N(0, H_{k-1})$

optimality result follows from KKT conditions: $X = H_k$ satisfies

$$X^{-1} = H_{k-1}^{-1} \frac{1}{2}(s\nu^T + \nu s^T), \quad Xs = y, \quad X \succ 0$$

with

$$\nu = \frac{1}{s^T y}\left(2H_{k-1}^{-1}y - \left(1 + \frac{y^T H_{k-1}^{-1} y}{y^T s}\right)s\right)$$

Davidon-Fletcher-Powell (DFP) update

switch H_{k-1} and X in objective on previous page

$$\begin{array}{ll} \min & \operatorname{tr}(H_{k-1}^{-1} X^{-1}) - \log\det(H_{k-1}^{-1} X^{-1}) - n \\ s.t. & Xs = y \end{array}$$

- minimize relative entropy between $N(0, H_{k-1})$ and $N(0, X)$
- problem is convex in X^{-1} (with constraint written as $s = X^{-1}y$)
- solution is 'dual' of BFGS formula

$$H_k = \left(I - \frac{ys^T}{s^T y}\right) H_{k-1} \left(I - \frac{sy^T}{s^T y}\right) + \frac{yy^T}{s^T y}$$

(known as DFP update)

predates BFGS update, but is less often used

Limited memory quasi-Newton methods

main disadvantage of quasi-Newton method is need to store H_k or H_k^{-1}

Limited-memory BFGS (L-BFGS): do not store H_k^{-1} explicitly

- instead we store the m (e.g., $m = 30$) most recent values of

$$s_j = x^{(j)} - x^{(j-1)},\ y_j = \nabla f(x^{(j)}) - \nabla f(x^{(j-1)})$$

- we evaluate $\triangle x = H_k^{-1} \nabla f(x^{(k)})$ recursively, using

$$H_j^{-1} = (I - \frac{s_j y_j^T}{s_j^T y_j}) H_{j-1}^{-1} (I - \frac{y_j s_j^T}{s_j^T y_j}) + \frac{s_j s_j^T}{s_j^T y_j},$$

  for $j = k, k-1, \cdots, k-m+1$, assuming, for example, $H_{k-m}^{-1} = I$
- cost per iteration is $O(nm)$, storage is $O(nm)$

References

- J. Nocedal and S. J. Wright, Numerical Optimization (2006), chapters 6 and 7
- J. E. Dennis and R. B. Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear Equations (1983)